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The primary objective of SAIC was to develop an unstructured grid algorithm and code that dynamically adapts to the computed solution of the time dependent Euler equations of gasdynamics in two and three spatial dimensions. Important requirements that were imposed on the algorithm were: robustness, accuracy, efficiency, flexibility, and adaptability. The main research and code development effort was focused on achieving these objectives; extensive testing and code validation effort was undertaken to demonstrate the code's performance for realistic CFD problems. The method is accurate in all flow regimes from subsonic to hypersonic. The main achievement was the development of the AUGUST code (Adaptive Unstructured Grid Upwind Second Order for Triangles). AUGUST is implemented for solution of Euler's equations on dynamically adaptive triangular or tetrahedral grids. The code fully implements the Second-Order Godunov method, allowing accurate and robust numerical solution of Euler equations of gas dynamics. A new method was developed for Direct Dynamic Grid Refinement (DDR). The AUGUST code was also implemented for multiphase, multicomponent flows. A combined structured/unstructured version of the AUGUST code was also developed. The AUGUST code was extensively validated for a wide range of problems and has proven to be a robust tool.

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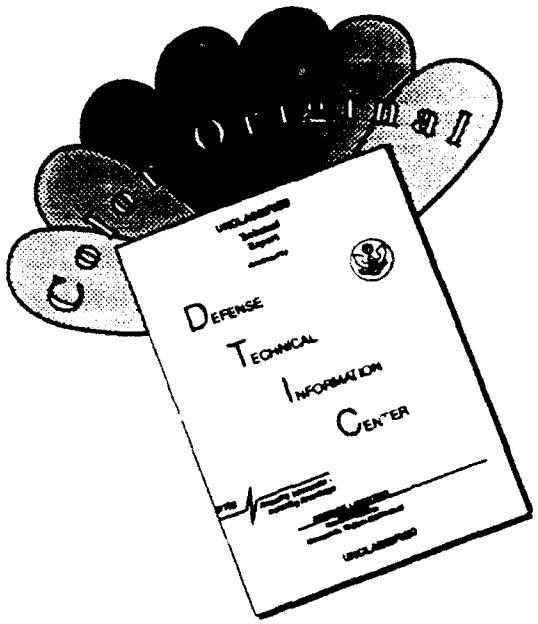

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EXECUTIVE SUMMARY

This progress report documents the effort conducted at SAIC from 15 October 1990 through 31 May 1993, under DARPA and AFOSR contract #F49620-89-C-0087 entitled "UUGM Code Development".

Scope of Research

The primary objective of SAIC was to develop an unstructured grid algorithm and code that dynamically adapts to the computed solution of the time dependent Euler equations of gasdynamics in two and three spatial dimensions. Important requirements that were imposed on the algorithm were: robustness, accuracy, efficiency, flexibility, and adaptability. The main research and code development effort was focused on achieving these objectives; extensive testing and code validation effort was undertaken to demonstrate the code's performance for realistic CFD problems. The method is accurate in all flow regimes from subsonic to hypersonic.

Achievements

The main achievement was the development of the AUGUST code (Adaptive Unstructured Grid Upwind Second Order for Triangles). AUGUST is implemented for solution of Euler's equations on dynamically adaptive triangular or tetrahedral grids. The code fully implements the Second-Order Godunov method, allowing accurate and robust numerical solution of Euler equations of gas dynamics.

A new method was developed for Direct Dynamic Grid Refinement (DDR). This method allows grid refinement in arbitrary regions of the computational domain, using only one level of undirectness in the logical data structure. The DDR is an integral part of the AUGUST solver and allows manipulation of the grid as a part of the solution. The adapted grid is not only more refined in the adaptation regions of the flow but is also improved structurally due to a refinement algorithm.

The AUGUST code was also implemented for multiphase, multicomponent flows. We used a multiple-fluid description, where a separate set of conservation laws is used to describe every flow component. In our approach Lagrangian tracers are used to describe sparse or discrete flow components that do not form a continuum. Use of unstructured triangular grids allows adjustment of the grid resolution to the accuracy requirements in the flow subdomains.

A combined structured/unstructured version of the AUGUST code was also developed. Following this approach the unstructured adaptive grid is used only in the flow regions requiring adaptation or description of the complex geometry elements. The structured grid is used to simulate the larger part of the computational domain. This approach has allowed us to capitalize on the advantages of both structured and unstructured grid approaches. Using the structured/unstructured grid version of the

AUGUST code, we simulated the shock wave focusing problem for the reflector used for extracorporeal shock-wave lithotripsy. In this simulation, we showed that the solution smoothly transits through the interfaces between the grids, maintaining the same accuracy and resolution.

The AUGUST code was extensively validated for a wide range of problems and has proven to be a robust tool. The code was initiated at the start of the UUGM project and has now evolved into a production code that is used for many applied problems. The list of applications includes potential flow past an ellipse, hypersonic flow past a flat plate, shock diffraction over single and double wedges, mine explosions under vehicles, pulsed detonation engines, shock focusing in air, and nonideal airburst in multiphase media. The code has shown the required robustness and insensitivity to the initial user specified grid. The number of nodes required to obtain a high-quality solution is significantly smaller than for structured grid codes. This is particularly true for transient problems with complicated flows having discontinuities.

It is important to note that the AUGUST code obtains a high resolution solution with no "knobs." The various flow regimes, except those requiring a different definition of boundary and initial conditions, were simulated using the same code.

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1. INTRODUCTION

1.1 RECENT CFD DEVELOPMENT

Computational fluid dynamics (CFD) development over the past twenty years has truly been outstanding. The recent CFD developments that are particularly important are: 1) advances in flow solvers in all the regimes of fluid flow (very low speed and subsonic flows, transonic flow, supersonic and hypersonic flows), 2) advances in unstructured adaptive gridding techniques and, 3) advances in chemical and particle kinetic modeling for fluid flows. Developments in graphics and visualization, construction of graphical user interfaces (GUIs) and advances in large database management have also played an important role in the scale and complexity of problems that can now be realistically simulated by CFD techniques. SAIC has been involved in all aspects of these developments and is on the forefront of CFD technology development.

DARPA, NASA, DNA and DOE have for the most part been the largest benefactors of CFD development, and each agency today is actively pursuing CFD applications to real problems. Full 3-D unsteady flows about military and commercial aircraft are routinely simulated to assess aerodynamic performance characteristics, and where it used to require several hundred hours of CRAY CPU time it now takes minutes to an hour on a supercomputer or a like time on workstations, depending on the specifics of the problem being solved. The U.S. Marine Corps' latest initiative in the development of blast (due to land mines) resistant vehicles is being pursued successfully with the aid of full 3-D CFD simulations of land mine blast effects on truck configurations. The CFD technology developed in SAIC's UUGM contract is playing a leading role in this Marine Corps effort (see Section 3.4). Many other such examples of improvements in CFD performance exist. In view of this, it is quite appropriate to begin to transition CFD technology into other disciplines that can take advantage of realistic CFD based simulation.

1.2 UNSTRUCTURED MESHES IN COMPLEX GEOMETRIES

Current emphasis in CFD calls for solutions of applied physical problems for complex realistic geometries.[1] In addition to the inherent difficulties in describing the details of the complex three-dimensional geometry, the flow fields usually have an inhomogeneous structure. Regions of rapid change of the flow functions and chemical reactions will be embedded in regions where the flow gradients are relatively small. Accurate simulations of flows in regions with strong gradients is key to the overall accuracy of physical, chemical and biological simulations. For this reason most of the software and hardware computational resources are defined by the accuracy requirements of these flow regions and geometry of the computational domain.

Early CFD research was almost entirely concerned with the formulation the mathematical models of the flow and methods of solution. Mesh generation was regarded as secondary and meshes were developed for specific cases. During this early period very

significant improvements were made in the methods of integration of the partial differential equations of gasdynamics. Presently, as a result of steady improvement in the various integration techniques, the advantages which could be gained by using better flow solvers have become limited. On the other hand substantial progress is anticipated in the areas of grid generation and algorithm development.[2]

Currently, most numerical simulations employ structured meshes composed of quadrilaterals in two dimensions or hexahedra in three dimensions. However, it has become evident that the quadrilateral structured grids cannot satisfy the requirements of large scale numerical simulations over complex geometries in three dimensions. The physics of the flow about a complete aircraft is extremely complex. Yet the flow in many distinct regions and regimes may be represented by fairly well-known physical theories. Vortices shed by lifting surfaces are confined to fairly thin wake regions. Exhaust plumes can be initially approximated by regular bounding surfaces. Flow disturbances due to shocks are confined to thin discontinuities. Boundary layers are restricted to near-wall regions. Each of these flow regions requires different theories, different resolution and different numerical algorithms. This diversity of computational requirements cannot be satisfied by the quadrilateral structured grids.

Recently proposed alternatives to quadrilateral grids use triangles in two dimensions and tetrahedra in three dimensions. For these grids the mesh will generally lose its structure, allowing a new degree of flexibility in treating complex geometries.[3,4] Unstructured grids can relatively easily be adapted to follow flow features, thereby increasing the solution accuracy. The result has been the development of adaptive refinement techniques which have been used with great success for two dimensional simulations on unstructured triangular grids. These methods have resulted in the resolution of previously difficult details in the evolving flows over complex configurations.

However, it is not a trivial task to adapt this approach to three-dimensional simulations. One of the problems is the generation of the adaptive grid. Since the grid is constructed from the volume elements (tetrahedra) the moving front is made up of a surface of triangular faces. It should be noted that this moving front can and will change its shape during the computation as time evolves. It is necessary to take care when determining the intersections of planar faces, and to ensure that no overlapping of tetrahedra occurs.

2. UUGM: UNIVERSAL CFD SIMULATION ENVIRONMENT

The Ultimate Unstructured Grid Method (UUGM) represents a new approach to the computational domain discretization. The principal advantage of the method is most apparent for simulations of complicated flow regimes with physical and chemical processes over bodies with complex geometries in three dimensions.

The usual technique employed in regridding is called hierarchical dynamic refinement (H refinement). The idea here is to retain a history of the original grid and the

subdivisions needed to change it into the current grid, so that it is always possible to retrace these steps and get back to previous grids. While this feature is useful in modeling reversible processes, it is generally unnecessary, and it increases overhead costs. Our implementation (Direct Dynamic Refinement) is Markovian, in the sense that the way regridding is done depends only on the current grid and flow conditions.

The other distinguishing feature is the use of the Second-order Godunov method to solve the Euler equations of gasdynamics. The philosophy behind it is to treat the local values of the dependent variables at every point on the grid as initial conditions for a Riemann problem, and to use the resultant solution of that problem to calculate the fluxes of material, momentum, and energy from one cell to the rest. Previous implementations of this method were confined to structured meshes.

2.1 MATHEMATICAL MODEL AND INTEGRATION ALGORITHM

We consider a system of two-dimensional Euler equations written in conservation law form as

$$\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}=0, \tag{2.1}$$

where

$$U=\begin{vmatrix}\rho\\ \rho u\\ \rho v\\ e\end{vmatrix},\quad F=\begin{vmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ u(e+p)\end{vmatrix},\quad G=\begin{vmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ v(e+p)\end{vmatrix}.$$

Here u, v are the x, y velocity vector components, p is the pressure, ρ is the density and e is total energy of the fluid. We assume that the fluid is an ideal gas and the pressure is given by the equation of state,

$$p=(\gamma-1)\left[e-\left(\frac{\rho}{2}\right)(u^2+v^2)\right], \tag{2.2}$$

where γ is the ratio of specific heats and is typically taken as 1.4 for air. It is assumed that an initial distribution of the fluid parameters is given at $t = 0$, and the boundary conditions defining a unique solution are specified for the computational domain.

The system of governing equations in Eq. (2.1) can be written as

$$\frac{\partial U}{\partial t}+\nabla\cdot Q=0, \tag{2.3}$$

where Q represents the convective flux vector. Integrating Eq. (2.3) over space and using Gauss' theorem produces the expression

$$\frac{\partial}{\partial t}\int_{\Omega} U\, dA + \oint_{\partial\Omega} Q \cdot dl = 0, \tag{2.4}$$

where $dl = ndl$, n is the unit normal vector in the outward direction, and dl is the element of length on the boundary of the domain. Here Ω is the domain of computation and $\partial\Omega$ is the boundary of this domain.

We seek a solution to the system of Eq. (2.1) in the computational domain, which is decomposed in part into triangles with arbitrary connectivity and in part into rectangles using a logically structured grid. We use the advantage of the unstructured grid (Refs. 5-8) to describe the curved boundary of the computational domain and areas that need increased local resolution; this covers a small part of the total computational domain. The largest area of the computational domain is decomposed by the structured grid. The numerical technique for solving Euler's equation on an unstructured grid is described in Refs. 9-11, and the technique for the structured grid is described in Ref. 9. These numerical techniques apply some of the ideas that were introduced in Refs. 13-14. The structured and unstructured codes apply the center-based formulation, i.e., the primitive variables are defined in the center of the cell, which makes the cell the integration volume, while the fluxes are computed across the edges of the cell. The basic algorithmic steps of the Second-Order Godunov method can be defined as follows:

1. Find the value of the gradient at the baricenter of the cell for each gasdynamic parameter U_i;

2. Find the interpolated values of U at the edges of the cell using the gradient values;

3. Limit these interpolated values based on the monotonicity condition;[13]

4. Subject the projected values to the characteristics constraints;[14]

5. Solve the Riemann problem applying the projected values at the two sides of the edges;

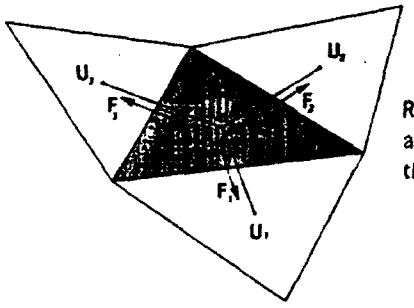
6. Update the gas dynamic parameter U according to the conservation equations (1) applying to the fluxes computed and the current timestep.

As was recommended in Ref. 11, we prefer the version based on triangle centers over the vertex-based version of the code. For the same unstructured grid, a center-based algorithm will result in smaller control volumes than a vertex-based. In addition, for the Second-Order Godunov solver, implementation of the boundary conditions is more straightforward and accurate for the center-based algorithm than in the vertex-based version. These two factors, along with the effects of grid connectivity, strongly affect the algorithm accuracy and performance and are the main reasons for the superiority of the center-based version over the vertex version.

Equation (2.4) can be discretized for each element (cell) in the domain

$$\frac{(U_i^{n+1} - U_i^n)}{\Delta t} A_i = \sum_{j=1}^{M} Q_j^n \cdot n_j \, \Delta L_j , \tag{2.5}$$

where A_i is the area of the cell; Δt is the marching timestep; U_i^n and U_i^{n+1} are the primitive variables at the center of the cell at time n and at the updated $(n + 1)$st timestep; Q_j is the value of the fluxes across the boundaries on the circumference of the cell where n_j is the unit normal vector to the boundary edge j, and ΔL_j is the length of the boundary edge j. The fluxes Q_j^n are computed applying the Second-Order Godunov algorithm, and Eq. (2.5) is used to update the physical primitive variables u_i according to computed fluxes for each marching timestep Δt. The marching timestep is subjected to the Courant-Friedrichs-Lewy (CFL) constraint.



Representative triangular cell in the mesh and its neighbors showing fluxes across the edges

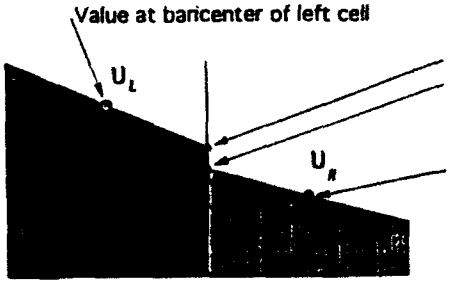


Figure 2.1.1 Representative triangular cell in the mesh showing fluxes and projected values

To obtain second-order spatial accuracy, the gradient of each primitive variable is computed in the baricenter of the cell. This gradient is used to define the projected values of primitive variables at the two sides of the cell edge, as shown in Fig. 2.1.1. The gradient is approximated by a path integral

$$\int_{\Omega} \nabla U_i^{\text{cell}} \, dA = \oint_{\partial\Omega} U_j^{\text{edge}} \, dl . \tag{2.6}$$

The notation is similar to the one used for Eq. (2.5), except that the domain Ω is a single cell and U_i and U_j are values at the baricenter and on the edge respectively. The gradient is estimated as

$$\nabla U_i^{\text{cell}} = \frac{1}{A} \sum_{j=1}^{3} U_j^{\text{edge}} \, n_j \, \Delta L_j \tag{2.7}$$

where U_j^{edge} is an average value representing the value of primitive variable for edge j.

The gradients that are computed at each baricenter are used to project values for the two sides of each edge by piecewise linear interpolation. The interpolated values are subjected to monotonicity constraints.[3] The monotonicity constraint ensures that the interpolated values do not create new extrema.

The monotonicity limiter algorithm can be written in the following form

$$U_{\text{proj}}^{\text{edge}} = U_i^{\text{cell}} + \phi \nabla U_i \cdot \Delta \boldsymbol{r} \tag{2.8}$$

where $\Delta \boldsymbol{r}$ is the vector from the baricenter to the point of intersection of the edge with the line connecting the baricenters of the cells over the two sides of this edge. Here ϕ is the coefficient that limits the gradient ∇U_i.

First we compute the maximum and minimum values of the primitive variable in the ith cell and its three neighboring cells that share common edges (see Fig. 2.1.1):

$$\left.\begin{aligned} U_{\text{cell}}^{\max} &= \max\left(U_k^{\text{cell}}\right) \\ U_{\text{cell}}^{\min} &= \min\left(U_k^{\text{cell}}\right) \end{aligned}\right\} k = i, 1, 2, 3. \tag{2.9}$$

The limiter can be defined as

$$\phi = \min\left\{1, \phi_k^{lr}\right\}, k = 1,2,3 \tag{2.10}$$

where the superscript lr stands for left and right of the three edges (6 combinations altogether); ϕ_k^{lr} is defined by

$$\phi_k^{lr} = \frac{\left[1 + \operatorname{sgn}\left(\Delta U_k^{lr}\right)\right] \Delta U_{\text{cell}}^{\max} + \left[1 - \operatorname{sgn}\left(\Delta U_k^{lr}\right)\right] \Delta U_{\text{cell}}^{\min}}{2 \Delta U_k^{lr}}, \quad k = 1, 2, 3 \tag{2.11}$$

where $\Delta U_k^{lr} = \nabla U_i^{lr} \cdot \Delta \boldsymbol{r}_k$ and

$$\left.\begin{aligned} \Delta U_{\text{cell}}^{\max} &= U_{\text{cell}}^{\max} - U_i^{\text{cell}} \\ \Delta U_{\text{cell}}^{\min} &= U_{\text{cell}}^{\min} - U_i^{\text{cell}} \end{aligned}\right\}. \tag{2.12}$$

To obtain second-order accuracy in time and space, we subject the projected values of the left and right side of the cell edge to characteristic constraints following Ref. 4. The one-dimensional characteristic predictor is applied to the projected values at the half timestep $t^n + \Delta t/2$. The characteristic predictor is formulated in the local system of coordinates for the one-dimensional Euler equation. We illustrate the implementation of

the characteristic predictor in the direction of the unit vector $\mathbf{n}_c$. The Euler equations for this direction can be written in the form

$$W_t + A(W)W_{nc} = 0; \tag{2.13}$$

$$W = \begin{Bmatrix} \tau \\ u \\ p \end{Bmatrix}; \; A(W) = \begin{pmatrix} u & -\tau & 0 \\ 0 & u & \tau \\ 0 & \rho c^2 & u \end{pmatrix}, \tag{2.14}$$

where $\tau = \rho^{-1}$, ρ denotes density, u, p are the velocity and pressure. The matrix $A(W)$ has three eigenvectors ($l\#$, $r\#$) (l for left and r for right, where # stands for +, 0, –) associated with the eigenvalues $\lambda^+ = u + c, \lambda^\circ = u, \lambda^- = u - c$.

An approximation of the value projected to an edge, accurate to second order in space and time, can be written as

$$\begin{aligned} W_{i+\Delta r}^{n+1/2} &\approx W_i^n + \frac{\Delta t}{2}\frac{\partial W}{\partial t} + \Delta r \frac{\partial W}{\partial r_{nc}} \\ &\approx W_i^n + \left[\Delta r - \frac{\Delta t}{2} A(W_i)\right]\frac{\partial W}{\partial r_{nc}}. \end{aligned} \tag{2.15}$$

An approximation to $W_{i+\Delta r}^{n+1/2}$ can be written as

$$W_{i+\Delta r}^{n+1/2} = W_i + \left(\Delta \mathbf{r}_i - \frac{\Delta t}{2}\left(M_x M_n\right)\mathbf{n}_c\right)\cdot \nabla W_i, \tag{2.16}$$

where

$$\left(\mathrm{M_x\, M_n}\right) = \begin{cases} \max\left(\lambda_i^+, 0\right) & \text{for the cell on the left of the edge} \\ \min\left(\lambda_i^-, 0\right) & \text{for the cell on the right of the edge.} \end{cases} \tag{2.17}$$

The gradients applied in the process of computing the projected values at $t^n + \Delta t/2$ are subjected to the monotonicity limiter.

Following the characteristic predictor described above, the full Riemann problem is solved at the edge. The solution of the Riemann problem defines the flux $Q^{n+1/2}$ through the edge. The fluxes through the edges of triangles are then integrated (Eq. 2.5), thus giving an updated value of the variables at t^{n+1}. One of the advantages of this algorithm is that calculation of the fluxes is done over the largest loop in the system (the loop over edges) and can be vectorized or parallelized. This leads to an efficient algorithm.

We have carried out an extensive and painstaking series of tests in the course of developing and implementing the algorithm. Most of these used a standard benchmark, the exploding diaphragm or "Sod problem" (Fig. 2.1.2). In this problem two regions containing an ideal gas at different densities and pressure are separated by an infinitely thin interface (the diaphragm). A shock wave, a rarefaction wave, and a contact discontinuity propagate away from that point at different speeds when this diaphragm is instantaneously removed. The Riemann solution yields an analytical solution in terms of simple waves which can be compared with the numerical approximation.

We used this problem as a testbed to compare structured vs. unstructured grids, first-order vs. second-order Godunov schemes, schemes with and without limiters, etc. For example, Fig. 2.1.2 shows that the solution obtained with an unstructured grid is noticeably better than that obtained with a structured grid.

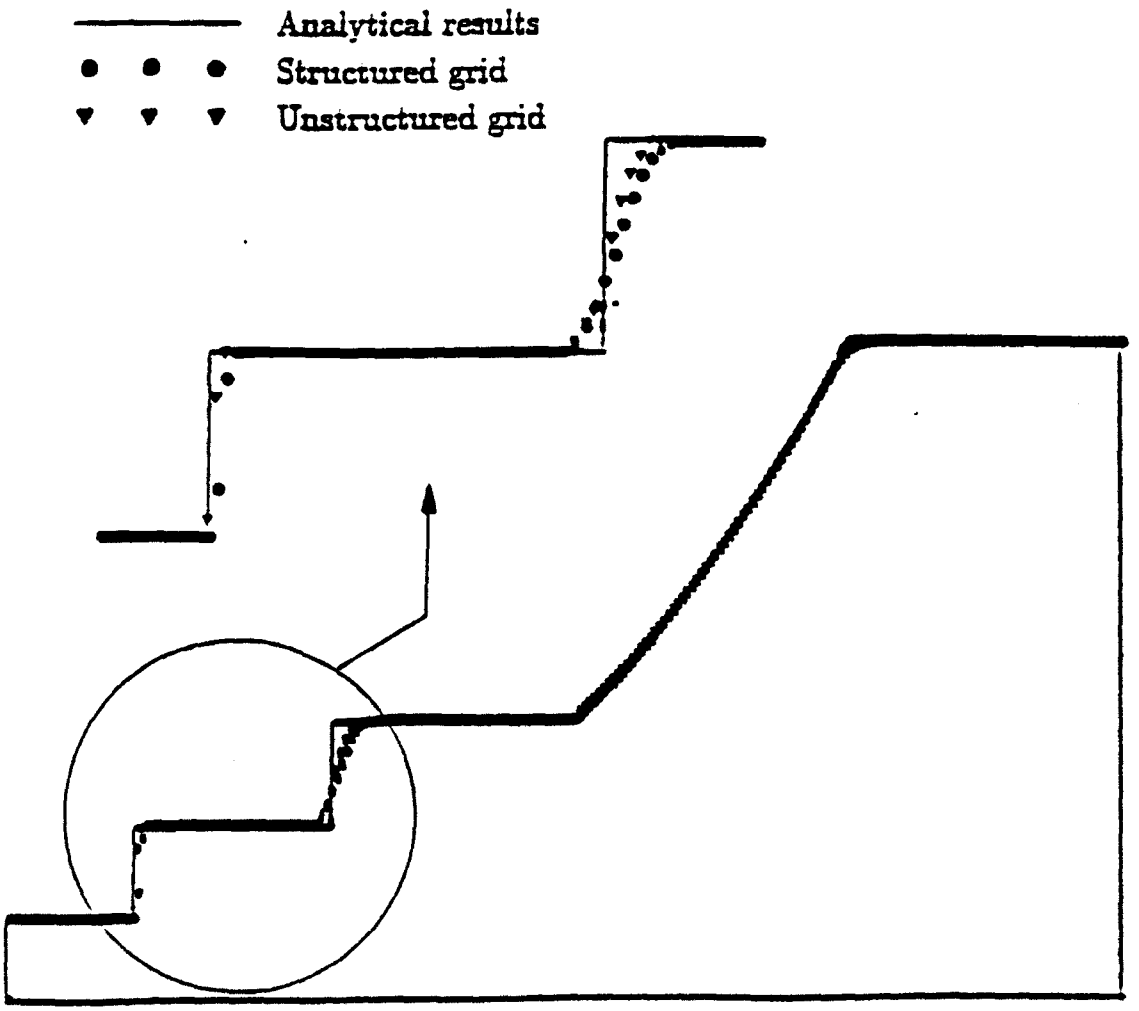


Figure 2.1.2 Density profile comparison between analytical results and results obtained by applying the second-order Godunov algorithm using structured or unstructured grids.

2.2 MULTIPHASE MULTICOMPONENT REACTIVE FLOW

Multiphase multicomponent reacting flows (MPMCRF) consist of material media (continua and particles) dispersed in a flow varying in space and time. Two basic approaches can be used to describe MPMCRFs, heterogeneous and homogeneous phase descriptions. For homogeneous mixtures one assumes that each mixture component occupies the same volume with other mixture components on an equal basis ($V_1=V_2=\ldots=V_n=V$). This approach is justified for an interpenetrating mixture of gases or a dilute suspension of particles in a gas. In a heterogeneous description of a suspension, each component occupies only part of the global volume ($V_1+V_2+\ldots+V_n=V$). Therefore in the mathematical description of the heterogeneous suspensions, in addition to the density of the i-th component ρ_i one needs to introduce the fractional volume of the components:

$$\phi_1 + \phi_2 + .. \phi_N = 1 \quad (\phi_i > 0), \tag{2.18}$$

which allows us to define the real density of each of the components as $\sigma_i = \frac{\rho_i}{\phi_i}$.

Consider a chemically reacting system containing an *N*-component gaseous phase and one solid particle phase. The conservation equations can be written as follows:[3]

Conservation of Mass

Global continuity for gaseous phase:

$$\frac{\partial \rho_g}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho_g u_{(g)j}\right) = I_g . \tag{2.19}$$

Continuity of N-1 species or components of gaseous phase:

$$\frac{\partial Y^l}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho_g Y^l\left(u_{(g)j} + V^l_j\right)\right] = \omega^l + I^l_g . \tag{2.20}$$

Continuity for solid particle phase:

$$-\frac{\partial \rho_p}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho_p u_{(p)j}\right) = -I_p . \tag{2.21}$$

In the above equation of mass conservation, ρ_g is the partial gas density. The gas volume fraction is ϕ_g. The relation between partial gas density and material density σ_g is $\rho_g = \phi_g \sigma_g$. Similarly, we define the partial phase density ρ_p and material density σ_p. The relation between the two is then $\rho_p = \phi_p \sigma_p$. We assume volume conservation, which is

$$\phi_g + \phi_p = 1. \tag{2.22}$$

The species diffusion velocity V_i^l is calculated through Fick's law:

$$V_i^l = -\frac{D}{Y^l}\frac{\partial Y^l}{\partial x_i}, \tag{2.23}$$

where D is the diffusion coefficient. Finally, we assume mass conservation in all chemical reactions:

$$\sum_l^N w_i^l = 0 \quad \text{and} \quad I_p = -\sum_l^N I_g^l = -I_g. \tag{2.24}$$

Conservation of Momentum

Conservation of momentum for the gaseous phase:

$$\begin{aligned}&\frac{\partial\left(\rho_g u_{(g)i}\right)}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho_g u_{(g)i} u_{(g)j} + \delta_{ij}\phi_g p_g\right] \\ &= \frac{\partial}{\partial x_j}\left[\left(\mu' - \frac{2}{3}\mu\right)\frac{\partial u_{(g)k}}{\partial x_k}\delta_y + \mu\left(\frac{\partial u_{(g)i}}{\partial x_j} + \frac{\partial u_{(g)i}}{\partial x_i}\right)\right] \\ &- F_i^{(p)} + I_p u_{(p)i}.\end{aligned} \tag{2.25}$$

Conservation of momentum for the particle phase:

$$\frac{\partial\left(\rho_p u_{(p)i}\right)}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho_p u_{(p)i} u_{(p)j} + \delta_{ij}\phi_p p_p\right] = \frac{\partial}{\partial x_j}\left(\tau_{(p)ij}\right) + F_i^{(p)} - I_p u_{(p)i}. \tag{2.26}$$

In the above momentum conservation equations, p_p and p_g are the pressure of the solid particle and gaseous phases respectively, $F_i^{(p)}$ represents the interaction force between the two phases, and $\tau_{(p)ij}$ is the stress tensor for the particle phase, to be determined by experimental or empirical correlations.

For the gaseous phase, the stress tensor can be written as

$$\tau_{(g)ij} = -p\delta_{ij} + \left(\mu' - \frac{2}{3}\mu\right)\frac{\partial u_k}{\partial x_k}\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \tag{2.27}$$

where μ is the dynamic viscosity and μ' is the second viscosity coefficient.

Conservation of Energy

The governing equation for conservation of energy for the gaseous phase is usually written

$$\frac{\partial\left[\rho_g\left(e_g+0.5u_{(g)i}u_{(g)i}\right)\right]}{\partial t}+\frac{\partial}{\partial x_j}\left[\rho_g u_{(g)j}\left(e_g+0.5u_{(g)i}u_{(g)i}\right)+\phi_g p_g u_{(g)j}\right]$$
$$=-\frac{\partial q_{(g)j}}{\partial x_j}+Q_g+\frac{\partial}{\partial x_j}\left(u_{(g)i}\left[\left(\mu'-\frac{2}{3}\mu\right)\frac{\partial u_{(g)k}}{\partial x_k}\delta_{ij}+\mu\left(\frac{\partial u_{(g)i}}{\partial x_i}\right)\right]\right) \qquad (2.28)$$
$$-F_{(p)i}u_{(p)i}+Q_p.$$

The equation for conservation of energy for the particle phase has the form

$$\frac{\partial}{\partial t}\left[\rho_p\left(C_s T_p+0.5u_{(p)i}\right)\right]+\frac{\partial}{\partial x_j}\left[\rho_p u_{(p)j}\left(C_s T_p+0.5u_{(p)i}u_{(p)i}\right)+\phi_p u_{(p)j}p_p\right]$$
$$=-\frac{\partial q_{(p)j}}{\partial x_j}+\frac{\partial}{\partial x_j}\left(u_{(p)j}\tau_{(p)ij}\right)+F_i^{(p)}u_{(p)i}-Q_p. \qquad (2.29)$$

In the conservation of energy, $\frac{\partial q_{(g)j}}{\partial x_j}$ and $\frac{\partial q_{(p)j}}{\partial x_j}$ are the heat flux gradients in the jth direction in the gaseous and particle phases, respectively. Q_p is the energy source due to heterogeneous chemical reactions (between the gaseous and particle phases), plus heat transfer between the two phases. Here $Q_g=\sum_{i=1}^{N}\left(-\omega_i\Delta h_{fi}^{\circ}\right)$ is the energy source due to homogeneous (gaseous) chemical reactions, which is defined in the chemical reaction model.

Conservation of Number of Particles

An equation for total conservation of particles is given by

$$\frac{\partial n_p}{\partial t}+\frac{\partial}{\partial x_j}\left(n_p u_{(p)j}\right)=0. \qquad (2.30)$$

Equation of State

The equation of state for all gases can be put into the generic form

$$e_g=f_g\left(p_g,\sigma_g,Y^1,\cdots,Y^N\right), \qquad (2.31)$$

where for an ideal gas the form is

$$e_g = \frac{p_g}{\sigma_g(\gamma_g - 1)} \tag{2.32}$$

and

$$p_g = \sigma_g R_u T_g \sum_{i=1}^{N} \frac{Y^i}{W^i}. \tag{2.33}$$

An equation of state for the particle phase can be written in symbolic form as

$$p_p = f(\sigma_p, T_p), \tag{2.34}$$

where the exact form of Eq. (2.34) that is to be used in a numerical simulation depends on experimental data or results from physical approximations.

In the above equations, γ_g is the ratio of specific heats of the gaseous mixture and R_u is the universal gas constant.

Chemical Reaction Model

A phenomenological chemical reaction model for the gaseous phase (including M chemical reactions) has been formulated as

$$\omega^i = W^i \sum_{k=i}^{M} \left(\nu_k'^{(1)} - \nu_k^{(1)}\right) B_k T^{\alpha k} \exp\left(\frac{E_{ak}}{R_u T_g}\right) \prod_{j=1}^{N} \left(\frac{X^j p_g}{R_u T_g}\right)^{\nu_{jk}}. \tag{2.35}$$

Similarly, a phenomenological heterogeneous (for gas and particle phases) chemicals reaction model can be written symbolically as

$$I_{(p)} = f(T_p, P_p, \ldots), \tag{2.36}$$

and again the exact form of Eq. (2.36) will depend on experimental data or approximations from physical models.

The following nomenclature defines the symbols used in the above system of equations (2.19) - (2.36): B – chemical reaction collision frequency factor; C_S – specific heat for solid particle; e – internal energy; D – mass diffusion coefficient; E_{ak} – activation energy for the kth reaction; F_i – interphase force in ith direction; I – source function generated by chemical reaction; p_g – gas pressure; q_i – heat flux in the ith direction; R_u – universal gas constant; t – time; T – temperature; u_i – velocity in ith direction; V_i – species diffusion velocity in ith direction; W^i – molecular weight of ith component of gas; x_i – coordinate in ith direction; X^i – mode fraction of ith component of gas; Y^i – mass fraction of ith component of gas; α – temperature exponent of the kth reaction; γ – ratio of specific heat; λ – thermal conductivity of gas; μ – dynamic viscosity of gas; μ' – second

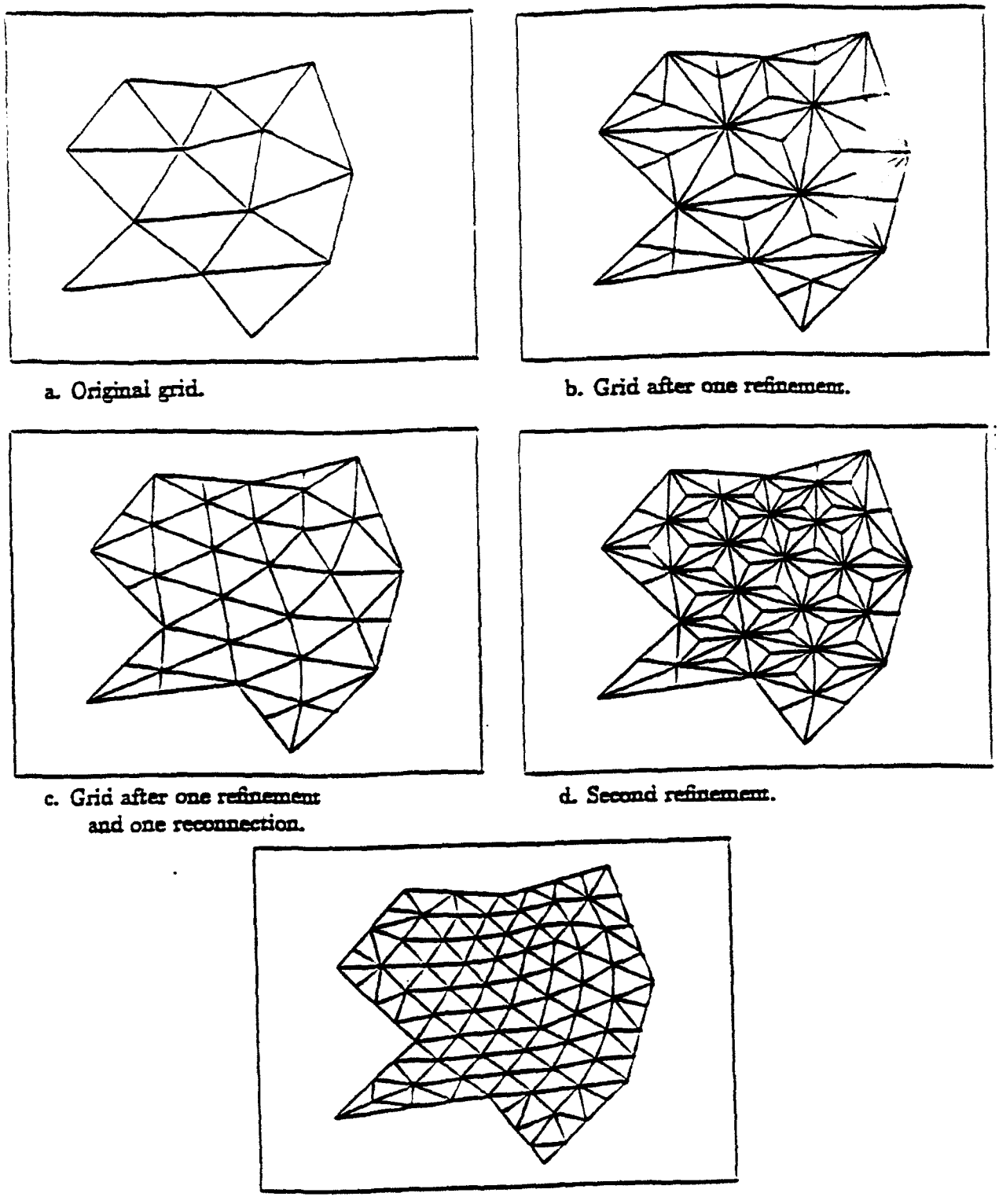
viscosity coefficient of gas; τ_{ij} – stress tensor; ω^{l} – mass rate of production of species i; ρ – density; $v_{i,k}$ – stoichiometric coefficient for species i appearing as a reactant in the kth reaction; $v'_{i,k}$ – stoichiometric coefficient for species i appearing as a product in the kth reaction; ϕ – volume fraction; σ – material density. Subscripts are defined as follows: g – gas phase; p – particle phase; i,j,k, – direction indexes; l – species index. Superscripts refer to species type.

The comprehensive mathematical model and system of equations given above for an MPMCRF simulation of advanced material synthesis processes is based on volume averaging, assuming that each phase or component can be described by continuous flow. Such averaging leads to a loss of information that can be recovered by appropriate closure relations. The closure relations such as interphase forces, chemical reaction models and the equations of state are usually developed from correlations involving experimental data or from simple physical or chemical models describing interphase or intraphase interactions. Such correlations are generally only valid within the range of known experimental data; the choice of appropriate closure models reflects the understanding of the underlying physical and chemical nature of the system to be simulated.

2.3 DIRECT DYNAMIC REFINEMENT METHOD FOR UNSTRUCTURED TRIANGULAR GRIDS

As stated, an unstructured grid is very well suited to implement boundary conditions on complex geometrical shapes and to refine the grid if necessary. This feature of the unstructured triangular grid is compatible with efficient use of memory resources. The adaptive grid enables the code to capture moving shocks and large-gradient flow features with high resolution. The memory resources available can be very efficiently distributed in the computational domain to accommodate the resolution needed to capture the main features of the solution's physical property. Dynamic refinement controls the resolution priorities. These priorities can be set according to the physical features that the user wishes to emphasize in the simulation. The user has control over the resolution of the physical features, without being restricted to the initial grid. The alternative to Direct Dynamic Refinement is the hierarchical dynamic refinement[6] (H refinement) that keeps a history of the initial grid (mother grid) and the subdivision of each level (daughter grids). In the H refinement method, it is necessary to keep overhead information on the level of each triangle subdivision, and double indirect indexing is required to keep track of the H refinement process. As mentioned, H refinement relies heavily on the initial grid as it subdivides the mother grid, and returns to that grid after the passage of the shock.

The Direct Dynamic Refinement (DDR) method for capturing the shock requires the refinement to be in the region ahead of the shock. This requirement minimizes the dissipation in the interpolation process when assigning values to the new triangles created in the refined region. Additionally, it requires that the coarsening of the grid be done after the passage of the shock. The interpolation and extrapolation in the refinement and coarsening of the grid is done in the region where the flow features are smooth.



a. Original grid.

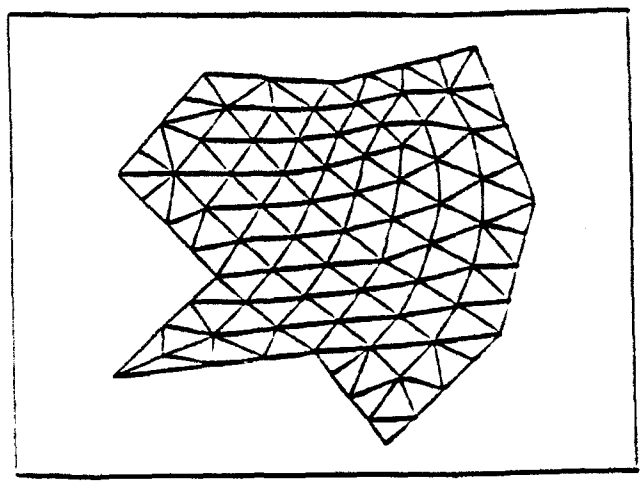
b. Grid after one refinement.

c. Grid after one refinement and one reconnection.

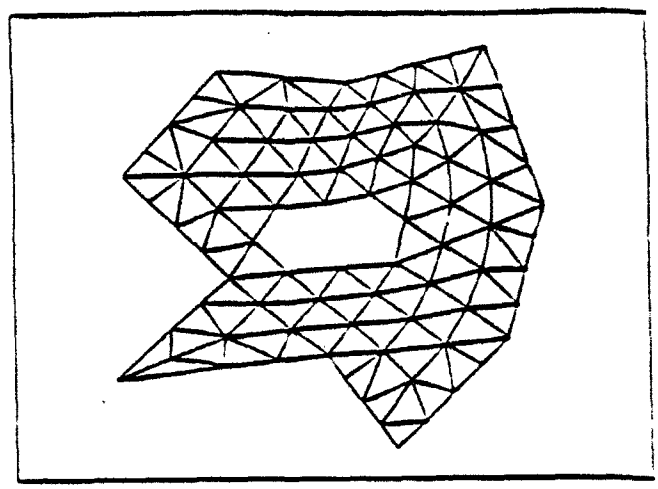
d. Second refinement.

e. Second reconnection.

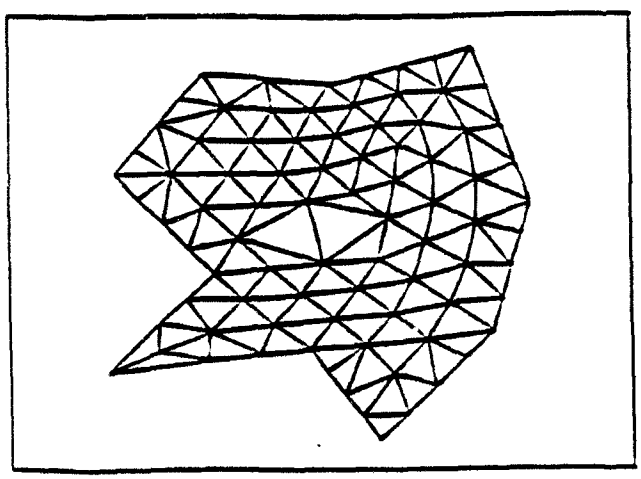
Figure 2.3.1 Illustration of the grid refinement process.



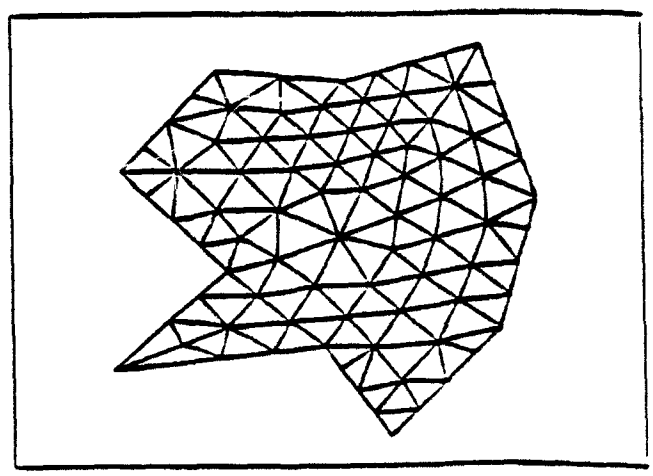
a. Original grid.



b. Point removal.



c. Constructing of new cells.



d. Grid after reconnection and relaxation.

Figure 2.3.2 Illustration of the grid coarsening process.

The physics of the problem is involved in the process that identifies the region of refinement and coarsening. Error criteria can be derived that will allow grid adaptation to stationary or moving pressure or density discontinuities, region of high vortical activity, etc. There should be an error indicator specially suited to capture and identify the region of importance for each of the physics features to be resolved.

The original FUGGS algorithm reported in Ref. 9 was modified to enable adaptivity of the grid in the course of the computation. In AUGUST, we have implemented an algorithm with multiple criteria for capturing a variety of features that might exist in the physics of the problem to be solved. To identify the location of a moving shock, we use the flux of total energy into triangles. The fluxes entering and leaving triangles are the most accurate physical variables computed by the Godunov algorithm for solving the Euler equations, and are used to update the physical variables for each timestep in each triangle. A shock wave means that there is a "step-function" change in the cell that is caused by an influx of energy, momentum or density. Stationary shocks can be identified by density gradients that are computed in the course of implementing the Second-Order Godunov algorithm.

In Fig. 2.3.1, we illustrate the basic process of refinement accomplished in the DDR. The original grid is shown in Fig. 2.3.1a. Figure 2.3.1b illustrates a one-step scheme refinement in which a new vertex is introduced into a triangular cell, forming three new cells. This is followed by reconnection, which modifies the grid as demonstrated in Fig. 2.3.1c. The process of refinement and reconnection can be continued until the necessary grid resolution is achieved, as illustrated in Figs. 2.3.1d and 2.3.1e. This direct approach to the grid refinement provides extreme flexibility in resolving local flow features. A similar simple method is applied to grid coarsening. In the first step of coarsening the marked vertices, all associated elements of the grid are simply removed, as shown in Fig. 2.3.2a. During the second step, this void in the grid is filled with new larger triangles (Fig. 2.3.2b) and then reconnected as shown in Fig. 2.3.2c. When a very large increase of the local grid density is required, these simple algorithms of grid addition and deletion can create triangles with an unacceptably large aspect ratio. To avoid this condition for very large grid densities (when the area of the triangles in the dense region is reduced to less than 2% of the initial area), we introduced local grid relaxation immediately after the grid deletion procedure.

AUGUST has proven to be a very robust and efficient algorithm capable of computing transient phenomena, and with the ability to sense the region of physical interest and resolve it by refining and coarsening the grid as needed.

2.4 STRUCTURED/UNSTRUCTURED COMPOSITE GRIDS

Structured rectangular grids allow the construction of numerical algorithms that perform an efficient and accurate integration of fluid conservation equations. The efficiency of these schemes results from the extremely low storage overhead needed for domain decomposition and the efficient and compact indexing that also defines domain

connectivity. These two factors allow code construction based on a structured domain decomposition that can be highly vectorized and parallelized. Integration in physical space on orthogonal and uniform grids produces the highest possible accuracy of the numerical algorithms. The disadvantage of structured rectangular grids is that they cannot be used for decomposition of computational domains with complex geometries.

The early developers of computational methods realized that, for many important applications of Computational Fluid Dynamics (CFD), it is unacceptable to describe curved boundaries of the computational domain using the stair-step approximation available with the rectangular domain decomposition technique. To overcome this difficulty, the techniques of boundary-fitted coordinates were developed. With these techniques, the computational domain is decomposed into quadrilaterals that can be fitted to the curved domain boundaries. The solution is then obtained in the physical space using the geometrical information defining the quadrilaterals, or in the computational coordinate system that is obtained by transformation of the original domain into a rectangular domain. The advantage of this technique is that it employs the same indexing method as the rectangular structured domain decomposition methods that also serve to define domain connectivity. The boundary-fitted coordinate approach leads to efficient codes, with approximately a 4:1 penalty in terms of memory requirement per cell as compared with rectangular domain decomposition. However, this approach is somewhat restricted in its domain decomposition capability, since distortion or large size variations of the quadrilaterals in one region of the domain leads to unwanted distortions or increased resolution in other parts of the domain. An example of this is the case of structured body fitted coordinates used for simulations of flows over a profile with sharp trailing edges. In this case, increased resolution in the vicinity of the trailing edge leads to increased resolution in the whole row of elements connected to the trailing edge elements.

The most effective methods of domain decomposition developed to overcome this disadvantage are those using unstructured triangular grids. These methods were developed to cope with very complex computational domains. The unstructured grid method, while efficient and powerful in domain decomposition, results in codes that must store large quantities of information defining the grid geometry and connectivity, and have large computational and storage overheads. As a rule, an unstructured grid code requires greater storage by a factor of 10, and will run about 20 times slower per cell per iteration than a structured rectangular code.

Unstructured grid methods are used to their best advantage when combined with grid adaptivity. This feature usually allows dynamic decomposition of the computational domain subregions, thus leading to an order-of-magnitude reduction in the number of cells for some problems, as compared to the unstructured grid lacking this adaptive capability. However, this advantage is highly dependent on the problem solved. Adaptive unstructured grids have an advantage over the unadaptive unstructured domain decomposition if the area of high-resolution domain decomposition is less than one tenth of the global area of the computational domain. This explains why the adaptive unstructured method may be extremely effective for solutions with multiple shock waves

in complex geometries, but becomes extremely inefficient when high resolution is needed in a substantial area of the computational domain.

Our approach to domain decomposition combines the structured and unstructured methods for achieving better efficiency and accuracy. Under this method, structured rectangular grids are used to cover most of the computational domain, and unstructured triangular grids are used only to patch between the rectangular grids (Fig. 2.4.1) or to conform to the curved boundaries of the computational domain (Fig. 2.4.2). In these figures, an unstructured triangular grid is used to decompose the regions of the computational domain that have a simple geometry.

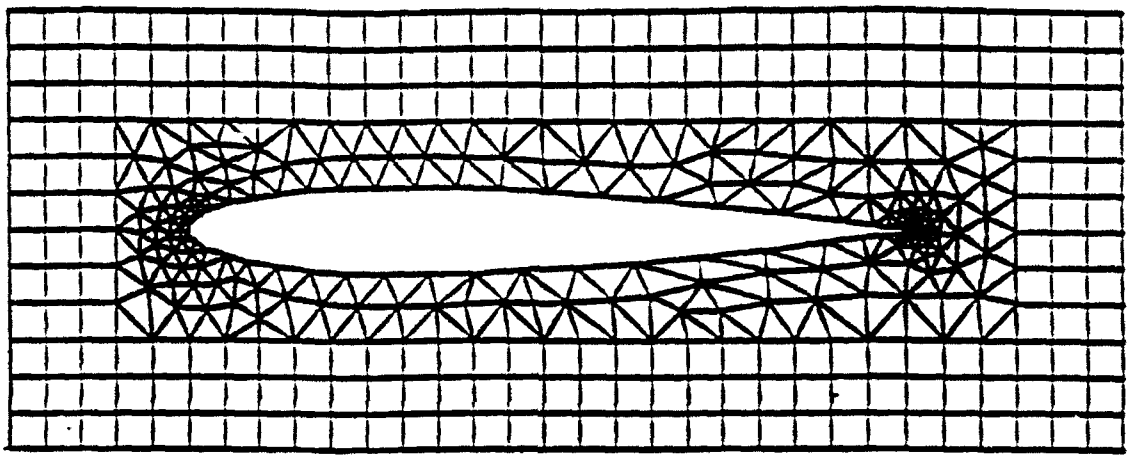


Figure 2.4.1 A possible candidate configuration for hybrid structured/unstructured domain decomposition.

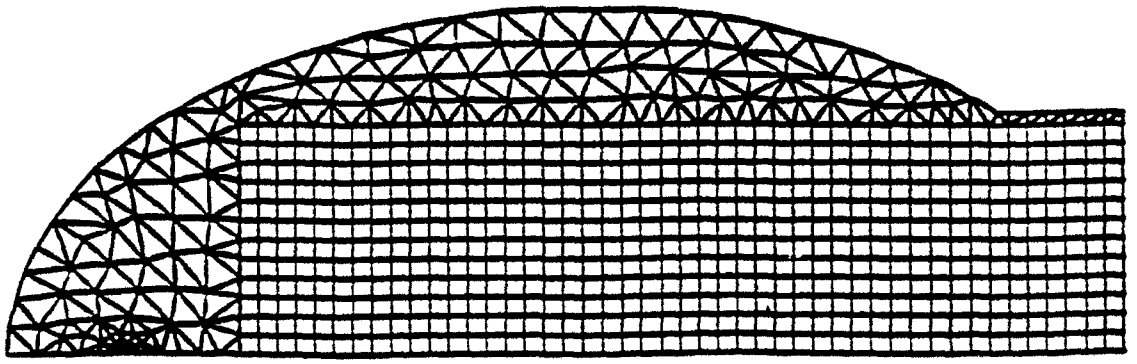


Figure 2.4.2 Hybrid structured/unstructured grid used to simulate ellipsoidal reflector, showing adaptation to curved boundaries.

2.5 THREE-DIMENSIONAL CAPABILITY

Once the 2D capability was fully developed, we initiated the development of a fully 3D CFD adaptive unstructured simulation capability. This part of our effort is not yet documented in published material.

The first step in solving a 3D CFD problem is to discretize the computational domain into tetrahedra. The grid generation is a recognized bottleneck in the time it takes to evaluate an aerodynamic configuration.[15] One could even argue that it represents the most time-consuming portion of the evaluation process. There are a handful of codes that are capable of gridding any given domain into tetrahedra. In order to shorten the part to our objective of achieving a 3D adaptive solver capability, we decided to make use of an existing grid generator to provide the initial grid.

OCTREE,[16] which was developed at Rensselaer Polytechnic Institute (RPI), is a Finite Octree 3D grid generator that provides the initial grid for our adaptive solver. The productivity of a 3D grid generator is a function of the complexity of the surfaces that define the domain of computation. Usually, this task is the most time-consuming and painful for the user. OCTREE does not have a CAD/CAM package to assist the user in defining the surfaces of the geometry to be gridded. Nevertheless, OCTREE is a very robust and reliable grid generator.

The OCTREE algorithm is based on the concept of dividing the computational domain into octants. In each step, the code defines three planes that halve the domain in each of the three dimensions, thus dividing the volume into eight octants. Those three planes intersect the surfaces of the geometry, defining vertices. All the vertices are collected and sorted into topological loops. If the vertices are not sufficient to define correct topological loops, the code will subdivide the corresponding octant into eight smaller octants until the topology is fully resolved. The user is allowed to specify the level of the local octree subdivision he wishes to resolve. Once the code subdivides the volume into the level of octree specified by the user or needed to resolve the local geometrical details, the code defines tetrahedra to fill the volume of the computation domain. The code provides the user with an option that improves the quality of the tetrahedra by smoothing and eliminating the very small ones.

As stated, OCTREE provides the initial grid for the 3D solver. The adaptivity of the mesh is controlled by specific physical features that the user defines based on the physics of the problem to be solved. The adaptivity of the mesh automatically traces the physical features in the simulation and refines and coarsens the mesh accordingly to the criteria and the resolution specified by the user.

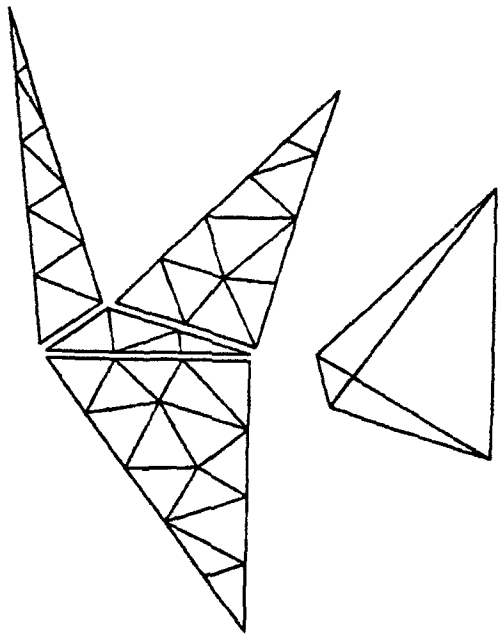


Figure 2.5.1 An elongated tetrahedron can be refined using smaller tetrahedra that are nearly regular.

The target tetrahedra are refined by first subdividing each of the four surfaces into smaller triangles that satisfy the resolution set by the user. There are no constraints on the way each face is subdivided. Each edge of the face is subdivided according to the local resolution needed, and the points along the edges are connected to construct the best triangles possible. The code adds points inside the face along with points on the edges to achieve an adequate triangulation of the faces. The triangles of the four faces of the target tetraheda are used to define smaller tetrahedra that will fill the volume. If needed, the code will add points inside the volume of the target tetrahedron to achieve the best tetrahedra possible. The code has the ability to reconnect tetrahedra to improve quality. The reconnection is done by pulling out an edge, sorting all the tetrahedra connected to this edge, deleting these tetrahedra and filling the void with better shaped tetrahedra.

Figure 2.5.1 shows how the subdivision process can fill an irregular (elongated) tetrahedron with smaller tetrahedra that are nearly equilateral. (This is not the case with H refinement.) Figure 2.5.2 shows points used to create octree refinement to grid a problem involving surface-mine blast effects on the underside of a truck. Figure 2.5.3 is the corresponding tetrahedral grid. The calculated overpressures on the surface of the truck underbody for an eight-pound explosive are shown in Sec. 3.4.

The algorithm used to solve the 3D gasdynamic equations is an immediate extension of the 2D case described in Sec. 2.1. Thus, Eq. (2.6) is replaced by

$$\int_{\Omega} \nabla U_i^{\text{cell}} \, dV = \int_{\partial\Omega} U_j^{\text{face}} \, d\mathbf{S}, \tag{2.6'}$$

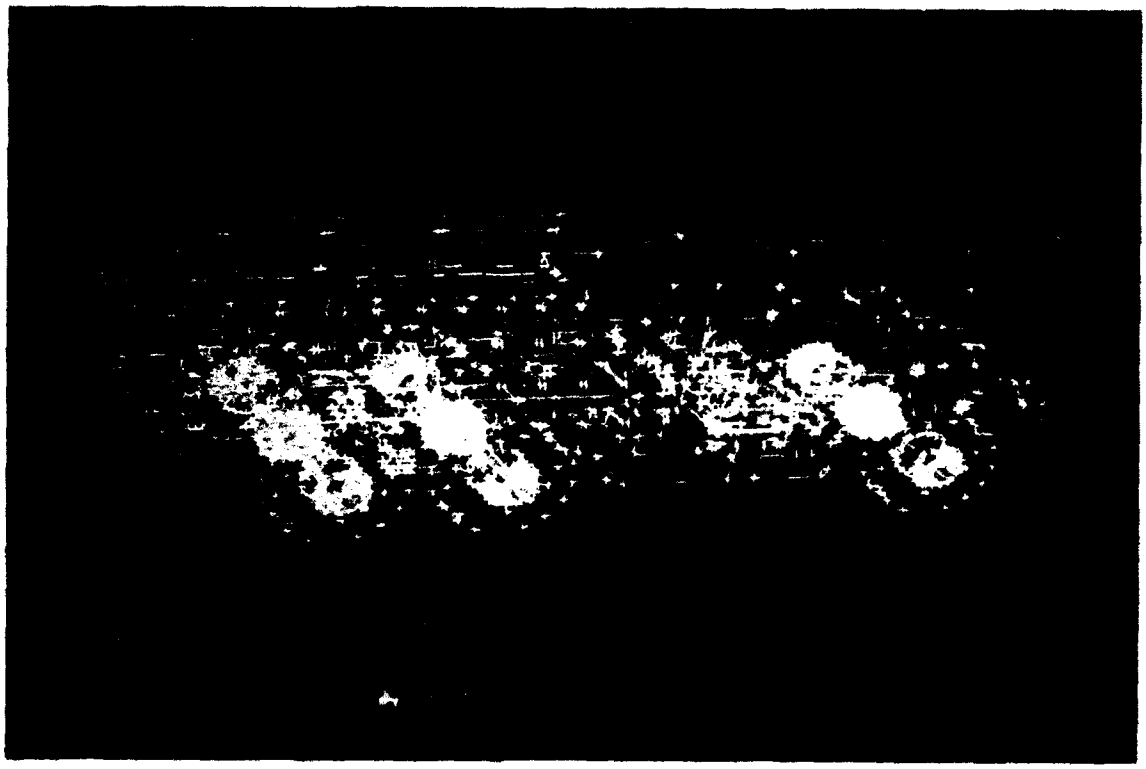


Figure 2.5.2 Points used to define structure of vehicle.

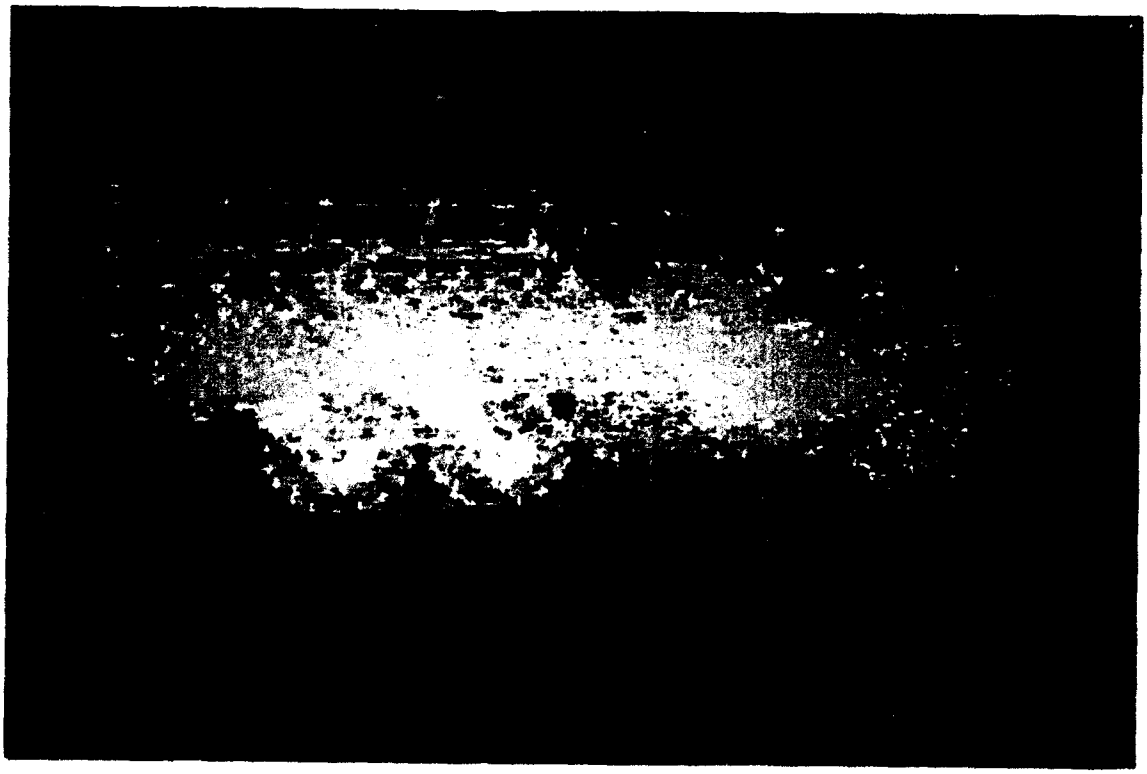


Figure 2.5.3 Tetrahedral grid generated by Finite Octree method.

where now Ω and $\partial\Omega$ are the volume and surface of a tetrahedron, and dV and dS are the corresponding differential elements. Its finite-difference approximation is

$$\nabla U_i^{\text{cell}} = \frac{1}{V} \sum_{j=1}^{4} \tilde{U}_j^{\text{face}} \, \mathbf{n}_j \, \Delta S_j , \tag{2.7'}$$

where the summation is over the four faces and $\mathbf{n}_j$ is the normal to the jth face with surface area dS_j. In the equations corresponding to Eqs. (2.9) - (2.11), the range 1, 2, 3 is replaced by 1, 2, 3, 4. Equations (2.12) - (2.16) are formally unchanged, and Eq. (2.17) becomes

$$\left(\mathrm{M}_x \, \mathrm{M}_n\right) = \begin{cases} \max\left(\lambda_i^+, 0\right) & \text{for the cell on the left of the edge} \\ \min\left(\lambda_i^-, 0\right) & \text{for the cell on the right of the edge.} \end{cases} \tag{2.17'}$$

3. APPLICATIONS

The AUGUST code was extensively validated for a wide range of known CFD problems and has been shown to be a robust simulation tool. It has been utilized on a variety of problems which span flow regimes ranging from low subsonic Mach numbers to hypersonic Mach numbers (Table 3.1).

Appendix C contains a complete collection and description of the CFD problems addressed during the UUGM research. Additional details of the AUGUST code are contained in SAIC's progress report for the UUGM DARPA program, submitted in November 1991. Here we briefly describe the most noteworthy applications.

It is worth underscoring again that in the past it was necessary to use a sequence of codes as well as numerical parameter adjustment to bridge the gap in flow phenomena occurring in different flow regimes. An important point to be made here is that the AUGUST code allows robust, accurate and efficient solutions across these different regimes without the necessity of adjusting coefficients to enhance convergence accuracy or efficiency.

Table 3.1 AUGUST Applications

Problem	Activity
1. Calculation of potential flow about an ellipse.	Reported at the 4th International Symposium on Computational Fluid Dynamics, Davis, CA, Sept 1991.
2. Hypersonic flow past a flat plate.	Reported at AIAA Reno Meeting (AIAA-90-0699), 1990.

Problem	Activity
3. Shock on wedge with adaptive gridding.	Reported at the Free Lagrange Conference, Jackson Lake, WY, 1990.
4. Simulation of mine explosion under a vehicle.	Performed for U.S. Army Corps of Engineers, Ft. Belvoir, VA.
5. Simulation of pulsed detonation engine.	Published in J. of Propulsion and Power Nov/Dec 1991 Vol. 7 (6) pp. 857-865 and AIAA Meeting, Reno, NV 1992.
6. Shock focusing in air using structured/unstructured grids.	Presented at the ICAM Conference, Rutgers, NJ, June 1992.
7. Nonideal airburst calculations for multiphase media.	Performed for the Defense Nuclear Agency, Alexandria, VA.
8. Flow in the SARL wind tunnel.	Performed for Wright-Patterson AFB.
9. Simulation of a shock on a double wedge.	Presented at the Army workshop on Adaptive Methods for PDEs, RPI, March 1992.
10. Supersonic spray coating devices.	To be published.
11. Nanomaterial synthesis.	Published in Surf. Coating Tech. **49**, 387-393 (1991).
12. Dusty flow over a cylinder.	To be published in AIAA Journal.
13. Image processing.	Presented at SPIE conference on Applications of Digital Image Processing, San Diego, July 1991.
14. Multiphase detonation.	Published in Combust. Sci. Tech. **89**, 201-218 (1993).

3.1 POTENTIAL FLOW OVER AN ELLIPSE

One of the outstanding early CFD computational challenges (from the point of view that no satisfactory solution had been obtained) was associated with simulating subsonic (Mach 0.2 and less) flow over a symmetric elliptical airfoil using the Euler equations (Fig. 3.1.1). All previous attempts to compute the flow over such an ellipse resulted in spurious lift and drag values that were significantly larger than the classical

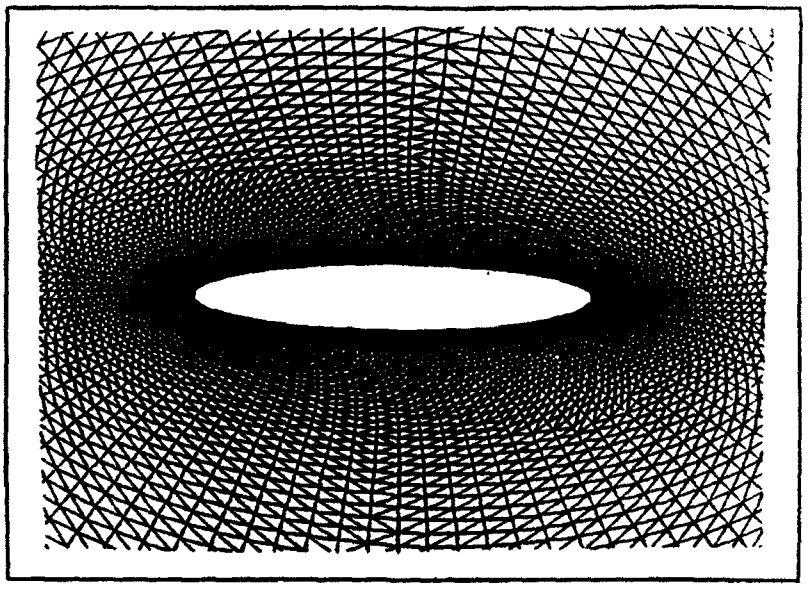


Figure 3.1.1 The grid used for simulating the flow over an ellipse.

potential flow solution. The potential flow result should have been closely approximated if there were no numerical viscosity present. This test case is important because, in transitioning from an Euler solver to a full Navier-Stokes solver, one needs confidence that the artificial (numerical) viscosity will not dominate the physical viscosity included in the Reynolds' stress terms. As shown in Appendix C-1, use of an earlier version of the AUGUST code, the Fast Unstructured Grid Godunov Solver (FUGGS) code provided solutions to this test case that were very close to the potential flow solution. Other attempts resulted in lift and drag values that were off by several orders of magnitude compared with the SAIC FUGGS results. The results described here were prepared for a poster presented to Dr. Arje Nachman, SAIC's UUGM AFOSR program monitor and Dr. James Crowley, SAIC's UUGM DARPA program manager.

3.2 HYPERSONIC FLOW PAST A FLAT PLATE

To demonstrate the versatility of the method for the entire range of flow regimes we have simulated a hypersonic flow test problem. One of the advantages of the Godunov methods is that over the whole range of calculations performed (low subsonic flow, supersonic flow, unsteady flow with strong shock, or hypersonic flow at Mach number M=32) it is unnecessary to change or adjust the numerical algorithm. In Ref. 17 the performance of first- and second-order Godunov methods was analyzed for hypersonic flow regimes. There, as a test problem, an analytical solution was used for a hypersonic flow around a flat plate of finite thickness. This solution was obtained based on the analogy between hypersonic flow over a flat plate of finite thickness and a strong planar explosion. Here we use an expression from Ref. 17 which defines the shape of the shock wave as a function of plate thickness d; γ is the adiabatic coefficient, and α is a nondimensional scale factor related to the energy released at the stagnation point.

$$Y_{SHOCK} = \left(\frac{1}{2} D_f \frac{dx^2}{2} \right)^{1/3}$$

where D_f is a coefficient of order unity,

$$a = k_1 (\gamma - 1)^{k_2 + k_3 \ln(\gamma - 1)}$$

with $k_1 = 0.36011$, $k_2 = 1.2537$, and $k_3 = -0.1847$.

As a direct comparison we solved the hypersonic flow problem for the same set of conditions as in Ref. 17:

$$U_\infty = 10011 \text{ m/sec}, \; p = 98.72 \text{ Pa}, \; \rho = 1.24 \times 10^{-3} \text{ kg/m}^3, \text{ and } \gamma = 1.2.$$

The grid used for this simulation is shown in Fig. 3.2.1a. This grid has ≈ 5500 vertices and its spatial resolution at the leading edge of the plate is of the same order as that of a 300 x 60 rectangular grid used in Ref. 5.

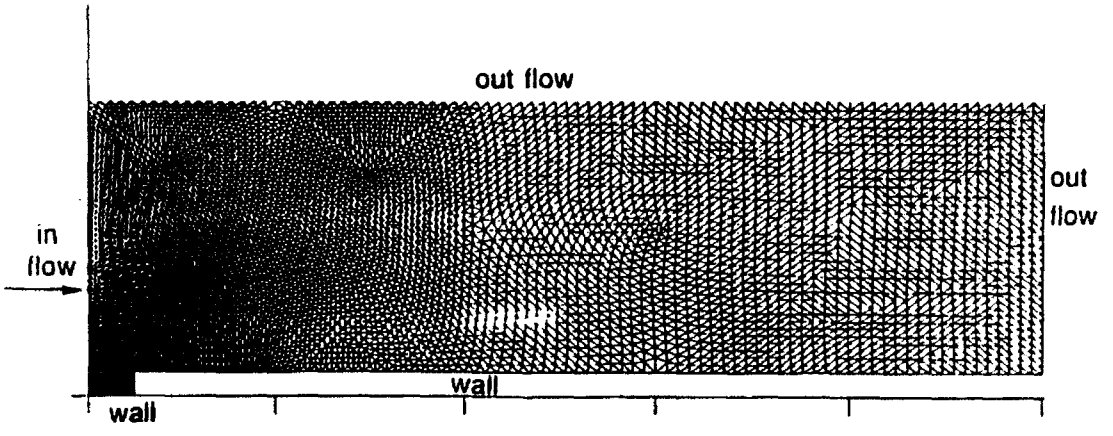


Figure 3.2.1a Grid for simulation of hypersonic flow over a flat plate.

Figure 3.2.1b shows results for this simulation in the form of pressure contours. Figure 3.2.1b also represents the location of the analytically calculated shock front by a discrete line (squares). The shock resolution and accuracy or its location are comparable to that obtained in Ref. 17 even though our triangular grid has less than one third as many nodes as the rectangular grid used in Ref. 17. This is because in constructing the triangular grid we had the flexibility to place the highest concentration of nodes in the area of the leading edge where the main properties of the flow are established.

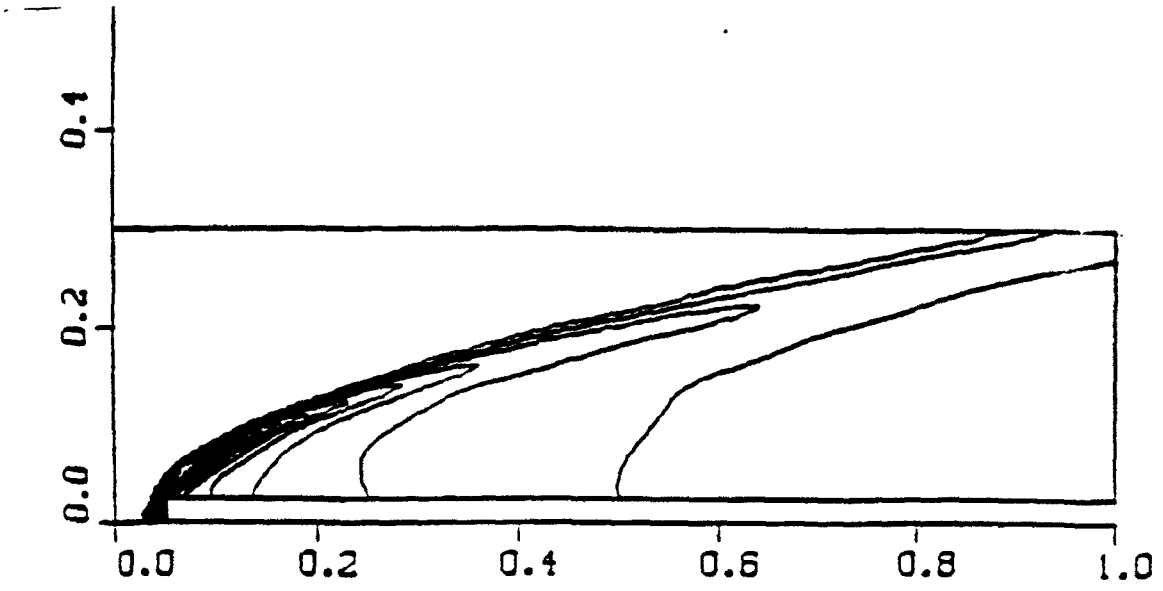


Figure 3.2.1b Second order solution for a flat plate, pressure contours. Mach = 32: 5509 grid vertices: $P_{max} = 5.0 \times 10^4$ Pa, $P_{min} = 98.7$ Pa.

3.3 SHOCK ON WEDGE WITH ADAPTIVE GRIDDING

An unstructured grid is very suitable for implementing boundary conditions on complex geometrical shapes and refining the grid if necessary. This feature of the unstructured triangular grid is compatible with efficient usage of memory resources. The adaptive grid enables the code to capture moving shocks and large-gradient flow features with high resolution. The memory resources available can be very efficiently distributed in the computational domain to accommodate the resolution needed to capture the main features of the physical property of the solution.

One strategy for doing this is called hierarchical dynamic refinement (H refinement). It keeps a history of the initial grid (other grid) and the subdivision of each level (daughter grid). H refinement subdivides the initial grid into two or four triangles in each level, and keeps track of the number of subdivision levels each triangle has undertaken. In the H refinement method, one has to keep overhead information on the level of each triangle subdivision, and needs double indirect indexing to keep track of the H refinement process. This slows down the computation by partially disabling the vectorization of the code. As mentioned, H refinement relies heavily on the initial grid as it subdivides the mother grid and returns back to it after the passage of the shock.

AUGUST and its predecessor FUGGS use a second-order Godunov solver on an unstructured grid. The refinement strategy incorporated in these codes is called Direct Dynamic Refinement. For shock capturing, Direct Dynamic Refinement basically requires

the refinement to be in the region ahead of the shock. This requirement minimizes the dissipation in the interpolation process when assigning values to the new triangles created in the refined region. Additionally, it requires that the coarsening of the grid should be done after the passage of the shock. In principle, the interpolation and extrapolation in the refinement and coarsening of the grid are done in the region where the flow features are smooth.

FUGGS was used with direct dynamic refinement to solve the transient behavior of the flow entering a channel with a wedge (prism) having an inclination of 27°. The flow enters the channel from the left with Mach number 8.7. A sequence of snapshots illustrates the density contours, and the grid for each timestep is given in Figs. 3.3.1a - 3.3.3a (contour plots) and 3.3.1b - 3.3.3b (grid). These figures clearly demonstrate the automatic adaptation of the grid to the moving shocks and the ability to capture the detailed physics of the simulation with very high resolution and minimal memory requirements. The initial grid can clearly be seen to the right of the shock ("ahead") in the early stage of the shock propagation from left to right. The coarsening algorithm is able to produce a reasonable mesh in the region trailing the shock as shown in the figures.

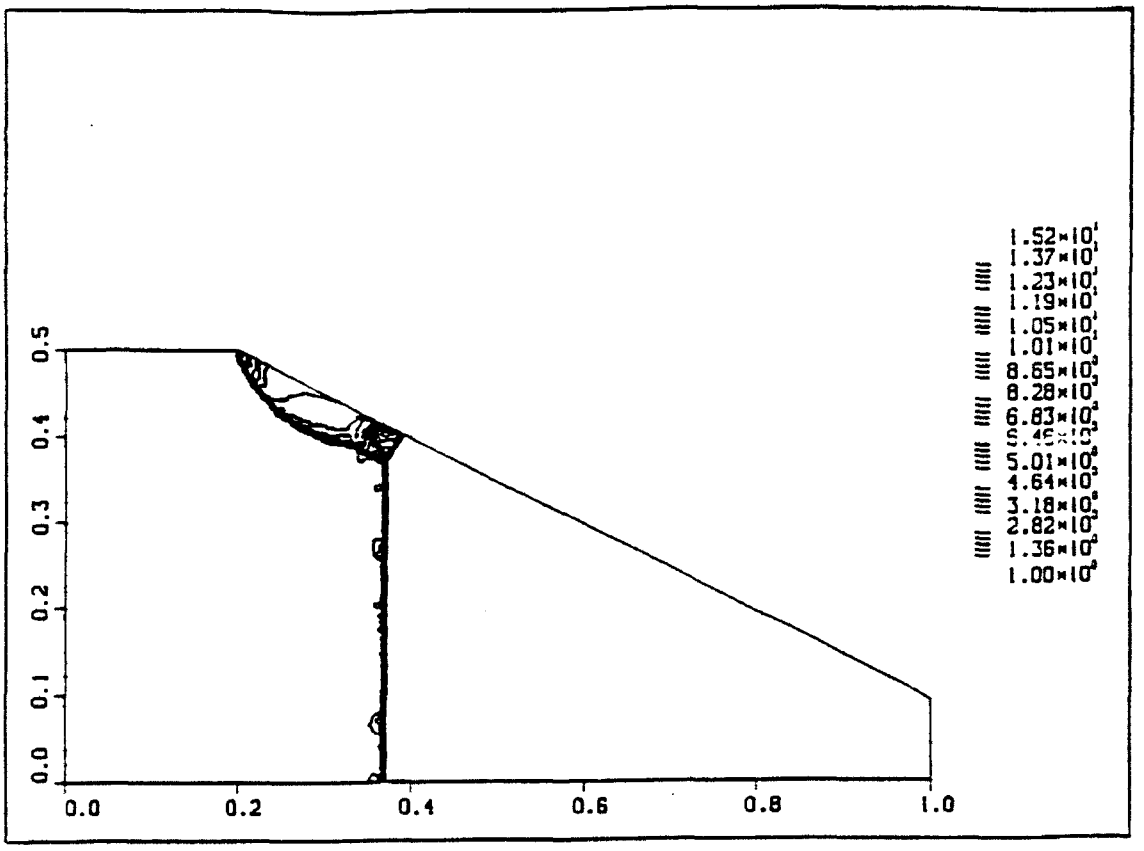


Figure 3.3.1a Density contours at early time for shock in planar channel (M = 8.7, wedge angle = 27°).

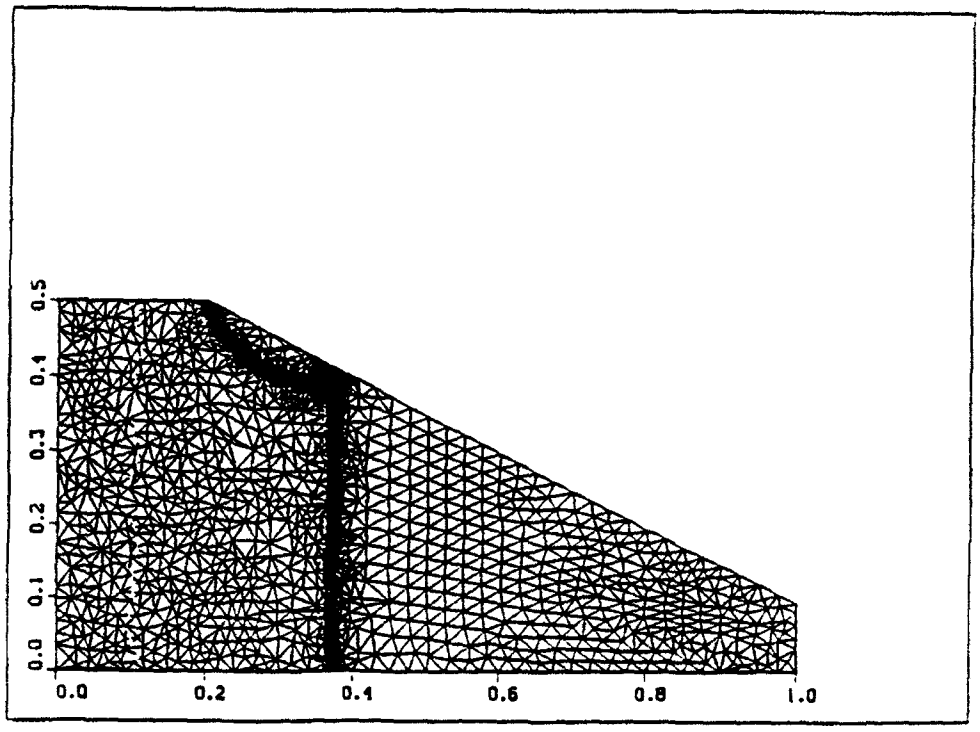


Figure 3.3.1b Grid at early time for shock in planar channel
(M = 8.7, wedge angle = 27°).

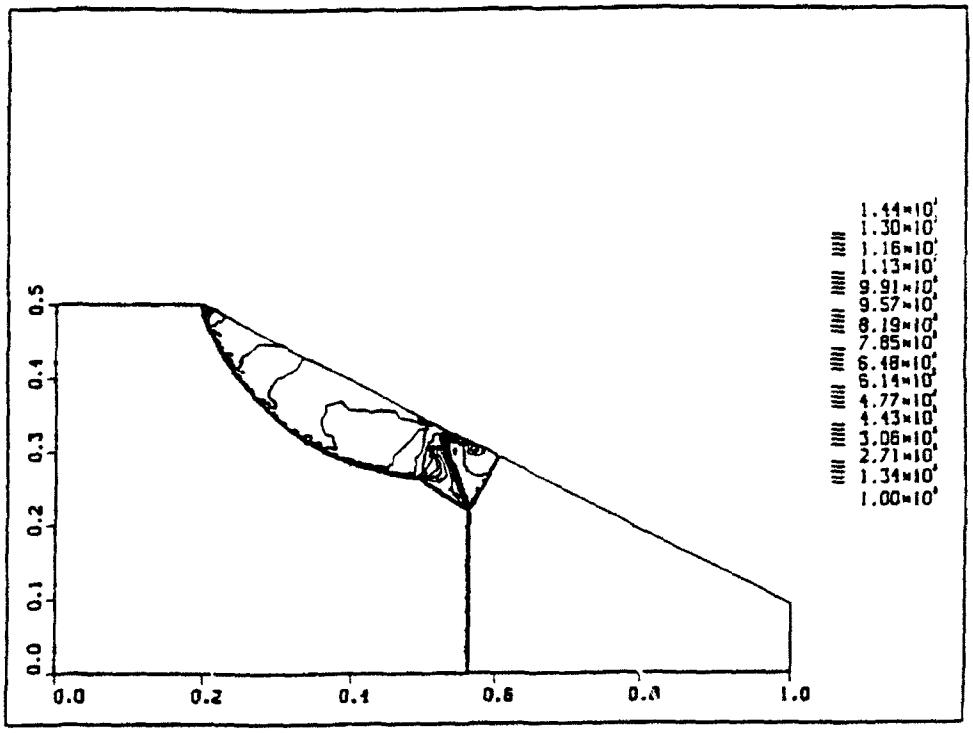


Figure 3.3.2a Density contours at intermediate time for shock in planar channel
(M = 8.7, wedge angle = 27°).

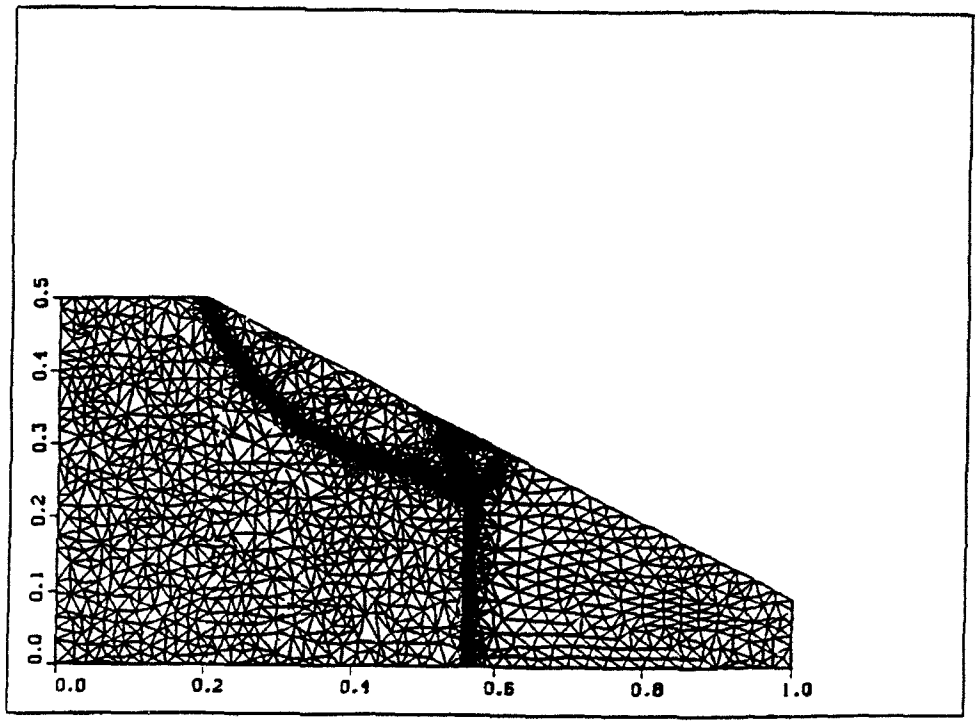


Figure 3.3.2b Grid at intermediate time for shock in planar channel (M = 8.7, wedge angle = 27°).

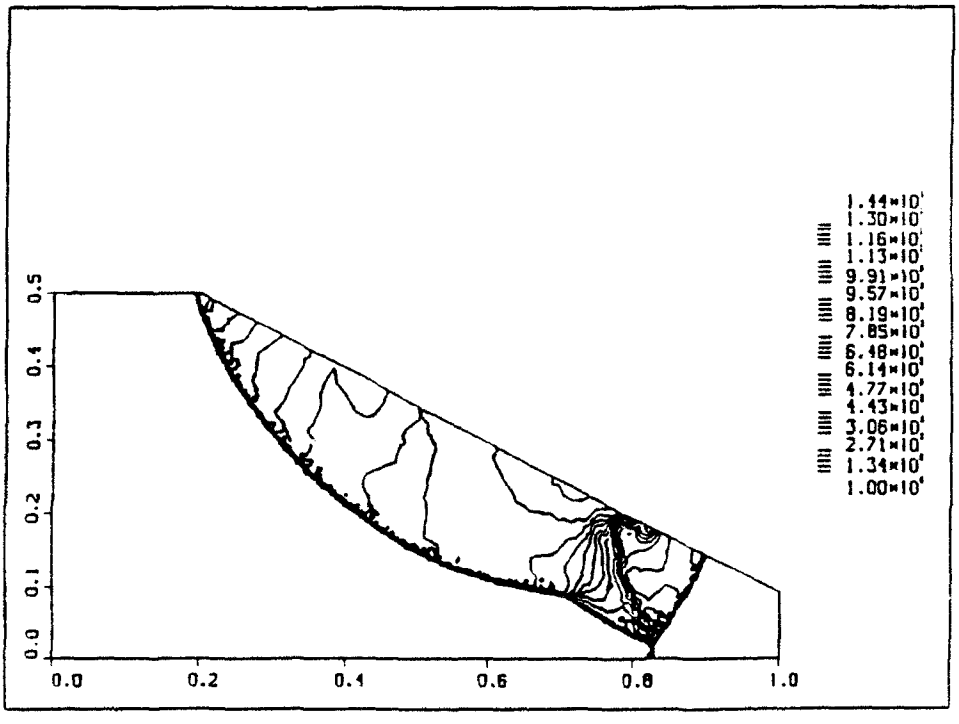


Figure 3.3.3a Density contours at late time for shock in planar channel (M = 8.7, wedge angle = 27°).

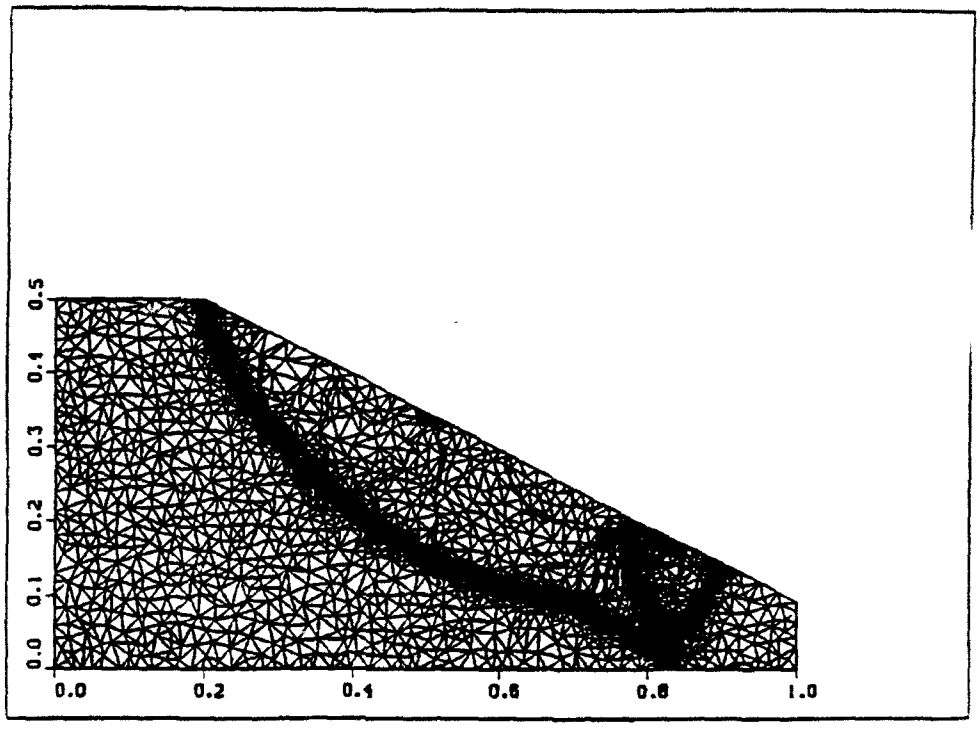


Figure 3.3.3b Grid at late time for shock in planar channel
(M = 8.7, wedge angle = 27°).

3.4 MINE EXPLOSION UNDER VEHICLE

The main objective of this joint Marine-Army program was the development of vehicles hardened against antitank (AT) land mines. The basic vehicle is the M925 5-ton cargo truck. Numerical simulations were used to determine the dynamic loads produced by the AT mine detonation on the cargo bed and other structural elements of the truck.

The algorithms, techniques and codes developed under the UUGM program provided two key elements necessary for the numerical simulations for this project: a) flexibility in describing the very complex geometry of the truck; b) high resolution-calculation of the shocks and other discontinuities using an adaptive unstructured grid. A version of the AUGUST-2D code developed under the UUGM program is being used for the analysis of blast resistance of different truck geometries.

We have carried out four such calculations, using four, eight, eight, and 20 pounds of C-4 explosive. These employed fixed (nonadaptive) meshes with 30,000 (4-1b case), 21,000 (8-lb cases).

A one- or two-dimensional calculation was performed to produce the initial blast profiles laid down on the three-dimensional grid. Aside from the amount of explosive, the calculations differed in the following ways: all but the 4-lb blast were centered beneath

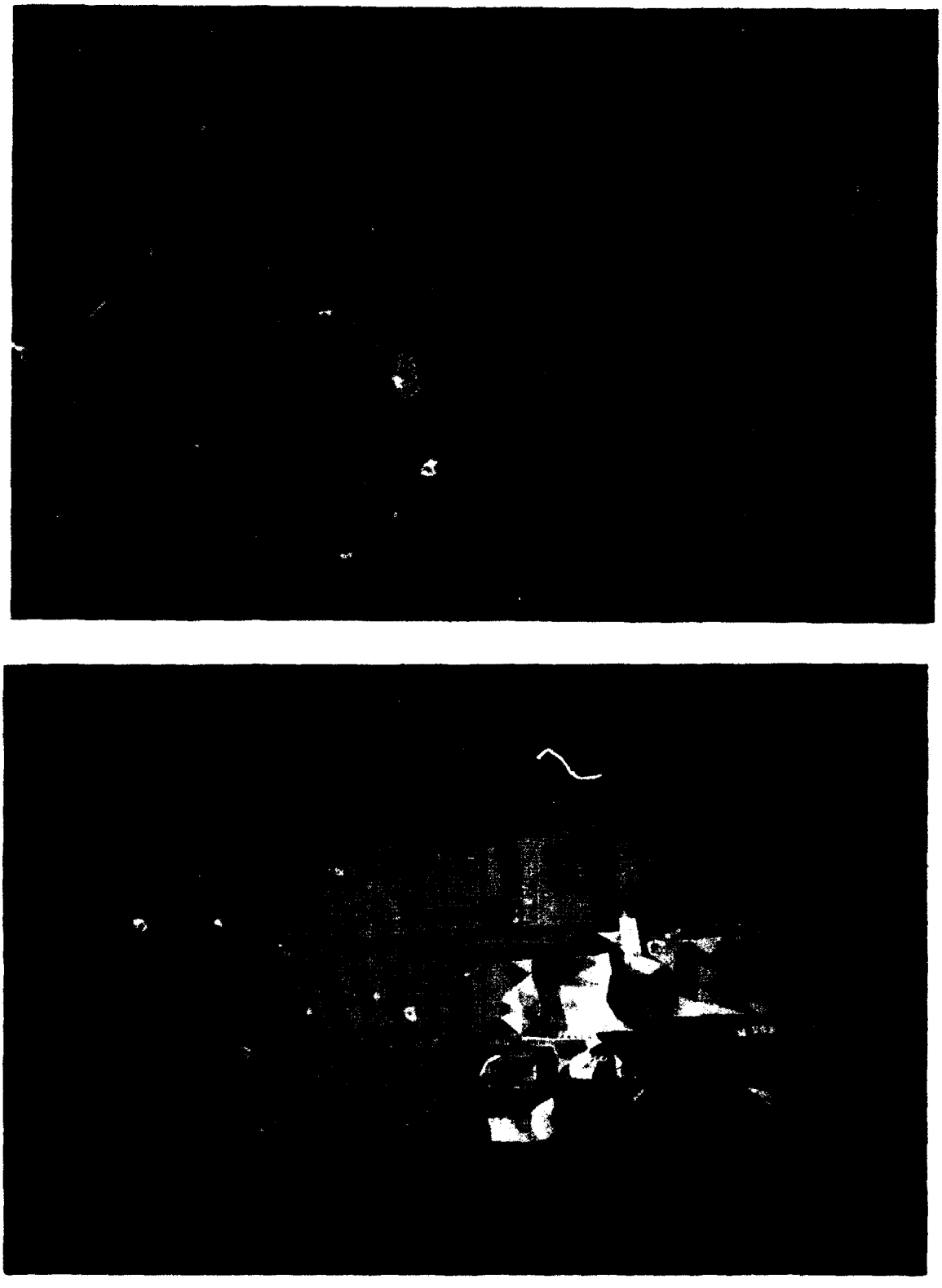


Figure 3.4.1 Two views of interaction between mine blast and M925 cargo truck: pressure contours at t = 0.574 msec.

the left front wheel of the truck (the 4-lb blast was situated 70 cm further back); for the first 8-lb case a crater with diameter 60 cm and depth 30 cm was situated underneath the blast.

All but the second 8-lb case used an ideal-gas equation of state with $\lambda = 7/5$ for the air and detonation products. Twenty pressure "sensors" positioned on the mesh at points corresponding to the pressure gauges used in actual field tests were used to record the pressure and impulse histories there for comparison with the experimental data.

The calculations were run out to about 4.5 msec. The pressure stations closest to ground level and to the blast center exhibited peaks up to ~ 10^3 psi. In some cases multiple peaks were present, corresponding to reflected shocks.

An example of the domain decomposition of the computational grid for a typical mine-truck interaction problem is shown in Fig. 2.5.2. In Fig. 2.5.3 the unstructured triangular grid is used to describe a cross section of an M925 cargo truck. Use of unstructured grids allows detailed description of the truck geometry. Figure 3.4.2 shows results of the simulation in the form of pressure contours overlaid on the unstructured grid, viewed from two different directions halve a millisecond after the detonation.

At Ft. Belvoir's request, SAIC also assessed the damage to a mine-clearing plow due to a single detonation of an AT mine at close range during the Desert Storm operation. At that time, Ft. Belvoir RDEC had responsibility for support of countermine activity in the Desert Storm operation.

To simulate the plow-mine blast interaction, SAIC used computational capabilities partially developed under the UUGM program. Use of unstructured triangular grids again enables detailed description of the plow geometry and use of Direct Dynamic grid Adaptation method allows detailed simulation of the complex pattern of the shock wave reflections.

In Fig. 3.4.2 the initial stage of the blast-plow cross section interaction is shown in the form of pressure contours overlaid on the dynamically adapting grids. In Fig. 3.4.3 a more advanced stage of the blast-structure interaction is shown in the same format as in Fig. 3.4.2. The adaptive grid allows high resolution of a complex blast interaction phenomena.

SAIC has also simulated the structural response of the plow to the dynamic load that is defined by the gas dynamic simulations described above. In Figs. 3.4.4a - d results are shown for the plow deformation in response to dynamic load. Recent experimental assessment of the plow damage showed that SAIC predictions correctly described blast damage to the plow.

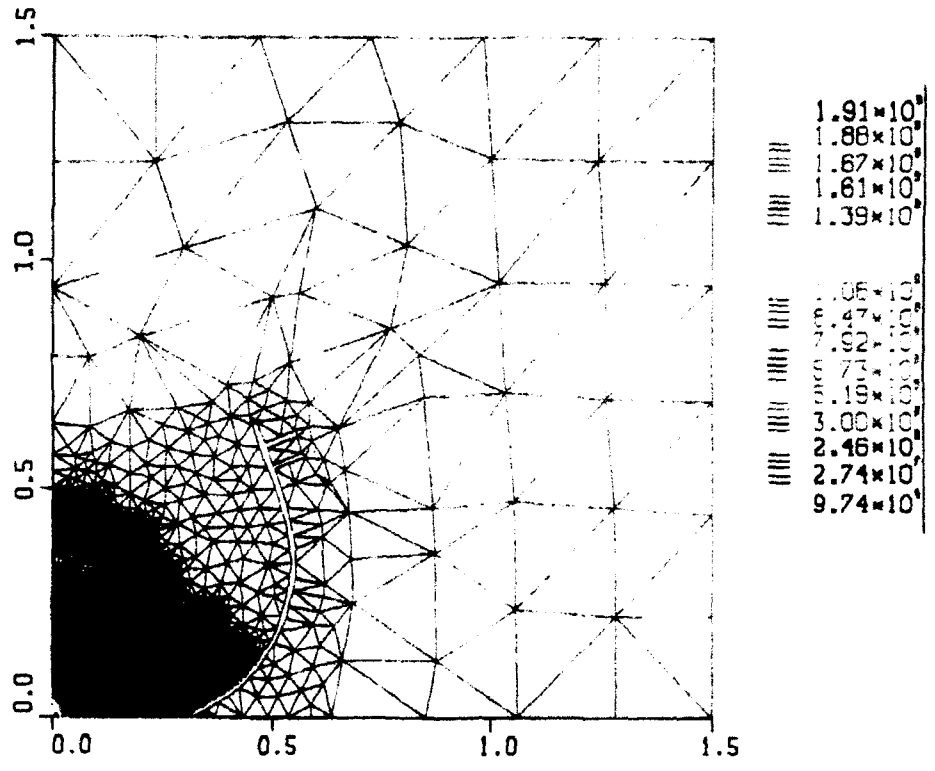


Figure 3.4.2 Blast – plow interaction: pressure contours in initial stage.

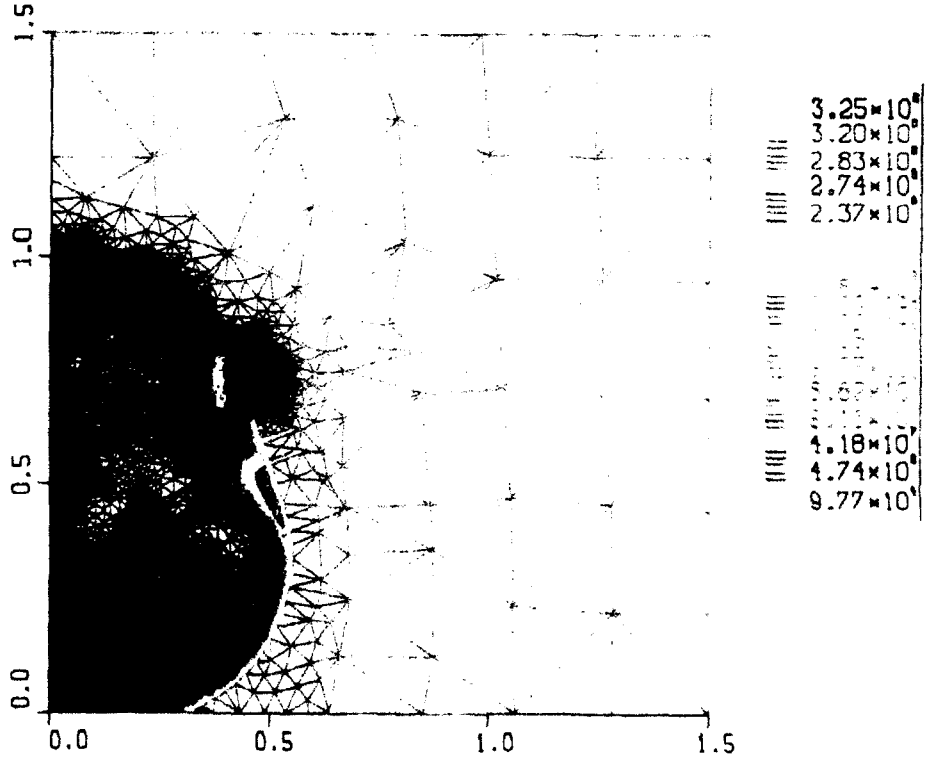


Figure 3.4.3 Blast – plow interaction: pressure contours in advanced stage

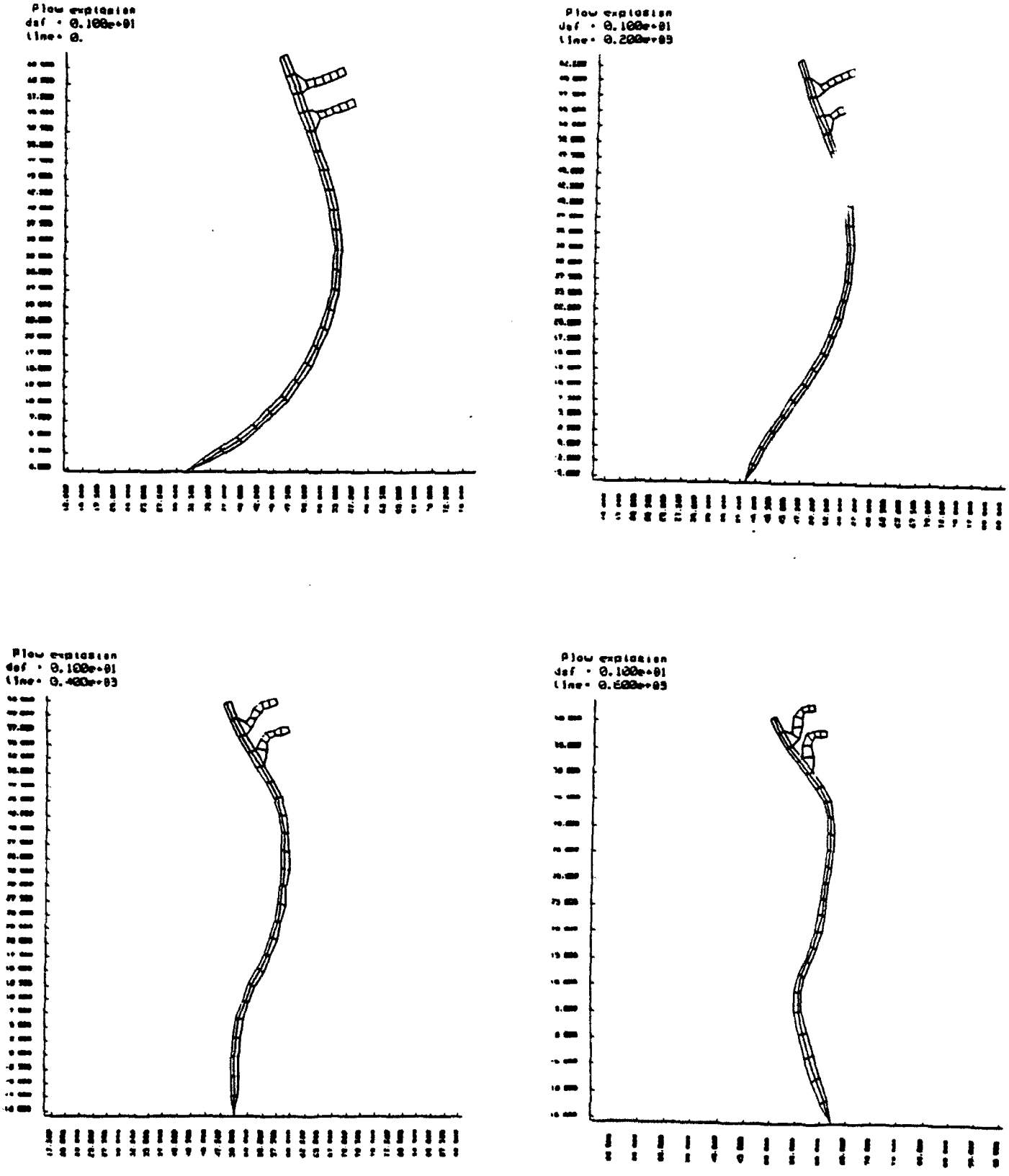
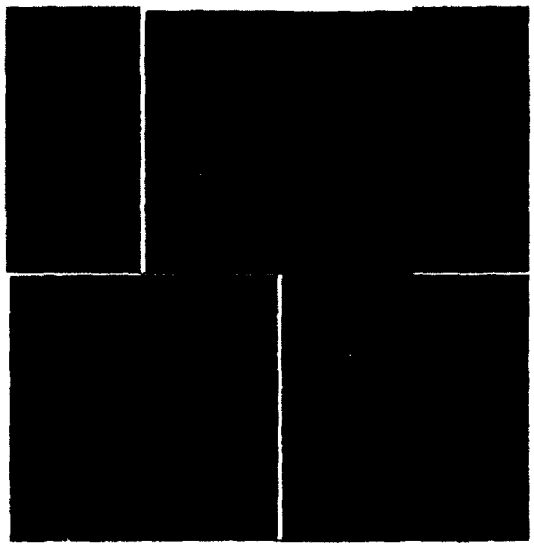
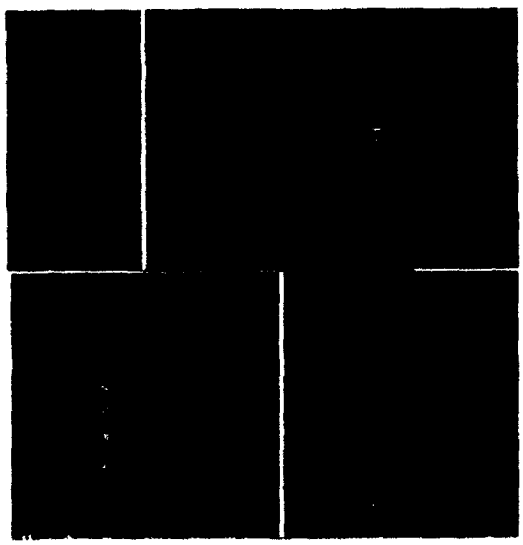


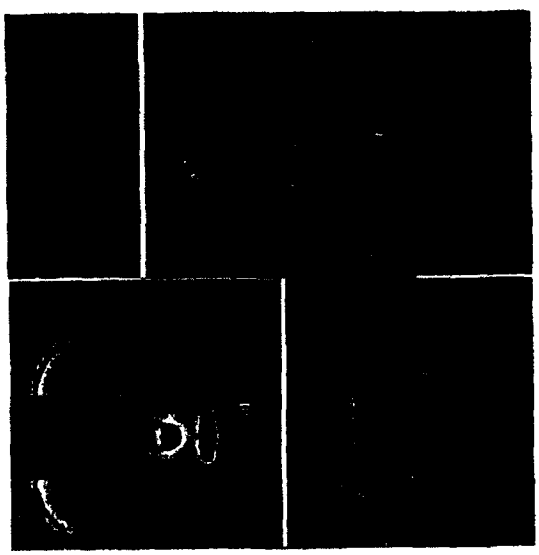
Figure 3.4.4 Structural response of the plow to blast load:
a) $t = 0$; b) $t = 200$ msec; c) $t = 400$ msec; d) $t = 600$ msec.



a. Predetonation stage



b. Detonation



c. Detonation product expansion

Figure 3.5.1 Pulsed detonation engine simulation: flow tracers.

3.5 PULSED DETONATION ENGINE

The main objective was the development of a revolutionary propulsion concept based on intermittent detonative combustion. Development of this concept will result in a new class of engines with performance surpassing those of small turbines at significantly reduced cost. SAIC's PDE research was noted in a recent article [Aviation Week, October 28, 1991, pages 68-89]. The PDE is currently considered as a candidate concept for numerous propulsion systems including the air-to-air missile, cruise missile, RPV engine, high altitude UAVs and others.

The codes developed under the UUGM program have enabled SAIC to conduct a detailed study of the PDE concept. The unstructured grids used in the simulations allowed us to describe the complex geometries of the detonation chamber and air inlets for a full missile configuration. Adaptive gridding allowed efficient and accurate simulation of the detonation and resulting shock waves interacting with the thrust-producing surfaces of the engine.

In Fig. 3.5.1 results are shown for the simulation of the PDE detonation cycle for a Mach 2 missile. Lagrangian flow tracers are used to track air and fuel trajectories in the engine. The figures demonstrate the sequence of stages in one PDE cycle. Shown in Figs. 3.5.1a-c are the fuel mixing stage, the detonation stage and the detonation products discharge stage, respectively. Detailed CFD analysis of various geometries and flow regimes allowed us to develop an understanding of the parametric dependence of the fundamental variables that determine the PDE performance.

3.6 SHOCK FOCUSING IN AIR

Research relating to focusing of shock and acoustic waves is of considerable practical interest for application to extracorporeal shock-wave lithotripsy (ESWL). A schematic of the cross section of such a reflector is shown in Fig. 3.6.1. Strong acoustic waves are generated in the left focal point of the ellipsoid by an instantaneous release of energy and are refocused at the right focal point. Ideally, focusing should be based on waves of acoustic intensity, since the nonlinear reflections of strong shock waves lead to significant distortions in wave propagation and impair simple geometrical focusing.

Figure 3.6.1 shows the computational domain and grid for the ellipsoidal reflector. Figure 3.6.2 shows the simulation results at time $t = 1.21 \times 10^{-6}$sec. At this stage, the wave front that propagated to the left has undergone full reflection and the reflected wave propagates in the direction of the incident wave to the right. Figure 3.6.3 shows the pressure contours ($t = 8.41 \times 10^{-4}$sec) when the maximum focused pressure is obtained in the system. The incident front has left the computational domain, and the maximum pressure occurs in a small volume in the vicinity of the right focal point. The maximum focused pressure has reached 1.37×10^{5} Pa and is located 11 mm to the right of the focal point of the ellipsoid. In all the figures presented, the method of composite domain decomposition works extremely well, producing seamless solutions at the interfaces.

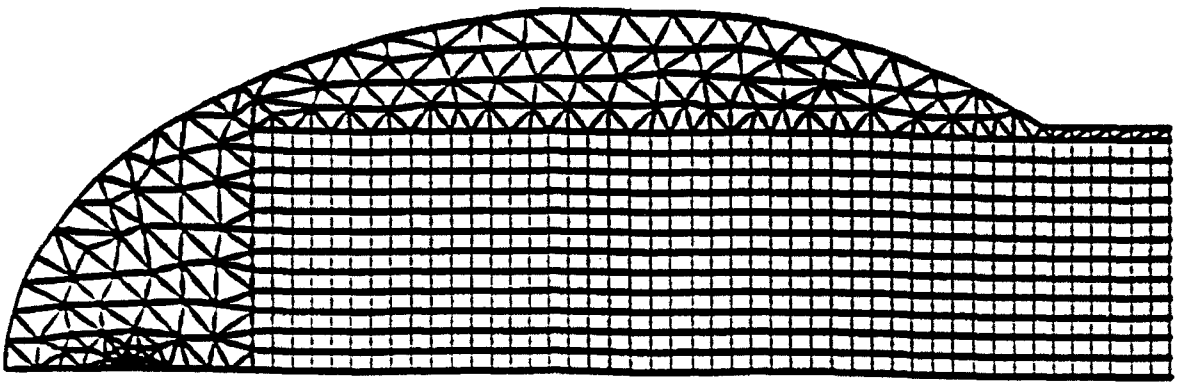


Figure 3.6.1a Hybrid structured/unstructured grid
used for numerical simulation of ellipsoidal reflector.

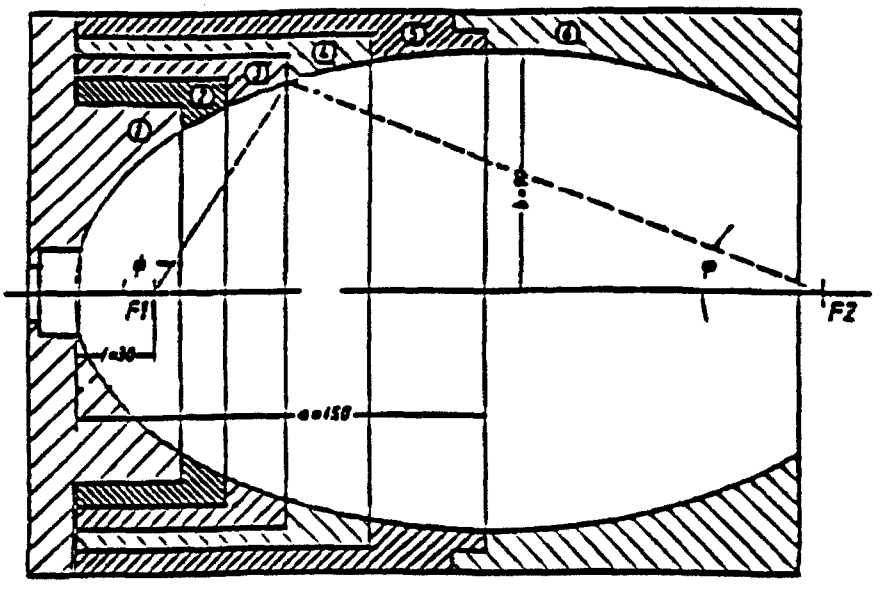


Figure 3.6.1b A schematic drawing of the center cross section of the ellipsoidal reflector.

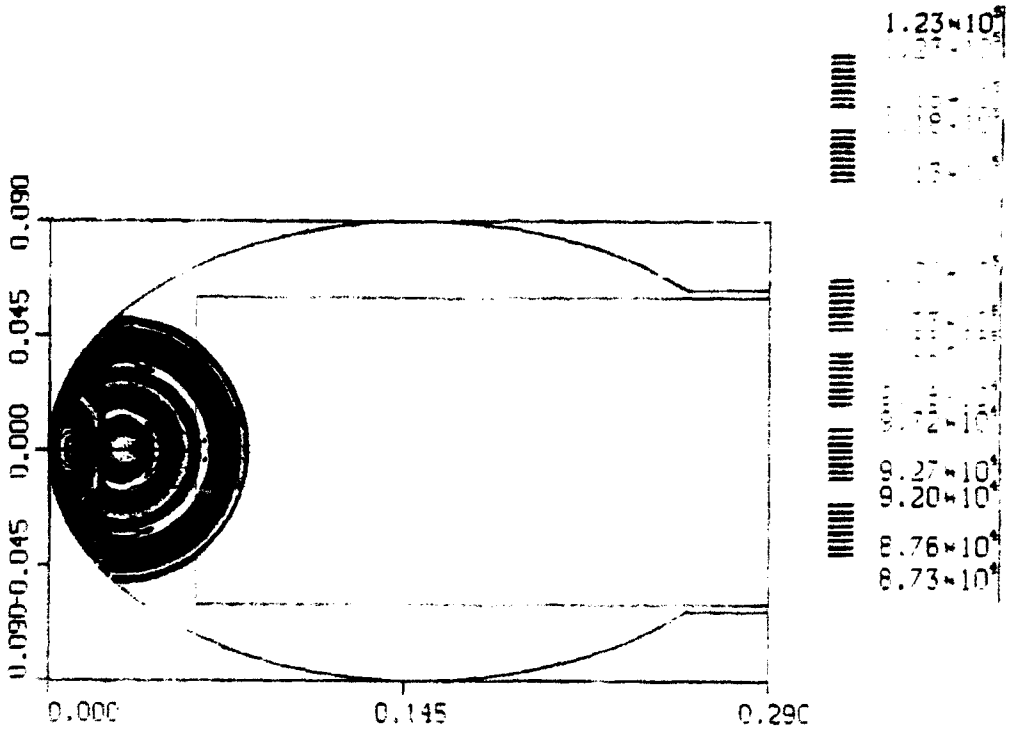


Figure 3.6.2 Pressure contours at time t = 1.21×10^{-6}sec showing the incident wave as reflected from the reflector wall.

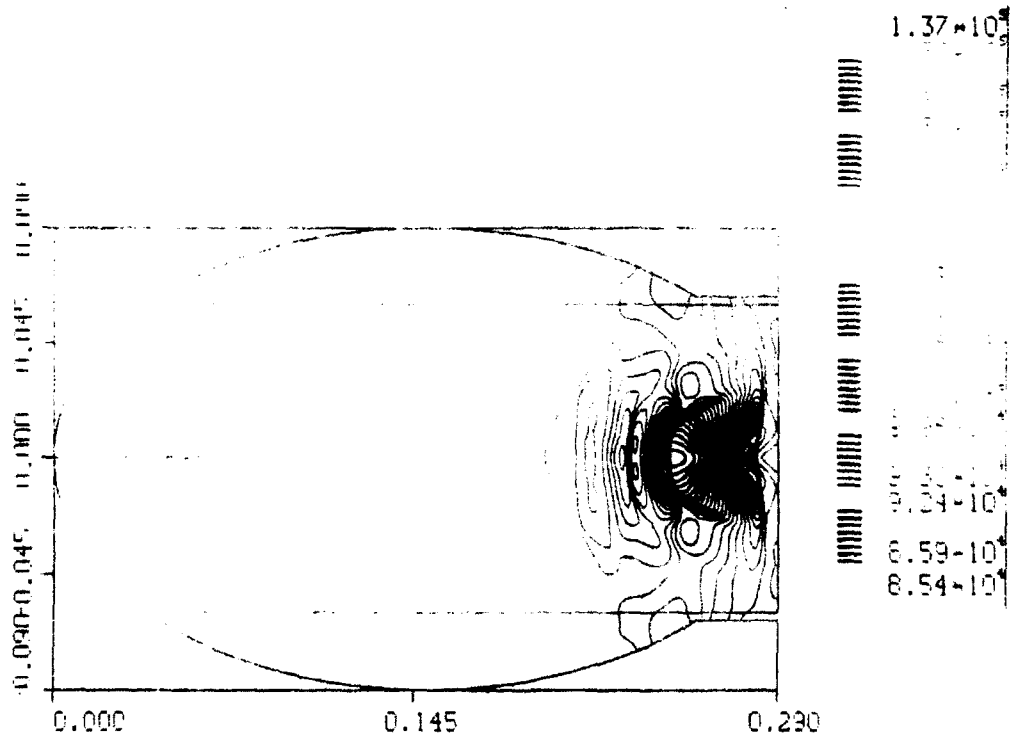


Figure 3.6.3 Pressure contours at time t = 8.41×10^{-4}sec showing the stage at which the maximum focused pressure is obtained.

3.7 NONIDEAL AIRBURST IN MULTIPHASE MEDIA

The main objective was to advance the understanding of the formation dynamics and microphysics of the multiphase flow of clouds developing as a result of a nuclear explosion. A main difficulty in analysis of nuclear cloud formation is the necessity to take into account physical phenomena that are interdependent and occur on vastly different scales. At about 30 seconds after a nuclear detonation, the cloud can be 4 km high and the shock wave will be at the distance of 10 km. The multiphase interactions that occur on a scale of 10-100 meters are very important and have to be accounted for.

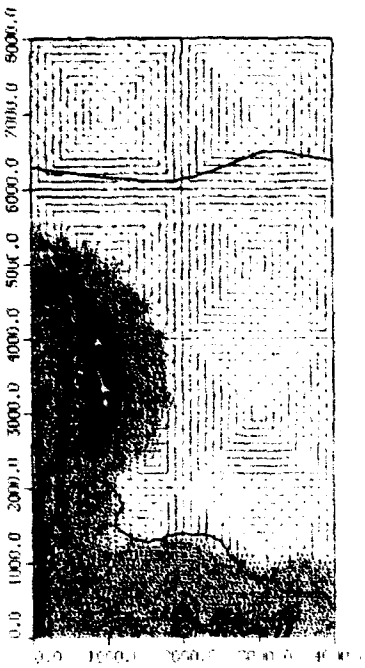
SAIC has developed a multiphase, multicomponent version of the AUGUST-2D code developed under the UUGM program. We use an explicit method for the solution of the multiphase flow described by equivalent Euler equations, and an implicit integration for simulation of the particle-fluid interactions. The grid adaptivity allows efficient and accurate simulation of this multiphase phenomenon. The grid adaptivity is used for adjusting the spatial scale of the domain decomposition to the scale required for accurate simulation of various physical interactions. Other code improvements such as introduction of the real-gas equation of state and Lagrangian particle tracing were employed to enable simulations and analysis of this complicated phenomena.

In Fig. 3.7.1a the computational domain and grid are shown for the nuclear cloud simulation. In this figure the temperature contours are overlaid on the unstructured grid. In Fig. 3.7.1b the particle density contours are shown for the same stage of the cloud evolution as in Fig. 3.7.1a. In Fig. 3.7.1c particle radius is shown for the same stage of the cloud evolution, and Fig. 3.7.1d shows locations of the Lagrangian tracers that mark evolution of the detonation products.

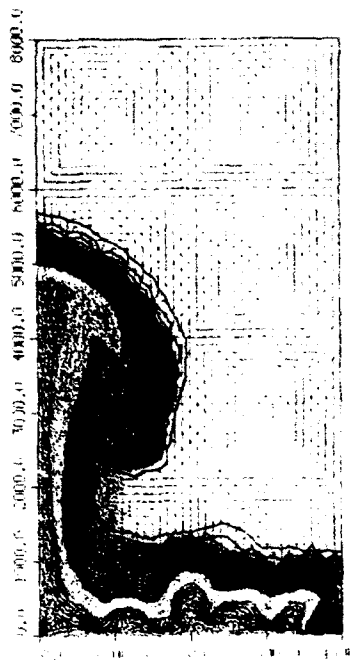
3.8 FLOW IN THE SARL WIND TUNNEL

One of the problems to which AUGUST 3D has been applied is that of modeling the SARL wind tunnel at Wright Laboratory. This example is a good test of the use of the Second-Order Godunov method to do nearly incompressible flow calculations. To illustrate the results, Fig. 3.8.1 shows the grid used for simulating the flow. The calculation was performed by specifying the inflow and outflow parameters and running the simulation to convergence. The run was performed at SAIC on the Stardent workstation and repeated on an Iris at FIMM. Figures 3.8.2 and 3.8.3 show the pressure levels in the tunnel. The results were visualized using AVS.

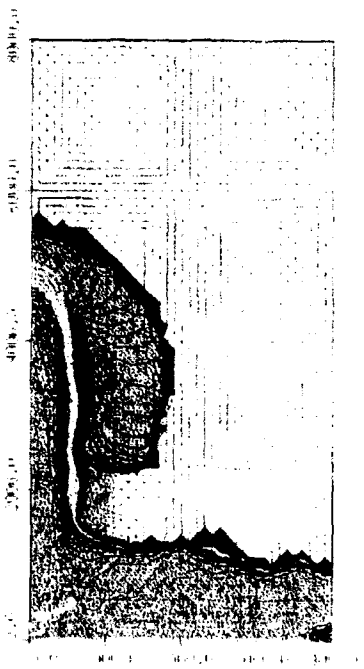
Figures 3.8.1 and 3.8.2 show two views of the pressure contours generated in a calculation of subsonic flow (Mach number 0.05). The results were confirmed by comparison with those obtained using a code with a structured grid, and by checking them against measurements.



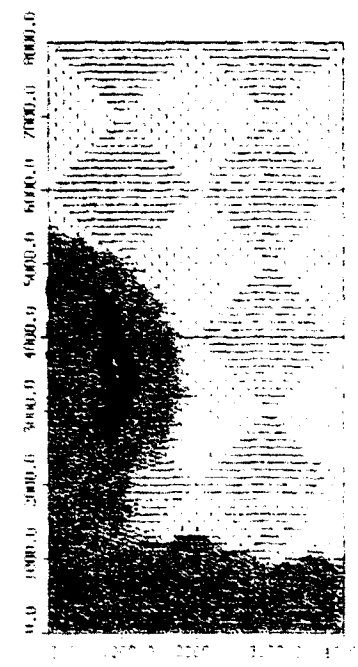
a. Temperature contours and grid.



b. Particle density.



c. Particle radius.



d. Lagrangian traces.

Figure 3.7.1 Formation of a radiative cloud. Multiphase simulation.

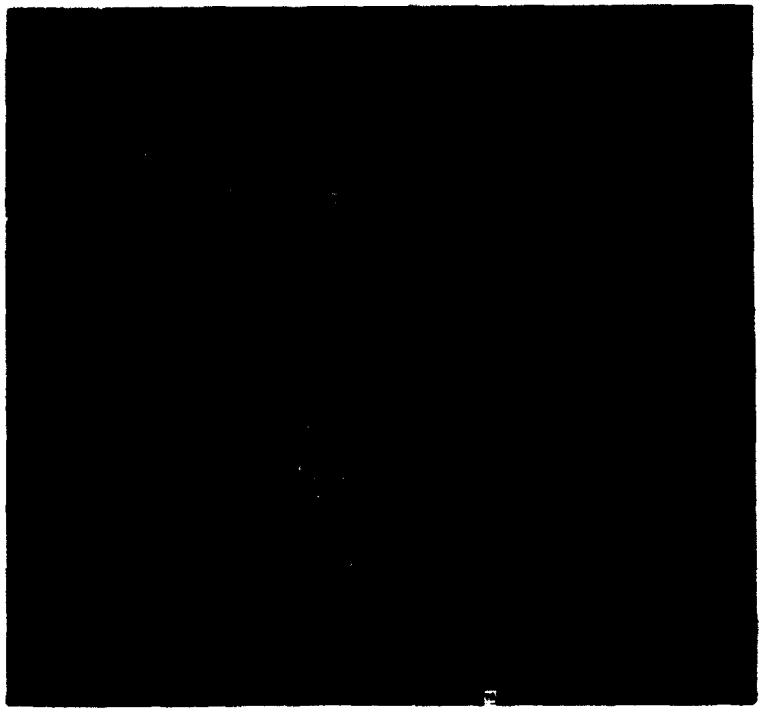


Figure 3.8.1 The unstructured grid used to simulate the SARL wind tunnel.

Figure 3.8.2 The pressure contours from the simulation of the SARL wind tunnel.

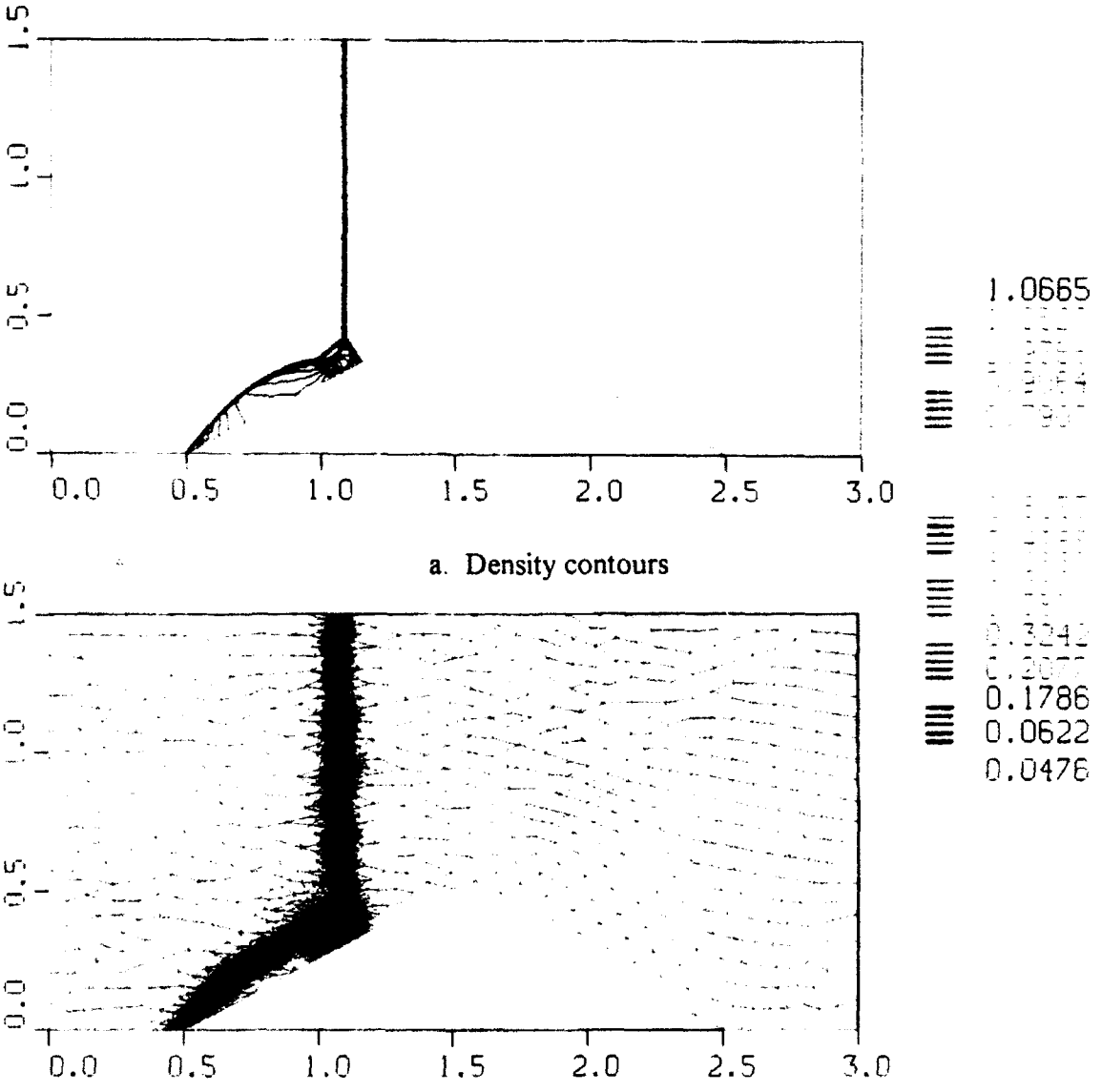
3.9 SHOCK ON DOUBLE WEDGE

A much more complicated problem, which has been extensively studied to benchmark and validate Euler solvers, is flow over a double wedge. This problem contains multiple fluid phenomena and is a stringent test for any solver. It includes shock formation, a Mach stem, rarefaction, a slip line, vortex generation and rollup, and is transient in nature. To validate our direct dynamic refinement method in AUGUST, we simulated a Mach 2.85 shock wave propagating in a channel and impinging on a symmetric 45° wedge, and also a Mach 8.7 shock impinging on a symmetric 27° wedge.

Both of these compared well with experimental results. Figure 3.9.1 shows an interferogram taken from Glaz et al.,[17] showing the M = 8.7 shock interacting with the front surface of the 27° wedge. Our results are shown in Figs. 3.9.2 - 3.9.4. The first of these illustrates the grid and density when the shock is on top of the wedge. The shock is well resolved and the grid is well adapted in the vicinity of important features and coarsened in the region that the shock has passed through. The next two figures show the evolution of the flow and the grid after the wedge where comparison can be made with the experimental results. AUGUST produces no artificial features and recovers the phenomenology seen in the experiment.

Figure 3.9.1 Experimental interferogram of a shock hitting a 45° corner at $M_S = 2.85$.

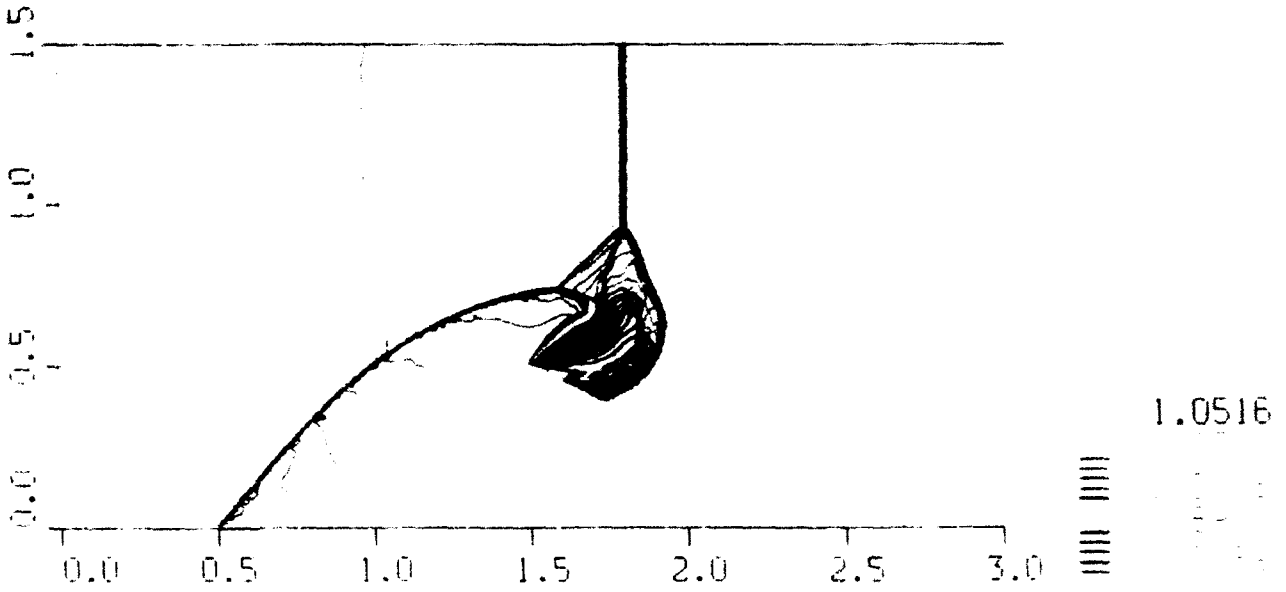
In the figures showing the triangular grids, the area of a triangle in the dense region of the grid is roughly 100 times smaller than the area of a triangle in the initial grid. The figures show that the grid adaptivity is capable of capturing the flow gradients including shocks, contact discontinuities and slip lines. Formation of a triple point of the Mach reflection, slip line and strong vortex formation are seen in Fig. 3.9.2a. In fairness, most of the flow phenomena that is captured by AUGUST have also been captured by other CFD schemes.[18] However, the accuracy estimated for the AUGUST numerical calculations in this example is on the order of 4%, equal to the accuracy of the experimental observations.



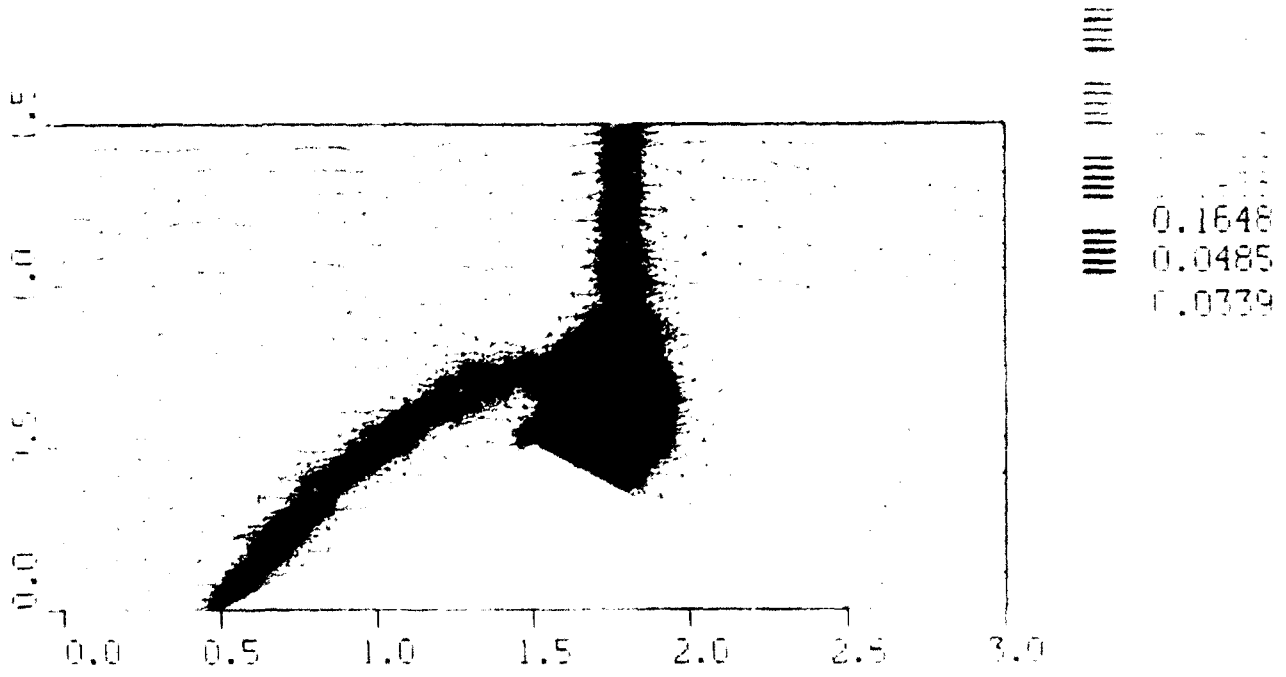
a. Density contours

b. Adaptive grid, 15,123 vertices

Figure 3.9.2 Interaction of a Mach 8.7 planar shock wave with a 27° double ramp: Mach reflection stage.

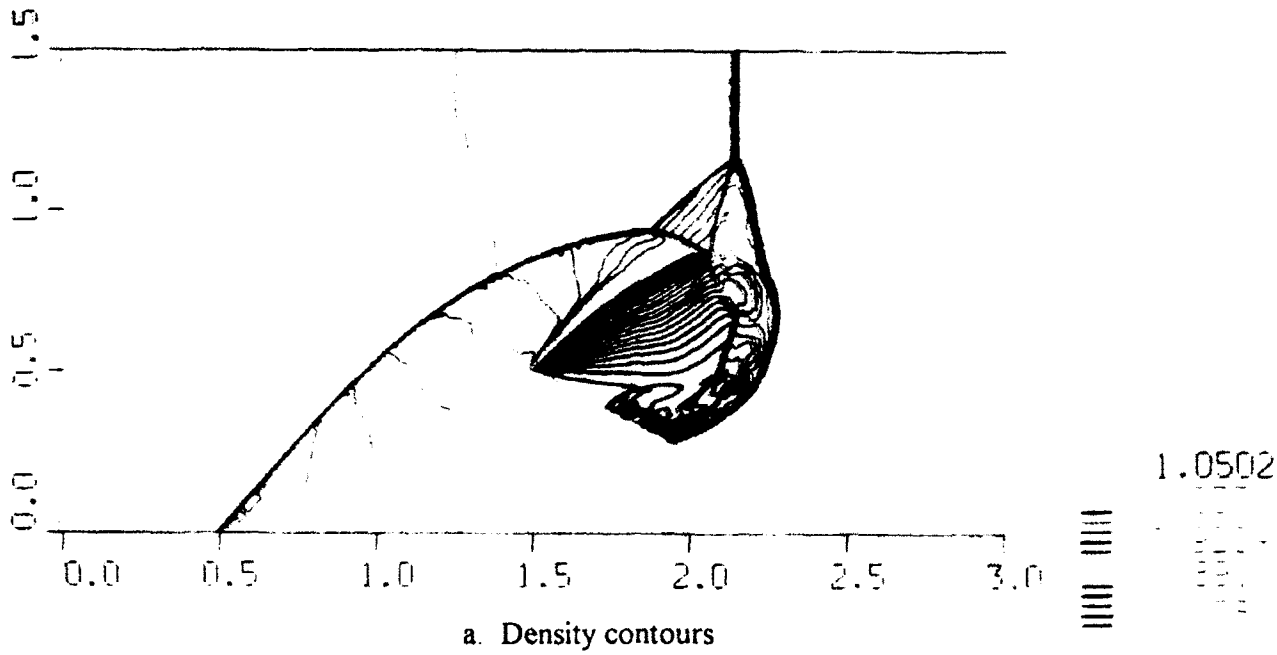


a. Density contours

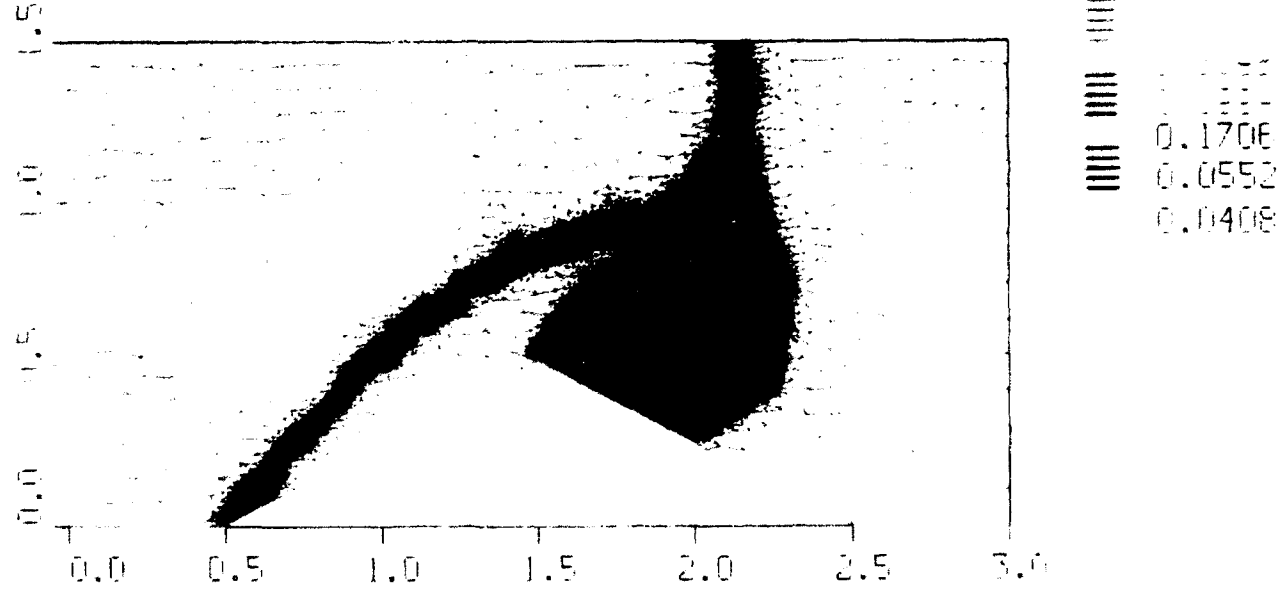


b. Adaptive grid, 27,132 vertices

Figure 3.9.3 Interaction of Mach 8.7 planar shock wave with a 27° double ramp: start of the diffraction stage.



a. Density contours



b. Adaptive grid, 46,462 vertices

Figure 3.9.4 Interaction of Mach 8.7 planar shock wave with a 27° double ramp: shock diffraction stage.

3.10 SUPERSONIC SPRAY COATING DEVICES

In this section we present the results of an application of the UUGM sim- ɔn technology to a sample problem involving spray-coating devices. Here we only tre ıe aerodynamic flow of particles in a high temperature gas which is moving supersc ly; we consider a reasonably complex geometry including a simulated surface tha: the substrate to be coated. The details of the surface interaction resulting in depos: ..ı are not treated in this example.

In Fig. 3.10.1 the computational domain and grid are shown for a model supersonic jet sprayer device that includes reactor nozzle, solid particle injector, and expansion nozzle. Also shown in Figure 3.10.1 is a perforated flat surface substrate placed in the flow field. The high-velocity high-temperature flow stream exiting the reactor nozzle accelerates the injected particles. The particles are heated during acceleration, melt, then expand with the flow in the nozzle, gain more speed, and finally impinge onto the surface. Details of the flow-surface interaction (here without boundary layers taken into account) will strongly affect the uniformity with which the surface will be "coated" by the particles carried by the flow.

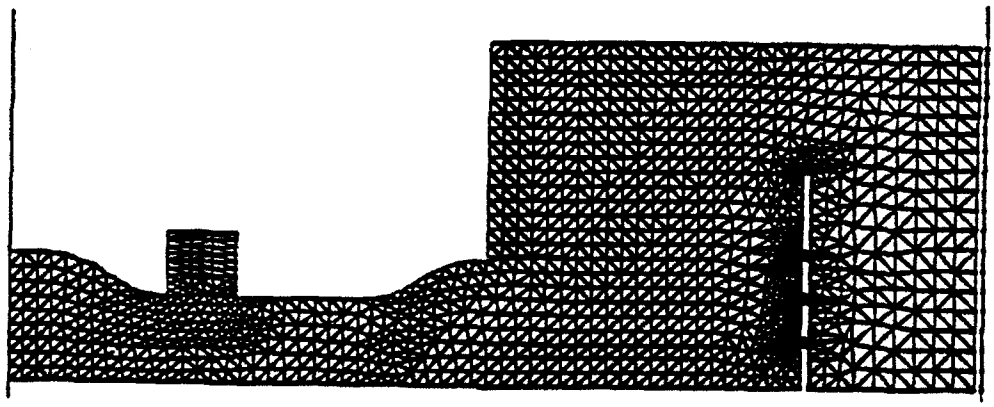


Figure 3.10.1 The figure shows the initial computational grid for the jet spray simulation demonstration. Shown are the nozzle, injection region and target surface depicted as a flat plate with perforations, oriented perpendicular to the mean spray flow. The boundary conditions used for the sample simulation were: V_g = 1000 m/sec, ρ_g = 0.1 kg/m^3, T_g = 3500 K at the inlet of the reactor nozzle; V_g = 1500 m/sec, ρ_g = 0.3 kg/m^3, T_g = 1500 K, V_p = 1500 m/sec, T_p = 1500 K, N_p = 2000 at the inlet of the reactor nozzle.

To trace the motion of the particles in the plasma spray device and the interaction pattern with the target surface we have injected Lagrangian "marker" particles (massless but moving with the local flow speed) in the particle injector flow stream. In Fig. 3.10.2 results are shown in the form of marker particle locations. To monitor the particle temperatures we have introduced particle coloring, where the color defines the local particle temperature. Thus one can evaluate the evolution of the particle temperature by observing the particle color transition. This coloring scheme can be used to show other parameters such as particle residence time or density. This represents a simple method of visualization that we have used successfully in past UUGM simulations.

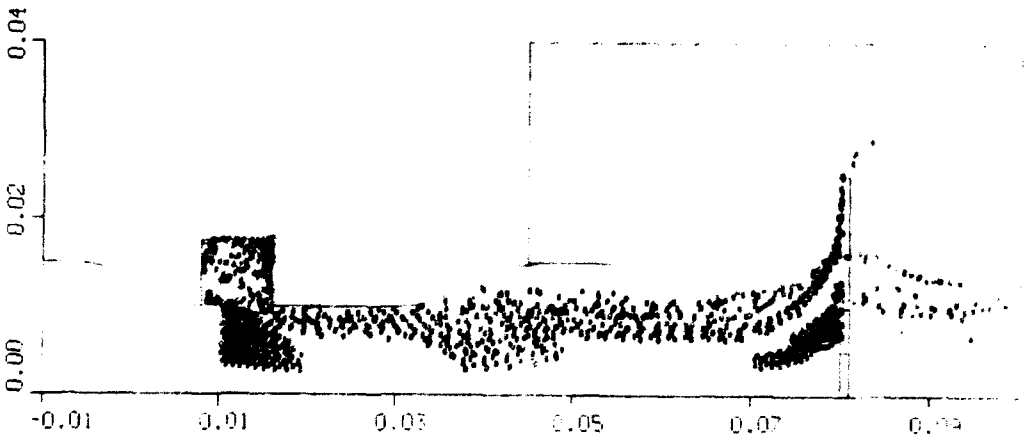


Figure 3.10.2 Lagrangian marker particles are shown in color representing the evolution of injected particle temperature as a function of particle position and time in the jet spray stream.

In Fig. 3.10.3 simulation results for the steady state are presented in the form of gas temperature contours for the jet spray system. Here it is possible to observe a very large temperature variation in the nozzle. The cold gas that is injected with the particles remains at the edge of the jet stream. At the same time the main jet cools through the expansion in the nozzle from 3500°K to 2000°K, and then undergoes a series of expansions and compressions in the system of shock waves created by overexpansion of the supersonic jet. Figure 3.10.3 also shows a nonuniform temperature distribution on the surface that is partially created by the gas flow through the perforated holes.

In Figs. 3.10.4 and 3.10.5 simulation results are shown for the density and pressure contours. Here we can observe the formation of several diamond-shaped shock structures as a result of supersonic flow over expansion. However, for the flow regimes in our simulation these shocks do not lead to a higher rate of mixing by injected cold gas with particles and the main hot gas stream. This can be noticed in the density contours, where one clearly observes that the high-density cold gas does not penetrate the main hot jet flow. By changing the condition (injection pressure, angle of entry, etc.) of the injected flow one can improve mixing, thus achieving higher particle temperatures and velocity.

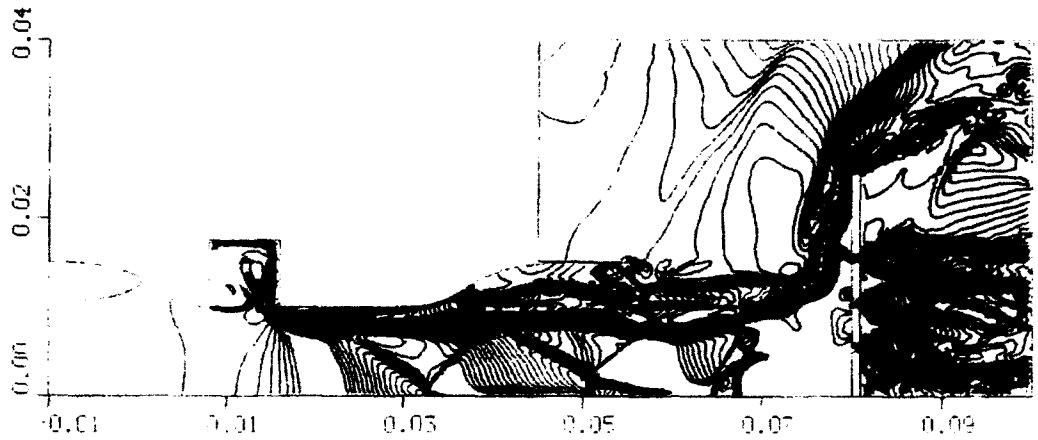


Figure 3.10.3 Gas temperature contours in the jet spray stream. The maximum temperature is 3500°K and the minimum is 600°K.

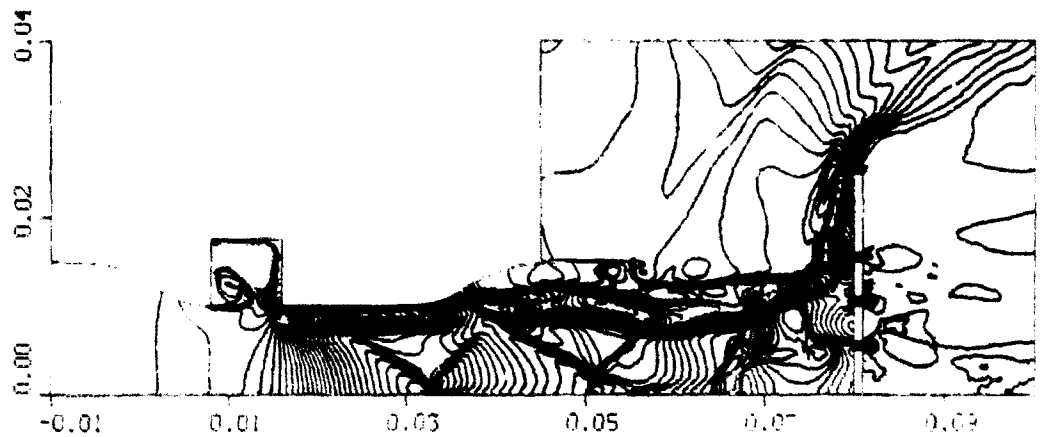


Figure 3.10.4 Gas density contours in the jet spray stream. The injected stream and the main flow mix poorly. The diamond patterns describe the shock wave pattern resulting from the flow's overexpansion.

Figure 3.10.5 Pressure contours in the jet spray stream. The diamond patterns show that supersonic flow is maintained near the vicinity of the target surface.

3.11 DUSTY FLOW OVER A CYLINDER

A numerical study of two-phase compressible flow has been performed for the reflection and diffraction of a shock wave propagating over a semicircular cylinder in a dusty gas. The following model was used to derive the governing equations:

(1) The gas is air and is assumed to be ideal;

(2) The particles do not undergo a phase change because for the particles considered here (sand) the phase transition temperature is much higher than the temperatures typical for the simulated cases;

(3) The particles are solid spheres of uniform diameter and have a constant material density;

(4) The volume occupied by the particles is negligible;

(5) The interaction between particles can be ignored;

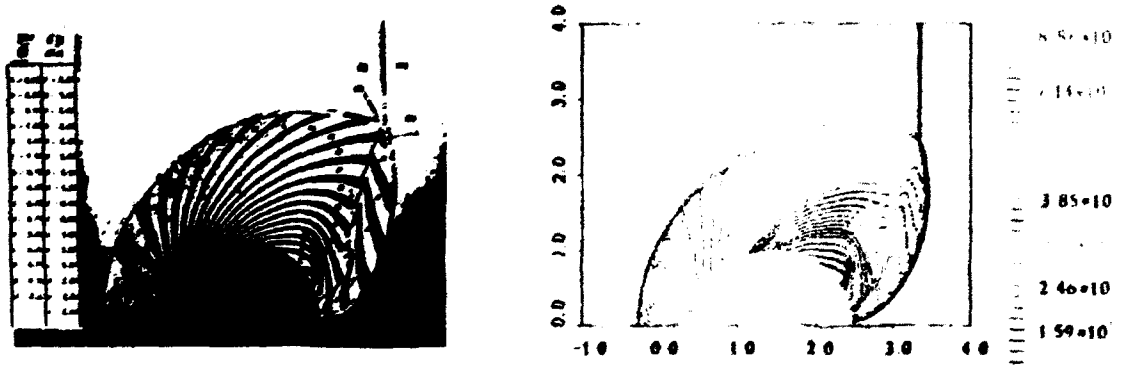
(6) The only force acting on the particles is drag and the only mechanism for heat transfer between the two phases is convection. The weight of the solid particles and their buoyant force are negligibly small compared to the drag force;

(7) The particles have a constant specific heat and are assumed to have a uniform temperature distribution inside each particle.

Under the above assumptions, separate equations of continuity, momentum, and energy are written for each phase. The interaction effects between the two phases appear as source terms on the right-hand sides of the governing equations. The two phases are coupled by interactive drag force and heat transfer.

The objectives of the study were (a) to solve the two-phase compressible flow field and compare the simulation with available experimental results; (b) to observe and investigate the reflection and diffraction wave patterns when a shock wave propagates over a semicircular cylinder in a dusty gas, with particle radius and loading as parameters.

To test the accuracy of the two-dimensional computation, we first computed the pure gas flow case of shock wave reflection and diffraction over a semicircular cylinder. We then compared the simulation with experimental results. Shock wave reflection on a wedge has been extensively studied by many researchers (see e.g., review papers of Ben-Dor and Dewey[18] and Hornung.[19] As one can see from Fig. 3.11.1, the results show excellent quantitative and qualitative agreement between the numerical simulation and experimental results.



(a) (b)

Figure 3.11.1 Comparison for $M_S = 2.8$ pure-gas flow: (a) interferogram from experiment; (b) density contours from present calculation.

In the two-phase simulation a planar shock with $M_S = 2.8$ propagates into an area of dusty gas and impinges on a semicircular cylinder. The interface between pure air and dusty air is located at $x = 0.0$ of the computational domain. The area of the dusty air contains a semicylinder with a radius of 1m. The size of the computational domain, initial parameters of the gas, parameters of the incoming shock, size of the semicylinder and its location in the computational domain, are the same as in the reflection and diffraction simulation in the pure gas case. The main objective of this set of simulations was to study the effects of particle size and particle loading on the parameters of the reflected and diffracted shock waves.

The first set of simulation results is shown for the case with dust parameters r_p = 10μm and $\rho_p = 0.25$ kg/m^3. The gas parameters and the parameters of the incoming shock wave were the same as in the pure gas case presented above. In Figs. 3.11.2a and 3.11.2b, the particle density and gas density contours are shown at the stage where significant diffraction has taken place and the shock front is approaching the trailing edge of the cylinder. To study the influence of particle loading on the dynamics of reflection and diffraction, we have simulated the case with a dust density of $\rho_p = 0.76$ kg/m^3 and with r_p = 10μm. To examine the effect of particle size on the reflection-diffraction process, we simulated a case where the particle loading and gas flow conditions were the same as in the previous case with particle density $\rho_p = 0.76$ kg/m^3, but the particle size was r_p = 50μm (Fig. 3.11.3).

On the basis of these calculatrions we reached the following conclusions:

(1) For a two-dimensional pure-gas flow, numerical results agree well with existing experimental data qualitatively and quantitatively, indicating that the gas phase is accurately simulated by the adaptive grid technique;

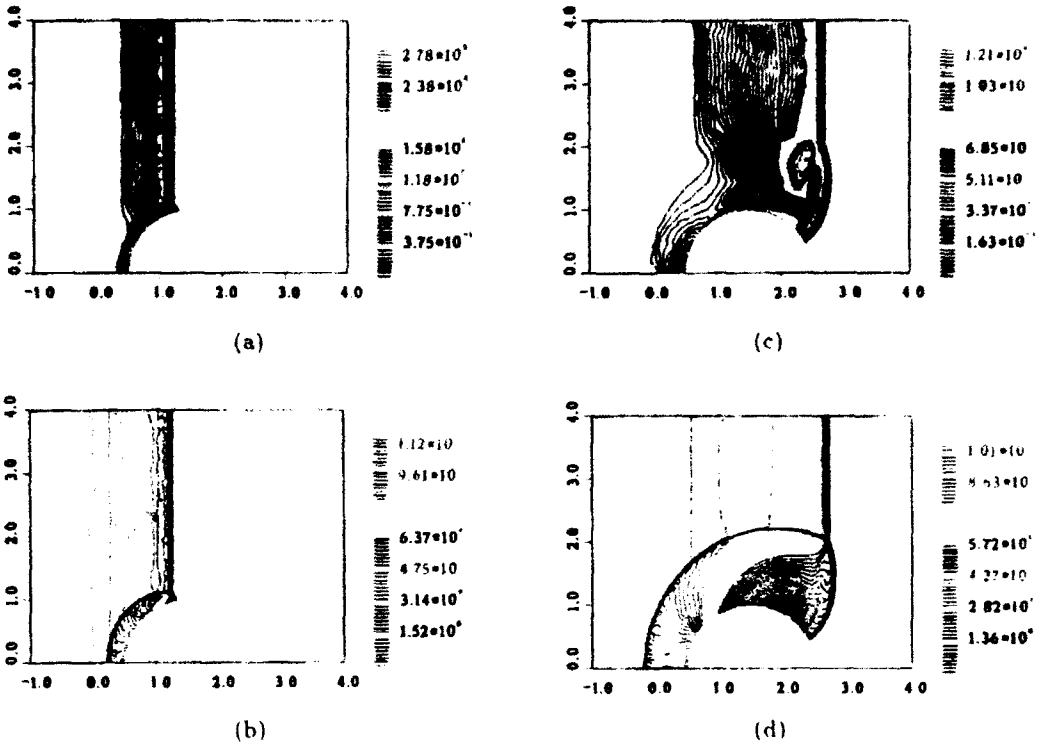


Figure 3.11.2 Density contours for the case $M_s = 2.8$, $\rho_p = 0.25$ kg/m^3, $r_p = 10\mu$m at two different times: (a) particle density at t_1, (b) gas density at t_1; c) particle density at t_2, (d) gas density at t_2.

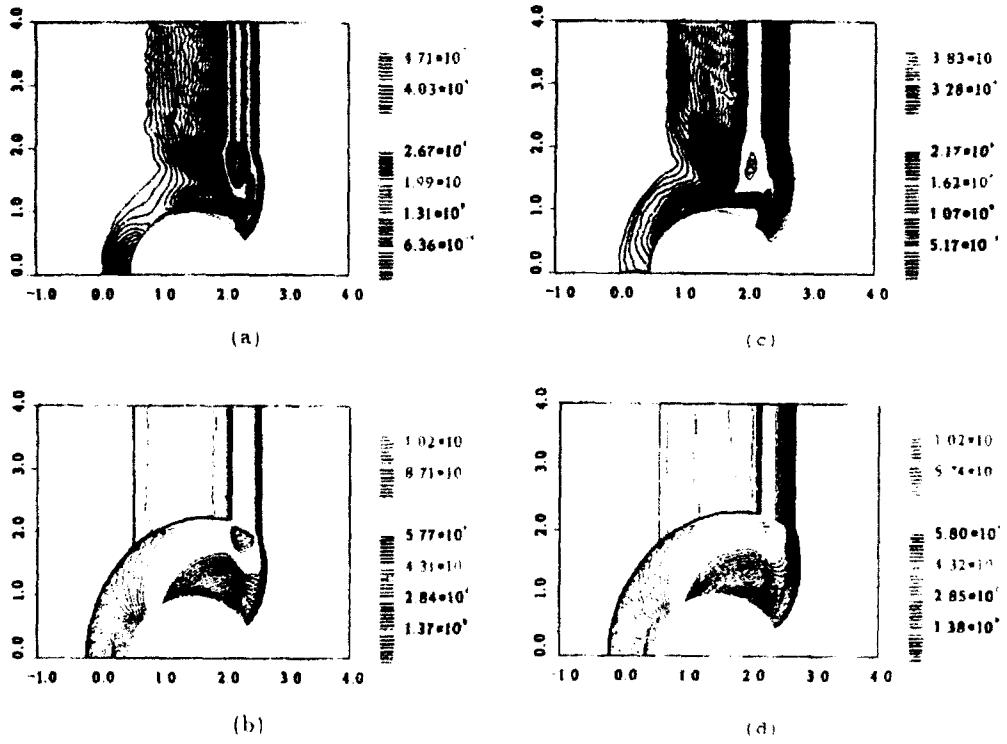


Figure 3.11.3 Density contours for the case $M_s = 2.8$, $\rho_p = 0.76$ kg/m^3, for two different particle sizes: (a) particle density and (b) gas density for $r_p = 10\mu$m; c) particle density and (d) gas density for $r_p = 50\mu$m.

(2) Particles in the gas can have a profound effect on the shock wave reflection and diffraction pattern, which is a function of particle size and loading. The less the particle loading, the less the influence of particle on the flow field;

(3) In the three simulation cases, particles accumulate behind the "back shoulder" of the semicircular cylinder due to the effect of particle inertia and the rarefaction wave;

(4) For different particle sizes at fixed particle loading, the larger particle will have a longer relaxation zone and less accumulation at the "back shoulder" and behind the incident shock. The gas density contours show a less distinguishable slip line in the small particle case than in the large particle case.

3.12 IMAGE PROCESSING

Very recently, there have been exploratory efforts in image processing based on nonlinear methods. If the purpose of an enhancement process is to highlight the edges of an image, then the technique used in the frequency domain is usually highpass filtering. An image can be blurred, however, by attenuating the high-frequency component of its Fourier transform. Since edges and other abrupt changes in the gray levels are associated with high-frequency components, image sharpening can be achieved in the frequency domain by a highpass filtering process, which attenuates the low-frequency without disturbing high-frequency information in the Fourier transform. The primary problem with this technique is that an ideal discontinuity has an infinite spectrum of frequencies associated with it. When filtering is applied, some frequencies are cut off, leading to a loss of edges in the image.

In computational fluid dynamics (CFD) similar problems exist in simulating flows with discontinuities. The problem of simulating flows with discontinuities is less forgiving, since an incorrect calculation usually leads to a complete distortion of the flow field. This has led CFD scientists to develop sophisticated algorithms that identify and preserve discontinuities while integrating the flow field in the computational domain. In the image domain, sharpening is usually done by differentiation. The most commonly used methods involve the use of either gradients or second derivatives of the pixel information. Central differencing is usually used to calculate the derivatives. CFD research has shown that this strategy will lead in many cases to smearing of the flow discontinuities (analog of the image edges in image enhancement).

A new and unique image sharpening method based on computational techniques developed for AUGUST has been developed. Preliminary experience shows that it can enhance image edges and deconvolve images with random noise. This indicates a potential application for image deconvolution from sparse and noisy data resulting from measurements of backscattered laser-speckle intensity.

The Second-Order Godunov Method used in AUGUST was developed from an understanding of the phenomenology of signal propagation in gasdynamical systems. The numerical algorithm implementing this method is not analytical and contains a set of steps that can be regarded as wave filters. These filters are designed to not smear the discontinuity (edge), suppress the spurious oscillations, and propagate the relevant signals through the system. The following algorithmic steps are performed to advance the solution for a single iteration in the Second-Order Godunov Method:

1. Local Extrapolation
2. Monotonicity Constraint
3. Characteristics Constraint
4. Riemann Problem Solution
5. Integration

Most of these steps have an analog in conventional image processing methods. Here we will give an explanation of the function of each algorithmic step of the Second-Order Godunov Method and where applicable, will point to its possible analog in conventional signal processing techniques.

Step 1 consists of extrapolation of the values in the computational grid (pixel) cell to the edges of the cell. Linear or nonlinear extrapolation can be used. This step is analogous to the standard edge-sharpening techniques used in image processing, with one important difference: the extrapolation is done not for the value itself but for its flux (change of value across cell boundary).

Step 2 includes a monotonicity constraint for the values at the cell edges. This is analogous to the nonlinear technique of locally monotonic regression only recently introduced for signal processing.

Step 3 subjects the values at the edges to the constraints derived from a solution of the one-dimensional characteristics. This step assures that the values at the edges have not been extrapolated from directions inconsistent with the characteristic solutions. This prevents extrapolation as well as smearing or overshoot of the discontinuities. For the image-processing application, this can be regarded as a form of automatic edge detection step where the shock waves are associated with the edges of an image.

Step 4 uses an exact solution of the system of the gasdynamic equations for calculation of the flux values based on the extrapolated values of the parameters at the left and right side of the edges. This step has no analogy in image processing. However, since the analytical solution includes discontinuities, an exact calculation of the flux at the edge location is allowed, even if this flux is calculated through a discontinuity.

Step 5 consists of finite-volume integration of the system of conservation laws. Here, the image is effectively treated as a flow field: the flux integration serves as a smoothing filter from the image perspective.

The effect of these steps is equivalent to the application of a unique filter stack with proven properties of discontinuity preservation and robustness.

The field of gray scale intensity of an image can be translated into a flow field. To every image pixel we assign to the corresponding cell of the computational domain values of the gasdynamical parameters proportional to the values of the gray scale. Our understanding of the basic gasdynamical processes plays a major role in completing the analogy. Appropriate mapping of the image gray scale intensity into a flow field creates conditions favorable for the formation or enhancement of field discontinuities. For example, a shock wave reflecting from a wall or a contact surface can increase in strength, or two colliding flow streams will produce a contact surface that will become stronger in time. If we have a numerical technique to resolve these discontinuities accurately, then with successive numerical integration of the flow field, the discontinuities will sharpen as the solution evolves in time. Then by inverse mapping of the flow field to the image gray scale field, we can reconstruct an enhanced image.

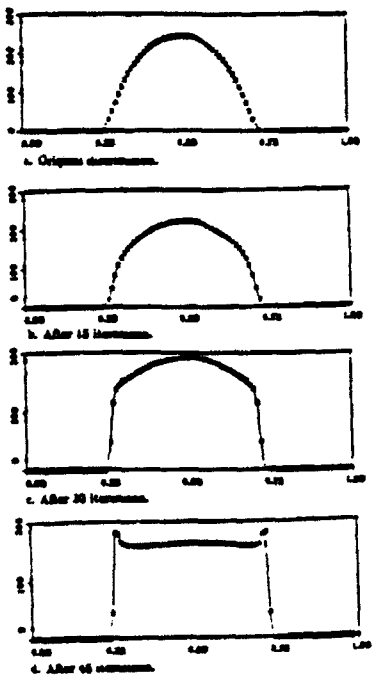


Figure 3.12.1 Edge enhancement for a sinusoidal distribution without noise.

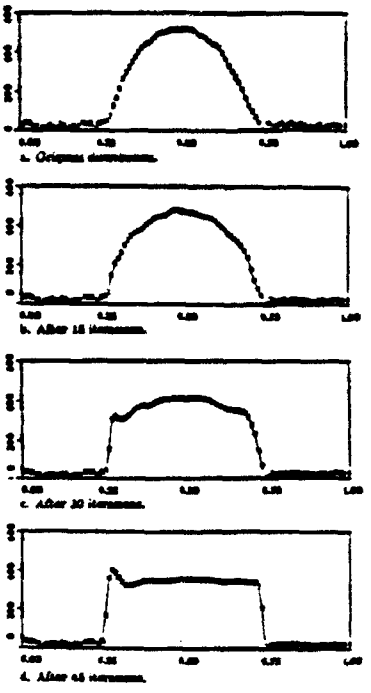


Figure 3.12.2 Edge enhancement for a sinusoidal distribution with 10% intensity random noise.

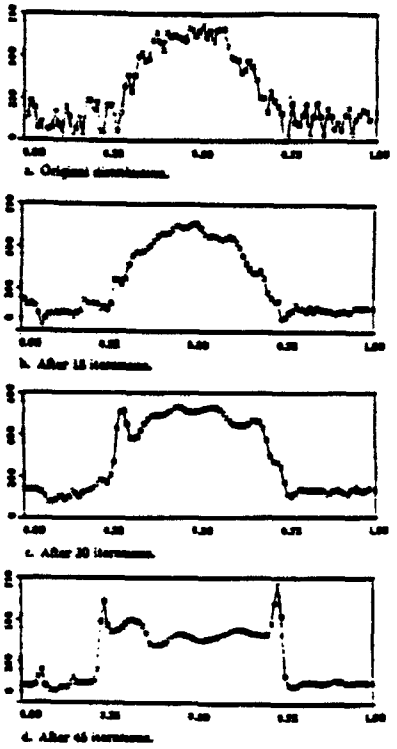


Fig. 3.12.3 Edge enhancement for a sinusoidal distribution with 50% intensity random noise.

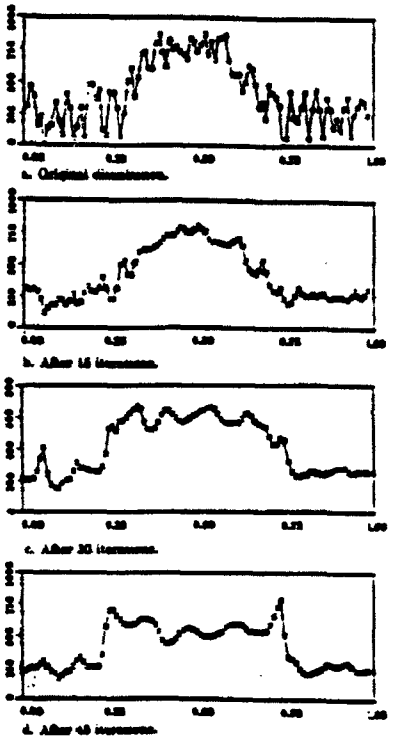


Fig. 3.12.4 Edge enhancement for a sinusoidal distribution with 100% intensity random noise.

Applications have been made to two-dimensional images derived from satellite reconnaissance and gamma-ray medical diagnostics (see Appendix C). Note that the images shown there are distorted by the xerographic process used to reproduce these illustrations, which also act as a nonlinear filter but is not tuned to these images.

Analogous extensions of nonlinear CFD techniques can be used for image compression.

3.13 DETONATION IN A MULTIPHASE MEDIUM

In this study the main subjects were the initiation, propagation, and structure of detonations occurring when combustible particles are intentionally or unintentionally dispersed into the air. Formation of this potentially explosive dust environment and the properties of its detonation are of significant practical interest in view of its destructive or creative effects. Previous experimental and theoretical studies of these phenomena addressed only homogeneous particle/oxidizer mixtures. However, intentional or accidental processes of the explosive dust dispersion always lead to inhomogeneous particle density distribution.

On the other hand, some industrial methods of explosive forming rely on detonation of explosive powder. This powder can be deposited as a thin layer over the surface area of the forming metal, with a residual concentration in the vicinity of the layer.

When the detonation wave is generated in a homogeneous mixture by "direct initiation," it starts with a strong blast wave from the initiating charge. As the blast wave decays, combustion of the reactive mixture behind its shock front starts to have a larger role in support of the shock wave motion. When the initial explosion energy exceeds some critical value, transition to steady state detonation occurs. In explosive dust mixtures with a nonuniform particle density, the initiation dynamics is significantly more complicated. The critical initiation energy sufficient for one of the explosive particle density regions is not necessarily adequate for other regions. We have demonstrated that the phenomenology of these interactions is distinctly different from the classical studies of multilayer detonations in gases. This is primarily because the energy content of adjacent layers in a typical multigas layer experiment varies by a factor of two or four, whereas the energy content in explosive dust/air mixtures can vary by several orders of magnitude.

At present the physics of the energy release mechanisms in solid particles/air mixtures is not clearly understood. This can be attributed to the obvious difficulties of making a direct non-obtrusive measurement in the optically thick environment typical for this system. The chemical processes of single-particle combustion, which mainly occur in the gaseous phase, are significantly faster than the physical processes of particle gasification or disintegration. Thus, in the multiphase mixtures, the rate of energy release is mostly determined by physics of particle disintegration. It is very difficult to describe the details of particle disintegration in the complex environment prevalent behind the shock or detonation wave. Fortunately, in most cases of multiphase detonation, only the main features of the particle disintegration dynamics need to be captured to describe the phenomena.

In this work we considered solid particles consisting of explosive material. Two-dimensional simulations were done for the system of low particle density concentration clouds and ground layers formed by high concentrations of the RDX powder. We examined three cases of ground layer density distribution: a fourth power distribution with 12 mm above ground with a maximum density on the ground of 800 kg/m^3; a uniform 25-mm layer with a density of 100 kg/m^3; and a 12-mm uniform layer with a density of 250 kg/m^3. In all these cases, the weight of the condensed phase per unit area was the same, which allowed examination of the effects of the particle density distribution on detonation wave parameters.

Figure 3.13.1 shows a setup for a typical two-dimensional simulation. Here the computational domain is 25cm × 25cm. The explosive powder density is distributed according to the 4th power law of the vertical distance, starting from the ground where the density is 800 kg/m^3, and rising to 1.2cm, where the density is 0.75 kg/m^3. From this point to 25cm height, the density is constant and equal to 0.75kg/m^3. The density distribution is uniform in the x direction.

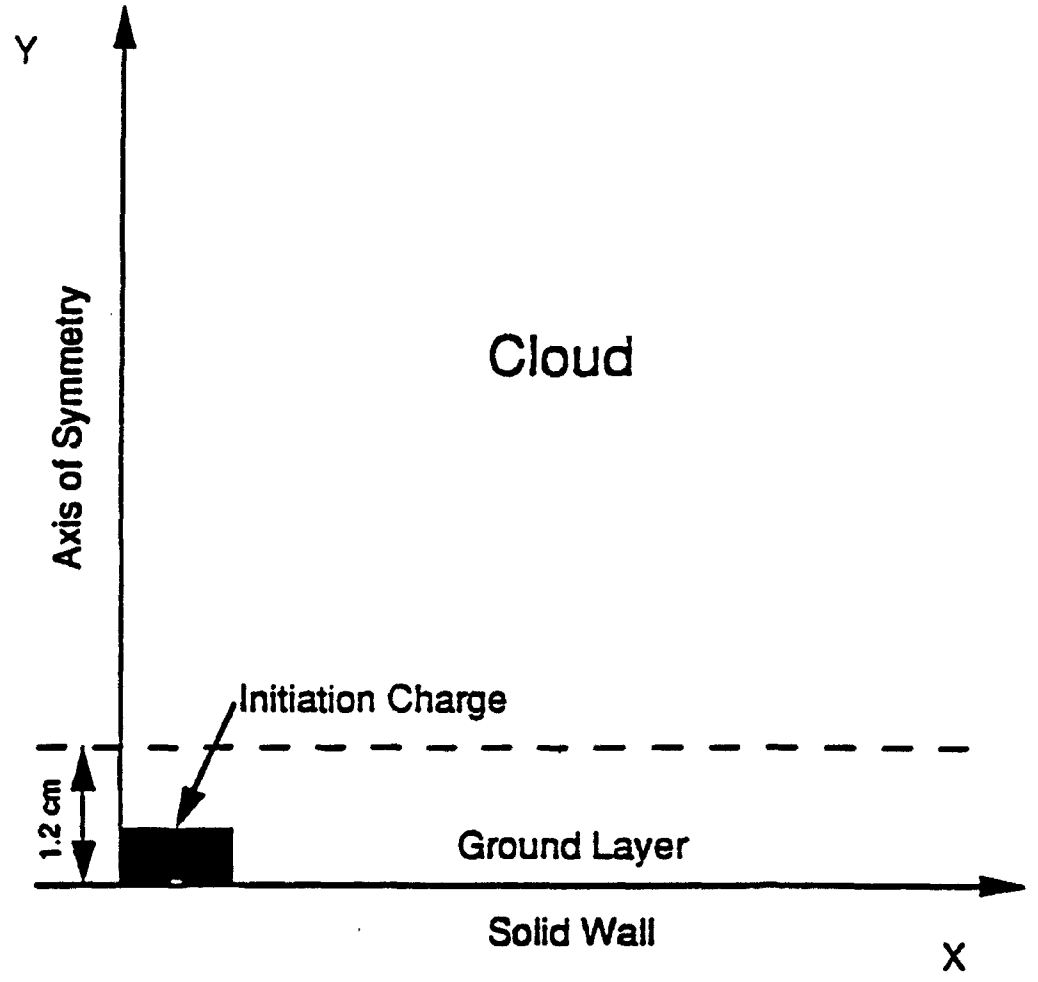


Figure 3.13.1 Computational domain and boundary conditions.

In all three cases, the detonation wave in the cloud in the computational domain was significantly overdriven and did not play an important role. We estimated that the self-sustained regime of the detonation wave in the cloud for the examined cloud concentrations can occur only at the distances of 2-3m above ground. At the same time, the particle density distribution in the layer determines the dynamics of the detonation wave as well as the pressure on the ground.

In all three two-dimensional simulations, we observed a very distinctive shape of the detonation wave front in the vicinity of the layer. In this area, the overdriven detonation in the cloud is preceding the detonation wave in the ground layer. This feature of the detonation front can be explained by the fact that the energy released in the ground layer detonation wave produces a faster propagating shock wave in the dilute cloud than in the ground layer which is heavily loaded with solid particles. However, these structures were not observed experimentally, and more studies are needed to examine their parameters.

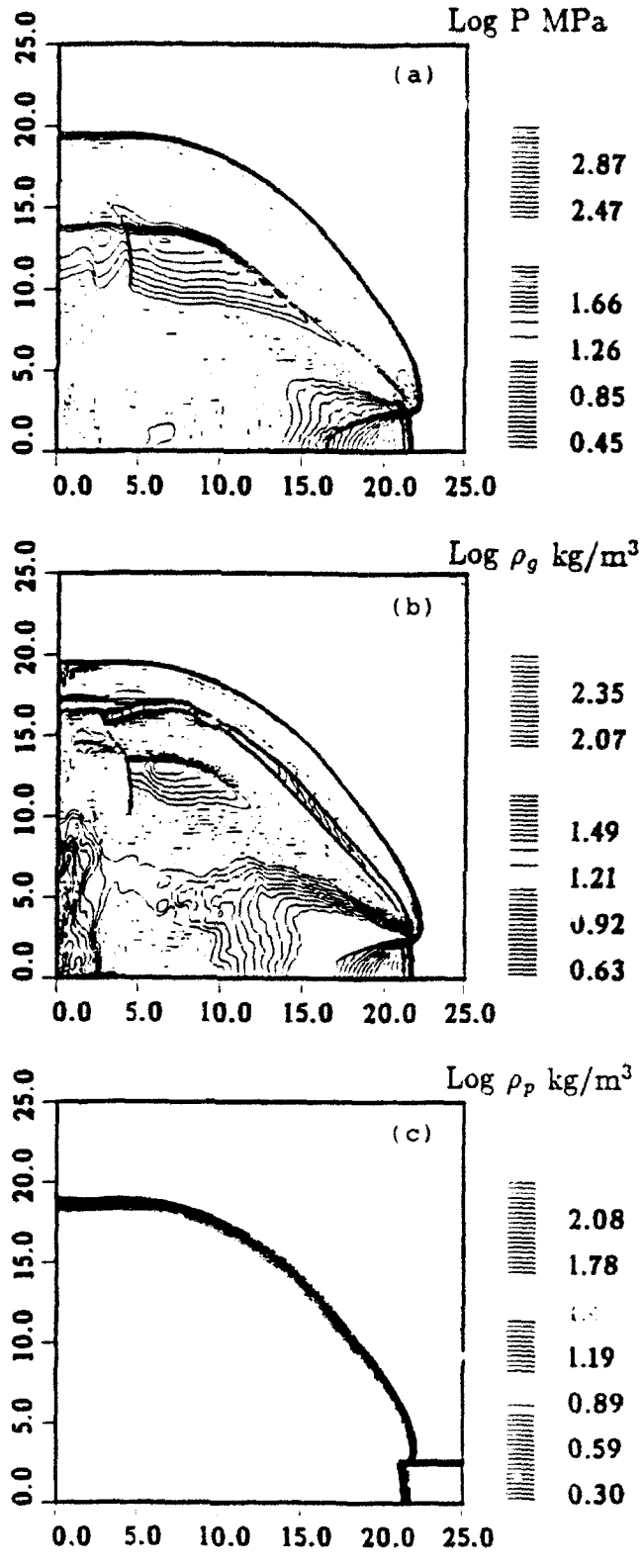


Figure 3.13.2 Explosive initially localized in 2.5-cm layer at constant density of 100 kg/m^3. Density in the cloud is 0.75 kg/m^3. (a), (b), and (c) are gas pressure, gas density, and particle density at 66 μsec, respectively.

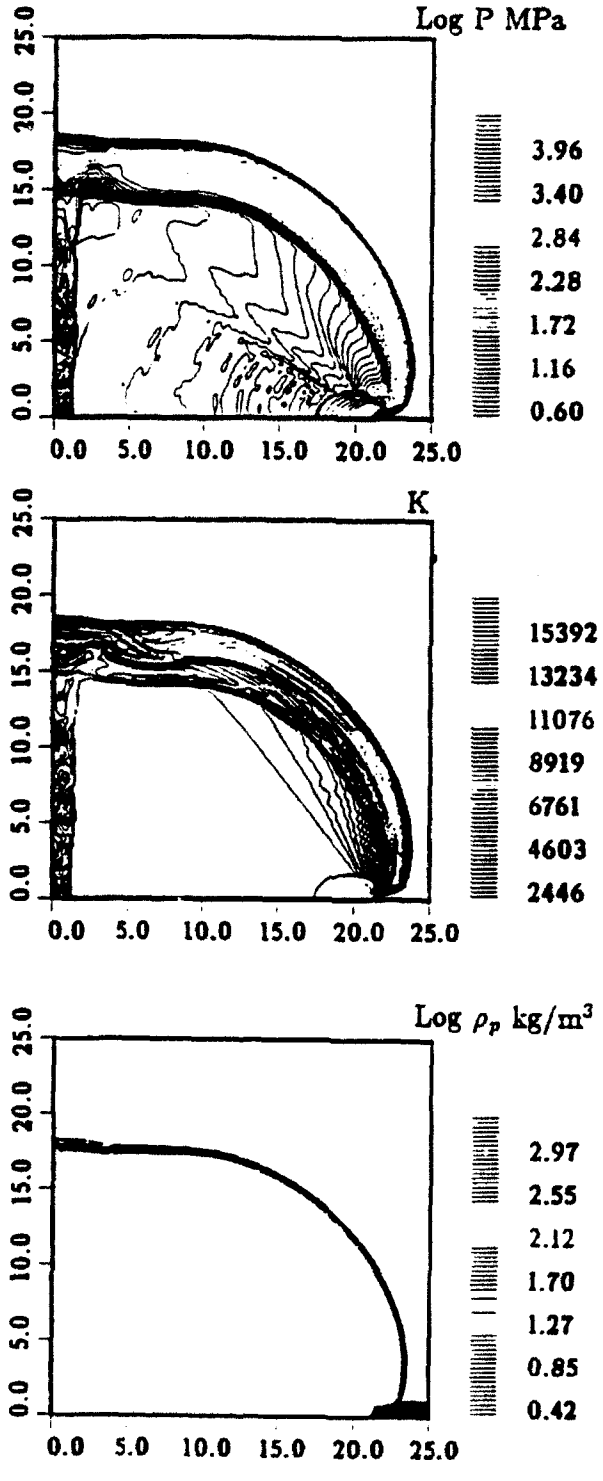


Figure 3.13.3 Particle density distributed in layer in accordance with the fourth power of height. Gas pressure, temperature, and particle density at 55 μsec, respectively.

4. CONCLUSIONS

The AUGUST-2D and AUGUST-3D adaptive unstructured CFD simulation codes, developed under SAIC's UUGM (through a contract form ARPA's Applied and Computational Mathematics Program) program have been tested through the set of standard CFD benchmark test cases and have been applied to a wide range of practical problems for a variety of end-users. In most cases where these codes have been applied, significant improvements in accuracy, resolution, and ease of use have been noted. Use of the Second Order Godunov flow solver algorithm has provided a robust capability to treat low Mach number subsonic-to high Mach number hypersonic flow problems within one simulation code without the necessity of tuning the flow solver via adjustable parameters. In addition, the extension of the AUGUST family of codes to treat multiphase, multicomponent reactive flow phenomena provides the capability, for the first time, of simulating a wide variety of physically interesting and challenging problems that are rich in physics-chemical phenomena. The range of these problems includes: 1) full 3D flows about complex aircraft in all flight regimes (except rarefied flows), 2) shock-body interactions, 3) chemically reacting flows typical in combustion problems, and 4) detonation phenomena found in explosives, shock tubes, and specific applications to such devices as the pulsed detonation engine.

SAIC's UUGM program has resulted in over 20 publications in various stages of preparation, and numerous presentations at U.S. and international technical meetings, conferences, and workshops. The AUGUST family of simulation codes is presently being applied to several current materials development and synthesis areas of research. In particular, the ability of the AUGUST codes to capture the complex geometry of material synthesis reactor configurations, resolve the complex flow patterns, and treat the complex physics and chemistry of the synthesis process provides a simulation and modeling tool that is useful for design of such process reactors, analyse and evaluate experimental results, and (depending on successful benchmarking) provide a process control tool based on validated models. SAIC intends to exploit this capability in future programs.

SAIC's Applied Physics Operation, Hydrodynamic Modeling Division staff members performed the work under the DARPA UUGM program. Dr. Shmuel Eidelman and Dr. William Grossmann were co-program managers. Important contributions were made by Drs. Itzhak Lottati, Xiaolong Yang, Marty Fritts, Adam Drobot, Ahron Friedman, and Michael Kress. SAIC's UUGM team would like to acknowledge the support and interest of Dr. James Crowley (ARPA ACMP program manager), Drs. Lois Auslander and Helena Wisniewski (previously DARPA ACMP program managers), and Dr. Arje Nachman (AFOSR) who served as the ARPA agent for the UUGM program.

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APPENDIX A

CODE DESCRIPTION

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CODE DESCRIPTION

A.1 AUGUST (2D)

The subroutines in the AUGUST code are organized here as they appear in the listing in Appendix B. A brief description indicates the function performed by each subroutine.

TABLE A.1

LIST OF SUBROUTINES

1. **MAIN**	Governing program for AUGUST. Reads input files and sets the mode for the computation.
2. **HYDRFL**	Computes the fluxes at interfaces by applying the Godunov algorithm to solve the Riemann problem across the interface.
3. **HYDRMN**	Controls the computation. The integration of the fluxes and update of the physical variables, adaptation of the grid and writing to output files are performed in this subroutine.
4. **GEOMTR**	Calculates the geometrical quantities not provided by the input data file but needed for the computational algorithm. GEOMTR is only used once for starting a new simulation.
5. **UPDATE**	Reads the input file for a new simulation and calls GEOMTR to update the geometrical variables needed to perform the computation.

6. **UPGRAD**	Called if a restart run is performed. Will read the appropriate file written at the end of the previous run.
7. **GRADNT**	Computes the gradient of the physical variables to improve the prediction of those variables for the two sides of the interface. The gradients are subjected to the monotonicity condition that limits the projected values, thus preventing new maxima-minima from being caused artificially by interpolation (IOPORD = 2). Calls FCHART in order to compute projected values at the half timestep associated with the local characteristics of the flow.
8. **GRDFLX**	Computes the gradient of the pressure and Mach number in each cell. This information is used as an error indicator for the adaptation needed in a steady state solution.
9. **FIRST**	The equivalent of GRADNT if run in a first order mode (IOPORD = 1). Using FIRST assumes that the physical variables are constant in each cell. Takes care of the boundary conditions if the interface is a boundary.
10. **FCHART**	Computes the projected values at a half timestep for the two sides of the interface based on the local characteristics of the flow. Called by GRADNT, it modifies the projected values for the two sides of the interface and assigns them to the correct location in memory. Takes care of the boundary conditions if the interface is a boundary.

11. **PRLCTN**	Determines particle cell location in the initial phase of tracing a group of particles.
12. **PRPTHC**	Advances the position of each particle, assuming that the particle has the flow velocity of the cell. PRPTHC will find the cell location of the particle after it advances by the timestep of the computation.
13. **VERCEN**	Places an additional vertex at the center of a specified cell to refine the size of the cell by a factor of three.
14. **DISECT**	Places an additional vertex at the middle of a specified edge to refine the size of the two cells adjacent to the edge by a factor of two. This method of refinement is used only on the edges lying on the boundaries of the computational domain.
15. **DYNPTN**	Tests and flags the cells for specified refinement criteria. DYNPTN is called only if the parameter IOPADD = 1. Will start the refinement procedure by calling VERCEN and DISECT and will call DYYPTN for further refinement. This insures that the buffer zone ahead of the shock is resolved according to the specified area criteria (AREADD).
16. **DYYPTN**	Refines the cells flagged by DYNPTN by calling VERCEN and DISECT until the area of each flagged cell meets the area criteria specified by the parameter AREADD.

17. **INTPTN**	Refines the cells in the inlet region. Prepares the inlet region for the introduction of a shock wave. This initial refinement is essential to prevent additional refinement of the grid in the presence of a shock wave. It is called only if the parameters ICOND=0 and IOPTN= 2 (solution for transient phenomena).
18. **DELPTN**	Tests and flags the cells for the specified criteria for coarsening. DELPTN is called only if parameter IOPDEL = 1.
19. **RELAXY**	Relaxes the vertices of the cells that were created in the process of deleting a vertex.
20. **VERDEL**	Deletes a specified vertex.
21. **RECNC**	Tests two cells adjacent to the specified edge. Compares them to the two cells that can be created if this edge is flipped to pass between the other two vertices of the quadrilateral containing the original two cells. If the tests result in a better quality triangle, then RECNC will swap the edge.
22. **EOS**	Applies Gilmore equation of state to compute $\gamma = c_p/c_v$, giving the internal energy and density of the fluid in a cell. This option is controlled by the parameter IOPEOS = 1.
23. **LIFTDR**	A diagnostic to compute the lift, drag, and transfer momentum developed in the configuration. Takes into account all boundary edges that are specified as 5. It is controlled by the parameter IOPLFT = 1.

All of the data input and initiation of a run (or a restart run) is performed in MAIN. The actual simulation is controlled by HYDRMN, which is called from MAIN. At the completion of a run, control is returned to MAIN and a successful termination prints the message STOP 777.

MAIN contains one name list (file no. 2) and requires an input file that contains tne grid data description (file no. 16). The data organization for the grid file is described in Appendix A. There are five files that should be included: CINT00.H, CMSH00.H, CPHS10.H, CPHS20.H, CHYD00.H.

NAMELIST/DATA	ICOND	ICONP	ITRIGR	IOPTN
	XMCHIN	RIN	PIN	ALFA
	HRGG	IHRN	NTIME	MDUMP
	NDUMP	KDUMP	IOSPCL	IOPLFT
	IOPRCN	IOPORD	IOPBYN	IAXSYM
	IOPEOS	MPRTCL	IOPINT	IOPADD
	IOPDEL	AREADD	AREDEL	IWINDW
	ISTATC			

VARIABLE	PURPOSE
ICOND	= 0 READ INPUT GRID FOR A NEW SIMULATION = 1 READ THE GRID FROM PREVIOUS RUN

ICOND = 0:

MAIN will read the initial grid definition stored in file number 16. The current setting is to read the input file as provided by Smart, a two dimensional triangular grid generator that runs interactively on the Macintosh personal computer.

MAIN will call UPDATE, which will call GEOMTR. GEOMTR will compute essential geometrical parameters that are not provided by file 16. All geometrical information is dumped into output files (8 and 88) so that ICOND=0 is used only once at the beginning of a new simulation.

ICOND = 1:

MAIN will call UPGRAD, which will call one of the output files (8 or 88) written by the previous run. This will load the geometrical definition of the grid (either 8 or 88---they are identical). Writing identical files provides a backup in the event that the job terminates for lack of time while in the process of writing to one of those output files.

VARIABLE	PURPOSE
ICONP	= 0 PRIMITIVE VARIABLES INITIALIZED = 1 VARIABLES READ FROM PREVIOUS RUN

ICONP = 0:

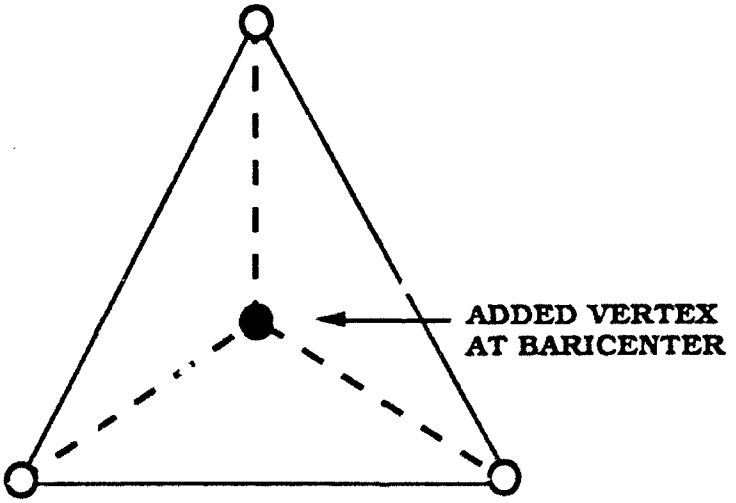
Initialize the primitive variables in computational domain with an initial value specified by the user. The two options set by the code are controlled by IOPTN.

ICONP = 1:

The flow field condition reads in files 8 or 88 and provides a followup run set from the previous run.

VARIABLE	PURPOSE
ITRIGR	= 0 USING THE INPUT GRID AS THE INITIAL GRID = 1 THE INPUT GRID TRIPLED BY ADDING AN EXTRA VERTEX IN EACH TRIANGLE

ITRIGR = 1: The original grid cells will be tripled by adding an extra vertex in the baricenter of each triangle. This option can be triggered at the beginning of a simulation only (ICOND = 0).



VARIABLE	PURPOSE
IOPTN	= 1 SOLUTION FOR STEADY STATE = 2 SOLUTION FOR TRANSIENT PHENOMENA

There are two choices available to set the initial condition of the problem.

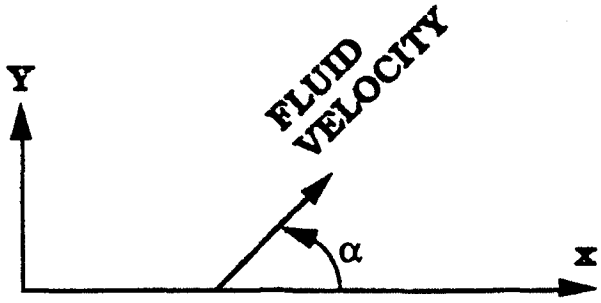
IOPTN = 1.

Assign the conditions at the inlet to the computational domain. This is the fastest way to get a steady state solution for the conditions specified at the inlet. In this option, PIN (pressure), RIN (density) and XMCHIN (Mach number) are assigned to the pressure density and velocity (the speed of sound is computed in the code) and imposed at the inlet boundaries.

IOPTN = 2.

Used if a shock wave is to be simulated moving from the inlet (edge boundary 8) to the outlet (edge boundary 7). For this setting, specify PIN (ambient pressure in the chamber), RIN (ambient density in the chamber) and XMCHIN (upstream Mach number). The code will use the normal shock wave relations for an adiabatic flow of a completely perfect fluid to compute the static-pressure ratio across the shock P_2/P_1 and the density ratio ρ_2/ρ_1, and the ratio of the Mach number across the shock M_2/M_1. These computed quantities are applied to set correctly the condition on the pressure density and velocity at the inlet boundary.

VARIABLE	PURPOSE
ALPHA	THE DIRECTION OF INFLOW IN DEGREES RELATIVE TO A RIGHT HAND COORDINATE SYSTEM. ALPHA = 0 MEANS FLOW FROM LEFT TO RIGHT.



The velocity computed by the code according to the input data provided by the user is split (projected) in the X and Y directions by using α.

VARIABLE	PURPOSE
HRGG	INITIAL γ IN THE EQUATION OF STATE. THE CODE RUNS USING THE IDEAL EQUATION OF STATE AS A BASELINE AND SHOULD BE MODIFIED IF SOMETHING ELSE IS DESIRED. IOPEOS=1 WILL TRIGGER THE USE OF GILMORE EQUATION OF STATE.

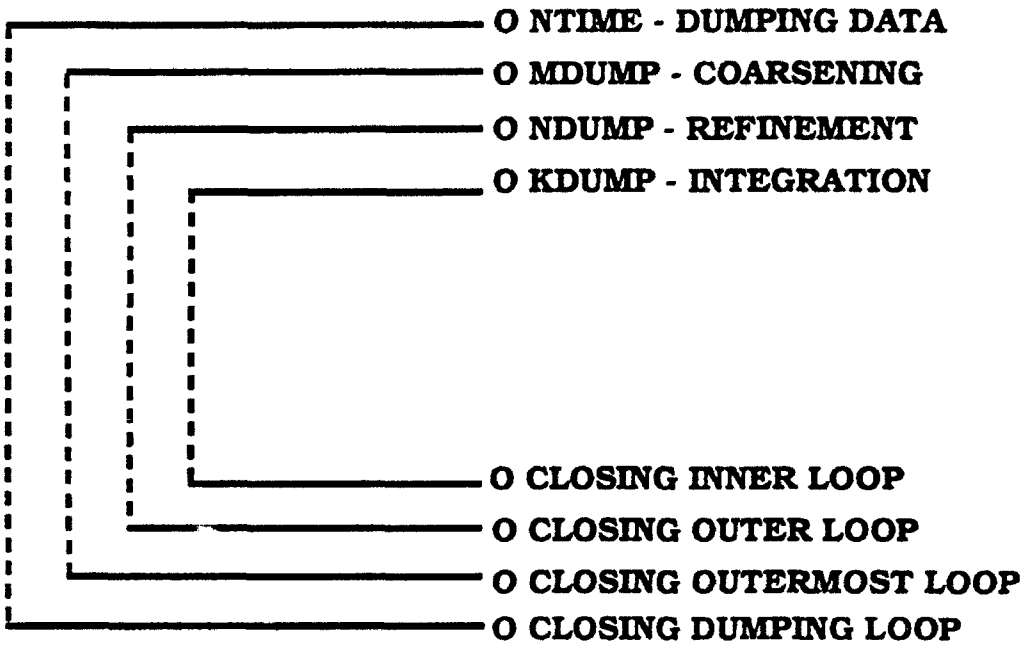
VARIABLE	PURPOSE
IHRN	NUMBER OF ITERATIONS IN THE RIEMANN SOLVER TO FIND THE DIAPHRAGM SOLUTION. (THREE TO FOUR SHOULD BE USED AND INCREASED ONLY FOR A VERY HIGH MACH NUMBER CASES.)

VARIABLE	PURPOSE
NTIME	NUMBER OF REPEATS FOR THE INTEGRATION/ REFINEMENT/COARSENING SEQUENCE. AN OUTPUT DUMP IS DONE FOR EVERY SEQUENCE REPEAT.

VARIABLE	PURPOSE
MDUMP	NUMBER OF OUTERMOST LOOP ITERATIONS IN THE CALCULATION WHERE COARSENING OF THE GRID IS PERFORMED EVERY SEQUENCE REPEAT.

VARIABLE	PURPOSE
NDUMP	NUMBER OF OUTER LOOP ITERATIONS IN THE CALCULATION WHERE REFINING IS DONE FOR EVERY SEQUENCE REPEAT WITHOUT COARSENING.

VARIABLE	PURPOSE
KDUMP	NUMBER OF ITERATIONS PERFORMED WITH NO REFINEMENT OR COARSENING. THE INNER LOOP OF THE CALCULATION. IF KDUMP = 0, KDUMP WILL BE SET BY THE CODE AUTOMATI-CALLY ACCORDING TO THE SETTING OF THE VARIABLE AREADD.



VARIABLE	PURPOSE
IOSPCL	= 0 NOT USING REDEFINITION OF POINTS ON THE BOUNDARY = 1 USING REDEFINITION OF POINTS ON THE BOUNDARY

IOSPCL = 1: Modifies the definition of points along the boundary according to a presetting in the code. The setting currently will redefine the points along the edge boundary 5 to exactly match NACA0012 airfoil shape. This is done to redefine points on a boundary that has an analytical definition of points, but where these points have been dislocated by a refining procedure.

VARIABLE	PURPOSE
IOPLFT	= 0 THE COMPUTATION OF LIFT DRAG AND MOMENT TURNED OFF = 1 THE COMPUTATION OF LIFT DRAG AND MOMENT TURNED ON

Set IOPLFT = 1 if integral quantities need to be computed. The current setting will calculate the lift, drag and moment on edge boundary 5.

VARIABLE	PURPOSE
IOPRCN	= 0 A GLOBAL SWAPPING (RECONNECTION) PROCEDURE IS OFF = 1 A GLOBAL SWAPPING (RECONNECTION) PROCEDURE IS ON

This swapping is done by calling subroutine RECNC. It is used only in a new simulation (ICOND = 0).

VARIABLE	PURPOSE
IOPORD	= 1 THE CODE WILL RUN FIRST ORDER GODUNOV METHOD = 2 THE CODE WILL RUN SECOND ORDER GODUNOV METHOD

IOPORD = 1 Subroutine FIRST is called.

IOPORD = 2 Subroutine GRADNT is called.

VARIABLE	PURPOSE
IOP[illegible]YN	= 0 NO BUOYANCY EFFECTS ARE COMPUTED = 1 BUOYANCY EFFECTS IN THE X DIRECTION ARE COMPUTED = 2 BUOYANCY EFFECTS IN THE Y DIRECTION ARE COMPUTED

The buoyancy effect applies the gravity acceleration as g = 9.81.

VARIABLE	PURPOSE
IAXSYM	= 0 THE CODE WILL RUN IN A PURE TWO DIMENSIONAL MODEL = 1 THE CODE WILL RUN IN AN AXISYMMETRICAL MODE (X AS THE AXIS OF SYMMETRY) = 2 THE CODE WILL RUN IN AN AXISYMMETRICAL MODE (Y AS THE AXIS OF SYMMETRY)

VARIABLE	PURPOSE
IOPEOS	= 0 THE CODE WILL RUN WITH CONSTANT γ = 1 THE CODE WILL RUN WITH VARIABLE γ USING THE EQUATION OF STATE FOR AIR

IOPEOS = 0: The initial γ is not changed and is kept constant across the computational domain at all times (with value set by HRGG).

IOPEOS = 1: The γ of each cell will be modified according to local internal energy and density. Thus, if IOPEOS = 1, the actual pressure and density should be input (in the appropriate dimension). Otherwise (IOPEOS=0), a normalized pressure and density of unity can be used for simulation.

VARIABLE	PURPOSE
MPRTCL	= 0 NO PARTICLE TRACING = 1 THE CODE WILL TRACE PARTICLES

MPRTCL = 1: The ability to trace particles will be turned on. Initially PRLCTN is called to identify the cell location of each particle. For each time step, PRPTHC will be called to update the cell location of each particle if it is relocated, assuming the particle moves at the same velocity as the fluid.

The initial location of the particles is defined in MAIN.

VARIABLE	PURPOSE
IOPINT	= 0 DOES NOT PREPARE A BUFFER ZONE. = 1 INITIALLY PREPARE A BUFFER ZONE AHEAD OF EDGE BOUNDARY 8

For simulating transient phenomena, the refining of the grid is done in the region ahead of the shock. In this way, we avoid interpolating in a region where large gradients reside. IOPINT = 1 will refine the region of the inlet flow to prepare a buffer zone (edge boundary 8). If refining is needed in another region, subroutine INTPTN should be modified accordingly.

VARIABLE	PURPOSE
IOPADD	= 0 THE REFINEMENT PROCEDURE IS TURNED OFF = 1 THE REFINEMENT PROCEDURE IS TURNED ON

VARIABLE	PURPOSE
IOPDEL	= 0 THE COARSENING PROCEDURE IS TURNED OFF = 1 THE COARSENING PROCEDURE IS TURNED ON

VARIABLE	PURPOSE
AREADD	SPECIFIES THE MINIMUM AREA VALUE THAT A TRIANGLE SHOULD HAVE AFTER REFINEMENT. SPECIFIED AS A FRACTION OF THE AVERAGE TRIANGLE AREA OF THE INITIAL GRID. THIS REFERENCE AREA IS KEPT CONSTANT THROUGH THE WHOLE SIMULATION.

VARIABLE	PURPOSE
AREDEL	SPECIFIES THE MAXIMUM VALUE THAT A TRIANGLE SHOULD HAVE AFTER COARSENING DEFINED AS A FRACTION OF THE REFERENCE AREA.

VARIABLE	PURPOSE
IWINDW	= 0 NO RESTRICTION ON THE REGION FOR REFINING THE GRID = 1 SETTING A WINDOW FOR REFINING THE GRID

IWINDW = 1: The user can specify a region in which the refinement process will take place. Otherwise, the refinement takes place everywhere in the computational domain.

VARIABLE	PURPOSE
ISTATC	= 0 THE ADAPTATION WILL BE DONE ON A MOVING WAVE = 1 THE ADAPTATION WILL BE DONE ON A STEADY STATE CONDITION

Because the criteria for refinement in the presence of a static shock are not suited to treating a moving shock, the code sets different error indicators for adapting the grid for the two cases.

ISTATC = 0

The energy and density net fluxes across each cell are tested for sensing the level of activity. This method is a very good error indicator for sensing transient phenomena as traveling shocks.

ISTATC = 1

The pressure and Mach gradients in each cell are tested for sensing steady state shocks.

The gradient of density is always tested as a third criteria for making sure that static shocks are not ignored in computing a transient flow.

HYDRFL

Computes the fluxes across interfaces when the conditions for both sides are given. The fluxes are computed assuming a shock solution at a broken diaphragm simulated by the presence of the interface. The conditions existing on the two sides of the diaphragm will define the condition of the flow at the diaphragm location. These conditions are computed by solving the Riemann problem using the Godunov algorithm. The condition at the diaphragm defines the flux of energy, mass, and momentum passing across the interface. The Euler conservation law is applied to conserve energy, mass, and momentum crossing interfaces from one cell to the other.

Quantity	Side 1	Diaphragm (Interface)	Side 2
Density	ρ_1	ρ	ρ_2
Pressure	P_1	P	P_2
Velocity Perpendicular to Interface	u_1	u	u_2
Velocity Parallel to Interface	v_1	v	v_2

HYDRMN

Controls the code and the iteration loops. It calls HYDRFL to find the interface fluxes. These fluxes are integrated to update the physical variables in each cell. If adaptation of the grid is required, HYDRMN will set the criteria for controlling the adaptation of the grid. The refining (DYNPTN, DYYPTN) and coarsening (DELPTN) of the grid is invoked by HYDRMN. HYDRMN also controls the output by writing the necessary information on files for post processing data and for restarting the AUGUST code at a later time. It also manages print file diagnostics.

GEOMTR

Calculates geometrical variables that are not supplied by the input data and are needed to run the code. For example, it will compute:

1) Area of the cells;
2) Length of the edges;
3) Unit vector perpendicular to the edge. (For boundary edges, this unit vector is direct from the computational domain outward);
4) Unit vector directed from the baricenter of the left cell to the baricenter of the right cell. For boundary edges, the unit vector is perpendicular to the edge (from left cell outward).

The code will change the direction of the boundary edges so that all are arranged counterclockwise and the associated computational cell is always on the left side. GEOMTR is called once in the beginning of a new simulation.

UPDATE

Called in the beginning of a new simulation for setting geometrical variables not provided by the input data. (It calls GEOMTR.)

UPGRAD

Called if the run is a restart. UPGRAD will read the appropriate file (either 8 or 88) dumped by the previous run.

GRADNT

Compute the gradients of the physical variables in each cell. These computed gradients, along with the physical values at the baricenters, are applied using linear interpolation to predict the values on the interface.

The computed gradients are subjected to the monotonicity condition, ensuring that the projected values are bounded by the value of each quatity in the three adjacent cells, and to make sure that no new maxima or minima occurs. The projection of quantities to the interface improves the results from the code and provides second order accuracy in space.

GRADNT calls FCHART, which computes the projected values at the interfaces at the half timestep level according to the local characteristics of the flow in each cell bordering the interface cell. The assignment of values at the two sides of each interface is done at the end of FCHART. This same loop will also impose the boundary conditions for the interfaces at the boundaries of the computational domain.

GRDFLX

Computes the gradient of the Mach value and pressure gradient in each cell. These gradients are applied if the adaptation is done on a steady state converged solution. These variables, in addition to the computed density gradient, provide the criteria for adaptation if it is necessary to refine the grid for steady state problems.

FIRST

Assigns flow quantities to each side of an edge. These are based on the values at the baricenter of the triangles on either side of the edge. FIRST uses a first order approximation to find the values at the edge.

The user can specify FIRST or GRADNT by choosing 1 or 2 for the parameter IOPORD.

FCHART

Called by GRADNT to compute the values projected at the interfaces at the half timestep. These calculations are done by applying the local velocity characteristics in each cell. This projection in time improves the results and makes the code second order accurate in time.

PRLCTN

Identifies the initial cell location of each particle. Called once after specifying the starting location of each particle to be traced.

PRPTHC

Advances the particle position by the marching timestep. It finds the new cell location if a particle crosses an interface. The assumption is that the particles move at the fluid velocity.

VERCEN

Introduces a new vertex at the baricenter of the designated cell during the refinement process.

DISECT

Introduces a new vertex at the middle of a designated edge.

DYNPTN

Tests the cells according to the refining criteria and flags each cell which requires refinement. The flagged cells are refined in DYYPTN. The refinement is subjected to geometrical constraints on the cell shape to retain a high better quality refined grid.

The user can specify a window in the computational domain for refinement. The parameter to trigger this option is IWINDW = 1. For specifying the actual window, it may be necessary for the user to alter this subroutine and provide a definition of the geometrical area to be refined.

DYYPTN

Traces the cells that are flagged for refinement by DYNPTN. It subdivides them until each one of the refined cells meets the area refinement criteria of AREADD. Because each loop of refinement is restricted to a one-third reduction in cell area (calling VERCEN), DYYPTN will perform the necessary number of loops to meet the area reduction specified for refinement. AREADD is a fraction of the average area of the initial grid. This reference area is kept constant and fixes the minimum resolution in the simulation domain.

INTPTN

Performs the initial refinement of the grid before the initialization. The assumption is that a shock wave is introduced through the inlet boundary. Consequently, INTPTN will test for the inflow boundary interface and will refine the appropriate cells. (Note: It is not recommended that the code automatically refine the grid in the inlet region in the presence of a shock wave. If a shock wave is not introduced through the inlet, INTPTN should be modified to accommodate the change of the initial condition.)

DELPTN

Tests the cells according to coarsening criteria and flags them. Each triangle is tested to determine which vertex of the triangle is most appropriate for removal. This vertex is removed by calling VERDEL. DELPTN cannot delete nodes that have the status JV(1,IV) = 3. It is therefore recommended that nodes at sharp corners or nodes on important boundaries that are curved, be flagged as JV(1,IV) = 3.

RELAXY

Relaxes the cells that are created in the process of deleting a vertex. The relaxation procedure relocates the designated vertex to the mass center of the surrounding vertices.

LAPLAC

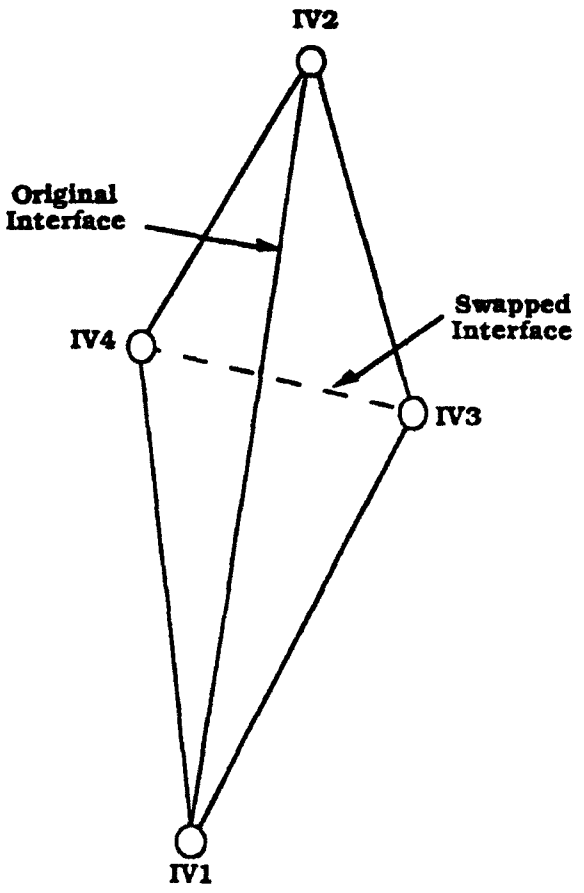
Computes the Laplacian of the pressure and density.

VERDEL

Deletes a designated vertex.

RECNC

Tests the possibility of swapping the designated interface to create two triangles of better quality than the original two.



EOS

Computes γ using to the equation of state for air (Gilmore equation of state), given the density and internal energy of the air. The user may choose to apply the equation of state by setting IOPEOS = 1.

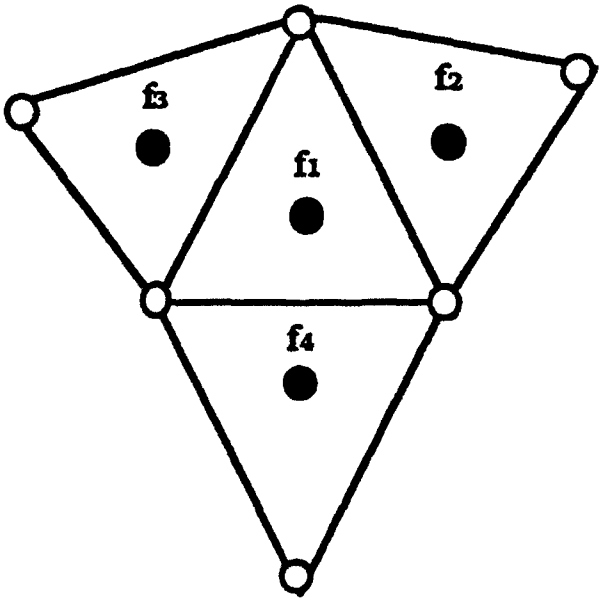
LIFTDR

Computes integral quantity diagnostics on any configuration. The integral quantities are lift, drag, and momentum and are found on boundary interfaces designated as 5.

GRADNT

Computes the gradient of a scalar variable at the center of a cell. It uses a least squares technique to interpolate the values at the center of four triangles (the cell and its three adjacent triangles) to fit (four equations with three unknowns).

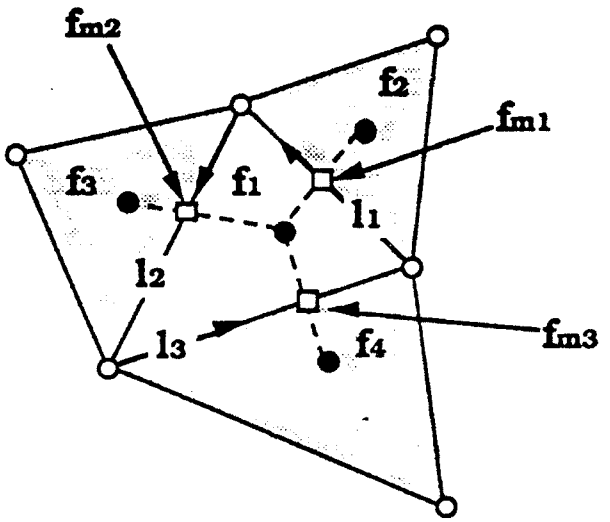
$$f = a_0 + a_1 x + a_2 y$$



Those gradients are subjected to a monotonicity limiter that ensures no new minima or maxima are produced artificially in the projected values at the interfaces.

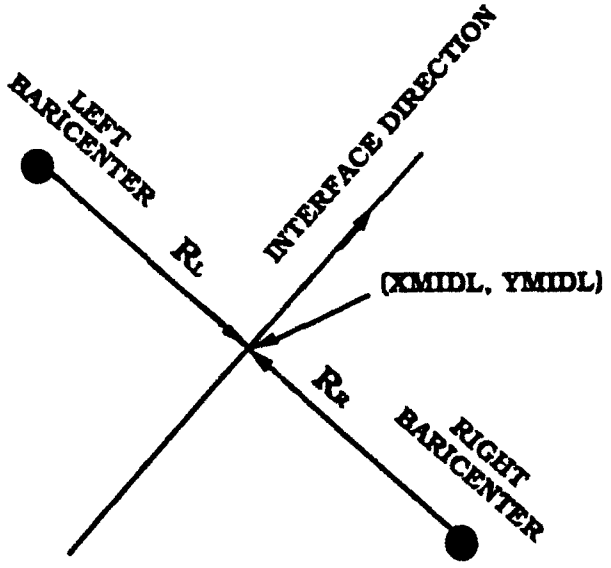
The monotonicity algorithm involves the following steps

1)	find maximum and minimum of f_1, f_2, f_3, f_4 $f_{max} = \text{Max}(f_1, f_2, f_3, f_4)$ $f_{min} = \text{Min}(f_1, f_2, f_3, f_4)$
2)	compute $\Delta f_{max} = f_{max} - f_1$ $\Delta f_{min} = f_{min} - f_1$
3)	compute incremental projected values at the interfaces $f_{mjR} - f_R = \nabla f_R \cdot \bar{r}_{jR}$ $f_{mjL} - f_L = \nabla f_L \cdot \bar{r}_{jL}$



$$\Delta f_{mjR} = f_{mjR} - f_R = \nabla f_R \cdot \bar{r}_{jR}$$
$$\Delta f_{mjL} = f_{mjL} - f_L = \nabla f_L \cdot \bar{r}_{jL}$$

where j stands for every interface of the cell and fmj is the interpolated value at the middle of the interface.



4) compute the limiter by calculating the minimum of indicator for each edge of the three edges of the cell.

$$\text{right to the interface RUVPR} = \frac{(1 + \text{sign } \Delta f_{mjR})\,\Delta f_{max} + (1 - \text{sign } \Delta f_{mjR})\Delta f_{min}}{2\,\Delta f_{mjR}}$$

$$\text{left to the interface RUVPL} = \frac{(1 + \text{sign } \Delta f_{mjL})\,\Delta f_{max} + (1 - \text{sign } \Delta f_{mjL})\Delta f_{min}}{2\,\Delta f_{mjL}}.$$

This formulation ensures that

$$\text{if} \begin{cases} \Delta f_{mj} > 0 \text{ RUVP} = \dfrac{\Delta f_{max}}{\Delta f_{mj}} \\ \Delta f_{mj} < 0 \text{ RUVP} = \dfrac{\Delta f_{min}}{\Delta f_{mj}} \end{cases}.$$

the outcome of RUVP is always positive. If RUVP > 1 then the projected value at the interfaces will introduce a new minimum or maximum relative to the values at the baricenters of the appropriate cells.

Select the minimum between the six values for RUVP (two for every one of the three interfaces of the cell) not exceeding unity. The selected minimum

of RUVP is the required limiter. The gradient is multiplied by this limiter that is always less or equal to unity.

FCHART

Computes the projected values at the half time step level based on the local characteristics of the flow. This process extends the accuracy of the code to be second-order in time as well as in space.

The characteristic projection consists of several steps.

1) Calculate the velocity of sound in the two cells bordering the designated interface

CNLEFT = $\sqrt{\gamma_L \cdot P_L/\rho_L}$ sound speed in left cell

CNRIGT = $\sqrt{\gamma_R \cdot P_R/\rho_R}$ sound speed in right cell

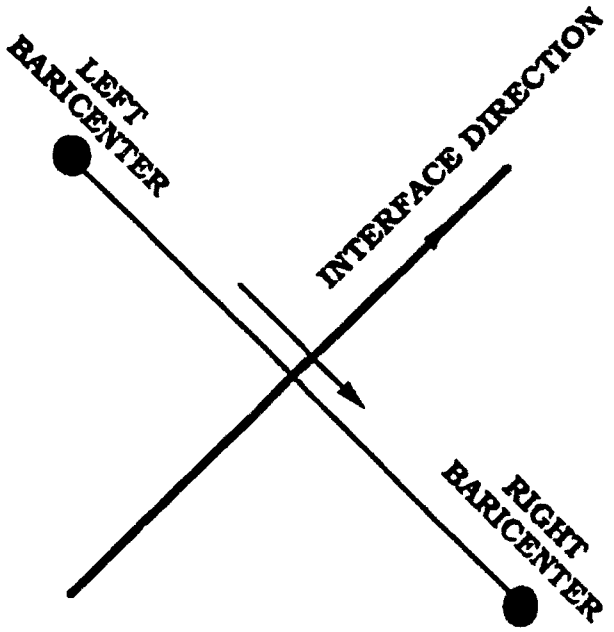
UVLEFT = $\bar{U}_L \cdot \bar{t}$ velocity of fluid at the left cell projected in $\bar{t}$ direction

UVRIGT = $\bar{U}_R \cdot \bar{t}$ velocity of fluid at the right cell projected in $\bar{t}$ direction

where

$$\bar{t} = XXN \cdot \bar{i} + YYN \cdot \bar{j}$$

$$\bar{U} = U \cdot \bar{i} + V \cdot \bar{j}$$



2) To compute the interpolated left and right projected values at time $t^N + \Delta t/2$, we calculate the distances that the disturbances generated from the baricenter of the cells, traveling toward the interface:

$$ZZLEFT = (UVLEFT + CNLEFT) \cdot \Delta t/2$$

$$ZZRIGT = - (UVRIGT - CNRIGT) \cdot \Delta t/2$$

If ZZLEFT or ZZRIGT is negative they are reset to zero.

3) Calculate the distances that the flow will travel if it were to flow at the velocity of each of the local characteristics:

$$ZOLEFT = UVLEFT \cdot \Delta t/2$$

$$ZORIGT = - UVRIGT \cdot \Delta t/2$$

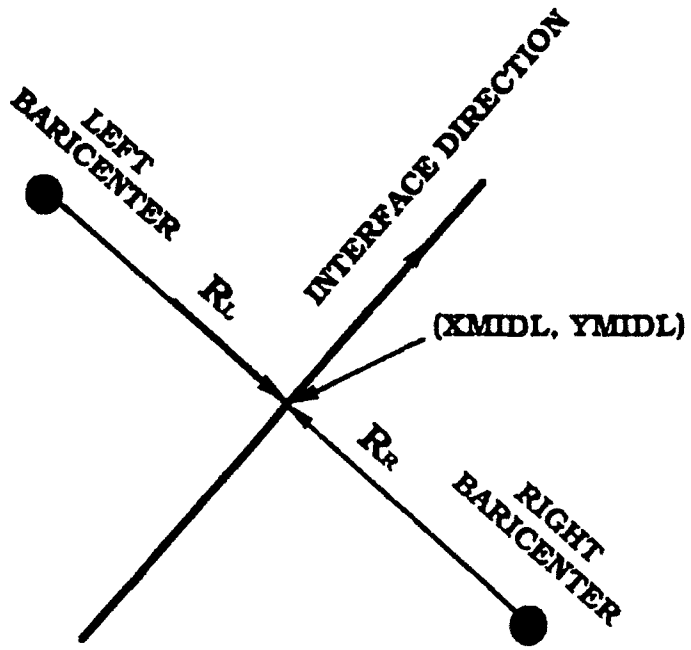
$$ZPLEFT = (UVLEFT + CNLEFT) \cdot \Delta t/2$$

$$ZPRIGT = -(UVRIGT + CNRIGT) \cdot \Delta t/2$$

$$ZMLEFT = (UVLEFT - CNLEFT) \cdot \Delta t/2$$

$$ZMRIGT = -(UVRIGT - CNRIGT) \cdot \Delta t/2.$$

4) Calculate the projected values of the nonconservative variables (density, velocity component (perpendicular and tangential to the interface), and pressure).



For the left cell:

Density HRRL = $\rho_L + \bar{\nabla}\rho_L \cdot (\bar{r}_L - ZZLEFT \cdot \bar{t})$

Perpendicular Velocity HUUL = $U_L + \bar{\nabla}U_L \cdot (\bar{r}_L - ZZLEFT \cdot \bar{t})$

Tangential Velocity	HVVL	=	$V_L + \bar{\nabla}V_L \cdot (\bar{r}_L - ZZLEFT \cdot \bar{t})$
Pressure	HPPL	=	$P_L + \bar{\nabla}P_L \cdot (\bar{r}_L - ZZLEFT \cdot \bar{t})$
	GMTLFT	=	$\rho_L \cdot HRRL \cdot HPPL$

For the right cell:

Density	HRRR	=	$\rho_R + \bar{\nabla}\rho_R \cdot (\bar{r}_R - ZZRIGT \cdot \bar{t})$
Perpendicular velocity	HUUR	=	$U_R + \bar{\nabla}U_R \cdot (\bar{r}_R - ZZRIGT \cdot \bar{t})$
Tangential velocity	HVVR	=	$V_R + \bar{\nabla}V_R \cdot (\bar{r}_R - ZZRIGT \cdot \bar{t})$
Pressure	HPPR	=	$P_R + \bar{\nabla}P_R \cdot (\bar{r}_R - ZZRIGT \cdot \bar{t})$
	GMTRGT	=	$\rho_R \cdot HRRR \cdot HPPR$

For the left cell, taking into account the following characteristics:

- For UVLEFT + CNLEFT:

$$UUU = \bar{\nabla}U_L \cdot (ZPLEFT - ZZLEFT)\,\bar{t}$$

$$PPP = \bar{\nabla}P_L \cdot (ZPLEFT - ZZLEFT)\,\bar{t}$$

$$UPLFT = -0.5 \cdot \left(UUU + PPP/\sqrt{GMTLFT}\right) / \sqrt{GMTLFT}$$

If UVLEFT + CNLEFT is negative, UPLFT is reset to zero.

- For UVLEFT – CNLEFT:

$$UUU = \bar{\nabla}U_L \cdot (ZMLEFT - ZZLEFT) \cdot \bar{t}$$

$$PPP = \bar{\nabla}P_L \cdot (ZMLEFT - ZZLEFT) \cdot \bar{t}$$

$$UM...T = 0.5 \cdot (UUU - PPP/\sqrt{GMTLFT}) / \sqrt{GMTLFT}$$

if l LEFT - CNLEFT is negative, UPLFT is reset to zero.

- For UVLEFT:

$$PPP = \bar{\nabla} P_L \cdot (ZOLEFT - ZZLEFT) \cdot \bar{t}$$

$$RRRR = \rho_L + \bar{\nabla} \rho_L \cdot (\bar{r}_L - ZOLEFT) \cdot \bar{t}$$

$$URLFT = PPP/GMTLFT + 1/HRRL - 1/RRRR$$

If UVLEFT is negative, URLEFT is reset to zero.

For the right cell, taking into account the following characteristics:

- For UVRIGT + CNRIGT:

$$UUU = \bar{\nabla} U_R \cdot (ZZRIGT - ZPRIGT) \bar{t}$$

$$PPP = \bar{\nabla} P_R \cdot (ZZRIGT - ZPRIGT) \bar{t}$$

$$UPRGT = -0.5 \cdot \left(UUU + PPP/\sqrt{GMTRGT}\right) /\sqrt{GMTRGT}$$

If UVRIGT + CNRIGT is positive, UMRGT is reset to zero.

- For UVRIGT – CNRIGT:

$$UUU = \bar{\nabla} U_R \cdot (ZZRIGT - ZMRIGT) \cdot \bar{t}$$

$$PPP = \bar{\nabla} P_R \cdot (ZZRIGT - ZMRIGT) \cdot \bar{t}$$

$$UMRGT = 0.5 \cdot \left(UUU - PPP/\sqrt{GMTRGT}\right) /\sqrt{GMTRGT}$$

If UVRIGT - CNRIGT is positive, UMRGT is reset to zero.

- For UVRIGT:

$$PPP = \bar{\nabla} P_R \cdot (ZZRIGT - ZORIGT) \cdot \bar{t}$$

$$RRRR = \rho_R + \bar{\nabla} \rho_R \cdot (\bar{r}_R + ZORIGT) \cdot \bar{t}$$

$$URRGT = PPP/GMTRGT + 1/HRRR - 1/RRRR$$

If UVRIGT - CNRIGT is positive, URRGT is reset to zero.

The projected values will be:

$$
\begin{aligned}
RRL &= 1/(1/HRRL - (UPLFT + UMLFT + URLFT)) \\
UUL &= HUUL + (UPLFT - UMLFT)\sqrt{GMTLFT} \\
VVL &= HVVL + (UPLFT - UMLFT)\sqrt{GMTLFT} \\
PPL &= HPPL + (UPLFT + UMLFT)\, GMTLFT \\
RRR &= 1/(1/HRRR - (UPRGT + UMRGT + URRGT)) \\
UUR &= HUUR + (UPRGT - UMRGT)\sqrt{GMTRGT} \\
VVR &= HVVR + (UPRGT - UMRGT)\sqrt{GMTRGT} \\
PPR &= HPPR + (UPRGT + UMRGT) \cdot GMTRGT.
\end{aligned}
$$

Those values are the assigned condition for the two sides of the interface. If the interface is a boundary, the right condition is determined according to the type of boundary.

DYNPTN & DYYPTN

DYNPTN applies three distinct criteria to test cells to determine their need for refinement. They are as follows:

For unsteady dynamic simulation

1) total energy flux entering or leaving a cell
2) total density flux entering or leaving a cell
3) density gradient in each cell.

For steady state simulation

1) Pressure gradient in each cell
2) Mach number gradient in each cell
3) density gradient in each cell.

Cells that meet one of those three criteria are flagged, and are actually subdivided in DYYPTN until they meet the area criteria set for refinement (AREADD). The code will compute the maximum of each of the three criteria and set a 5% of the maximum or higher to the refinement criteria for the fluxes and 3% for the gradient. These criteria work extremely well for moving waves.

It should be noted that those error indicators and their levels are set according to the actual simulated condition. For different cases, other error indicators and level settings might be more appropriate than the above.

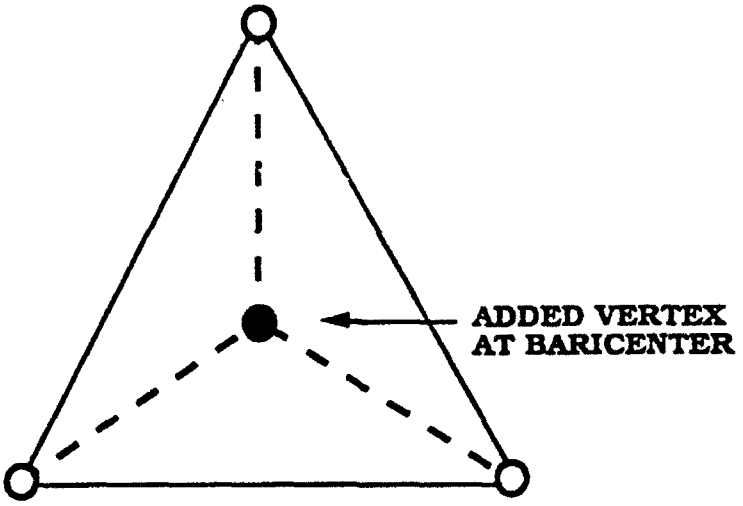
DELPTN

Tests the cells for coarsening criteria. The same criteria that refines the grid are applied to coarsen the grid but in a different setting. Each cell that has less than 5% of the fluxes and less than 3% of the gradient criteria is eligible for coarsening. The code will test the cell flagged for coarsening and will choose one of the three vertices of the cell for deletion by determining which of the three has the smallest aspect ratio. (The aspect ratio is defined as the ratio between the height emerging from the node and its corresponding base.) There are vertices that cannot be removed, such as corners or vertices that preserve the original shape of the boundaries (JV(1,IV) = 3).

After the vertex is deleted, a relaxing procedure is performed on the vertices surrounding the deleted vertex, as well as a swapping procedure to improve the quality of the triangles constructed in the deletion procedure.

VERCEN

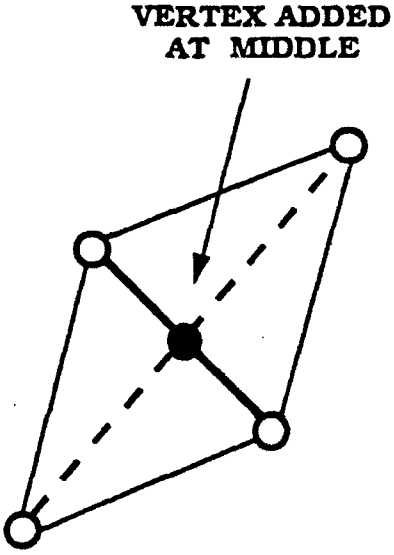
Adds an additional vertex at the baricenter of the designated cell.



VERCEN assigns one of the three new triangles the number of the original triangle and will add two more at the end of cells table. A new vertex plus three new interfaces are added at the end of the associated tables.

DISECT

Adds a new vertex at the middle of the designated edge.



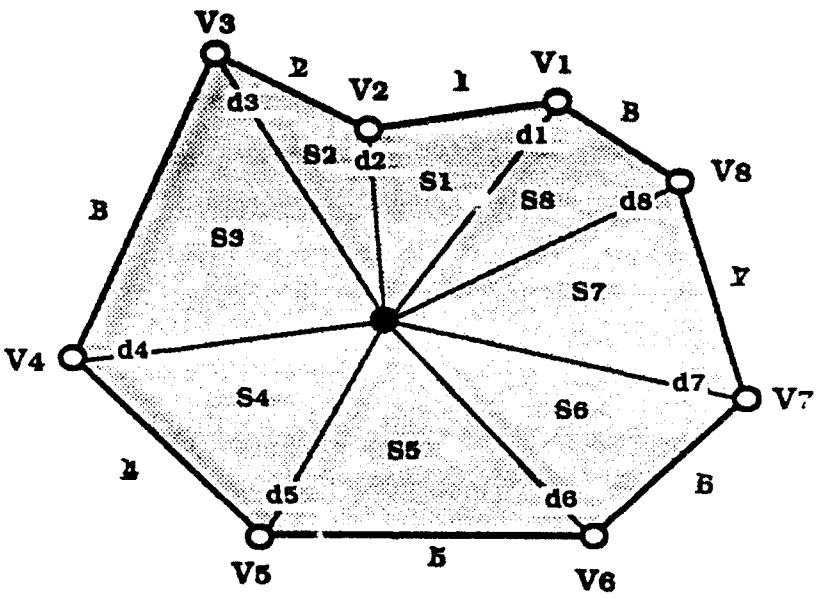
DISECT will add one new vertex, three new edges and two new triangles, all of which are added at the end of the corresponding tables (vertices, edges and cells).

VERDEL

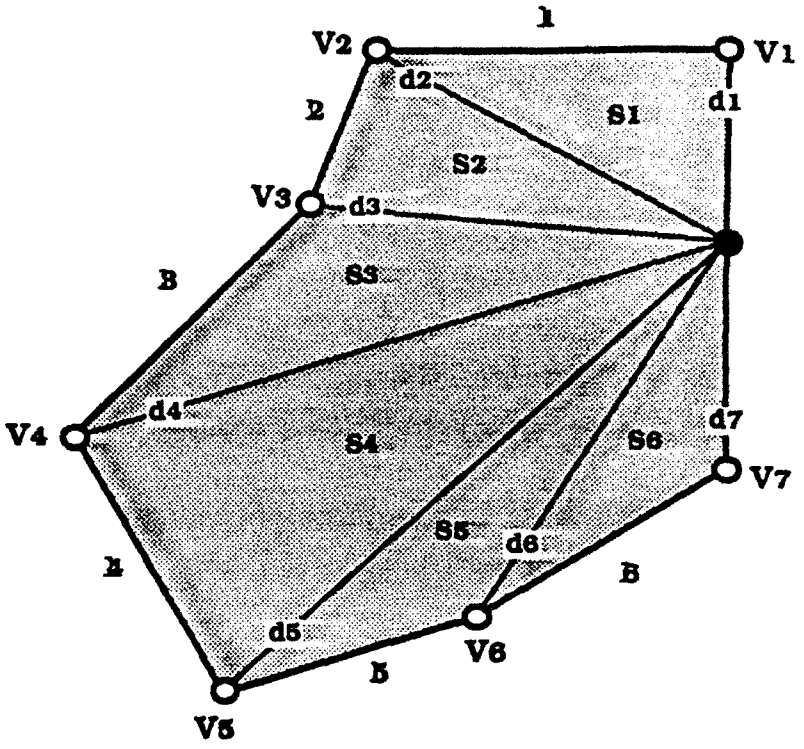
Forces deletion of a designated vertex. There are two types of vertices: deletion of a vertex in the interior of the computational domain and deletion of a vertex on the boundary. The steps of deleting a vertex are:

1) Identify the edges and cells surrounding the designated vertex in the computational domain

Interior Vertex to be Deleted



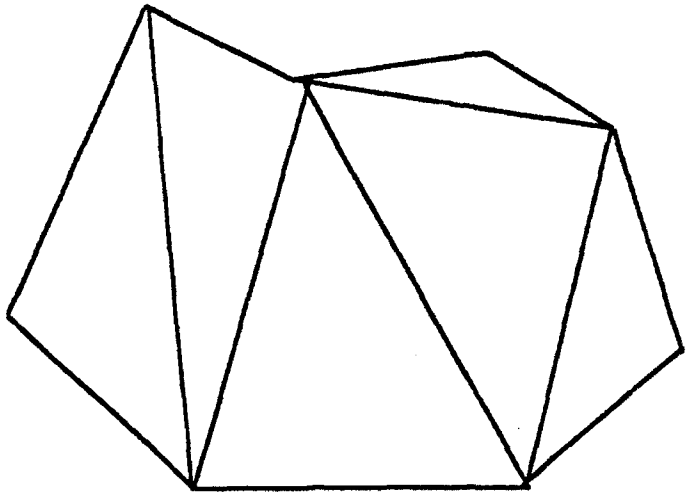
and on the boundary.



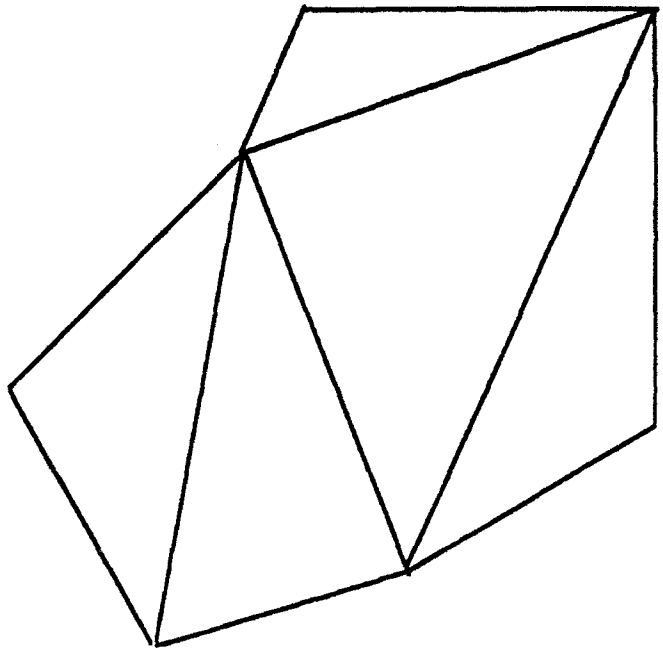
Deletion is more difficult and needs more computational resources than addition. The new vertices edges and cells being added are stacked at the bottom of the corresponding tables while undergoing deletion is always a member in the table. In order not to leave gaps in the table, a more complicated procedure was developed to replace the deleted member by the member at the bottom of the table.

2) Once the vertex, edges and cells joining the designated vertex are deleted we rezone the void (polygon) without adding new vertices. The adding of the new edges and cells are stacking at the end of the corresponding tables.

Interior Vertex



Boundary Vertex



3) A relaxation procedure is performed on the vertices of the polygon (void). This procedure improve the quality of the cells that fill the void.

4) A swap procedure is performed on the new edges that were added in the process of filling the void.

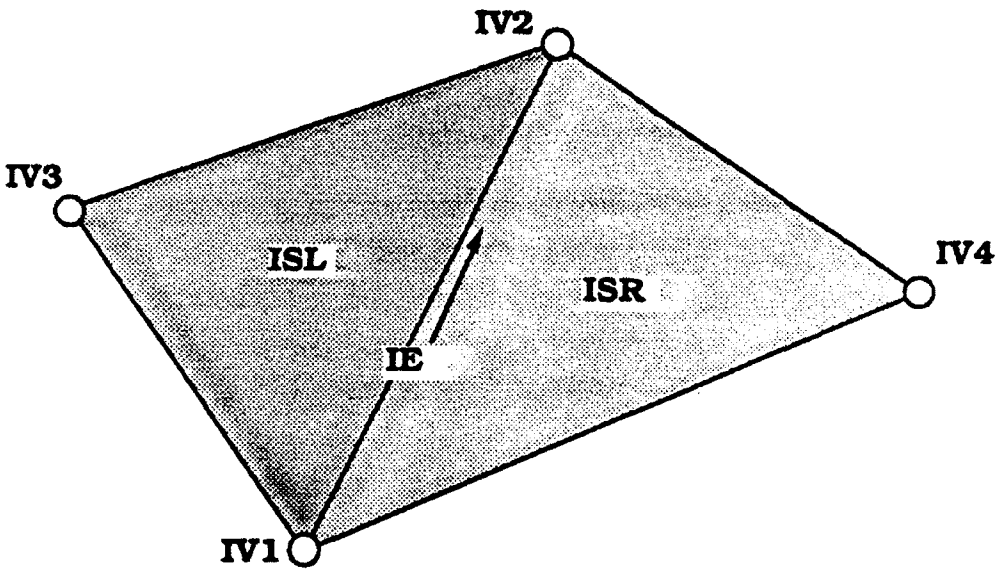
A.1.1 Pre-Processor for the Unstructured Grid

The input geometrical data for AUGUST should provide the following data:

1) Number of:
   - vertices (NV)
   - flagged vertices (NVM)
   - edges (NE)
   - cells (NS)
2) A table of vertices specifying:
   - number of vertex (IV)
   - x coordinate (XV(1,IV))
   - y coordinate (XV(2,IV)).
3) A table of flagged vertices that cannot be removed by the coarsening process:
   - number of vertex (IV)
   - status of vertex (JV(1, IV))

   The only status of vertex that is currently implemented is the flagging node that does not allow removal:
   - JV(1,IV)=3
4) A table of edges specifying:
   - number of edges (IE)
   - vertex number indicating the beginning of the edge (JE(1,IE))
   - vertex number indicating the end of the edge (JE(2,IE))
   - cell number indicating the cell at the left of the edge (JE(3,IE))
   - cell number indicating the cell at the right of the edge (JE(4,IE))
   - number associated with the status of the edge (JE(5,IE))

If JE(5,IE)=0, the edge is an ordinary edge inside the computational domain.
If JE(5,IE)≠0, the edge lies on the boundary of the domain. The labeling number will indicate what type of boundary to be applied through this edge.



IV1 = JE(1,IE) vertex indicating the beginning of the edge
IV2 = JE(2,IE) vertex indicating the end of the edge

The direction of the edge is defined from IV1 to IV2.

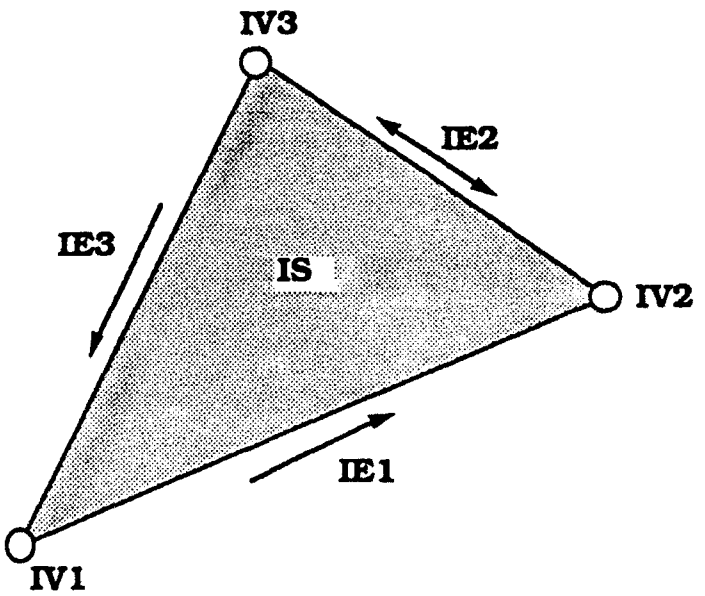
ISL = JE(3,IE)	left triangle
ISR = JE(4,IE)	right triangle
IJE5 = JE(5,IE)	status of the edge
IJE5 = 5	simulating wall conditions
IJE5 = 6	simulating wall conditions
IJE5 = 7	simulating supersonic outlet conditions
IJE5 = 8	simulating supersonic inlet conditions

5) A table of cells specifying:

number of cells (IS)
number of first edge (JS(4,IS))
number of second edge (JS(5,IS))
number of third edge (JS(6,IS))

The sign of JS(4,IS), JS(5,IS), JS(6,IS) indicates whether the direction of the edge is counterclockwise (positive) or clockwise (negative).

The three associated vertices for the triangle JS(1,IS), JS(2,IS), JS(3,IS) are defined by the code in GEOMTR.



The three vertices of the cell are ordered in a counterclockwise arrangement.

IV1 = JS(1,IS)	first vertex
IV2 = JS(2,IS)	second vertex
IV3 = JS(3,IS)	third vertex
IE1 = JS(4,IS)	First edge of the triange directed from IV1 to IV2 (IE1 is positive).
IE2 = JS(5,IS)	Second edge directed originally from IV3 to IV2. (IE2 will be negative because its direction is clockwise)
IE3 = JS(6,IS)	Third edge directed originally from IV3 to IV1 (IE3 is positive)

A.1.2 Post-Processor for the Unstructured Grid

Postprocessing for visualization of the results on an unstructured grid is done in two different codes. The first code, DRAWBF, reads the data as dumped by AUGUST and performs the whole load of computation necessary to produce the information needed for the graphic.

The second code DRAWAF reads the data file written by DRAWBF and uses the DISSPLA software to produce the image on the screen. Breaking the postprocessing job into two separate codes enables the user to run the two codes on different machines.

DRAWBF

Reads an input data file produced by AUGUST and will read another input data file (drawbf.d) specifying the option that the user chooses to have processed.

The input data file drawbf.d specifies the window of the computational domain chosen by the user to be processed. This window is specified by XMIN, XMAX, DX and YMIN, YMAX, DY, where XMIN, XMAX, YMIN, YMAX, will specify the lower and upper limit of the region to be drawn. DX and DY will be parameters for DISSPLA to subdivide the axis into tick marks.

DISSPLA is constrained to seven colors. To extend the number of contour levels, the code can be set to draw a couple of levels in each color (7 x **NLEV** where **NLEV** is the number of levels for each color).

The user should specify the variable he wants to draw:

IHYD = 1 is density,
= 2 is velocity in the x direction
= 3 is velocity in the y direction
= 4 is pressure
= 5 is gamma (γ)
= 6 is Mach number
= 7 is entropy
= 8 is a vector plot of the velocity field
= 9 is a plot of the location of particles

The last parameter that the user should specify is IREC. IREC specifies how many dumps are in the input file produced by AUGUST. If IREC=0, the user will get as many figures as the number of dumps produced by AUGUST. Otherwise, the user will get the figure corresponding to IREC specified in the input file.

Subroutine NEXTREC reads a whole dump from the input file (written by AUGUST). It will make sure that the allocation of memory is adequate according to the number of vertices, edges and triangles to be processed. If the memory allocation is not adequate, the code will stop with an explanatory message.

Subroutine LOADF loads the portion of data needed according to the specification of the window and according to the specified IHYD into the appropriate matrices in the code.

Subroutine PHYDR produces the data for the contour plots.

Subroutine VECTOR produces the data for the vector plot of the velocity field.

Subroutine TRACER produces the data for the location of particles.

DRAWAF

DRAWAF reads an input data file (drawbf.k) produced by DRAWBF and another input file (drawaf.d) that specifies the format chosen for display.

The parameters specified in drawaf.d are:

IFMESH = 0: No grid is drawn.

IFMESH = 1: Grid is drawn.

IOPTON = 0: A single frame is drawn.

IOPTON = 1: Two frames are drawn, one for the grid and one for displaying results. The frame for the grid is drawn even if IFMESH=0, but in this case the frame will stay empty.

IOPTON = 2: Identical with IOPTN=1 except the level on the bar chart is written in engineering format (XE+Y). As in the former, it is written keeping a four decimal digit.

ICONFG = 0: The basic dimension for the frames is specified as 6.0 x 3.0 inches (in the x and y axis, respectively). The code makes sure that the proportionality of the frame matches the physical window to be drawn, so that the figure will not be distorted. This is done by redefining the x or y dimension of the frame accordingly, but not to exceed the 6.0 x 3.0 on the screen (ICONFG=0 should be picked if IOPTON > 0 and a two-frame drawing is desired).

ICONFG>0: The same as ICONFG=0 except that the basic dimensions are defined now as 6.0 x 6.0 inches. This option should be specified if a one frame drawing is desired.

Caption 1
Caption 2

The user can specify a header for the drawing composed of two lines to be specified as Caption 1 and Caption 2 in the input file.

The standard drawing includes the number of vertices, edges and cells as well as the Mach number, lift, drag, moment, angle of attack (for drawing diagnostics for a wing profile). An indication of the nature of the results that appear on the drawing is also included, i.e., the physical variables drawn are identified by the parameter passing from DRAWBF.

It should be noted that the format of the output drawing is very easily redesigned to meet the needs of an individual user.

1. Read geometrical data defining the initial grid. The current format is set to read data file from Smart (two dimension grid generator).
2. Read geometrical data defining the grid read from a file dumped by a previous run of the code.
3. Initialize the physical variables according to IOPTN (either steady state or moving shock wave). If a different initial setting is needed, it should replace the current setting.
4. Read the physical variables from a file dumped by a previous run.

A.2 AUGUSTT (3D)

The subroutines in the AUGUSTT code are organized here as they appear in the listing in Appendix B. A brief description indicates the function performed by each subroutine.

TABLE A.2.1

LIST OF SUBROUTINES

The subroutines in the AUGUST code are organized here as they appear in the listing in Appendix B. A brief description indicates the function performed by each subroutine.

1. MAIN	Governing program for AUGUST. Reads input files and sets the mode for the computation.
2. HYDRFL	Computes the fluxes at interfaces by applying the Godunov algorithm to solve the Riemann problem across the interface.
3. HYDRMN	Controls the computation. The integration of the fluxes and update of the physical variables and writing to output files are performed in this subroutine.
4. GEOMTR	Calculates the geometrical quantities not provided by the input data file but needed for the computational algorithm. GEOMTR is only used once for starting a new simulation.
5. UPDATE	Reads the input file for a new simulation and calls GEOMTR to update the geometrical variables needed to perform the computation.
6. UPGRAD	Called if a restart run is performed. Will read the appropriate file written at the end of the previous run.

7. GRADNT	Computes the gradient of the physical variables to improve the prediction of those variables for the two sides of the interface. The gradients are subjected to the monotonicity condition that limits the projected values, thus preventing new maxima-minima to be caused artificially by interpolation (IOPORD = 2). Calls FCHART in order to compute projected values at the half timestep associated with the local characteristics of the flow.
8. FIRST	The equivalent of GRADNT if run in a first order mode (IOPORD = 1). Using FIRST assumes that the physical variables are constant in each cell. Takes care of the boundary conditions if the interface is a boundary.
9. FCHART	Computes the projected values at a half timestep for the two sides of the interface based on the local characteristics of the flow. Called by GRADNT, it modifies the projected values for the two sides of the interface and assigns them to the correct location in memory. Takes care of the boundary conditions if the interface is a boundary.

The MAIN Program

All of the data input and initiation of a run (or a restart run) is performed in MAIN. The actual simulation is controlled by HYDRMN, which is called from MAIN. At the completion of a run, control is returned to MAIN and a successful termination prints the message STOP 777.

MAIN contains one name list (file no. 2) and requires an input file that contains the grid data description (file no. 16). The data organization for the

grid file is described in Appendix A. The following files should be included: DMSH00.H, DPHSϕ0.H, DHYD00.H.

NAMELIST/DATA	ICOND	ICONP	IOPTN
	XMCHIN	RIN	PIN
	ALFA	HRGG	IHRN
	NTIME	NDUMP	IOPORD

VARIABLE	PURPOSE
ICOND	= 0 READ INPUT GRID FOR A NEW SIMULATION = 1 READ THE GRID FROM PREVIOUS RUN

ICOND = 0:

MAIN will read the initial grid definition stored in file number 16. The current setting is to read the input file as provided by Smart, a two-dimensional triangular grid generator that runs interactively on a Macintosh personal computer.

MAIN will call UPDATE, which will call GEOMTR. GEOMTR will compute essential geometrical parameters that are not provided by file 16. All geometrical information is dumped into output files (8 and 88) so that ICOND=0 is used only once at the beginning of a new simulation.

ICOND = 1:

MAIN will call UPGRAD, which will call one of the output files (8 or 88) written by the previous run. This will load the geometrical definition of the grid (either 8 or 88---they are identical). Writing identical files provides a backup in the event that the job terminates for lack of time while in the process of writing to one of those output files.

VARIABLE	PURPOSE
ICONP	= 0 PRIMITIVE VARIABLES INITIALIZED = 1 VARIABLES READ FROM PREVIOUS RUN

ICONP = 0: Initialize the primitive variables in computational domain with an initial value specified by the user. The two options set by the code are controlled by IOPTN.

ICONP = 1: The flow field condition reads in files 8 or 88 and provides a follow-up run set from the previous run.

VARIABLE	PURPOSE
IOPTN	= 1 SOLUTION FOR STEADY STATE = 2 SOLUTION FOR TRANSIENT PHENOMENA

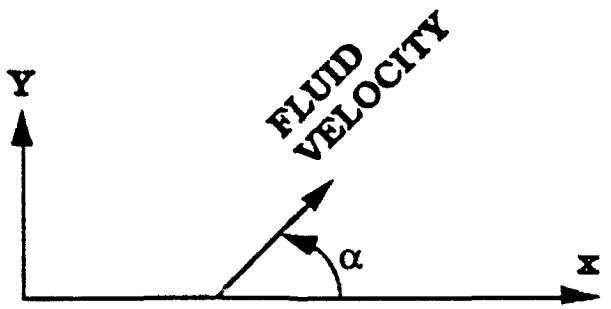
There are two choices available to set the initial condition of the problem.

IOPTN = 1: Assign the conditions at the inlet to the computational domain. This is the fastest way to get a steady-state solution for the conditions specified at the inlet. In this option, PIN (pressure), RIN (density) and XMCHIN (Mach number) are assigned to the pressure density and velocity (the speed of sound is computed in the code) and imposed at the inlet boundaries.

IOPTN = 2:

Used if a shock wave is to be simulated moving from the inlet (edge boundary 8) to the outlet (edge boundary 7). For this setting, specify PIN (ambient pressure in the chamber), RIN (ambient density in the chamber) and XMCHIN (upstream Mach number). The code will use the normal shockwave relations for an adiabatic flow of a completely perfect fluid to compute the static-pressure ratio across the shock P2/P1 and the density ratio r2/r1, and the ratio of the Mach number across the shock M2/M1. These computed quantities are applied to set correctly the condition on the pressure density and velocity at the inlet boundary.

VARIABLE	PURPOSE
ALFA	THE DIRECTION OF INFLOW IN DEGREES RELATIVE TO A RIGHT-HAND COORDINATE SYSTEM. ALFA = 0 MEANS FLOW FROM LEFT TO RIGHT.



The velocity computed by the code according to the input data provided by the user is split (projected) in the X and Y directions by using α.

VARIABLE	PURPOSE
HRGG	INITIAL γ IN THE EQUATION OF STATE. THE CODE RUNS USING THE IDEAL EQUATION OF STATE AS A BASELINE AND SHOULD BE MODIFIED IF SOMETHING ELSE IS DESIRED. IOPEOS=1 WILL TRIGGER THE USE OF GILMORE EQUATION OF STATE.

VARIABLE	PURPOSE
IHRN	NUMBER OF ITERATIONS IN THE RIEMANN SOLVER TO FIND THE DIAPHRAGM SOLUTION. (THREE TO FOUR SHOULD BE USED AND THE NUMBER INCREASED ONLY FOR VERY HIGH MACH NUMBER CASES.)

VARIABLE	PURPOSE
NTIME	NUMBER OF REPEATS FOR THE INTEGRATION SEQUENCE. AN OUTPUT DUMP IS DONE FOR EVERY SEQUENCE REPEAT.

VARIABLE	PURPOSE
NDUMP	NUMBER OF OUTER LOOP ITERATIONS IN THE CALCULATION WHERE REFINING IS DONE FOR EVERY SEQUENCE REPEAT WITHOUT COARSENING.

VARIABLE	PURPOSE
IOPORD	= 1 THE CODE WILL RUN FIRST ORDER GODUNOV METHOD = 2 THE CODE WILL RUN SECOND ORDER GODUNOV METHOD

IOPORD = 1 Subroutine FIRST is called.

IOPORD = 2 Subroutine GRADNT is called.

HYDREL

Computes the fluxes across interfaces when the conditions for both sides are given. The fluxes are computed assuming a shock solution at a ruptured diaphragm simulated by the presence of the interface. The conditions existing on the two sides of the diaphragm will define the condition of the flow at the diaphragm location. These conditions are computed by solving the Riemann problem using the Godunov algorithm. The condition at the diaphragm defines the flux of energy, mass, and momentum passing across the interface. The Euler conservation law is applied to conserve energy, mass, and momentum crossing interfaces from one cell to the other.

Quantity	Side 1	Diaphragm (Interface)	Side 2
Density	ρ_1	ρ	r_2
Pressure	P_1	P	P_2
Velocity Perpendicular to Interface	u_1	u	u_2
Velocity Parallel to Interface	v_1	v	v_2
Velocity Parallel to Interface to Construct a Right-Hand Coordinate System (u, v, w,)	w_1	w	w_2

HYDRMN

Controls the code and the iteration loops. It calls HYDRFL to find the interface fluxes. These fluxes are integrated to update the physical variables in each cell. If adaptation of the grid is required, HYDRMN also controls the output by writing the necessary information on files for postprocessing data and for restarting the AUGUST code at a later time. It also manages print file diagnostics.

GEOMTR

Calculates geometrical variables that are not supplied by the input data and are needed to run the code. For example, it computes:

1) distances between baricenters of adjoining cells;
2) the location of the intersection between the line joining adjacent baricenter cells and the interface.

The code changes the direction of the boundary edges so that all are arranged counter clockwise and the associated computational cell is always on the left side. GEOMTR is called once in the beginning of a new simulation.

UPDATE

Called in the beginning of a new simulation for setting geometrical variables not provided by the input data. (It calls GEOMTR.)

UPGRAD

Called if the run is a restart. UPGRAD will read the appropriate file (either 8 or 88) dumped by the previous run.

GRADNT

Compute the gradients of the physical variables in each cell. These computed gradients, along with the physical values at the baricenters, are applied using linear interpolation to predict the values on the interface.

The computed gradients are subjected to the monotonicity condition, ensuring that the projected values are bounded by the value of each quantity in the three adjacent cells, and to make sure that no new maxima or minima occur. The projection of quantities to the interface improves the results from the code and provides second order accuracy in space.

GRADNT calls FCHART, which computes the projected values at the interfaces at the half timestep level according to the local characteristics of the flow in each cell bordering the interface cell. The assignment of values at the two sides of each interface is done at the end of FCHART. This same loop also imposes the boundary conditions for the interfaces at the boundaries of the computational domain.

FIRST

Assigns flow quantities to each side of an edge. These are based on the values at the baricenter of the triangles on either side of the edge. FIRST uses a first order approximation to find the values at the edge.

The user can specify FIRST or GRADNT by choosing 1 or 2 for the parameter IOPORD.

FCHART

Called by GRADNT to compute the values projected at the interfaces at the half timestep. These calculations are done by applying the local velocity characteristics in each cell. This projection in time improves the results and makes the code second order accurate in time.

GRADNT

Computes the gradient of a scalar variable at the center of a cell. The gradient theorem is applied for each cell.

$$\int_{\text{volume}} \nabla \cdot dv = \oint_{\text{four surfaces}} f \, \bar{n} \, ds$$

Those gradients are subjected to a monotonicity limiter that ensures no new minima or maxima are produced artificially in the projected values at the interfaces.

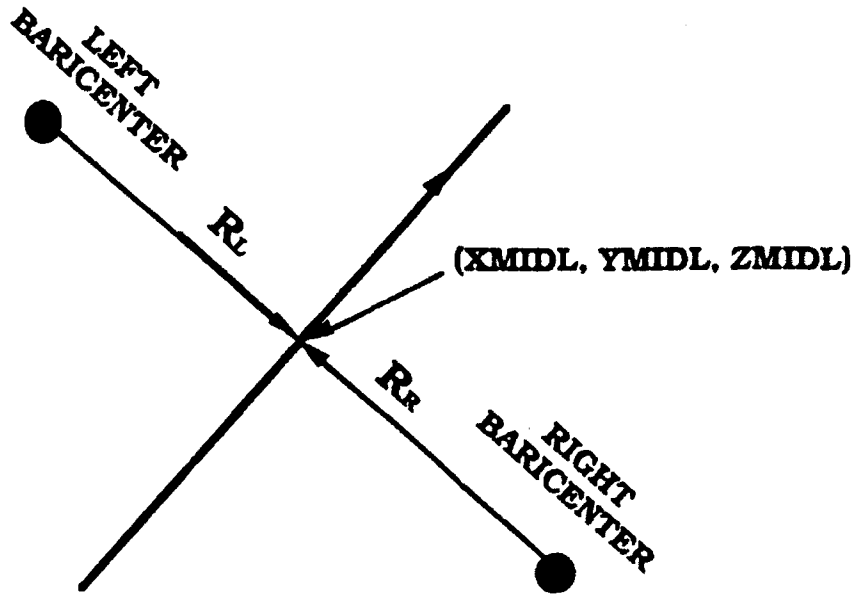
The monotonicity algotithm involves the following steps.

1)	find maximum and minimum of f_1, f_2, f_3, f_4, f_5 $f_{max} = \text{Max}\ (f_1, f_2, f_3, f_4, f_5)$ $f_{min} = \text{Min}\ (f_1, f_2, f_3, f_4, f_5)$
2)	compute $\Delta f_{max} = f_{max} - f_1$ $\Delta f_{min} = f_{min} - f_1$
3)	compute incremental projected values at the interfaces $f_{mjR} - f_R = \bar{\nabla} f_R \cdot \bar{r}_{jR}$ $f_{mjL} - f_L = \bar{\nabla} f_L \cdot \bar{r}_{jL}$

$$Df_{mjR} = f_{mjR} - f_R = \bar{\nabla} f_R \cdot \bar{r}_{jR}$$

$$Df_{mjL} = f_{mjL} - f_L = \bar{\nabla} f_L \cdot \bar{r}_{jL}$$

where j stands for every interface of the cell and fmj is the interpolated value at the middle of the interface.



4) compute the limiter by calculating the minimum of indicator for each edge of the four surfaces of the cell.

$$\text{right to the interface RUVPR} = \frac{(1 + \text{sign } \Delta f_{mjR})\, \Delta f_{max} + (1 - \text{sign } \Delta f_{mjR})\Delta f_{min}}{2\, \Delta f_{mjR}}$$

$$\text{left to the interface RUVPL} = \frac{(1 + \text{sign } \Delta f_{mjL})\, \Delta f_{max} + (1 - \text{sign } \Delta f_{mjL})\Delta f_{min}}{2\, \Delta f_{mjL}}.$$

This formulation ensures that:

$$\text{if} \begin{cases} \Delta f_{mj} > 0 \text{ RUVP} = \dfrac{\Delta f_{max}}{\Delta f_{mj}} \\ \Delta f_{mj} < 0 \text{ RUVP} = \dfrac{\Delta f_{min}}{\Delta f_{mj}} \end{cases}.$$

the outcome of RUVP is always positive. If RUVP > 1 then the projected value at the interfaces will introduce a new minima or maxima as compared to the values at the baricenters of the appropriate cells.

Select the minimum between the six values for RUVP (two for every one of the three interfaces of the cell) not exceeding unity. The selected minimum of RUVP is the required limiter. The gradient is multiplied by this limiter that is always less or equal to unity.

B CHART

Computes the projected values at the half timestep level based on the local characteristics of the flow. This process extends the accuracy of the code to be second-order in time as well as in space.

The characteristics projection consists of several steps.

1) Calculate the velocity of sound in the two cells bordering the designated interface:

$CNLEFT = \sqrt{\gamma_L \cdot P_L/\rho_L}$ sound speed in left cell

$CNRIGT = \sqrt{\gamma_R \cdot P_R/\rho_R}$ sound speed in right cell

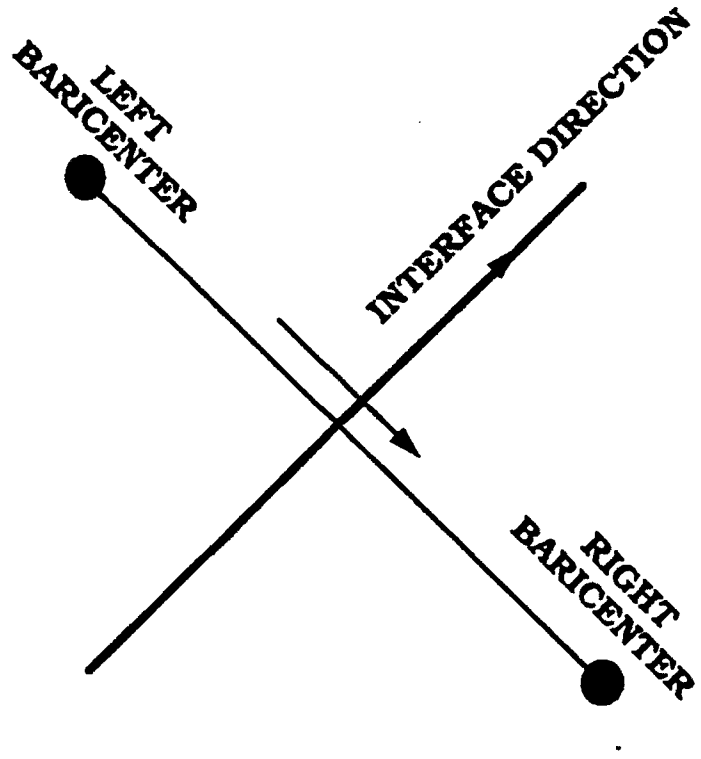
$UVLEFT = \bar{UL} \cdot \bar{t}$ velocity of fluid at the left cell projected in $\bar{t}$ direction

$UVRIGT = \bar{UR} \cdot \bar{t}$ velocity of fluid at the right cell projected in $\bar{t}$ direction

where:

$$\bar{t} = XXN \cdot \bar{i} + YYn \cdot \bar{j} + zzn\, \bar{k}$$

$$\bar{U} = U \cdot \bar{i} + v \cdot \bar{j} + w \cdot \bar{k}$$



2) To compute the interpolated left and right projected values at time tN + Dt/2, we calculate the distances that the disturbances generated from the baricenter of the cells, traveling toward the interface:

$$ZZLEFT = (UVLEFT + CNLEFT) \cdot \Delta t/2$$

$$ZZRIGT = - (UVRIGT - CNRIGT) \cdot \Delta t/2$$

If ZZLEFT or ZZRIGT are negative they are reset to zero.

3) Calculate the distances that the flow will travel if it were to flow at the velocity of each of the local characteristics:

$$ZOLEFT = UVLEFT \cdot \Delta t/2$$

$$ZORIGT = - UVRIGT \cdot \Delta t/2$$

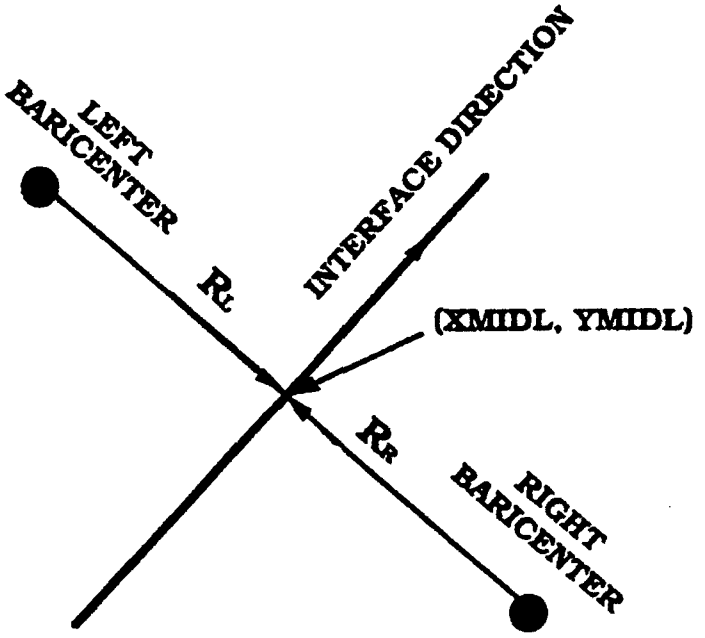
$$ZPLEFT = (UVLEFT + CNLEFT) \cdot \Delta t/2$$

$$ZPRIGT = - (UVRIGT + CNRIGT) \cdot \Delta t/2$$

$$ZMLEFT = (UVLEFT - CNLEFT) \cdot \Delta t/2$$

$$ZMRIGT = -(UVRIGT - CNRIGT) \cdot \Delta t/2.$$

4) Calculate the projected values of the nonconservative variables (density, velocity component (perpendicular and tangential to the interface), and pressure).



For the left cell:

Density	HRRL	=	$\rho_L + \bar{\nabla}\rho_L \cdot (\bar{r}_L - ZZLEFT \cdot \bar{t})$
Perpendicular Velocity	HUUL	=	$U_L + \bar{\nabla}U_L \cdot (\bar{r}_L - ZZLEFT \cdot \bar{t})$
Tangential Velocity	HVVL	=	$V_L + \bar{\nabla}V_L \cdot (\bar{r}_L - ZZLEFT \cdot \bar{t})$
Pressure	HPPL	=	$P_L + \bar{\nabla}P_L \cdot (\bar{r}_L - ZZLEFT \cdot \bar{t})$
	GMTLFT	=	$\rho_L \cdot HRRL \cdot HPPL$

For the right cell:

Density	HRRR	=	$\rho_R + \bar{\nabla}\rho_R \cdot (\bar{r}_R - ZZRIGT \cdot \bar{t})$
Perpendicular velocity	HUUR	=	$U_R + \bar{\nabla}U_R \cdot (\bar{r}_R - ZZRIGT \cdot \bar{t})$
Tangential velocity	HVVR	=	$V_R + \bar{\nabla}V_R \cdot (\bar{r}_R - ZZRIGT \cdot \bar{t})$
Pressure	HPPR	=	$P_R + \bar{\nabla}P_R \cdot (\bar{r}_R - ZZRIGT \cdot \bar{t})$
	GMTRGT	=	$\rho_R \cdot HRRR \cdot HPPR$

For the left cell, taking into account the following characteristics:

- For (UVLEFT + CNLEFT):

  $UUU = \bar{\nabla}U_L \cdot (ZPLEFT - ZZLEFT)\,\bar{t}$

  $PPP = \bar{\nabla}P_L \cdot (ZPLEFT - ZZLEFT)\,\bar{t}$

  $UPLFT = -0.5 \cdot \left(UUU + PPP/\sqrt{GMTLFT}\right) \;/\sqrt{GMTLFT}$

  If UVLEFT + CNLEFT is negative, UPLFT is reset to zero.

- For UVLEFT – CNLEFT:

  $UUU = \bar{\nabla}U_L \cdot (ZMLEFT - ZZLEFT) \cdot \bar{t}$

  $PPP = \bar{\nabla}P_L \cdot (ZMLEFT - ZZLEFT) \cdot \bar{t}$

  $UMLFT = 0.5 \cdot (UUU - PPP/\sqrt{GMTLFT}\,) \,/\, \sqrt{GMTLFT}$

  If UVLEFT - CNLEFT is negative, UPLFT is reset to zero.

- For UVLEFT:

  $PPP = \bar{\nabla}P_L \cdot (ZOLEFT - ZZLEFT) \cdot \bar{t}$

$$RRRR = \rho_L + \bar{\nabla}\rho_L \cdot (\bar{r}_L - ZOLEFT) \cdot \bar{t}$$

URLFT = PPP/GMTLFT + 1/HRRL - 1/RRRR

If UVLEFT is negative, URLEFT is reset to zero.

For the right cell, taking into account the following characteristics:

- For UVRIGT + CNRIGT:

$$UUU = \bar{\nabla}U_R \cdot (ZZRIGT - ZPRIGT)\ \bar{t}$$

$$PPP = \bar{\nabla}P_R \cdot (ZZRIGT - ZPRIGT)\ \bar{t}$$

$$UPRGT = -0.5 \cdot \left(UUU + PPP/\sqrt{GMTRGT}\right) /\sqrt{GMTRGT}$$

If UVRIGT + CNRIGT is positive, UMRGT is reset to zero.

- For UVRIGT - CNRIGT:

$$UUU = \bar{\nabla}U_R \cdot (ZZRIGT - ZMRIGT) \cdot \bar{t}$$

$$PPP = \bar{\nabla}P_R \cdot (ZZRIGT - ZMRIGT) \cdot \bar{t}$$

$$UMRGT = 0.5 \cdot \left(UUU - PPP/\sqrt{GMTRGT}\right) /\sqrt{GMTRGT}$$

If UVRIGT - CNRIGT is positive, UMRGT is reset to zero.

- For UVRIGT:

$$PPP = \bar{\nabla}P_R \cdot (ZZRIGT - ZORIGT) \cdot \bar{t}$$

$$RRRR = \rho_R + \bar{\nabla}\rho_R \cdot (\bar{r}_R + ZORIGT) \cdot \bar{t}$$

URRGT = PPP/GMTRGT + 1/HRRR - 1/RRRR

If UVRIGT - CNRIGT is positive, URRGT is reset to zero.

The projected values will be:

RRL = 1/(1/HRRL - (UPLFT + UMLFT + URLFT))

$$UUL = HUUL + (UPLFT - UMLFT)\sqrt{GMTLFT}$$

$$VVL = HVVL + (UPLFT - UMLFT)\sqrt{GMTLFT}$$
$$PPL = HPPL + (UPLFT + UMLFT)\,GMTLFT$$
$$RRR = 1/(1/HRRR - (UPRGT + UMRGT + URRGT))$$
$$UUR = HUUR + (UPRGT - UMRGT)\sqrt{GMTRGT}$$
$$VVR = HVVR + (UPRGT - UMRGT)\sqrt{GMTRGT}$$
$$PPR = HPPR + (UPRGT + UMRGT)\cdot GMTRGT.$$

Those values are the assigned condition for the two sides of the interface. If the interface is a boundary, the right condition is determined according to the type of boundary.

A.2.1 Preprocessor for the Three-Dimensional Unstructured Grid

The input geometrical data for AUGUST should provide the following data:

1) Number of vertices (NV)

2) A table of vertices specifying:
   number of vertex (IV)
   x coordinate (XV(1,IV))
   y coordinate (XV(2,IV))
   z coordinate (XV(3,IV).

3) Number of edges (NE)

4) A table of edges specifying
   number of edges (IE)
   vertex number indicating the beginning of the edge (JE(1,IE))
   vertex number indicating the end of the edge (JE(2,IE))

   IV1 = JE(1,IE) vertex indicating the beginning of the edge

   IV2 = JE(2,IE) vertex indicating the end of the edge

The direction of the edge is defined from IV1 to IV2.

5) Number of sides (NS)

6) A table of sides (triangles) specifying:

number of sides (IS)
number of first vertice (JS(1,IS))
number of second vertices (JS(2,IS))
number of third vertices (JS(3,IS))
number of first edge (JS(4,IS))
number of second edge (JS(5,IS))
number of third edge (JS(6,IS))

The sign of JS(4,IS), JS(5,IS), JS(6,IS) indicates whether the direction of the edge is counter clockwise (positive) or clockwise (negative).

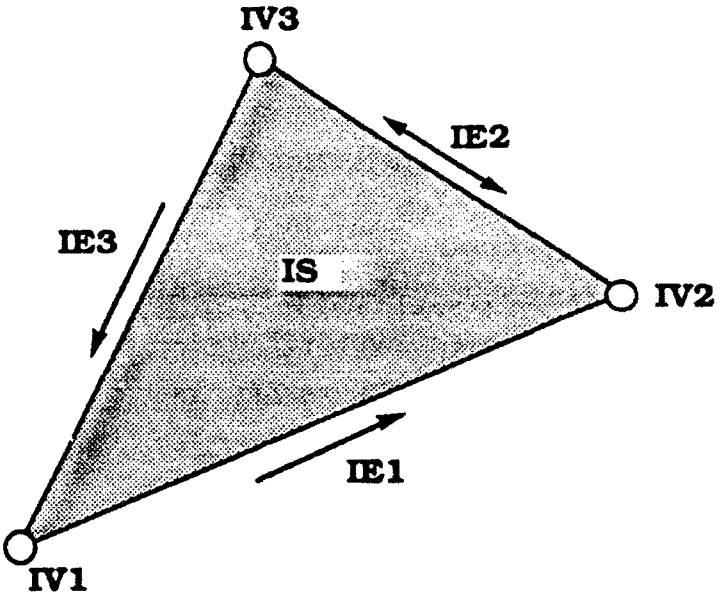
tetrahedra on left to the side (JS(7,IS))

tetrahedra on right to the side (JS(8,IS))

Number associated with the status of the side (JS(9,IS)).

if JS(9,IS) = 0 the side is an ordinary side inside the computational domain.

if JS(9,IS) $\neq$ 0 the side lies on the boundary of the domain. The labeling number will indicate what type of boundary to applied through this side.



The three vertices of the side are ordered in a counter clockwise arrangement.

IV1 = JS(1,IS)	first vertex
IV2 = JS(2,IS)	second vertex
IV3 = JS(3,IS)	third vertex
IE1 = JS(4,IS)	First edge of the triangle directed from IV1 to IV2 (IE1 is positive).
IE2 = JS(5,IS)	Second edge directed originally from IV3 to IV2. (IE2 will be negative because its direction is clockwise.)
IE3 = JS(6,IS)	Third edge directed originally from IV3 to IV1 (IE3 is positive).
IC1 =JS(7,IS)	tetrahedra on the left
IC2 = JS(8,IS)	tetrahedra on the right

The normal to the side is directed from IC1 toward IC2. If the side is a boundary, the normal is always from the computational domain pointing outside (out of the fluid domain). The three vertices are ordered in a counter clockwise direction opposite to the direction of the normal to the side. For a boundary side, IC2 will be always zero.

IJS = JS(9,IS)	Status of the side
IJS9 = 6	Simulating wall conditions
IJS9 = 7	Simulating supersonic outlet conditions
IJS9 = 8	Simulating supersonic inlet conditions.

7) A table of sides specifying:
x coordinate of baricenter of side (XS(1,IS))
y coordinate of baricenter of side (XS(2,IS))
z coordinate of baricenter of side (XS(3,IS))
area of side (XS(4,IS))

8) A table of sides specifying:
the three component of the vector normal to the side:

$$\vec{N} = XN(IS)\,\vec{i} + yN(IS)\,\vec{J} + ZN(IS)\vec{k}$$

the three component of the parallel vector tangential to the side:

$$\vec{P} = XP(IS)\,\vec{r} + YP(IS) + ZP(IS)\vec{k}$$

the three component of the parallel vector tangential to the side:

$$T = XT(IS)\,\vec{r} + YT(IS)\,\vec{j} + ZT(IS)\,\vec{k}$$

where $\vec{P} \times \vec{T} = \vec{N}$ (the normal, perpendicular and parallel vectors form a local right-handed coordinate system).

9) number of cells (tetrahedrals) (NC)

10) A table of cells specifying:
Number of cells (IC)
Number of first vertex (JC(1,IC))
Number of second vertex (JC(2,IC))
Number of third vertex (JC(3,IC))
Number of fourth vertex (JC(4,IC))
Number of the first side (JC(5,IC))
Number of the second side (JC(6,IC))

Number of the third side (JC(7,IC))

Number of the fourth side (JC(8,IC))

IV1 = JC(1,IC) first vertex

IV2 = JC(2,IC) second vertex

IV3 = JC(3,IC) third vertex

IV4 = JC(4,IC) fourth vertex

Seen from inside the tetrahedron. the first three vertices are counter clockwise around the large with the fourth vertex at the apex.

IS1 = JC(5,IC) first side

IS2 = JS(6,IC) second side

IS3 = JS(7,IC) third side

IS4 = JS(8,IC) fourth side

Face ISJ is opposite the IVJ vertex

11) A table of cells specifying:

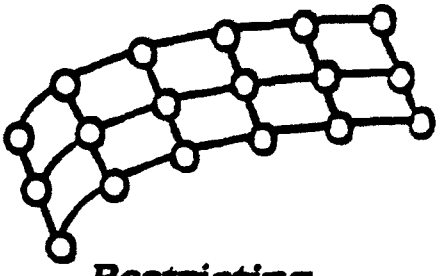
x coordinate of the baricenter of cell	(XC(1,IC))
y coordinate of the baricenter of cell	(XC(2,IC))
z coordinate of the baricenter of cell	(XC(3,IC))
Volume of the cell	(XC(4,IC))

A.2.2 Face(Triangle) information

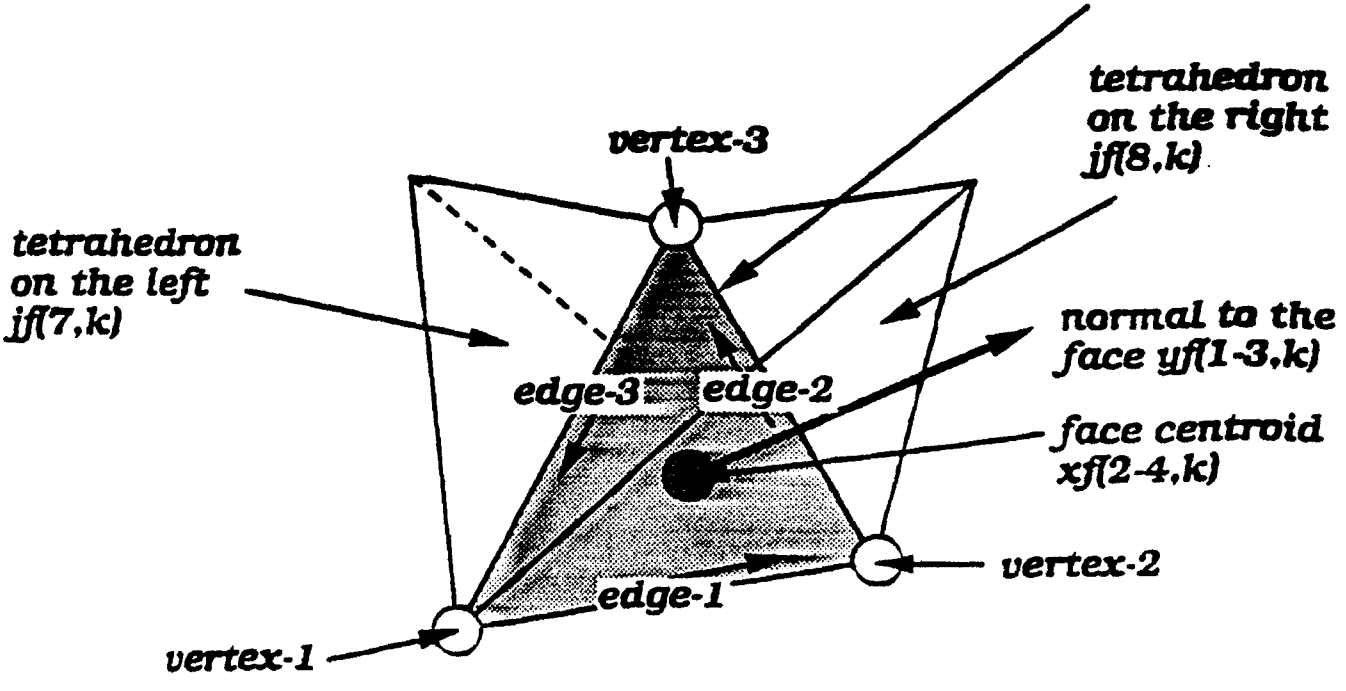
xf(1,k) - area of the kth face
xf(2,k) - x position of face centroid
xf(3,k) - y position of face centroid
xf(4,k) - z position of face centroid

yf(1,k) - x component of normal to face
yf(2,k) - y component of normal to face
yf(3,k) - z component of normal to face

jf(1,k) - the index of the first vertex
jf(2,k) - the index of the second vertex
jf(3,k) - the index of the third vertex
jf(4,k) - the signed index of the first edge
jf(5,k) - the signed index of the second edge
jf(6,k) - the signed index of the third edge
jf(7,k) - the index of the tetrahedron
to the left of face
jf(8,k) - the index of the tetrahedron
to the rigth of face
jf(9,k) - status of the kth face
s=0 face unrestricted
s=1 not used
s=2 face restricted to a surface
s=3 face is fixed
jf(10,k) - pointer to surface that
restricts the face.
jf(11,k) - the boundary condition for this face



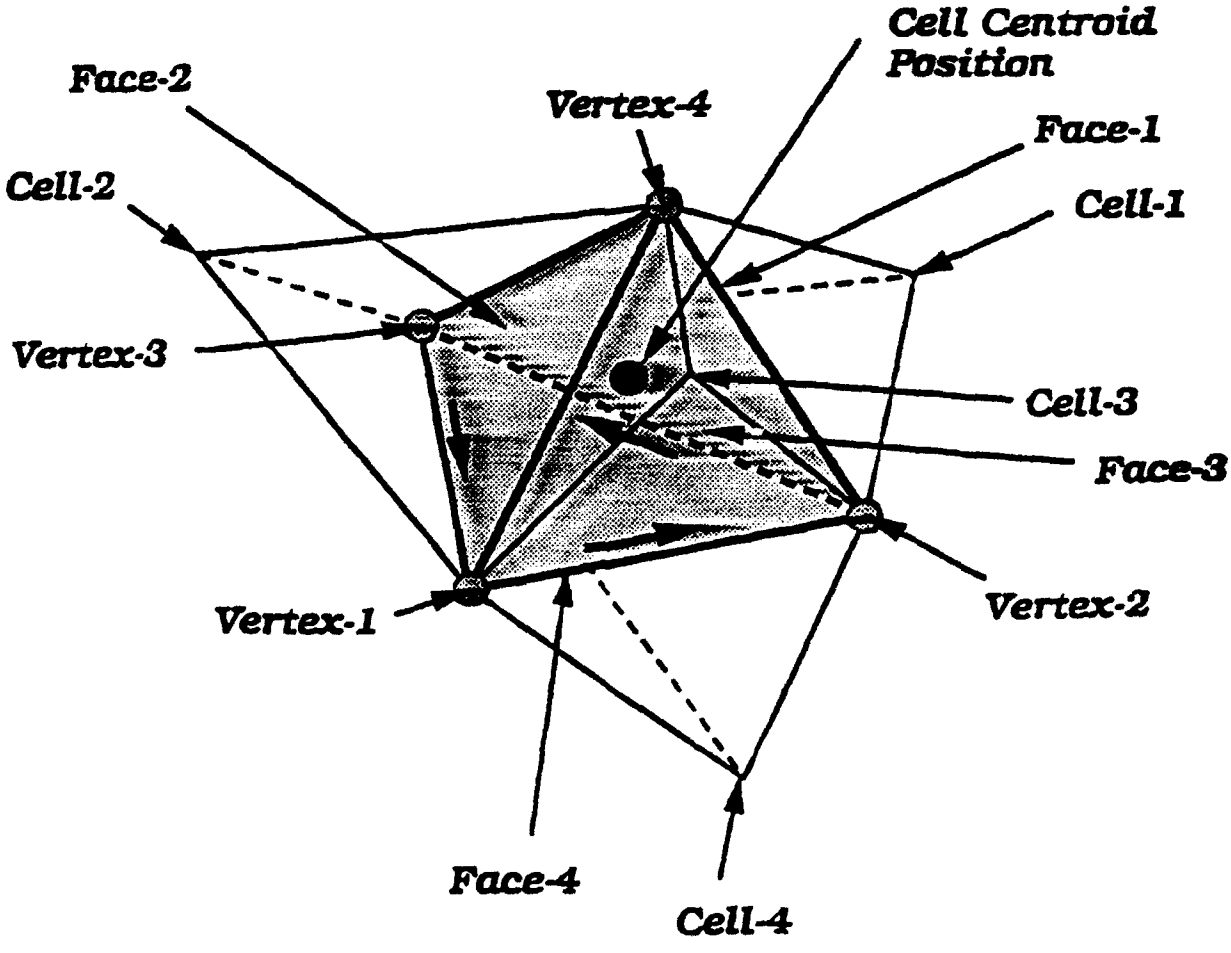
Restricting line/surface element jf(10,k) when jf(9,k)>0



Cell(Tetrahedral) information

xc(1.k) - x position of cell centroid
xc(2.k) - y position of cell centroid
xc(3.k) - z position of cell centroid
xc(4.k) - volume of cell

jc(1.k) - the index of the first base vertex
jc(2.k) - the index of the second base vertex
jc(3.k) - the index of the third base vertex
jc(4.k) - the index of fourth vertex opposite base
jc(5.k) - the index of face opposite first vertex
jc(6.k) - the index of face opposite first vertex
jc(7.k) - the index of face opposite secondvertex
jc(8.k) - the index of face opposite third vertex
jc(9.k) - the index of face opposite fourth vertex
jc(10.k) - the index of cell opposite first vertex
jc(11.k) - the index of cell opposite second vertex
jc(12.k) - the index of cell opposite third vertex
jc(13.k) - the index of cell opposite fourth vertex



APPENDIX B

LISTINGS

#	routine	page
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11	MATRLX	64
12	PSM	64
13	RYDRFL	19
14	UPGRAD	38
15	VOLMTETC	66
16	main	1

```
      PROGRAM AUGUSTT
C
C=====================================================================
C
C       The AUGUSTT Code
C
C                       -  Adaptive
C                       -  Unstructured
C                       -  Godunov
C                       -  Upwind
C                       -  Second order
C                       -  Triangular
C                       -  Three dimension
C
C                      The geometry structure comes from BERMUDA
C                      The solver is based on FUGGS
C
C
C       Version:   1.00      22 July, 1991
C
C       Authors:   Itzhak Lottati     (703)749-8648
C                  Shmuel Eidelman    (703)448-6491
C                  Adam Drobot        (703)734-5840
C
C                  Science Applications International Corporation
C                  Applied Physics Operation
C                  1710 Goodridge Drive
C                  McLean, Virginia 22102
C
C=====================================================================
C
C
C-----------------------------------------------------------------I
C                                                                 I
C     BERMUDA IS A MULTIDIMENSIONAL CODE WHICH IS BASED ON THE    I
C             USE OF TRIANGULAR GRIDS AS THE FUNDAMENTAL MESH     I
C             FOR FIELD LIKE QUANTITIES.  THE CODE REQUIRES       I
C             THAT ALL QUANTITIES ARE BASED AT THE BARICENTER     I
C             OF SIDES/TRIANGLES.                                 I
C                                                                 I
C             THE QUIP IS THAT THOSE WHO WORK ON BERMUDA          I
C             TRIANGLES ARE NEVER HEARD FROM AGAIN.               I
C                                                                 I
C             THE BASIC MODULES IN BERMUDA INCLUDE:               I
C                                                                 I
C                   A HYDRODYNAMICS CODE                        I
C                         .BASED ON A FIRST ORDER GODUNOV       I
C                          METHOD OR A SECOND ORDER GODUNOV     I
C                          WITH MESH ADAPTATION.                I
C                                                                 I
C-----------------------------------------------------------------I
C
C     GRID SETUP TABLES AND THEIR MEANING:
C
C     ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C     +                                                          +
C     +  LIST OF VERTICES                                        +
C     +                                                          +
C     +       IV          - VERTEX INDEX                         +
C     +       XV(1,IV)    - X POSITION OF VERTEX                 +
C     +       XV(2,IV)    - Y POSITION OF VERTEX                 +
C     +       XV(3,IV)    - Z POSITION OF VERTEX                 +
C     +                                                          +
C     ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C
C     ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C     +                                                          +
C     +  LIST OF EDGES                                           +
C     +                                                          +
C     +       IE          - EDGE INDEX                           +
C     +       JE(1,IE)    - INDEX OF LOWER EDGE VERTEX           +
C     +       JE(2,IE)    - INDEX OF UPPER EDGE VERTEX           +
C     +       JE(3,IE)    - INDEX OF LEFT  SIDE                  +
```

```
C     +       JE(4,IE)    - INDEX OF RIGHT SIDE                 +
C     +       XE(1,IE)    - LENGTH OF EDGE                      +
C     +       XE(2,IE)    - DISTANCE BETWEEN ADJOINING SIDE     +
C     +                     POINTS.                             +
C     +                                                         +
C     +-------------------------------------------------------+
C
C     +-------------------------------------------------------+
C     +                                                       +
C     +  LIST OF SIDES                                        +
C     +                                                       +
C     +       IS          - SIDE INDEX                        +
C     +       JS(1,IS)    - INDEX OF FIRST  VERTEX            +
C     +       JS(2,IS)    - INDEX OF SECOND VERTEX            +
C     +       JS(3,IS)    - INDEX OF THIRD  VERTEX            +
C     +                                                       +
C     +       THE VERTICES RUN AROUND THE SIDE IN ORDER       +
C     +       COUNTER-CLOCKWISE FASHION                       +
C     +                                                       +
C     +       JS(4,IS)    - INDEX OF THE FIRST  EDGE          +
C     +       JS(5,IS)    - INDEX OF THE SECOND EDGE          +
C     +       JS(6,IS)    - INDEX OF THE THIRD  EDGE          +
C     +                                                       +
C     +       THE EDGES ARE ARRANGED IN COUNTER-iCLOCKWISE    +
C     +       FASHION. EDGE ONE RUNS FROM VERTEX-ONE TO       +
C     +       VERTEX-TWO ETC.. THE SIGN OF JS(4-6,IS) INDICATES +
C     +       IF EDGE DATA IS STORED THE SAME WAY. IF IT IS   +
C     +       JS>0 AND IT IS REVERSED JS<0                    +
C     +       JS(7,IS)    - INDEX OF CELL ON LEFT             +
C     +       JS(8,IS)    - INDEX OF CELL ON RIGHT            +
C     +                                                       +
C     +       XS(1,IS)     - X POSITION OF CENTROID OF TRIANGLE +
C     +       XS(2,IS)     - Y POSITION OF CENTROID OF TRIANGLE +
C     +       XS(3,IS)     - Z POSITION OF CENTROID OF TRIANGLE +
C     +       XS(4,IS)     - AREA OF TRIANGLE                 +
C     +       XS(5,IS)     - DISTANCE BETWEEN ADJOINING CELLS +
C     +                      POINTS CROSSING TRIANGLE IS      +
C     +                                                       +
C     +                                                       +
C     +-------------------------------------------------------+
C
C     +-------------------------------------------------------+
C     +                                                       +
C     +  LIST OF CELLS                                        +
C     +                                                       +
C     +       IC          - CELL INDEX                        +
C     +       JC(1,IC)    - INDEX OF FIRST  VERTEX            +
C     +       JC(2,IC)    - INDEX OF SECOND VERTEX            +
C     +       JC(3,IC)    - INDEX OF THIRD  VERTEX            +
C     +       JC(4,IC)    - INDEX OF FOURTH VERTEX            +
C     +                                                       +
C     +       THE CONVENTION FOR VERTICES IS THAT 1-3         +
C     +       ARE ARRANGED COUNTER-CLOCKWISE ABOUT THE        +
C     +       BASE AND THAT 4 IS AT THE APEX.                 +
C     +                                                       +
C     +       JC(5,IC)    - INDEX OF FIRST  SIDE              +
C     +       JC(6,IC)    - INDEX OF SECOND SIDE              +
C     +       JC(7,IC)    - INDEX OF THIRD  SIDE              +
C     +       JC(8,IC)    - INDEX OF FOURTH SIDE              +
C     +                                                       +
C     +       THE CONVENTION FOR SIDES IS THAT SIDE ONE COVERS +
C     +       THE SPACE BETWEEN VERTEX-ONE,VERTEX-TWO,AND THE +
C     +       VERTEX AT THE APEX ETC.. SIDE FOUR IS THE BASE  +
C     +                                                       +
C     +       XC(1,IC)    - X POSITION OF CELL POINT          +
C     +       XC(2,IC)    - Y POSITION OF CELL POINT          +
C     +       XC(3,IC)    - Z POSITION OF CELL POINT          +
C     +       XC(4,IC)    - CELL VOLUME.                      +
C     +                                                       +
C     +                                                       +
C     +-------------------------------------------------------+
C
C
C=============================================================
```

```
C
C --- DEFINITION FOR ALL HYDRODYNAMIC QUANTITIES ----------------------
C
C-------------------------------------------------------------------I
C                                                                   I
C     USE OF PARAMETERS:                                            I
C                                                                   I
C         MHQ     - MAXIMUM NUMBER OF HYDRO QUANTITIES.           I
C                                                                   I
C                                                                   I
C-------------------------------------------------------------------I
C
C*******************************************************************
C
      include     'dmsh00.h'
      include     'dhydm0.h'
      include     'dphsm0.h'
      include     'dmtrl0.h'
C
      REAL XX(600),PP(600),HR(600),
     .     UU(600),GG(600),AA(600),EE(600)
      DOUBLE PRECISION VOL1,VOL2,VOL3,VOL4,VOLL,XXI,YYI,ZZI
      DOUBLE PRECISION DEFVOL
      OPEN(2 ,FILE='data.dd',FORM='FORMATTED')
      OPEN(4 ,FILE='thermo.d',FORM='FORMATTED')
      OPEN(8 ,FILE='threed2.5',FORM='UNFORMATTED')
      OPEN(88 ,FILE='threed82',FORM='UNFORMATTED')
      OPEN(9 ,FILE='threed3',FORM='UNFORMATTED')
      OPEN(10,FILE='threed4',FORM='FORMATTED')
      OPEN(15,FILE='AVSfmhail.inp',FORM='FORMATTED')
      OPEN(14,FILE='AVSsmhail.inp',FORM='FORMATTED')
      OPEN(16,FILE='OUTPUT.MSH',FORM='FORMATTED')
      OPEN(26,FILE='EXPLSV.RND',FORM='FORMATTED')
      OPEN(17,FILE='ve0640.stv',FORM='FORMATTED')
      OPEN(18,FILE='f0640.stv',FORM='FORMATTED')
      OPEN(19,FILE='pr640.stv',FORM='FORMATTED')
      OPEN(11,FILE='truck.input.8b',STATUS='OLD'      )
C
C*******************************************************************
C
C      NAMELIST /DATA/ ICOND,ICONP,IOPTN,XMCHIN,RIN,PIN,ALFA,HRGG,IHRN,
C     .                NTIME,NDUMP,IOPORD
C
C-------------------------------------------------------------------I
C                                                                   I
C                                                                   I
C     --- MEANING OF NAMELIST VARIABLES:                            I
C                                                                   I
C     ICOND = 0 READ INPUT GRID FOR A NEW RUN                       I
C           = 1 READ THE GRID FROM PREVIOUS RUN                     I
C     ICONP = 0 PRIMITIVE VARIABLES SET TO ZERO                     I
C           = 1 VARIABLES READ FROM PREVIOUS RUN                    I
C     IOPTN = 1 SOLUTION FOR STEADY STATE,                          I
C           = 2 SOLUTION FOR TRANSIENT PHENOMENA                    I
C                                                                   I
C     XMCHIN = FOR TRANSIENT SHOCK CALCULATIONS(IOPTN=2)THIS VARIABLE I
C              IS USED TO SPECIFY THE UPSTREAM MACH NUMBER           I
C                                                                   I
C              RIN = THE AMBIENT DENSITY IN THE CHAMBER             I
C                                                                   I
C              PIN = THE AMBIENT PRESSURE IN THE CHAMBER            I
C                                                                   I
C              APPLYING NORMAL SHOCK WAVES RELATIONS FOR AN ADIABATIC I
C              FLOW RELATION STATIC-PRESSURE RATIO ACROSS THE SHOCK  I
C              AS WELL AS THE DENSITY RATIO AND MACH NUMBER RATIO    I
C              ARE COMPUTED TO SET CORRECTLY THE CONDITION AT THE    I
C              INLET EDGES( EDGE BOUNDARY 8 ) OF THE COMPUTATIONAL   I
C              DOMAIN                                               I
C                                                                   I
C              FOR STEADY STATE SHOCK CALCULATIONS(IOPTN=1)THIS IS THE I
C              INFLOW MACH NUMBER. ALL DOMAIN VELOCITIES ARE THEN    I
C              INITIALIZED WITH THIS VALUE.                         I
C                                                                   I
C              RIN = THE AMBIENT DENSITY AT INFINITY                I
```

```
222  222  C                                                                I  222
223  223  C              PIN = THE AMBIENT PRESSURE AT INFINITY             I  223
224  224  C                                                                 I  224
225  225  C              ALL COMPUTATIONAL DOMAIN ARE THEN INITIALIZED WITH  I  225
226  226  C              THOSE VALUES.                                      I  226
227  227  C                                                                 I  227
228  228  C     ALFA  = THE DIRECTION OF INFLOW IN DEGREES RELATIVE TO A RIGHT I  228
229  229  C             HAND COORDINATE SYSTEM. ALFA=0 MEANS FLOW FROM LEFT TO I  229
230  230  C             RIGHT. ALFA=90 MEANS FROM BOTTOM TO TOP. ALFA=-90 OR 270 I  230
231  231  C             MEANS FLOW FROM TOP TO BOTTOM ETC.                 I  231
232  232  C     HRGG  = INITIAL GAMMA IN THE EQUATION OF STATE             I  232
233  233  C             THE CODE RUNS USING THE AIR EQUATION AS A BASELINE AND I  233
234  234  C             SHOULD BE MODIFIED IF SOMETHING ELSE IS DESIRED.   I  234
235  235  C     IHRN  = NUMBER OF ITERATIONS IN THE RIEMANN SOLVER TO FIND THE I  235
236  236  C             DIAPHRAGM SOLUTION.(3 to 4 SHOULD BE USED AND INCREASED I  236
237  237  C             ONLY FOR HIGH MACH NUMBER CASES).                  I  237
238  238  C                                                                 I  238
239  239  C     NTIME = NUMBER OF REPEATS FOR THE INTEGRATION SEQUENCE.     I  239
240  240  C             AN OUTPUT DUMP IS DONE EVERY SEQUENCE REPEAT.      I  240
241  241  C     NDUMP = NUMBER OF ITERATIONS IN THE INNER LOOP             I  241
242  242  C                                                                 I  242
243  243  C        +_____________________ o NTIME - DUMPING DATA            I  243
244  244  C        I                                                        I  244
245  245  C        I            +_______ o NDUMP - INTEGRATION              I  245
246  246  C        I            I                                           I  246
247  247  C        I            I                                           I  247
248  248  C        I            +_______ o ..... INNER LOOP                 I  248
249  249  C        I                                                        I  249
250  250  C        +_____________________ o ..... DUMPING LOOP              I  250
251  251  C                                                                 I  251
252  252  C     IOPORD = 1 THE CODE WILL RUN FIRST ORDER GODUNOV METHOD      I  252
253  253  C            = 2 THE CODE WILL RUN SECOND ORDER GODUNOV METHOD     I  253
254  254  C                                                                 I  254
255  255  C-----------------------------------------------------------------I  255
256  256  C
257  257        ICOND = 0
258  258        ICONP = 0
259  259        IOPTN = 1
260  260        IEOS  = 1
261  261  C
262  262        XMCHIN = 2.5
263  263        RIN    = 1.25
264  264        PIN    = 101350.
265  265        RGAS   = 8314.3
266  266        GPERCC = .001
267  267  C
268  268        ALFA = 0.
269  269        HRGG = 1.4
270  270        IHRN = 4
271  271        NTIME = 12
272  272        NDUMP = 200
273  273        IOPORD = 2
274  274  C
275  275  C --- READ THE INPUT DATA ------------------------------------------
276  276  C
277  277  C       READ (2,DATA)
278  278  C
279  279  C --- PRINTOUT THE RUN PARAMETERS ----------------------------------
280  280  C
281  281        PRINT 101,    ICOND,ICONP,IOPTN,XMCHIN,RIN,PIN,ALFA,HRGG,IHRN,
282  282       .              NTIME,NDUMP,IOPORD
283  283  C
284  284  C --- SET RUN CONDITIONS AND PRINTOUT TO CONSOLE ---------------------
285  285  C
286  286  C     READING GRID DATA FROM EDGE.ZON
287  287  C
288  288        THIRD = 1. / 3.
289  289         IF( ICOND . EQ . 0 ) THEN
290  290  C
291  291         CALL UPDATE
292  292  C
293  293        ELSE
294  294  C
295  295         CALL UPGRAD
```

```
296   296  C
297   297         END IF
298   298         CALL MATRLA
299   299         CALL MATRLX
300   300  C
301   301  C --- INITIALIZATION OF THE PROBLEM
302   302  C
303   303            HRSM = 1.E-8
304   304            HRGP = HRGG + 1.
305   305            HRGM = HRGG - 1.
306   306            CF   = HRGP / ( 2. * HRGG )
307   307         TT = 0.
308   308  C
309   309         PIRAD = ATAN( 1. ) / 45.
310   310         ALPHA = ALFA * PIRAD
311   311         PRINT *,ALFA,PIRAD,ALPHA
312   312  C
313   313         COSS = COS( ALPHA )
314   314         SINN = SIN( ALPHA )
315   315         TANN = TAN( ALPHA )
316   316  C
317   317  C---------------------------------------------------------------------
318   318  C
319   319  C --- SET THE INITIAL VALUE FOR PRIMITIVE VARIABLES ------------------
320   320  C
321   321  C(2)>>>>
322   322          TLIMIT = .9
323   323          ITER = 6
324   324         IF( ICOND . EQ . 0 ) THEN
325   325           UVIN = XMCHIN * SQRT( HRGG * PIN / RIN )
326   326           UIN = UVIN * COSS
327   327           VIN = UVIN * SINN
328   328           WIN = 0.
329   329  C
330   330           DO 150 IC = 1 , NC
331   331              HYDV( IC , 1 ) = RIN
332   332              HYDV( IC , 2 ) = 0.
333   333              HYDV( IC , 3 ) = 0.
334   334              HYDV( IC , 4 ) = 0.
335   335              HYDV( IC , 5 ) = PIN
336   336              HYDV( IC , 6 ) = 1.E-6
337   337              HYDV( IC , 7 ) = 1.4
338   338              HYDV( IC , 8 ) = PIN / ( HYDV( IC , 7 ) - 1. )
339   339  C
340   340   150     CONTINUE
341   341           RADIUS = .0001
342   342           EXPLSV = 8.
343   343           DO IC = 1 , NC
344   344              XXI = XC( 1 , IC )
345   345              YYI = XC( 2 , IC )
346   346              ZZI = XC( 3 , IC )
347   347              RSS = SQRT( XXI * XXI + YYI * YYI + ZZI * ZZI )
348   348              IF( RSS . LT . RADIUS ) THEN
349   349                print*,xxi,yyi,zzi,radius
350   350                 HYDV( IC , 1 ) = EXPLSV * .4536 * .75 / 3.141569 /
351   351        .                          ( RADIUS * RADIUS * RADIUS )
352   352                 HYDV( IC , 6 ) = 1.
353   353                 HYDV( IC , 8 ) = HYDV( IC , 1 ) * 1080. * 4.185 *
354   354        .                                  1000. * 1.01 / .7
355   355         NITER = 0
356   356         DST = HYDV( IC , 1 ) * GPERCC
357   357         VOL = WMX * ( 1. - DST / FSX ) / DST / XGX
358   358         EMEO = HYDV( IC , 8 ) / HYDV( IC , 1 ) * WMX / RGAS
359   359  C
360   360         IYY = ( EMEO - EMEOX( 3 ) ) / RANGEX + 1
361   361         IYY = MAXO( 1 , MINO( IYY , 47 ) )
362   362  C
363   363         K = IYY + 2
364   364         IYY = IYY
365   365        . + INT( AMAX1( EMEO - EMEOX( K ) , 0.) / DYX( K ) )
366   366        . - INT( AMAX1( EMEOX( K + 1 ) - EMEO , 0. ) / DYX( K ) )
367   367         IYY = MAXO( 1, MINO( IYY , 47 ) )
368   368  C
369   369         K1 = IYY + 2
```

```
370   370         K2 = K1 + 1                                                    370
371   371         RT = ( EMEO - EMEOX( K1 ) ) / ( EMEOX( K2 ) - EMEOX( K1 ) )    371
372   372         T = TX( K1 ) + 100. * RT                                       372
373   373         CVM = CVMX( K1 ) + RT * ( CVMX( K2 ) - CVMX( K1 ) )            373
374   374         ERS = 0.                                                       374
375   375   C                                                                    375
376   376   10    CONTINUE                                                       376
377   377         P = RGAS * T / VOL / GPERCC                                    377
378   378         RGAMM1 = CVM                                                   378
379   379   C                                                                    379
380   380         X = COVX / VOL / ( ( T + THETAX ) ** ALFAX )                   380
381   381         Z = X * EXP( BETAX * X )                                       381
382   382         X = 1. + BETAX * X                                             382
383   383         RT = ALFAX * T / ( T + THETAX )                                383
384   384         ERS = ERS + RT * Z * T                                         384
385   385   C                                                                    385
386   386         IF ( ITER .EQ. NITER ) GO TO 20                                386
387   387   C                                                                    387
388   388         CVM = CVM * XGX + SCVX                                         388
389   389        *           + RT * Z * ( 2. - RT / ALFAX - RT * X )             389
390   390         T = T - AMIN1( ERS / CVM , TLIMIT * T )                        390
391   391   C                                                                    391
392   392         NITER = NITER + 1                                              392
393   393   C                                                                    393
394   394         RT = 0.01 * T                                                  394
395   395         K1 = RT                                                        395
396   396         K1 = MIN0 ( K1, 49 )                                           396
397   397         K1 = MAX0 ( K1, 3  )                                           397
398   398         K2 = K1 + 1                                                    398
399   399         RT = RT - K1                                                   399
400   400         CVM = CVMX(K1) + RT * ( CVMX( K2 ) - CVMX( K1 ) )              400
401   401         ERS = EMEOX( K1 ) + RT * ( EMEOX( K2 ) - EMEOX( K1 ) )         401
402   402         ERS = ERS - EMEO                                               402
403   403   C                                                                    403
404   404         GO TO 10                                                       404
405   405   C                                                                    405
406   406   20    CONTINUE                                                       406
407   407         P = P * ( 1. + Z )                                             407
408   408         RGAMM1 = ( RGAMM1 +                                            408
409   409        *           RT * Z * ( 2. - RT / ALFAX - RT * X ) ) / ( 1. + Z ) 409
410   410         X = X * Z / ( 1. + Z )                                         410
411   411         RGAMM1 = RGAMM1 / ( ( 1. - RT * X ) ** 2 + X * RGAMM1 )        411
412   412         ERS = ERS / EMEO                                               412
413   413         HYDV( IC , 7 ) = 1. / RGAMM1 + 1.                              413
414   414         HYDV( IC , 5 ) = P                                             414
415   415         END IF                                                         415
416   416         END DO                                                         416
417   417   C                                                                    417
418   418         XCOUNT = 0                                                     418
419   419         DO IC = 1 , NC                                                 419
420   420         RCOUNT = HYDV( IC , 8 ) + .5 * HYDV( IC , 1 ) *                420
421   421        .                   ( HYDV( IC , 2 ) * HYDV( IC , 2 ) +         421
422   422        .                     HYDV( IC , 3 ) * HYDV( IC , 3 ) +         422
423   423        .                     HYDV( IC , 4 ) * HYDV( IC , 4 ) )         423
424   424         XCOUNT = XCOUNT + XC( 4 , IC ) * RCOUNT                        424
425   425         END DO                                                         425
426   426          PRINT * ,XCOUNT                                               426
427   427             IIJJ=1                                                     427
428   428             IF(IIJJ.EQ.0) GO TO 1122                                   428
429   429   C     remove the followed IF statement for regular run               429
430   430   C      IF( IOPTN . EQ . 2 ) THEN                                     430
431   431   C      IF( IOPTN . EQ . 1 ) THEN                                     431
432   432   C                                                                    432
433   433             NX = 360                                                   433
434   434             DO 190 IX = 1 , NX                                         434
435   435                XX(IX) = (IX-.5)*.002                                   435
436   436   190       CONTINUE                                                   436
437   437             READ (11,1001) (PP(IX),IX=1,NX)                            437
438   438             READ (11,1001) (UU(IX),IX=1,NX)                            438
439   439             READ (11,1001) (HR(IX),IX=1,NX)                            439
440   440             READ (11,1001) (AA(IX),IX=1,NX)                            440
441   441             READ (11,1001) (GG(IX),IX=1,NX)                            441
442   442             READ (11,1001) (EE(IX),IX=1,NX)                            442
443   443   1001  FORMAT(6E12.5)                                                 443
```

```
444   444   C
445   445         ICOUNT = 0
446   446         DO 260 IC = 1 , NC
447   447   C        XXI = XC( 1 , IC ) + .2667
448   448            XXI = XC( 1 , IC ) + .1143
449   449            YYI = XC( 2 , IC ) - 1.96596
450   450   C        ZZI = XC( 3 , IC ) - 1.25
451   451            ZZI = XC( 3 , IC ) - 1.905
452   452            RSS = SQRT( XXI * XXI + YYI * YYI + ZZI * ZZI )
453   453            XYS = SQRT( XXI * XXI + YYI * YYI )
454   454   C
455   455            DO 270 IX = 1 , NX-1
456   456               XDD1 = XX( IX )
457   457               XDD2 = XX( IX+1 )
458   458               IF( RSS . GT . XDD1 . AND . RSS . LT . XDD2 ) THEN
459   459                  XKSI = ( RSS - XDD1 ) / ( XDD2 - XDD1 )
460   460                  ICOUNT = ICOUNT + 1
461   461   C
462   462                  HYDV(IC,1) = HR(IX) * (1.-XKSI) +
463   463        .                              HR(IX+1) * XKSI
464   464   C
465   465                  HYDUVW = UU(IX) * (1.-XKSI) +
466   466        .                           UU(IX+1) * XKSI
467   467                  HYDV(IC,4) = ZZI / RSS * HYDUVW
468   468                  HYDVUV = XYS / RSS * HYDUVW
469   469   C
470   470                  THETHA = ATAN2( YYI , XXI )
471   471                  HYDV(IC,2) = HYDVUV * COS( THETHA )
472   472                  HYDV(IC,3) = HYDVUV * SIN( THETHA )
473   473   C
474   474                  HYDV(IC,5) = PP(IX) * (1.-XKSI) +
475   475        .                              PP(IX+1) * XKSI
476   476   C              HYDV(IC,5) = 1.08*HYDV(IC,5)
477   477                  HYDV(IC,7) = GG(IX) * (1.-XKSI) +
478   478        .                              GG(IX+1) * XKSI
479   479                  HYDV(IC,6) = AA(IX) * (1.-XKSI) +
480   480        .                              AA(IX+1) * XKSI
481   481                  HYDV(IC,8) = EE(IX) * (1.-XKSI) +
482   482        .                              EE(IX+1) * XKSI
483   483   C
484   484                  GOTO 301
485   485               ENDIF
486   486    270     CONTINUE
487   487    301     CONTINUE
488   488         NITER = 6
489   489         IF(NITER.EQ.0) THEN
490   490         IF( HYDV( IC , 6 ) . LT . .2 ) THEN
491   491         DST = HYDV( IC , 1 ) * GPERCC
492   492         VOL = WMA * ( 1. - DST / FSA ) / DST / XGA
493   493         TT = HYDV( IC , 5 ) * VOL * GPERCC / RGAS
494   494   C
495   495         T = TT
496   496         RT = 0.01 * T
497   497         K1 = RT
498   498         K1 = MINO ( K1, 49 )
499   499         K1 = MAXO ( K1, 3  )
500   500         K2 = K1 + 1
501   501         RT = RT - K1
502   502         ENERGY = EMEOA( K1 ) + RT * ( EMEOA( K2 ) - EMEOA( K1 ) )
503   503         ENERGY = ENERGY * RGAS / WMA
504   504   C
505   505         DO ITER = 1 , NITER
506   506         X = COVA / VOL / ( T + THETAA ) ** ALFAA
507   507   C
508   508         BETAZX = BETAA * X
509   509         RT = X * EXP( BETAZX )
510   510         RTINV = 1. / ( 1. + RT )
511   511   C -   ERS IS THE FUNCTION, RT IS THE DERIVATIVE
512   512         ERS = T -  TT * RTINV
513   513         RT = 1. - TT * RTINV * RTINV * ALFAA * RT * ( 1. + BETAZX ) /
514   514        .                ( T + THETAA )
515   515         ERS = ERS / RT
516   516         T = T - ERS
517   517         END DO
```

```
518     518   C
519     519         RT = 0.01 * T                                                    519
520     520         K1 = RT                                                          520
521     521         K1 = MINO ( K1, 49 )                                             521
522     522         K1 = MAXO ( K1, 3  )                                             522
523     523         K2 = K1 + 1                                                      523
524     524         RT = RT - K1                                                     524
525     525         ENERGY = EMEOA( K1 ) + RT * ( EMEOA( K2 ) - EMEOA( K1 ) )        525
526     526   C                                                                      526
527     527         X = COVA / VOL / ( ( T + THETAA ) ** ALFAA )                     527
528     528         EX = EXP( BETAA * X )                                            528
529     529         Z = X * EX                                                       529
530     530         RT = ALFAA * T / ( T + THETAA )                                  530
531     531         ENERGY = ENERGY + RT * Z * T                                     531
532     532         HYDV( IC , 8 ) = ENERGY * RGAS / WMA                             532
533     533         EMEO = HYDV( IC , 8 ) / HYDV( IC , 1 ) * WMA / RGAS              533
534     534   C                                                                      534
535     535         IYY = ( EMEO - EMEOA( 3 ) ) / RANGEA + 1                         535
536     536         IYY = MAXO( 1 , MINO( IYY , 47 ) )                               536
537     537   C                                                                      537
538     538         K = IYY + 2                                                      538
539     539         IYY = IYY                                                        539
540     540        . + INT( AMAX1( EMEO - EMEOA( K ) , 0.) / DYA( K ) )              540
541     541        . - INT( AMAX1( EMEOA( K + 1 ) - EMEO , 0. ) / DYA( K ) )         541
542     542         IYY = MAXO( 1, MINO( IYY , 47 ) )                                542
543     543   C                                                                      543
544     544         K1 = IYY + 2                                                     544
545     545         K2 = K1 + 1                                                      545
546     546         RT = ( EMEO - EMEOA( K1 ) ) / ( EMEOA( K2 ) - EMEOA( K1 ) )      546
547     547         T = TA( K1 ) + 100. * RT                                         547
548     548         CVM = CVMA( K1 ) + RT * ( CVMA( K2 ) - CVMA( K1 ) )              548
549     549         ERS = 0.                                                         549
550     550   C                                                                      550
551     551         P = RGAS * T / VOL / GPERCC                                      551
552     552         RGAMM1 = CVM                                                     552
553     553         HYDV( IC , 7 ) = 1. / RGAMM1 + 1.                                553
554     554         HYDV( IC , 5 ) = P                                               554
555     555   C                                                                      555
556     556         ELSE                                                             556
557     557   C                                                                      557
558     558         DST = HYDV( IC , 1 ) * GPERCC                                    558
559     559         VOL = WMX * ( 1. - DST / FSX ) / DST / XGX                       559
560     560         TT = HYDV( IC , 5 ) * VOL * GPERCC / RGAS                        560
561     561   C                                                                      561
562     562         T = TT                                                           562
563     563         RT = 0.01 * T                                                    563
564     564         K1 = RT                                                          564
565     565         K1 = MINO ( K1, 49 )                                             565
566     566         K1 = MAXO ( K1, 3  )                                             566
567     567         K2 = K1 + 1                                                      567
568     568         RT = RT - K1                                                     568
569     569         ENERGY = EMEOX( K1 ) + RT * ( EMEOX( K2 ) - EMEOX( K1 ) )        569
570     570         ENERGY = ENERGY * RGAS / WMX                                     570
571     571   C                                                                      571
572     572         DO ITER = 1 , NITER                                              572
573     573         X = COVX / VOL / ( T + THETAX ) ** ALFAX                         573
574     574   C                                                                      574
575     575         BETAZX = BETAX * X                                               575
576     576         RT = X * EXP( BETAZX )                                           576
577     577         RTINV = 1. / ( 1. + RT )                                         577
578     578   C -   ERS IS THE FUNCTION, RT IS THE DERIVATIVE                        578
579     579         ERS = T -  TT * RTINV                                            579
580     580         RT = 1. - TT * RTINV * RTINV * ALFAX * RT * ( 1. + BETAZX ) /    580
581     581        .                 ( T + THETAX )                                  581
582     582         ERS = ERS / RT                                                   582
583     583         T = T - ERS                                                      583
584     584         END DO                                                           584
585     585   C                                                                      585
586     586         RT = 0.01 * T                                                    586
587     587         K1 = RT                                                          587
588     588         K1 = MINO ( K1, 49 )                                             588
589     589         K1 = MAXO ( K1, 3  )                                             589
590     590         K2 = K1 + 1                                                      590
591     591         RT = RT - K1                                                     591
```

```
592     592          ENERGY = EMEOX( K1 ) + RT * ( EMEOX( K2 ) - EMEOX( K1 ) )
593     593    C
594     594          X = COVX / VOL / ( ( T + THETAX ) ** ALFAX )
595     595          EX = EXP( BETAX * X )
596     596          Z = X * EX
597     597          RT = ALFAX * T / ( T + THETAX )
598     598          ENERGY = ENERGY + RT * Z * T
599     599          HYDV( IC , 8 ) = ENERGY * RGAS / WMX
600     600          VOL = WMX * ( 1. - DST / FSX ) / DST / XGX
601     601          EMEO = HYDV( IC , 8 ) / HYDV( IC , 1 ) * WMX / RGAS
602     602    C
603     603          IYY = ( EMEO - EMEOX( 3 ) ) / RANGEX + 1
604     604          IYY = MAXO( 1 , MINO( IYY , 47 ) )
605     605    C
606     606          K = IYY + 2
607     607          IYY = IYY
608     608         . + INT( AMAX1( EMEO - EMEOX( K ) , 0.) / DYX( K ) )
609     609         . - INT( AMAX1( EMEOX( K + 1 ) - EMEO , 0. ) / DYX( K ) )
610     610          IYY = MAXO( 1, MINO( IYY , 47 ) )
611     611    C
612     612          K1 = IYY + 2
613     613          K2 = K1 + 1
614     614          RT = ( EMEO - EMEOX( K1 ) ) / ( EMEOX( K2 ) - EMEOX( K1 ) )
615     615          T = TX( K1 ) + 100. * RT
616     616          CVM = CVMX( K1 ) + RT * ( CVMX( K2 ) - CVMX( K1 ) )
617     617          ERS = 0.
618     618    C
619     619    401   CONTINUE
620     620          P = RGAS * T / VOL / GPERCC
621     621          RGAMM1 = CVM
622     622    C
623     623          X = COVX / VOL / ( ( T + THETAX ) ** ALFAX )
624     624          Z = X * EXP( BETAX * X )
625     625          X = 1. + BETAX * X
626     626          RT = ALFAX * T / ( T + THETAX )
627     627          ERS = ERS + RT * Z * T
628     628    C
629     629          IF ( ITER .EQ. NITER ) GO TO 201
630     630    C
631     631          CVM = CVM * XGX + SCVX
632     632         *           + RT * Z * ( 2. - RT / ALFAX - RT * X )
633     633          T = T - AMIN1( ERS / CVM , TLIMIT * T )
634     634    C
635     635          NITER = NITER + 1
636     636    C
637     637          RT = 0.01 * T
638     638          K1 = RT
639     639          K1 = MINO ( K1, 49 )
640     640          K1 = MAXO ( K1, 3  )
641     641          K2 = K1 + 1
642     642          RT = RT - K1
643     643          CVM = CVMX(K1) + RT * ( CVMX( K2 ) - CVMX( K1 ) )
644     644          ERS = EMEOX( K1 ) + RT * ( EMEOX( K2 ) - EMEOX( K1 ) )
645     645          ERS = ERS - EMEO
646     646    C
647     647          GO TO 401
648     648    C
649     649    201   CONTINUE
650     650          P = P * ( 1. + Z )
651     651          RGAMM1 = ( RGAMM1 +
652     652         *           RT * Z * ( 2. - RT / ALFAX - RT * X ) ) / ( 1. + Z )
653     653          X = X * Z / ( 1. + Z )
654     654          RGAMM1 = RGAMM1 / ( ( 1. - RT * X ) ** 2 + X * RGAMM1 )
655     655          ERS = ERS / EMEO
656     656          HYDV( IC , 7 ) = 1. / RGAMM1 + 1.
657     657          HYDV( IC , 5 ) = P
658     658          END IF
659     659          END IF
660     660    260       CONTINUE
661     661    C
662     662    C(2)----
663     663          ELSE
664     664    C
665     665             XMSQR = XMCHIN * XMCHIN
```

```
      PINL = PIN
      RINL = RIN
      RINRTO = ( HRGG + 1. ) * XMSQR /
     .         ( ( HRGG - 1. ) * XMSQR + 2. )
      PINRTO = ( 2. * HRGG * XMSQR - ( HRGG - 1. ) ) /
     .                                 ( HRGG + 1. )
      PIN = PINRTO * PINL
      RIN = RINRTO * RINL
      YMCHIN = SQRT( ( ( HRGG - 1. ) * XMSQR + 2. ) /
     .               ( 2. * HRGG * XMSQR - ( HRGG - 1. ) ) )
      PRINT*,HRGG,RIN,PIN,YMCHIN
      PRINT*,HRGG,RINL,PINL,XMCHIN
      UVIN = XMCHIN * SQRT( HRGG * PINL / RINL ) -
     .       YMCHIN * SQRT( HRGG * PIN / RIN )
      UIN = UVIN * COSS
      VIN = UVIN * SINN
      WIN = 0.
C
      DO 155 IC = 1 , NC
         HYDV( IC , 1 ) = RINL
         HYDV( IC , 2 ) = UIN
         HYDV( IC , 3 ) = VIN
         HYDV( IC , 4 ) = WIN
         HYDV( IC , 5 ) = PINL
C
 155     CONTINUE
      ENDIF
C     remove the followed END IF for regular run
C      ENDIF
C      ENDIF
C(2)<<<<
C
1122  CONTINUE
      IF( ICOND . EQ . 0 ) THEN
      NPRTCL = 25
      XPRTCL(1,1) = .443
      XPRTCL(2,1) = 1.0414
      XPRTCL(3,1) = 1.4224
      XPRTCL(1,2) = -.002
      XPRTCL(2,2) = .3556
      XPRTCL(3,2) = 0.5842
      XPRTCL(1,3) = -.275
      XPRTCL(2,3) = -.3058
      XPRTCL(3,3) = -1.4224
      XPRTCL(1,4) = 2.032
      XPRTCL(2,4) = -.3048
      XPRTCL(3,4) = -4.572
      XPRTCL(1,5) = .3048
      XPRTCL(2,5) = .1016
      XPRTCL(3,5) = .3048
      XPRTCL(1,6) = .4572
      XPRTCL(2,6) = .1016
      XPRTCL(3,6) = .4572
      XPRTCL(1,7) = .6096
      XPRTCL(2,7) = .1016
      XPRTCL(3,7) = .3048
      XPRTCL(1,8) = .4572
      XPRTCL(2,8) = .1016
      XPRTCL(3,8) = .1524
      XPRTCL(1,9) = 1.3462
      XPRTCL(2,9) = .1016
      XPRTCL(3,9) = .3048
      XPRTCL(1,10) = 1.4986
      XPRTCL(2,10) = .1016
      XPRTCL(3,10) = .4572
      XPRTCL(1,11) = 1.651
      XPRTCL(2,11) = .1016
      XPRTCL(3,11) = .3048
      XPRTCL(1,12) = 1.4986
      XPRTCL(2,12) = .1016
      XPRTCL(3,12) = .1524
      XPRTCL(1,13) = .6096
      XPRTCL(2,13) = .7740
      XPRTCL(3,13) = 1.0668
```

```
740  740        XPRTCL(1,14) = .6096                                          740
741  741        XPRTCL(2,14) = .8138                                          741
742  742        XPRTCL(3,14) = .5334                                          742
743  743        XPRTCL(1,15) = 1.4224                                         743
744  744        XPRTCL(2,15) = .7740                                          744
745  745        XPRTCL(3,15) = 1.0668                                         745
746  746        XPRTCL(1,16) = 1.4224                                         746
747  747        XPRTCL(2,16) = .8128                                          747
748  748        XPRTCL(3,16) = .5334                                          748
749  749        XPRTCL(1,17) = -.3058                                         749
750  750        XPRTCL(2,17) = 1.3208                                         750
751  751        XPRTCL(3,17) = -.4318                                         751
752  752        XPRTCL(1,18) = .2032                                          752
753  753        XPRTCL(2,18) = .7590                                          753
754  754        XPRTCL(3,18) = 1.1898                                         754
755  755        XPRTCL(1,19) = .254                                           755
756  756        XPRTCL(2,19) = .1772                                          756
757  757        XPRTCL(3,19) = 1.1948                                         757
758  758        XPRTCL(1,20) = .9144                                          758
759  759        XPRTCL(2,20) = .4064                                          759
760  760        XPRTCL(3,20) = .9652                                          760
761  761        XPRTCL(1,21) = .2032                                          761
762  762        XPRTCL(2,21) = .7680                                          762
763  763        XPRTCL(3,21) = 1.1888                                         763
764  764        XPRTCL(1,22) = .1532                                          764
765  765        XPRTCL(2,22) = .7670                                          765
766  766        XPRTCL(3,22) = 1.1888                                         766
767  767        XPRTCL(1,23) = .1532                                          767
768  768        XPRTCL(2,23) = .7665                                          768
769  769        XPRTCL(3,23) = 1.1878                                         769
770  770        XPRTCL(1,24) = .1532                                          770
771  771        XPRTCL(2,24) = .7765                                          771
772  772        XPRTCL(3,24) = 1.1898                                         772
773  773        XPRTCL(1,25) = .1532                                          773
774  774        XPRTCL(2,25) = .7655                                          774
775  775        XPRTCL(3,25) = 1.1898                                         775
776  776        DO IK = 1 , NPRTCL                                            776
777  777        RMINN = 100000000.                                            777
778  778        DO IC = 1 , NC                                                778
779  779        I1=JC(1,IC)                                                   779
780  780        I2=JC(2,IC)                                                   780
781  781        I3=JC(3,IC)                                                   781
782  782        I4=JC(4,IC)                                                   782
783  783        XXI = XPRTCL( 1 , IK )                                        783
784  784        YYI = XPRTCL( 2 , IK )                                        784
785  785        ZZI = XPRTCL( 3 , IK )                                        785
786  786        CALL VOLMTETC ( I1, I2, I3, XXI, YYI, ZZI , VOL1 )            786
787  787        CALL VOLMTETC ( I1, I2, I4, XXI, YYI, ZZI , VOL2 )            787
788  788        CALL VOLMTETC ( I1, I3, I4, XXI, YYI, ZZI , VOL3 )            788
789  789        CALL VOLMTETC ( I2, I3, I4, XXI, YYI, ZZI , VOL4 )            789
790  790        XXI = XV( 1 , I4 )                                            790
791  791        YYI = XV( 2 , I4 )                                            791
792  792        ZZI = XV( 3 , I4 )                                            792
793  793        CALL VOLMTETC ( I1, I2, I3, XXI, YYI, ZZI , VOLL )            793
794  794        DEFVOL=DABS(VOL1)+DABS(VOL2)+DABS(VOL3)+DABS(VOL4)            794
795  795       .     -DABS(VOLL)                                              795
796  796        IF( DABS(DEFVOL/VOLL) . LT . .001 ) THEN                      796
797  797            IJKPRT(IK) = IC                                           797
798  798            PRINT*,ik,vol1,vol2,vol3,vol4                             798
799  799            PRINT*,ic,vol1,defvol,defvol/vol1                         799
800  800            PRINT*,(XV(kk,jc(1,ic)),kk=1,3)                           800
801  801            PRINT*,(XV(kk,jc(2,ic)),kk=1,3)                           801
802  802            PRINT*,(XV(kk,jc(3,ic)),kk=1,3)                           802
803  803            PRINT*,(XV(kk,jc(4,ic)),kk=1,3)                           803
804  804            PRINT*,(JS(9,jc(kk,ic)),kk=5,8)                           804
805  805        END IF                                                        805
806  806        END DO                                                        806
807  807        END DO                                                        807
808  808        DO IK = 1 , NPRTCL                                            808
809  809            IC = IJKPRT(IK)                                           809
810  810            ISS = JC(5,IC)                                            810
811  811        DO IKK = 5 , 8                                                811
812  812            IS = JC(IKK,IC)                                           812
813  813            IBC = JS(9,IS)                                            813
```

```
814     814           IF( I8C . EQ . 6 ) THEN                                  814
815     815            ISS = IS                                                815
816     816           END IF                                                   816
817     817         END DO                                                     817
818     818             IJKPRT(IK) = ISS                                       818
819     819         END DO                                                     819
820     820         END IF                                                     820
821     821   C                                                                821
822     822          PRINT * ,ICOND,ICONP                                      822
823     823   C                                                                823
824     824          IF( ICONP . EQ . 1 ) THEN                                 824
825     825          READ(8) RIN,PIN,RINL,PINL,UVIN,UIN,VIN,WIN,TT             825
826     826          PRINT *, RIN,PIN,RINL,PINL,UVIN,UIN,VIN,WIN,TT            826
827     827   C        READ (8) NPRTCL                                         827
828     828   C        IF(NPRTCL.GT.0)                                         828
829     829   C      . READ (8) (IJKPRT(IK),IK=1,NPRTCL)                       829
830     830          DO II = 1 , 5                                             830
831     831          READ(8) ((HYDV(IC,IK),IK=1,8),IC=1,NC)                    831
832     832          END DO                                                    832
833     833   C                                                                833
834     834         END IF                                                     834
835     835   C                                                                835
836     836         ZCOUNT = 0                                                 836
837     837         DO 380 IC = 1 , NC                                         837
838     838         RCOUNT = HYDV( IC , 8 ) + .5 * HYDV( IC , 1 ) *            838
839     839        .                    ( HYDV( IC , 2 ) * HYDV( IC , 2 ) +    839
840     840        .                      HYDV( IC , 3 ) * HYDV( IC , 3 ) +    840
841     841        .                      HYDV( IC , 4 ) * HYDV( IC , 4 ) )    841
842     842         ZCOUNT = ZCOUNT + XC( 4 , IC ) * RCOUNT                    842
843     843    380  CONTINUE                                                   843
844     844          YCOUNT = ZCOUNT - XCOUNT                                  844
845     845          PRINT * ,ZCOUNT,YCOUNT                                    845
846     846         CALL HYDRMN                                                846
847     847   C                                                                847
848     848   C --- EXIT POINT FROM PROGRAM ----------------------------------- 848
849     849   C                                                                849
850     850   C     --------                                                   850
851     851         STOP 777                                                   851
852     852   C     --------                                                   852
853     853   C                                                                853
854     854   C --- FORMATS ---------------------------------------------------- 854
855     855   C                                                                855
856     856   101   FORMAT(1H ,'ICOND=',I2,5X,'ICONP=',I2,5X,'IOPTN=',I2,/,1X,856
857     857        .           'XMCHIN=',F13.6,5X,'RIN=',F13.6,5X,'PIN=',F13.6,/,1X,857
858     858        .           'ALFA=',F13.6,5X,'HRGG=',F13.6,5X,'IHRN=',I2,5X,/,1X,858
859     859        .           'NTIME=',I2,5X,'NDUMP=',I5,5X,'IOPORD=',I2)    859
860     860                                                                    860
861     861          END                                                       861
862     862   C                                                                862
```

```
      SUBROUTINE HYDRFL
C
C-----------------------------------------------------------------I
C                                                                 I
C     HYDRFL IS A 2 DIMENSIONAL RIEMANN SOLVER THAT INTEGRATES    I
C           FLUXES ACROSS NORMAL INTERFACES TO UPDATE VERTICES    I
C           VARIABLES .                                           I
C                                                                 I
C-----------------------------------------------------------------I
C
      include     'dmsh00.h'
      include     'dhydm0.h'
      include     'dphsm0.h'
      include     'dmtrl0.h'
C
      REAL DELP(128),WSOP(128),WSOM(128),WS00(128),
     .     RSTAR(128),CSTAR(128),PMAX(128),PMIN(128)
      REAL RRIGHT(128),URIGHT(128),VRIGHT(128),PRIGHT(128)
      REAL RLEFTT(128),ULEFTT(128),VLEFTT(128),PLEFTT(128)
      REAL ENRGYI(128),ANRGYI(128)
C
C --- BEGIN LOOP OVER ALL EDGES IN THE DOMAIN ----------------------
C
      DO 280 IH = 1 , 6
      DO 280 IC = 1 , NC
      HYDFLX( IC , IH ) = 0.
 280  CONTINUE
C
      NS1 = 1
      NS2 = NOFVES( 1 )
      DO 110 INS = 1 , NVEES
C
C --- FETCH HYDRO QUANTITIES ---------------------------------------
C
      DO 120 IS = NS1 , NS2
          KS = IS - NS1 + 1
C
          RRR( KS ) = RR( IS )
          UUR( KS ) = UR( IS )
          VVR( KS ) = VR( IS )
          WWR( KS ) = WR( IS )
          PPR( KS ) = PR( IS )
          AAR( KS ) = AR( IS )
          EER( KS ) = ER( IS )
          GGR( KS ) = GR( IS )
C
          RRL( KS ) = RL( IS )
          UUL( KS ) = UL( IS )
          VVL( KS ) = VL( IS )
          WWL( KS ) = WL( IS )
          PPL( KS ) = PL( IS )
          AAL( KS ) = AL( IS )
          EEL( KS ) = EL( IS )
          GGL( KS ) = GL( IS )
C
 120  CONTINUE
C
      DO 130 KS = 1 , NOFVES( INS )
C
C --- THIS SECTION OF CODE SOLVES FOR "PSTAR" AND "USTAR" IN
C     THE RIEMANN PROBLEM USING NEWTON'S METHOD.
C
          WLEFT( KS ) = SQRT( GGL( KS ) * PPL( KS ) * RRL( KS ) )
          WRIGT( KS ) = SQRT( GGR( KS ) * PPR( KS ) * RRR( KS ) )
          WLESQ( KS ) = WLEFT( KS ) * WLEFT( KS )
          WRISQ( KS ) = WRIGT( KS ) * WRIGT( KS )
C
          PMIN( KS ) = AMIN1( PPL( KS ) , PPR( KS ) )
          PSML( KS ) = HRSM * PMIN( KS )
C
C --- FORM THE STARTING GUESS FOR THE SOLUTION ---------------------
C
          PSTAR( KS ) = ( WLEFT( KS ) * PPR( KS ) +
     .                    WRIGT( KS ) * PPL( KS ) -
```

```
      .                    WLEFT( KS ) * WRIGT( KS ) *
      .                  ( UUR( KS ) - UUL( KS ) ) /
      .                  ( WLEFT( KS ) + WRIGT( KS ) )
           PSTAR( KS ) = AMAX1( PSTAR( KS ) , PSML( KS ) )
  130  CONTINUE
C
           DO 140 I = 1 , IHRN
C
C --- BEGIN THE NEWTON ITERATION -----------------------------
C
      DO 150 KS = 1 , NOFVES( INS )
           CFFL = ( GGL( KS ) + 1. ) / ( 2. * GGL( KS ) )
           WLEFS( KS ) = ( 1. + CFFL * ( PSTAR( KS ) /
      .                              PPL( KS ) - 1. ) ) * WLESQ( KS )
           WLEFT( KS ) = SQRT( WLEFS( KS ) )
           ZLEFT( KS ) = 2. * WLEFT( KS ) * WLEFS( KS ) /
      .                    ( WLESQ( KS ) + WLEFS( KS ) )
           USTL( KS )  = UUL( KS ) -
      .                  ( PSTAR( KS ) - PPL( KS ) ) / WLEFT( KS )
  150  CONTINUE
C
      DO 152 KS = 1 , NOFVES( INS )
           CFFR = ( GGR( KS ) + 1. ) / ( 2. * GGR( KS ) )
           WRIFS( KS ) = ( 1. + CFFR * ( PSTAR( KS ) /
      .                              PPR( KS ) - 1. ) ) * WRISQ( KS )
           WRIGT( KS ) = SQRT( WRIFS( KS ) )
           ZRIGT( KS ) = 2. * WRIGT( KS ) * WRIFS( KS ) /
      .                    ( WRISQ( KS ) + WRIFS( KS ) )
           USTR( KS )  = UUR( KS ) +
      .                  ( PSTAR( KS ) - PPR( KS ) ) / WRIGT( KS )
  152  CONTINUE
C
      DO 160 KS = 1 , NOFVES( INS )
           DPST( KS )  = ZLEFT( KS ) * ZRIGT( KS ) *
      .                  ( USTR( KS ) - USTL( KS ) ) /
      .                  ( ZLEFT( KS ) + ZRIGT( KS ) )
           PSTAR( KS ) = PSTAR( KS ) - DPST( KS )
           PSTAR( KS ) = AMAX1( PSTAR( KS ) , PSML( KS ) )
  160     CONTINUE
C
  140     CONTINUE
C
C --- FORM FINAL SOLUTIONS -----------------------------------
C
      DO 170 KS = 1 , NOFVES( INS )
          CFFL = ( GGL( KS ) + 1. ) / ( 2. * GGL( KS ) )
          WLEFT( KS ) = SQRT( WLESQ( KS ) * ( 1. +
      .                  CFFL * ( PSTAR( KS ) / PPL( KS ) - 1. ) ) )
  170  CONTINUE
C
      DO 172 KS = 1 , NOFVES( INS )
          CFFR = ( GGR( KS ) + 1. ) / ( 2. * GGR( KS ) )
          WRIGT( KS ) = SQRT( WRISQ( KS ) * ( 1. +
      .                  CFFR * ( PSTAR( KS ) / PPR( KS ) - 1. ) ) )
  172  CONTINUE
C
      DO 180 KS = 1 , NOFVES( INS )
          USTAR( KS ) = ( PPL( KS ) - PPR( KS ) +
      .                    WLEFT( KS ) * UUL( KS ) +
      .                    WRIGT( KS ) * UUR( KS ) ) /
      .                  ( WLEFT( KS ) + WRIGT( KS ) )
  180  CONTINUE
C
      DO 190 KS = 1 , NOFVES( INS )
C
C --- BEGIN PROCEDURE TO OBTAIN FLUXES FROM REIMANN FORMALISM --
C
           IF( USTAR( KS ) . LE . 0.0 ) THEN
C
             RO( KS ) = RRR( KS )
             PO( KS ) = PPR( KS )
             UO( KS ) = UUR( KS )
             CO( KS ) = SQRT( HRGG * PPR( KS ) / RRR( KS ) )
             WO( KS ) = WRIGT( KS )
```

```
1011    149              GO( KS ) = GGR( KS )                                    1011
1012    150              ISN( KS ) = 1                                           1012
1013    151   C                                                                  1013
1014    152              ENRGYI( KS ) = EER( KS )                                1014
1015    153              ANRGYI( KS ) = AAR( KS )                                1015
1016    154              VGDNV( KS ) = VVR( KS )                                 1016
1017    155              WGDNV( KS ) = WWR( KS )                                 1017
1018    156   C                                                                  1018
1019    157            ELSE                                                      1019
1020    158   C                                                                  1020
1021    159              RO( KS ) = RRL( KS )                                    1021
1022    160              PO( KS ) = PPL( KS )                                    1022
1023    161              UO( KS ) = UUL( KS )                                    1023
1024    162              CO( KS ) = SQRT( HRGG * PPL( KS ) / RRL( KS ) )         1024
1025    163              WO( KS ) = WLEFT( KS )                                  1025
1026    164              GO( KS ) = GGL( KS )                                    1026
1027    165              ISN( KS ) = -1                                          1027
1028    166   C                                                                  1028
1029    167              ENRGYI( KS ) = EEL( KS )                                1029
1030    168              ANRGYI( KS ) = AAL( KS )                                1030
1031    169              VGDNV( KS ) = VVL( KS )                                 1031
1032    170              WGDNV( KS ) = WWL( KS )                                 1032
1033    171            END IF                                                    1033
1034    172    190   CONTINUE                                                   1034
1035    173   C                                                                  1035
1036    174          DO 200 KS = 1 , NOFVES( INS )                             1036
1037    175            DELP( KS ) = PSTAR( KS ) - PO( KS )                     1037
1038    176            WSOP( KS ) = ISN( KS ) * UO( KS ) + WO( KS ) / RO( KS ) 1038
1039    177            WSOM( KS ) = ISN( KS ) * UO( KS ) + CO( KS )            1039
1040    178    200   CONTINUE                                                   1040
1041    179   C                                                                  1041
1042    180          DO 210 KS = 1 , NOFVES( INS )                             1042
1043    181            IF( DELP( KS ) . GT . 0. ) THEN                         1043
1044    182              WSOO( KS ) = WSOP( KS )                               1044
1045    183            ELSE                                                    1045
1046    184              WSOO( KS ) = WSOM( KS )                               1046
1047    185            END IF                                                  1047
1048    186    210   CONTINUE                                                   1048
1049    187   C                                                                  1049
1050    188          DO 220 KS = 1 , NOFVES( INS )                             1050
1051    189   C                                                                  1051
1052    190   C --- USE OUTER STATE SOLUTION ------------------------------     1052
1053    191   C                                                                  1053
1054    192              PGDNV( KS ) = PO( KS )                                  1054
1055    193              UGDNV( KS ) = UO( KS )                                  1055
1056    194              CGDNV( KS ) = CO( KS )                                  1056
1057    195              RGDNV( KS ) = RO( KS )                                  1057
1058    196    220   CONTINUE                                                   1058
1059    197   C                                                                  1059
1060    198   C --- COMPUTE STARRED VALUES ---------------------------------     1060
1061    199   C                                                                  1061
1062    200          DO 230 KS = 1 , NOFVES( INS )                             1062
1063    201              RSTAR( KS ) = 1. / ( 1. / RO( KS ) - DELP( KS ) /     1063
1064    202         .                          ( WO( KS ) * WO( KS ) ) )       1064
1065    203              CSTAR( KS ) = SQRT( GO( KS ) * PSTAR( KS ) / RSTAR( KS ) )  1065
1066    204              WSOM( KS )  = ISN( KS ) * USTAR( KS ) + CSTAR( KS )   1066
1067    205    230   CONTINUE                                                   1067
1068    206   C                                                                  1068
1069    207          DO 240 KS = 1 , NOFVES( INS )                             1069
1070    208            IF( DELP( KS ) . GT . 0. ) THEN                         1070
1071    209              SPIN( KS ) = WSOP( KS )                               1071
1072    210            ELSE                                                    1072
1073    211              SPIN( KS ) = WSOM( KS )                               1073
1074    212            END IF                                                  1074
1075    213    240   CONTINUE                                                   1075
1076    214   C                                                                  1076
1077    215          DO 250 KS = 1 , NOFVES( INS )                             1077
1078    216   C                                                                  1078
1079    217          IF( WSOO( KS ) . GE . 0. ) THEN                           1079
1080    218              IF( SPIN( KS ) . GE . 0. ) THEN                       1080
1081    219   C                                                                  1081
1082    220   C --- USE THE STARRED STATE RESULTS ---------------------------    1082
1083    221   C                                                                  1083
1084    222                              RGDNV( KS ) = RSTAR( KS )               1084
```

```
                        UGDNV( KS ) = USTAR( KS )
                        CGDNV( KS ) = CSTAR( KS )
                        PGDNV( KS ) = PSTAR( KS )
            ELSE
C
C --- EVALUATE THE INSIDE RAREFACTION WAVE ---------------------
C
            CGDNV( KS ) = ( CSTAR( KS ) * 2. -
     .                      ISN( KS ) * USTAR( KS ) * ( GO( KS ) - 1. ) )
     .                                              / ( GO( KS ) + 1. )
            UGDNV( KS ) = - ISN( KS ) * CGDNV( KS )
            RGDNV( KS ) = ( CGDNV( KS ) / CO( KS ) ) **
     .                    ( 2. / ( GO( KS ) - 1. ) ) * RO( KS )
            PGDNV( KS ) = CGDNV( KS ) * CGDNV( KS ) * RGDNV( KS ) /
     .                                                GO( KS )
C
            END IF
C
          END IF
  250   CONTINUE
C
          DO 260 KS = 1 , NOFVES( INS )
              IS = KS + NS1 - 1
C
          ICL = JS( 7 , IS )
          ICR = JS( 8 , IS )
C
          CTT = SQRT( GO( KS ) * PGDNV( KS ) / RGDNV( KS ) )
          XSS = XS( 5 , IS )
          XYZ = 1. / XSS
C
          IATRB = JS( 9 , IS )
          IF( IATRB . EQ . 0 ) THEN
C
             XXN = ( XC( 1 , ICR ) - XC( 1 , ICL ) ) * XYZ
             YYN = ( XC( 2 , ICR ) - XC( 2 , ICL ) ) * XYZ
             ZZN = ( XC( 3 , ICR ) - XC( 3 , ICL ) ) * XYZ
C
          VEL =
     .        ( UGDNV( KS ) * XN( IS ) +
     .          VGDNV( KS ) * XP( IS ) +
     .          WGDNV( KS ) * XT( IS ) ) * XXN +
     .        ( UGDNV( KS ) * YN( IS ) +
     .          VGDNV( KS ) * YP( IS ) +
     .          WGDNV( KS ) * YT( IS ) ) * YYN +
     .        ( UGDNV( KS ) * ZN( IS ) +
     .          VGDNV( KS ) * ZP( IS ) +
     .          WGDNV( KS ) * ZT( IS ) ) * ZZN
C
          DTU = XSS / ( CTT + ABS( VEL ) )
          DTT = AMIN1( DTU , DTT )
C
          ELSE
C
             XXN = ( XYZMDL( 1 , IS ) - XC( 1 , ICL ) ) * XYZ
             YYN = ( XYZMDL( 2 , IS ) - XC( 2 , ICL ) ) * XYZ
             ZZN = ( XYZMDL( 3 , IS ) - XC( 3 , ICL ) ) * XYZ
C
          VEL =
     .        ( UGDNV( KS ) * XN( IS ) +
     .          VGDNV( KS ) * XP( IS ) +
     .          WGDNV( KS ) * XT( IS ) ) * XXN +
     .        ( UGDNV( KS ) * YN( IS ) +
     .          VGDNV( KS ) * YP( IS ) +
     .          WGDNV( KS ) * YT( IS ) ) * YYN +
     .        ( UGDNV( KS ) * ZN( IS ) +
     .          VGDNV( KS ) * ZP( IS ) +
     .          WGDNV( KS ) * ZT( IS ) ) * ZZN
C
          DTU = XSS / ( CTT + ABS( VEL ) )
          DTT = AMIN1( DTU , DTT )
C
          END IF
  260   CONTINUE
```

```
      C
            DO 270 KS = 1 , NOFVES( INS )
               IS = KS + NS1 - 1
      C
      C ... FLUX FOR DENSITY ..........................................
      C
            RO( KS ) = RGDNV( KS ) * UGDNV( KS )
      C
      C ... FLUX FOR MOMENTUM DENSITY .................................
      C
            UO( KS ) = PGDNV( KS ) * XN( IS ) +
           .              RO( KS ) * ( UGDNV( KS ) * XN( IS ) +
           .                           VGDNV( KS ) * XP( IS ) +
           .                           WGDNV( KS ) * XT( IS ) )
            CO( KS ) = PGDNV( KS ) * YN( IS ) +
           .              RO( KS ) * ( UGDNV( KS ) * YN( IS ) +
           .                           VGDNV( KS ) * YP( IS ) +
           .                           WGDNV( KS ) * YT( IS ) )
            WO( KS ) = PGDNV( KS ) * ZN( IS ) +
           .              RO( KS ) * ( UGDNV( KS ) * ZN( IS ) +
           .                           VGDNV( KS ) * ZP( IS ) +
           .                           WGDNV( KS ) * ZT( IS ) )
      C
      C ... FLUX FOR ENERGY DENSITY ...................................
      C
            PO( KS ) = UGDNV( KS ) * ( ENRGYI( KS ) +
           .      .5 * RGDNV( KS ) * ( UGDNV( KS ) * UGDNV( KS ) +
           .                           VGDNV( KS ) * VGDNV( KS ) +
           .                           WGDNV( KS ) * WGDNV( KS ) ) )
      C
      C ... FLUX FOR COMBUSTION INTERFACE TRACKING ....................
      C
            AO( KS ) = UGDNV( KS ) * RGDNV( KS ) * ANRGYI( KS )
      C
       270  CONTINUE
      C
            DO 290 IS = NS1 , NS2
               KS = IS - NS1 + 1
      C
             ICL = JS( 7 , IS )
             ICR = JS( 8 , IS )
      C
            IATRB = JS( 9 , IS )
            IF( IATRB . EQ . 0 ) THEN
      C
      C ... FLUX FOR DENSITY ..........................................
      C
            DLENG = XS( 4 , IS ) * RO( KS )
            HYDFLX( ICL , 1 ) = HYDFLX( ICL , 1 ) + DLENG
            HYDFLX( ICR , 1 ) = HYDFLX( ICR , 1 ) - DLENG
      C
      C ... FLUX FOR MOMENTUM DENSITY ( U DIRECTION ) .................
      C
            DLENG = XS( 4 , IS ) * UO( KS )
            HYDFLX( ICL , 2 ) = HYDFLX( ICL , 2 ) + DLENG
            HYDFLX( ICR , 2 ) = HYDFLX( ICR , 2 ) - DLENG
      C
      C ... FLUX FOR MOMENTUM DENSITY ( V DIRECTION ) .................
      C
            DLENG = XS( 4 , IS ) * CO( KS )
            HYDFLX( ICL , 3 ) = HYDFLX( ICL , 3 ) + DLENG
            HYDFLX( ICR , 3 ) = HYDFLX( ICR , 3 ) - DLENG
      C
      C ... FLUX FOR MOMENTUM DENSITY ( W DIRECTION ) .................
      C
            DLENG = XS( 4 , IS ) * WO( KS )
            HYDFLX( ICL , 4 ) = HYDFLX( ICL , 4 ) + DLENG
            HYDFLX( ICR , 4 ) = HYDFLX( ICR , 4 ) - DLENG
      C
      C ... FLUX FOR ENERGY DENSITY ...................................
      C
            DLENG = XS( 4 , IS ) * PO( KS )
            HYDFLX( ICL , 5 ) = HYDFLX( ICL , 5 ) + DLENG
            HYDFLX( ICR , 5 ) = HYDFLX( ICR , 5 ) - DLENG
```

```
1233     371   C                                                                 1233
1234     372   C ... FLUX FOR COMBUSTION INTERFACE TRACKING.....                 1234
1235     373   C                                                                 1235
1236     374         DLENG = XS( 4 , IS ) * AO( KS )                             1236
1237     375         HYDFLX( ICL , 6 ) = HYDFLX( ICL , 6 ) + DLENG               1237
1238     376         HYDFLX( ICR , 6 ) = HYDFLX( ICR , 6 ) - DLENG               1238
1239     377   C                                                                 1239
1240     378         ELSE                                                        1240
1241     379   C                                                                 1241
1242     380   C ... FLUX FOR DENSITY ..........................                 1242
1243     381   C                                                                 1243
1244     382         DLENG = XS( 4 , IS ) * RO( KS )                             1244
1245     383         HYDFLX( ICL , 1 ) = HYDFLX( ICL , 1 ) + DLENG               1245
1246     384   C                                                                 1246
1247     385   C ... FLUX FOR MOMENTUM DENSITY ( U DIRECTION ) .....             1247
1248     386   C                                                                 1248
1249     387         DLENG = XS( 4 , IS ) * UO( KS )                             1249
1250     388         HYDFLX( ICL , 2 ) = HYDFLX( ICL , 2 ) + DLENG               1250
1251     389   C                                                                 1251
1252     390   C ... FLUX FOR MOMENTUM DENSITY ( V DIRECTION ) .....             1252
1253     391   C                                                                 1253
1254     392         DLENG = XS( 4 , IS ) * CO( KS )                             1254
1255     393         HYDFLX( ICL , 3 ) = HYDFLX( ICL , 3 ) + DLENG               1255
1256     394   C                                                                 1256
1257     395   C ... FLUX FOR MOMENTUM DENSITY ( W DIRECTION ) .....             1257
1258     396   C                                                                 1258
1259     397         DLENG = XS( 4 , IS ) * WO( KS )                             1259
1260     398         HYDFLX( ICL , 4 ) = HYDFLX( ICL , 4 ) + DLENG               1260
1261     399   C                                                                 1261
1262     400   C ... FLUX FOR ENERGY DENSITY ....................                1262
1263     401   C                                                                 1263
1264     402         DLENG = XS( 4 , IS ) * PO( KS )                             1264
1265     403         HYDFLX( ICL , 5 ) = HYDFLX( ICL , 5 ) + DLENG               1265
1266     404   C                                                                 1266
1267     405   C ... FLUX FOR COMBUSTION INTERFACE TRACKING.....                 1267
1268     406   C                                                                 1268
1269     407         DLENG = XS( 4 , IS ) * AO( KS )                             1269
1270     408         HYDFLX( ICL , 6 ) = HYDFLX( ICL , 6 ) + DLENG               1270
1271     409   C                                                                 1271
1272     410         END IF                                                      1272
1273     411    290  CONTINUE                                                    1273
1274     412   C                                                                 1274
1275     413         NS1 = NS2 + 1                                               1275
1276     414         NS2 = NS2 + NOFVES( INS + 1 )                               1276
1277     415    110  CONTINUE                                                    1277
1278     416   C                                                                 1278
1279     417         RETURN                                                      1279
1280     418         END                                                         1280
1281     419   C                                                                 1281
```

```
      SUBROUTINE RYDRFL
C
C-----------------------------------------------------------------I
C                                                                 I
C     RYDRFL IS A 2 DIMENSIONAL RIEMANN SOLVER THAT INTEGRATES    I
C            FLUXES ACROSS NORMAL INTERFACES TO UPDATE VERTICES   I
C            VARIABLES .                                         I
C                                                                 I
C-----------------------------------------------------------------I
C
      include     'dmsh00.h'
      include     'dhydm0.h'
      include     'dphsm0.h'
      include     'dmtrl0.h'
C
      REAL DELP(128),WSOP(128),WSOM(128),WSO0(128),
     .     RSTAR(128),CSTAR(128),PMAX(128),PMIN(128)
      REAL RRIGHT(128),URIGHT(128),VRIGHT(128),PRIGHT(128)
      REAL RLEFTT(128),ULEFTT(128),VLEFTT(128),PLEFTT(128)
      REAL ENRGYI(128),ANRGYI(128)
C
C --- BEGIN LOOP OVER ALL EDGES IN THE DOMAIN ----------------------
C
      NS1 = 1
      NS2 = NOFVES( 1 )
      DO 110 INS = 1 , NVEES
C
C --- FETCH HYDRO QUANTITIES ---------------------------------------
C
      DO 120 IS = NS1 , NS2
          KS = IS - NS1 + 1
C
          ICL = JS( 7 , IS )
          IBC = JS( 9 , IS )
C
          RRL( KS ) = HYDV( ICL , 1 )
          UUL( KS ) = HYDV( ICL , 2 ) * XN( IS ) +
     .                HYDV( ICL , 3 ) * YN( IS ) +
     .                HYDV( ICL , 4 ) * ZN( IS )
          VVL( KS ) = HYDV( ICL , 2 ) * XP( IS ) +
     .                HYDV( ICL , 3 ) * YP( IS ) +
     .                HYDV( ICL , 4 ) * ZP( IS )
          WWL( KS ) = HYDV( ICL , 2 ) * XT( IS ) +
     .                HYDV( ICL , 3 ) * YT( IS ) +
     .                HYDV( ICL , 4 ) * ZT( IS )
          PPL( KS ) = HYDV( ICL , 5 )
          AAL( KS ) = HYDV( ICL , 6 )
          EEL( KS ) = HYDV( ICL , 8 )
          GGL( KS ) = HYDV( ICL , 7 )
C
          RRR( KS ) = RRL( KS )
          IF( IBC . EQ . 0 ) THEN
          UUR( KS ) = UUL( KS )
          ELSE
          UUR( KS ) = - UUL( KS )
          END IF
          VVR( KS ) = VVL( KS )
          WWR( KS ) = WWL( KS )
          PPR( KS ) = PPL( KS )
          AAR( KS ) = AAL( KS )
          EER( KS ) = EEL( KS )
          GGR( KS ) = GGL( KS )
C
 120  CONTINUE
C
      DO 130 KS = 1 , NOFVES( INS )
C
C --- THIS SECTION OF CODE SOLVES FOR "PSTAR" AND "USTAR" IN
C     THE RIEMANN PROBLEM USING NEWTON'S METHOD.
C
          WLEFT( KS ) = SQRT( GGL( KS ) * PPL( KS ) * RRL( KS ) )
          WRIGT( KS ) = SQRT( GGR( KS ) * PPR( KS ) * RRR( KS ) )
          WLESQ( KS ) = WLEFT( KS ) * WLEFT( KS )
          WRISQ( KS ) = WRIGT( KS ) * WRIGT( KS )
```

```
1356      75  C                                                                1356
1357      76            PMIN( KS ) = AMIN1( PPL( KS ) , PPR( KS ) )            1357
1358      77            PSML( KS ) = HRSM * PMIN( KS )                         1358
1359      78  C                                                                1359
1360      79  C --- FORM THE STARTING GUESS FOR THE SOLUTION ------------------ 1360
1361      80  C                                                                1361
1362      81            PSTAR( KS ) = ( WLEFT( KS ) * PPR( KS ) +              1362
1363      82           .                WRIGT( KS ) * PPL( KS ) -              1363
1364      83           .                WLEFT( KS ) * WRIGT( KS ) *            1364
1365      84           .              ( UUR( KS ) - UUL( KS ) ) ) /            1365
1366      85           .              ( WLEFT( KS ) + WRIGT( KS ) )            1366
1367      86            PSTAR( KS ) = AMAX1( PSTAR( KS ) , PSML( KS ) )        1367
1368      87     130  CONTINUE                                                  1368
1369      88  C                                                                1369
1370      89           . DO 140 I = 1 , IHRN                                   1370
1371      90  C                                                                1371
1372      91  C --- BEGIN THE NEWTON ITERATION -------------------------------- 1372
1373      92  C                                                                1373
1374      93           DO 150 KS = 1 , NOFVES( INS )                           1374
1375      94                CFFL = ( GGL( KS ) + 1. ) / ( 2. * GGL( KS ) )     1375
1376      95                WLEFS( KS ) = ( 1. + CFFL * ( PSTAR( KS ) /        1376
1377      96           .                          PPL( KS ) - 1. ) ) * WLESQ( KS ) 1377
1378      97                WLEFT( KS ) = SQRT( WLEFS( KS ) )                  1378
1379      98                ZLEFT( KS ) = 2. * WLEFT( KS ) * WLEFS( KS ) /     1379
1380      99           .                        ( WLESQ( KS ) + WLEFS( KS ) ) 1380
1381     100                USTL( KS )  = UUL( KS ) -                          1381
1382     101           .              ( PSTAR( KS ) - PPL( KS ) ) / WLEFT( KS ) 1382
1383     102     150  CONTINUE                                                  1383
1384     103  C                                                                1384
1385     104           DO 152 KS = 1 , NOFVES( INS )                           1385
1386     105                CFFR = ( GGR( KS ) + 1. ) / ( 2. * GGR( KS ) )     1386
1387     106                WRIFS( KS ) = ( 1. + CFFR * ( PSTAR( KS ) /        1387
1388     107           .                          PPR( KS ) - 1. ) ) * WRISQ( KS ) 1388
1389     108                WRIGT( KS ) = SQRT( WRIFS( KS ) )                  1389
1390     109                ZRIGT( KS ) = 2. * WRIGT( KS ) * WRIFS( KS ) /     1390
1391     110           .                        ( WRISQ( KS ) + WRIFS( KS ) ) 1391
1392     111                USTR( KS )  = UUR( KS ) +                          1392
1393     112           .              ( PSTAR( KS ) - PPR( KS ) ) / WRIGT( KS ) 1393
1394     113     152  CONTINUE                                                  1394
1395     114  C                                                                1395
1396     115           DO 160 KS = 1 , NOFVES( INS )                           1396
1397     116                DPST( KS )  = ZLEFT( KS ) * ZRIGT( KS ) *          1397
1398     117           .              ( USTR( KS ) - USTL( KS ) ) /            1398
1399     118           .              ( ZLEFT( KS ) + ZRIGT( KS ) )            1399
1400     119                PSTAR( KS ) = PSTAR( KS ) - DPST( KS )             1400
1401     120                PSTAR( KS ) = AMAX1( PSTAR( KS ) , PSML( KS ) )    1401
1402     121       160      CONTINUE                                           1402
1403     122  C                                                                1403
1404     123       140      CONTINUE                                           1404
1405     124  C                                                                1405
1406     125  C --- FORM FINAL SOLUTIONS --------------------------------- 1406
1407     126  C                                                                1407
1408     127           DO 170 KS = 1 , NOFVES( INS )                           1408
1409     128               CFFL = ( GGL( KS ) + 1. ) / ( 2. * GGL( KS ) )      1409
1410     129               WLEFT( KS ) = SQRT( WLESQ( KS ) * ( 1. +            1410
1411     130           .                 CFFL * ( PSTAR( KS ) / PPL( KS ) - 1. ) ) ) 1411
1412     131     170  CONTINUE                                                  1412
1413     132  C                                                                1413
1414     133           DO 172 KS = 1 , NOFVES( INS )                           1414
1415     134               CFFR = ( GGR( KS ) + 1. ) / ( 2. * GGR( KS ) )      1415
1416     135               WRIGT( KS ) = SQRT( WRISQ( KS ) * ( 1. +            1416
1417     136           .                 CFFR * ( PSTAR( KS ) / PPR( KS ) - 1. ) ) ) 1417
1418     137     172  CONTINUE                                                  1418
1419     138  C                                                                1419
1420     139           DO 180 KS = 1 , NOFVES( INS )                           1420
1421     140               USTAR( KS ) = ( PPL( KS ) - PPR( KS ) +             1421
1422     141           .                   WLEFT( KS ) * UUL( KS ) +           1422
1423     142           .                   WRIGT( KS ) * UUR( KS ) ) /         1423
1424     143           .                 ( WLEFT( KS ) + WRIGT( KS ) )         1424
1425     144     180  CONTINUE                                                  1425
1426     145  C                                                                1426
1427     146           DO 190 KS = 1 , NOFVES( INS )                           1427
1428     147  C                                                                1428
1429     148  C --- BEGIN PROCEDURE TO OBTAIN FLUXES FROM REIMANN FORMALISM -- 1429
```

```
1430     149  C                                                                  1430
1431     150            IF( USTAR( KS ) . LE . 0.0 ) THEN                        1431
1432     151  C                                                                  1432
1433     152              RO( KS ) = RRR( KS )                                   1433
1434     153              PO( KS ) = PPR( KS )                                   1434
1435     154              UO( KS ) = UUR( KS )                                   1435
1436     155              CO( KS ) = SQRT( HRGG * PPR( KS ) / RRR( KS ) )        1436
1437     156              WO( KS ) = WRIGT( KS )                                 1437
1438     157              GO( KS ) = GGR( KS )                                   1438
1439     158              ISN( KS ) = 1                                          1439
1440     159  C                                                                  1440
1441     160              ENRGYI( KS ) = EER( KS )                               1441
1442     161              ANRGYI( KS ) = AAR( KS )                               1442
1443     162              VGDNV( KS ) = VVR( KS )                                1443
1444     163              WGDNV( KS ) = WWR( KS )                                1444
1445     164  C                                                                  1445
1446     165            ELSE                                                     1446
1447     166  C                                                                  1447
1448     167              RO( KS ) = RRL( KS )                                   1448
1449     168              PO( KS ) = PPL( KS )                                   1449
1450     169              UO( KS ) = UUL( KS )                                   1450
1451     170              CO( KS ) = SQRT( HRGG * PPL( KS ) / RRL( KS ) )        1451
1452     171              WO( KS ) = WLEFT( KS )                                 1452
1453     172              GO( KS ) = GGL( KS )                                   1453
1454     173              ISN( KS ) = - 1                                        1454
1455     174  C                                                                  1455
1456     175              ENRGYI( KS ) = EEL( KS )                               1456
1457     176              ANRGYI( KS ) = AAL( KS )                               1457
1458     177              VGDNV( KS ) = VVL( KS )                                1458
1459     178              WGDNV( KS ) = WWL( KS )                                1459
1460     179            END IF                                                   1460
1461     180   190  CONTINUE                                                    1461
1462     181  C                                                                  1462
1463     182        DO 200 KS = 1 , NOFVES( INS )                               1463
1464     183            DELP( KS ) = PSTAR( KS ) - PO( KS )                     1464
1465     184            WSOP( KS ) = ISN( KS ) * UO( KS ) + WO( KS ) / RO( KS ) 1465
1466     185            WSOM( KS ) = ISN( KS ) * UO( KS ) + CO( KS )            1466
1467     186   200   CONTINUE                                                   1467
1468     187  C                                                                  1468
1469     188        DO 210 KS = 1 , NOFVES( INS )                               1469
1470     189          IF( DELP( KS ) . GT . 0. ) THEN                           1470
1471     190            WSOO( KS ) = WSOP( KS )                                 1471
1472     191          ELSE                                                      1472
1473     192            WSOO( KS ) = WSOM( KS )                                 1473
1474     193          END IF                                                    1474
1475     194   210  CONTINUE                                                    1475
1476     195  C                                                                  1476
1477     196        DO 220 KS = 1 , NOFVES( INS )                               1477
1478     197  C                                                                  1478
1479     198  C --- USE OUTER STATE SOLUTION ------------------------------     1479
1480     199  C                                                                  1480
1481     200            PGDNV( KS ) = PO( KS )                                  1481
1482     201            UGDNV( KS ) = UO( KS )                                  1482
1483     202            CGDNV( KS ) = CO( KS )                                  1483
1484     203            RGDNV( KS ) = RO( KS )                                  1484
1485     204   220  CONTINUE                                                    1485
1486     205  C                                                                  1486
1487     206  C --- COMPUTE STARRED VALUES ---------------------------------     1487
1488     207  C                                                                  1488
1489     208        DO 230 KS = 1 , NOFVES( INS )                               1489
1490     209            RSTAR( KS ) = 1. / ( 1. / RO( KS ) - DELP( KS ) /       1490
1491     210       .                                ( WO( KS ) * WO( KS ) ) )    1491
1492     211            CSTAR( KS ) = SQRT( GO( KS ) * PSTAR( KS ) / RSTAR( KS ) ) 1492
1493     212            WSOM( KS )  = ISN( KS ) * USTAR( KS ) + CSTAR( KS )     1493
1494     213   230  CONTINUE                                                    1494
1495     214  C                                                                  1495
1496     215        DO 240 KS = 1 , NOFVES( INS )                               1496
1497     216          IF( DELP( KS ) . GT . 0. ) THEN                           1497
1498     217            SPIN( KS ) = WSOP( KS )                                 1498
1499     218          ELSE                                                      1499
1500     219            SPIN( KS ) = WSOM( KS )                                 1500
1501     220          END IF                                                    1501
1502     221   240  CONTINUE                                                    1502
1503     222  C                                                                  1503
```

```
1504     223         DO 250 KS = 1 , NOFVES( INS )                                  1504
1505     224   C                                                                    1505
1506     225         IF( WSOO( KS ) . GE . 0. ) THEN                                1506
1507     226             IF( SPIN( KS ) . GE . 0. ) THEN                            1507
1508     227   C                                                                    1508
1509     228   C --- USE THE STARRED STATE RESULTS --------------------------       1509
1510     229   C                                                                    1510
1511     230                             RGDNV( KS ) = RSTAR( KS )                  1511
1512     231                             UGDNV( KS ) = USTAR( KS )                  1512
1513     232                             CGDNV( KS ) = CSTAR( KS )                  1513
1514     233                             PGDNV( KS ) = PSTAR( KS )                  1514
1515     234             ELSE                                                       1515
1516     235   C                                                                    1516
1517     236   C --- EVALUATE THE INSIDE RAREFACTION WAVE --------------------      1517
1518     237   C                                                                    1518
1519     238             CGDNV( KS ) = ( CSTAR( KS ) * 2. -                         1519
1520     239        .                    ISN( KS ) * USTAR( KS ) * ( GO( KS ) - 1. ) )  1520
1521     240        .                                          / ( GO( KS ) + 1. )  1521
1522     241             UGDNV( KS ) = - ISN( KS ) * CGDNV( KS )                    1522
1523     242             RGDNV( KS ) = ( CGDNV( KS ) / CO( KS ) ) **                1523
1524     243        .                  ( 2. / ( GO( KS ) - 1. ) ) * RO( KS )       1524
1525     244             PGDNV( KS ) = CGDNV( KS ) * CGDNV( KS ) * RGDNV( KS ) /    1525
1526     245        .                                                  GO( KS )     1526
1527     246   C                                                                    1527
1528     247             END IF                                                     1528
1529     248   C                                                                    1529
1530     249         END IF                                                         1530
1531     250    250  CONTINUE                                                      1531
1532     251   C                                                                    1532
1533     252         DO 260 KS = 1 , NOFVES( INS )                                  1533
1534     253             IS = KS + NS1 - 1                                          1534
1535     254             RR( IS ) = RGDNV( KS )                                     1535
1536     255             PR( IS ) = PGDNV( KS )                                     1536
1537     256    260  CONTINUE                                                      1537
1538     257   C                                                                    1538
1539     258         NS1 = NS2 + 1                                                  1539
1540     259         NS2 = NS2 + NOFVES( INS + 1 )                                  1540
1541     260    110  CONTINUE                                                      1541
1542     261   C                                                                    1542
1543     262         RETURN                                                         1543
1544     263         END                                                            1544
1545     264   C                                                                    1545
```

Thu Jul 1 14:17:00 1993 threed.f SUBROUTINE KYDRFL

```
1546       1         SUBROUTINE KYDRFL                                            1546
1547       2   C                                                                  1547
1548       3   C-------------------------------------------------------------I    1548
1549       4   C                                                             I    1549
1550       5   C      KYDRFL IS A 2 DIMENSIONAL RIEMANN SOLVER THAT INTEGRATES I    1550
1551       6   C             FLUXES ACROSS NORMAL INTERFACES TO UPDATE VERTICES I  1551
1552       7   C             VARIABLES .                                     I    1552
1553       8   C                                                             I    1553
1554       9   C-------------------------------------------------------------I    1554
1555      10   C                                                                  1555
1556      11         include     'dmsh00.h'                                       1556
1557      12         include     'dhydm0.h'                                       1557
1558      13         include     'dphsm0.h'                                       1558
1559      14         include     'dmtrl0.h'                                       1559
1560      15   C                                                                  1560
1561      16         REAL DELP(128),WSOP(128),WSOM(128),WSOO(128),                1561
1562      17        .     RSTAR(128),CSTAR(128),PMAX(128),PMIN(128)               1562
1563      18         REAL RRIGHT(128),URIGHT(128),VRIGHT(128),PRIGHT(128)         1563
1564      19         REAL RLEFTT(128),ULEFTT(128),VLEFTT(128),PLEFTT(128)         1564
1565      20         INTEGER NOFVEP(128)                                          1565
1566      21   C                                                                  1566
1567      22   C --- FETCH HYDRO QUANTITIES ----------------------------------    1567
1568      23   C                                                                  1568
1569      24         DO 120 KS = 1 , NPRTCL                                       1569
1570      25             IS = IJKPRT( KS )                                        1570
1571      26             ICL = JS( 7 , IS )                                       1571
1572      27             IBC = JS( 9 , IS )                                       1572
1573      28   C                                                                  1573
1574      29             RRL( KS ) = HYDV( ICL , 1 )                              1574
```

```
1575      30            UUL( KS ) = HYDV( ICL , 2 ) * XN( IS ) +                  1575
1576      31           .            HYDV( ICL , 3 ) * YN( IS ) +                  1576
1577      32           .            HYDV( ICL , 4 ) * ZN( IS )                    1577
1578      33            VVL( KS ) = HYDV( ICL , 2 ) * XP( IS ) +                  1578
1579      34           .            HYDV( ICL , 3 ) * YP( IS ) +                  1579
1580      35           .            HYDV( ICL , 4 ) * ZP( IS )                    1580
1581      36            WWL( KS ) = HYDV( ICL , 2 ) * XT( IS ) +                  1581
1582      37           .            HYDV( ICL , 3 ) * YT( IS ) +                  1582
1583      38           .            HYDV( ICL , 4 ) * ZT( IS )                    1583
1584      39            PPL( KS ) = HYDV( ICL , 5 )                               1584
1585      40            AAL( KS ) = HYDV( ICL , 6 )                               1585
1586      41            EEL( KS ) = HYDV( ICL , 8 )                               1586
1587      42            GGL( KS ) = HYDV( ICL , 7 )                               1587
1588      43  C                                                                   1588
1589      44            RRR( KS ) = RRL( KS )                                     1589
1590      45            IF( IBC . EQ . 0 ) THEN                                   1590
1591      46            UUR( KS ) = UUL( KS )                                     1591
1592      47            ELSE                                                      1592
1593      48            UUR( KS ) = - UUL( KS )                                   1593
1594      49            END IF                                                    1594
1595      50            VVR( KS ) = VVL( KS )                                     1595
1596      51            WWR( KS ) = WWL( KS )                                     1596
1597      52            PPR( KS ) = PPL( KS )                                     1597
1598      53            AAR( KS ) = AAL( KS )                                     1598
1599      54            EER( KS ) = EEL( KS )                                     1599
1600      55            GGR( KS ) = GGL( KS )                                     1600
1601      56  C                                                                   1601
1602      57   120   CONTINUE                                                     1602
1603      58  C                                                                   1603
1604      59          DO 130 KS = 1 , NPRTCL                                     1604
1605      60  C                                                                   1605
1606      61  C --- THIS SECTION OF CODE SOLVES FOR "PSTAR" AND "USTAR" IN        1606
1607      62  C     THE RIEMANN PROBLEM USING NEWTON'S METHOD.                    1607
1608      63  C                                                                   1608
1609      64            WLEFT( KS ) = SQRT( GGL( KS ) * PPL( KS ) * RRL( KS ) )   1609
1610      65            WRIGT( KS ) = SQRT( GGR( KS ) * PPR( KS ) * RRR( KS ) )   1610
1611      66            WLESQ( KS ) = WLEFT( KS ) * WLEFT( KS )                   1611
1612      67            WRISQ( KS ) = WRIGT( KS ) * WRIGT( KS )                   1612
1613      68  C                                                                   1613
1614      69            PMIN( KS ) = AMIN1( PPL( KS ) , PPR( KS ) )               1614
1615      70            PSML( KS ) = HRSM * PMIN( KS )                            1615
1616      71  C                                                                   1616
1617      72  C --- FORM THE STARTING GUESS FOR THE SOLUTION' ------------------   1617
1618      73  C                                                                   1618
1619      74            PSTAR( KS ) = ( WLEFT( KS ) * PPR( KS ) +                 1619
1620      75           .                WRIGT( KS ) * PPL( KS ) -                 1620
1621      76           .                WLEFT( KS ) * WRIGT( KS ) *               1621
1622      77           .              ( UUR( KS ) - UUL( KS ) ) ) /               1622
1623      78           .              ( WLEFT( KS ) + WRIGT( KS ) )               1623
1624      79            PSTAR( KS ) = AMAX1( PSTAR( KS ) , PSML( KS ) )           1624
1625      80   130   CONTINUE                                                     1625
1626      81  C                                                                   1626
1627      82            DO 140 I = 1 , IHRN                                       1627
1628      83  C                                                                   1628
1629      84  C --- BEGIN THE NEWTON ITERATION --------------------------------   1629
1630      85  C                                                                   1630
1631      86          DO 150 KS = 1 , NPRTCL                                     1631
1632      87               CFFL = ( GGL( KS ) + 1. ) / ( 2. * GGL( KS ) )        1632
1633      88               WLEFS( KS ) = ( 1. + CFFL * ( PSTAR( KS ) /           1633
1634      89           .                              PPL( KS ) - 1. ) ) * WLESQ( KS )  1634
1635      90               WLEFT( KS ) = SQRT( WLEFS( KS ) )                     1635
1636      91               ZLEFT( KS ) = 2. * WLEFT( KS ) * WLEFS( KS ) /        1636
1637      92           .                            ( WLESQ( KS ) + WLEFS( KS ) )  1637
1638      93               USTL( KS )  = UUL( KS ) -                             1638
1639      94           .               ( PSTAR( KS ) - PPL( KS ) ) / WLEFT( KS )  1639
1640      95   150   CONTINUE                                                     1640
1641      96  C                                                                   1641
1642      97          DO 152 KS = 1 , NPRTCL                                     1642
1643      98               CFFR = ( GGR( KS ) + 1. ) / ( 2. * GGR( KS ) )        1643
1644      99               WRIFS( KS ) = ( 1. + CFFR * ( PSTAR( KS ) /           1644
1645     100           .                              PPR( KS ) - 1. ) ) * WRISQ( KS )  1645
1646     101               WRIGT( KS ) = SQRT( WRIFS( KS ) )                     1646
1647     102               ZRIGT( KS ) = 2. * WRIGT( KS ) * WRIFS( KS ) /        1647
1648     103           .                            ( WRISQ( KS ) + WRIFS( KS ) )  1648
```

```
1649     104              USTR( KS )  = UUR( KS ) +                                  1649
1650     105             .                ( PSTAR( KS ) - PPR( KS ) ) / WRIGT( KS )  1650
1651     106      152  CONTINUE                                                       1651
1652     107      C                                                                  1652
1653     108           DO 160 KS = 1 , NPRTCL                                        1653
1654     109              DPST( KS )  = ZLEFT( KS ) * ZRIGT( KS ) *                  1654
1655     110             .              ( USTR( KS ) - USTL( KS ) ) /                1655
1656     111             .              ( ZLEFT( KS ) + ZRIGT( KS ) )                1656
1657     112              PSTAR( KS ) = PSTAR( KS ) - DPST( KS )                     1657
1658     113              PSTAR( KS ) = AMAX1( PSTAR( KS ) , PSML( KS ) )            1658
1659     114        160   CONTINUE                                                   1659
1660     115      C                                                                  1660
1661     116        140   CONTINUE                                                   1661
1662     117      C                                                                  1662
1663     118      C --- FORM FINAL SOLUTIONS ---------------------------------      1663
1664     119      C                                                                  1664
1665     120           DO 170 KS = 1 , NPRTCL                                        1665
1666     121              CFFL = ( GGL( KS ) + 1. ) / ( 2. * GGL( KS ) )             1666
1667     122              WLEFT( KS ) = SQRT( WLESQ( KS ) * ( 1. +                   1667
1668     123             .                  CFFL * ( PSTAR( KS ) / PPL( KS ) - 1. ) ) )  1668
1669     124      170  CONTINUE                                                       1669
1670     125      C                                                                  1670
1671     126           DO 172 KS = 1 , NPRTCL                                        1671
1672     127              CFFR = ( GGR( KS ) + 1. ) / ( 2. * GGR( KS ) )             1672
1673     128              WRIGT( KS ) = SQRT( WRISQ( KS ) * ( 1. +                   1673
1674     129             .                  CFFR * ( PSTAR( KS ) / PPR( KS ) - 1. ) ) )  1674
1675     130      172  CONTINUE                                                       1675
1676     131      C                                                                  1676
1677     132           DO 180 KS = 1 , NPRTCL                                        1677
1678     133              USTAR( KS ) = ( PPL( KS ) - PPR( KS ) +                    1678
1679     134             .                WLEFT( KS ) * UUL( KS ) +                  1679
1680     135             .                WRIGT( KS ) * UUR( KS ) ) /                1680
1681     136             .              ( WLEFT( KS ) + WRIGT( KS ) )                1681
1682     137      180  CONTINUE                                                       1682
1683     138      C                                                                  1683
1684     139           DO 190 KS = 1 , NPRTCL                                        1684
1685     140      C                                                                  1685
1686     141      C --- BEGIN PROCEDURE TO OBTAIN FLUXES FROM REIMANN FORMALISM --    1686
1687     142      C                                                                  1687
1688     143              IF( USTAR( KS ) . LE . 0.0 ) THEN                          1688
1689     144      C                                                                  1689
1690     145             .   RO( KS ) = RRR( KS )                                    1690
1691     146                 PO( KS ) = PPR( KS )                                   1691
1692     147                 UO( KS ) = UUR( KS )                                   1692
1693     148                 CO( KS ) = SQRT( HRGG * PPR( KS ) / RRR( KS ) )        1693
1694     149                 WO( KS ) = WRIGT( KS )                                 1694
1695     150                 GO( KS ) = GGR( KS )                                   1695
1696     151                 ISN( KS ) = 1                                          1696
1697     152      C                                                                  1697
1698     153                 VGDNV( KS ) = VVR( KS )                                1698
1699     154                 WGDNV( KS ) = WWR( KS )                                1699
1700     155      C                                                                  1700
1701     156              ELSE                                                       1701
1702     157      C                                                                  1702
1703     158                 RO( KS ) = RRL( KS )                                   1703
1704     159                 PO( KS ) = PPL( KS )                                   1704
1705     160                 UO( KS ) = UUL( KS )                                   1705
1706     161                 CO( KS ) = SQRT( HRGG * PPL( KS ) / RRL( KS ) )        1706
1707     162                 WO( KS ) = WLEFT( KS )                                 1707
1708     163                 GO( KS ) = GGL( KS )                                   1708
1709     164                 ISN( KS ) = - 1                                        1709
1710     165      C                                                                  1710
1711     166                 VGDNV( KS ) = VVL( KS )                                1711
1712     167                 WGDNV( KS ) = WWL( KS )                                1712
1713     168              END IF                                                    1713
1714     169      190  CONTINUE                                                       1714
1715     170      C                                                                  1715
1716     171           DO 200 KS = 1 , NPRTCL                                        1716
1717     172              DELP( KS ) = PSTAR( KS ) - PO( KS )                        1717
1718     173              WSOP( KS ) = ISN( KS ) * UO( KS ) + WO( KS ) / RO( KS )    1718
1719     174              WSOM( KS ) = ISN( KS ) * UO( KS ) + CO( KS )               1719
1720     175      200   CONTINUE                                                     1720
1721     176      C                                                                  1721
1722     177           DO 210 KS = 1 , NPRTCL                                        1722
```

```
1723    178          IF( DELP( KS ) . GT . 0. ) THEN                                  1723
1724    179            WSOO( KS ) = WSOP( KS )                                        1724
1725    180          ELSE                                                             1725
1726    181            WSOO( KS ) = WSOM( KS )                                        1726
1727    182          END IF                                                           1727
1728    183   210  CONTINUE                                                          1728
1729    184   C                                                                      1729
1730    185        DO 220 KS = 1 , NPRTCL                                           1730
1731    186   C                                                                      1731
1732    187   C --- USE OUTER STATE SOLUTION ----------------------------           1732
1733    188   C                                                                      1733
1734    189            PGDNV( KS ) = PO( KS )                                       1734
1735    190            UGDNV( KS ) = UO( KS )                                       1735
1736    191            CGDNV( KS ) = CO( KS )                                       1736
1737    192            RGDNV( KS ) = RO( KS )                                       1737
1738    193   220  CONTINUE                                                          1738
1739    194   C                                                                      1739
1740    195   C --- COMPUTE STARRED VALUES ------------------------------           1740
1741    196   C                                                                      1741
1742    197        DO 230 KS = 1 , NPRTCL                                           1742
1743    198            RSTAR( KS ) = 1. / ( 1. / RO( KS ) - DELP( KS ) /            1743
1744    199       .                          ( WO( KS ) * WO( KS ) ) )              1744
1745    200            CSTAR( KS ) = SQRT( GO( KS ) * PSTAR( KS ) / RSTAR( KS ) )   1745
1746    201            WSOM( KS )  = ISN( KS ) * USTAR( KS ) + CSTAR( KS )          1746
1747    202   230  CONTINUE                                                          1747
1748    203   C                                                                      1748
1749    204        DO 240 KS = 1 , NPRTCL                                           1749
1750    205          IF( DELP( KS ) . GT . 0. ) THEN                                1750
1751    206            SPIN( KS ) = WSOP( KS )                                      1751
1752    207          ELSE                                                           1752
1753    208            SPIN( KS ) = WSOM( KS )                                      1753
1754    209          END IF                                                         1754
1755    210   240  CONTINUE                                                          1755
1756    211   C                                                                      1756
1757    212        DO 250 KS = 1 , NPRTCL                                           1757
1758    213   C                                                                      1758
1759    214        IF( WSOO( KS ) . GE . 0. ) THEN                                  1759
1760    215            IF( SPIN( KS ) . GE . 0. ) THEN                              1760
1761    216   C                                                                      1761
1762    217   C --- USE THE STARRED STATE RESULTS ----------------------------      1762
1763    218   C                                                                      1763
1764    219                              RGDNV( KS ) = RSTAR( KS )                   1764
1765    220                              UGDNV( KS ) = USTAR( KS )                   1765
1766    221                              CGDNV( KS ) = CSTAR( KS )                   1766
1767    222                              PGDNV( KS ) = PSTAR( KS )                   1767
1768    223            ELSE                                                         1768
1769    224   C                                                                      1769
1770    225   C --- EVALUATE THE INSIDE RAREFACTION WAVE ---------------------      1770
1771    226   C                                                                      1771
1772    227            CGDNV( KS ) = ( CSTAR( KS ) * 2. -                           1772
1773    228       .                    ISN( KS ) * USTAR( KS ) * ( GO( KS ) - 1. ) )1773
1774    229       .                                          / ( GO( KS ) + 1. )    1774
1775    230            UGDNV( KS ) = - ISN( KS ) * CGDNV( KS )                      1775
1776    231            RGDNV( KS ) = ( CGDNV( KS ) / CO( KS ) ) **                  1776
1777    232       .                  ( 2. / ( GO( KS ) - 1. ) ) * RO( KS )        1777
1778    233            PGDNV( KS ) = CGDNV( KS ) * CGDNV( KS ) * RGDNV( KS ) /      1778
1779    234       .                                                  GO( KS )      1779
1780    235   C                                                                      1780
1781    236            END IF                                                       1781
1782    237   C                                                                      1782
1783    238        END IF                                                           1783
1784    239   250  CONTINUE                                                          1784
1785    240   C                                                                      1785
1786    241        DO 260 KS = 1 , NPRTCL                                           1786
1787    242            RR( KS ) = RGDNV( KS )                                       1787
1788    243            PR( KS ) = PGDNV( KS )                                       1788
1789    244   260  CONTINUE                                                          1789
1790    245   C                                                                      1790
1791    246        RETURN                                                           1791
1792    247        END                                                              1792
1793    248   C                                                                      1793
```

```
      SUBROUTINE HYDRMN
C
C-------------------------------------------------------------------I
C                                                                   I
C     HYDRMN IS A 2 DIMENSIONAL RIEMANN SOLVER THAT CALCULATES      I
C           FLUXES ACROSS NORMAL INTERFACES.                        I
C           IT IS CONFIGURED TO WORK IN EITHER TWO OR THREE         I
C           DIMENSIONAL SITUATIONS. THE HYDRODYNAMIC QUANTITIES     I
C           CAN BE SIDE OR VERTEX CENTERED FOR 2-D AND CELL OR      I
C           VERTEX CENTERED FOR 3-D. THE SPECIFIC USE IS BASED      I
C           ON THE CONTENTS OF "OPTHYD".                            I
C                                                                   I
C                                                                   I
C-------------------------------------------------------------------I
C
C     THE USE OF THE HYDRO VARIABLES IS AS FOLLOWS:
C
C     +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C     +                                                           +
C     +     HYDV(IV,IH) CONTAINS VERTEX CENTERED HYDRO-           +
C     +     DYNAMIC QUANTITIES. IT IS USED WITH ALL CASES.        +
C     +                                                           +
C     +     HYDE(IH,IE) CONTAINS EDGE   CENTERED HYDRO-           +
C     +     DYNAMIC FLUX QUANTITIES WITH ORIENTATION              +
C     +     DETERMINED BY THE "SIDE"  "VERTEX" OR "CELL  "        +
C     +     OPTIONS . IT IS USED FOR THE CASES WHERE              +
C     +     "OPTHYD" = "SIDE  2D" 2-D SIDE CENTERED               +
C     +              = "VERTEX2D" 2-D VERTEX CENTERED             +
C     +              = "VERTEX3D" 3-D VERTEX CENTERED             +
C     +                                                           +
C     +     HYDC(IC,IH) CONTAINS CELL   CENTERED HYDRO-           +
C     +     DYNAMIC QUANTITIES. IT IS USED FOR THE CASE           +
C     +     "OPTHYD" = "CELL  3D" 3-D CELL   CENTERED             +
C     +                                                           +
C     +                                                           +
C     +        IV   - VERTEX INDEX                                +
C     +        IS   - SIDE   INDEX                                +
C     +        IE   - EDGE   INDEX                                +
C     +        IC   - CELL   INDEX                                +
C     +        IH   - HYDRO  INDEX                                +
C     +                                                           +
C     +              1 = RO  DENSITY IN ***********               +
C     +              2 = UX  X VELOCITY ***********               +
C     +              3 = UY  Y VELOCITY ***********               +
C     +              4 = UZ  ************************             +
C     +              5 = PO  PRESSURE IN **********               +
C     +              6 = EN  ENERGY IN   **********               +
C     +                                                           +
C     +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C
      include     'dmsh00.h'
      include     'dhydm0.h'
      include     'dphsm0.h'
      include     'dmtrl0.h'
C
      REAL RRN(128),URN(128),VRN(128),WRN(128),EPN(128),
     .     ARN(128),XS2S(128),XSAR(128)
      REAL HYDVR(128),HYDVU(128),HYDVV(128),HYDVW(128),
     .     HYDVP(128)
      INTEGER NDUMMY1,NDUMMY2,NDUMMY3
      INTEGER IDUMMY(4),VDATA(2),FDATA(2)
      CHARACTER*31 VLABEL
      CHARACTER*32 FLABEL
      CHARACTER*6 CTRI, CTET
      INTEGER ISURF(400000)
C
      REAL CD1(4),CD2(4)
C
      NDUMMY1=1
      NDUMMY2=4
      NDUMMY3=0
      IDUMMY(1) = 0
      IDUMMY(2) = 0
      IDUMMY(3) = 0
```

```
      IDUMMY(4) = 0
      VDATA(1) = 1
      VDATA(2) = 1
      FDATA(1) = 1
      FDATA(2) = 4
      VLABEL=' pressure, new / m**2'
      FLABEL=' tets faces,'
      CTRI='  tri '
      CTET='  tet '
C      TLIMIT=TT
      TLIMIT=30.
C
       IJKNUM = 0
       IF( ICONP . EQ . 1 ) THEN
       REWIND 10
       REWIND 26
       READ (26,*) IJKNUM
       DO KKJ = 1 , IJKNUM
       READ (26,*) RO,(RRN(IK),IK=1,NPRTCL)
       WRITE (10,*) RO,(RRN(IK),IK=1,NPRTCL)
       END DO
       END IF
      DO 120 JT = 1 , NTIME
      IF(JT.GT.5) IEOS=0
C
        DO KK = 1 , 5
        DO IV = 1 , NV
        HNUM( IV , KK ) = 0.
        END DO
        END DO
      DO 140 ITT = 1 , NDUMP
C
C --- SELECT ORDER OF INTEGRATION ------------------------------------
C
      IF(IOPORD.EQ.1)THEN
         CALL FIRST
      ELSEIF(IOPORD.EQ.2)THEN
         CALL GRADNT
      ENDIF
C
      DTT = 1.E24
C
      CALL HYDRFL
C
      DTT = DTT * .4
      TT = TT + DTT
      PRINT *,JT,ITT,DTT,TT,NS
C
      NC1 = 1
      NC2 = NOFVEC( 1 )
      DO 110 INC = 1 , NVEEC
C
      DO 150 IC = NC1 , NC2
          KC = IC - NC1 + 1
          RRR( KC ) = HYDV( IC , 1 )
          UUR( KC ) = HYDV( IC , 2 )
          VVR( KC ) = HYDV( IC , 3 )
          WWR( KC ) = HYDV( IC , 4 )
          PPR( KC ) = HYDV( IC , 5 )
          AAR( KC ) = HYDV( IC , 6 )
C
          RRL( KC ) = HYDFLX( IC , 1 )
          UUL( KC ) = HYDFLX( IC , 2 )
          VVL( KC ) = HYDFLX( IC , 3 )
          WWL( KC ) = HYDFLX( IC , 4 )
          PPL( KC ) = HYDFLX( IC , 5 )
          AAL( KC ) = HYDFLX( IC , 6 )
C
          XS2S( KC ) = XC( 2 , IC )
          XSAR( KC ) = SVOLM( IC )
  150 CONTINUE
C
      DO 170 KC = 1 , NOFVEC( INC )
         IC = KC + NC1 - 1
```

```
1942     149          RRN( KC ) = RRR( KC )
1943     150          URN( KC ) = RRR( KC ) * UUR( KC )
1944     151          VRN( KC ) = RRR( KC ) * VVR( KC )
1945     152          WRN( KC ) = RRR( KC ) * WWR( KC )
1946     153          EPN( KC ) = HYDV( IC , 8 ) + .5 * RRR( KC ) *
1947     154         .                          ( UUR( KC ) * UUR( KC ) +
1948     155         .                            VVR( KC ) * VVR( KC ) +
1949     156         .                            WWR( KC ) * WWR( KC ) )
1950     157          ARN( KC ) = RRR( KC ) * AAR( KC )
1951     158    170   CONTINUE
1952     159    C --- COMPUTE THE SOURCE TERM FOR AXI SYMMETRY FLOW PROBLEM
1953     160    C --- IF THE FLOW IS NOT AXI SYMMETRY , COMMENT LOOP 160
1954     161    C
1955     162          DO 190 KC = 1 , NOFVEC( INC )
1956     163             IC = KC + NC1 - 1
1957     164          DTA = DTT * XSAR( KC )
1958     165    C
1959     166          RRLL = DTA * RRL( KC )
1960     167          UULL = DTA * UUL( KC )
1961     168          VVLL = DTA * VVL( KC )
1962     169          WWLL = DTA * WWL( KC )
1963     170          RRN( KC ) = RRN( KC ) - RRLL
1964     171    C
1965     172          URN( KC ) = URN( KC ) - UULL
1966     173    C
1967     174          VRN( KC ) = VRN( KC ) - VVLL
1968     175    C
1969     176          WRN( KC ) = WRN( KC ) - WWLL
1970     177    C
1971     178          PPLL = DTA * PPL( KC )
1972     179          EPN( KC ) = EPN( KC ) - PPLL
1973     180    C
1974     181          AALL = DTA * AAL( KC )
1975     182          ARN( KC ) = ARN( KC ) - AALL
1976     183    C
1977     184    190   CONTINUE
1978     185    C
1979     186          DO 195 IC = NC1 , NC2
1980     187             KC = IC - NC1 + 1
1981     188          HDUM           = 1. / RRN( KC )
1982     189          HYDV( IC , 1 ) = RRN( KC )
1983     190          HYDV( IC , 2 ) = URN( KC ) * HDUM
1984     191          HYDV( IC , 3 ) = VRN( KC ) * HDUM
1985     192          HYDV( IC , 4 ) = WRN( KC ) * HDUM
1986     193          HYDV( IC , 6 ) = ARN( KC ) * HDUM
1987     194    195   CONTINUE
1988     195    C
1989     196          DO 200 IC = NC1 , NC2
1990     197             KC = IC - NC1 + 1
1991     198          HYDV( IC , 8 ) = ( EPN( KC )  - .5 * HYDV( IC , 1 ) *
1992     199         .                   ( HYDV( IC , 2 ) * HYDV( IC , 2 ) +
1993     200         .                     HYDV( IC , 3 ) * HYDV( IC , 3 ) +
1994     201         .                     HYDV( IC , 4 ) * HYDV( IC , 4 ) ) )
1995     202    200   CONTINUE
1996     203    C
1997     204          IF( IEOS . EQ . 1 ) THEN
1998     205           TLIMIT = .9
1999     206           ITER = 6
2000     207           DO IC = NC1 , NC2
2001     208              KC = IC - NC1 + 1
2002     209    C
2003     210          NITER = 0
2004     211          IF( HYDV( IC , 6 ) . LE . .2 ) THEN
2005     212    C
2006     213          DST = HYDV( IC , 1 ) * GPERCC
2007     214          VOL = WMA * ( 1. - DST / FSA ) / DST / XGA
2008     215          EMEO = HYDV( IC , 8 ) / HYDV( IC , 1 ) * WMA / RGAS
2009     216    C
2010     217          IYY = ( EMEO - EMEOA( 3 ) ) / RANGEA + 1
2011     218          IYY = MAXO( 1 , MINO( IYY , 47 ) )
2012     219    C
2013     220          K = IYY + 2
2014     221          IYY = IYY
2015     222         . + INT( AMAX1( EMEO - EMEOA( K ) , 0.) / DYA( K ) )
```

```
2016  223        . - INT( AMAX1( EMEOA( K + 1 ) - EMEO , 0. ) / DYA( K ) )                2016
2017  224         IYY = MAXO( 1, MINO( IYY , 47 ) )                                       2017
2018  225   C                                                                             2018
2019  226         K1 = IYY + 2                                                            2019
2020  227         K2 = K1 + 1                                                             2020
2021  228         RT = ( EMEO - EMEOA( K1 ) ) / ( EMEOA( K2 ) - EMEOA( K1 ) )             2021
2022  229         T = TA( K1 ) + 100. * RT                                                2022
2023  230         CVM = CVMA( K1 ) + RT * ( CVMA( K2 ) - CVMA( K1 ) )                     2023
2024  231         ERS = 0.                                                                2024
2025  232   C                                                                             2025
2026  233         P = RGAS * T / VOL / GPERCC                                             2026
2027  234         RGAMM1 = CVM                                                            2027
2028  235         HYDV( IC , 7 ) = 1. / RGAMM1 + 1.                                       2028
2029  236         HYDV( IC , 5 ) = P                                                      2029
2030  237   C                                                                             2030
2031  238         ELSE                                                                    2031
2032  239   C                                                                             2032
2033  240         DST = HYDV( IC , 1 ) * GPERCC                                           2033
2034  241         VOL = WMX * ( 1. - DST / FSX ) / DST / XGX                              2034
2035  242         EMEO = HYDV( IC , 8 ) / HYDV( IC , 1 ) * WMX / RGAS                     2035
2036  243   C                                                                             2036
2037  244         IYY = ( EMEO - EMEOX( 3 ) ) / RANGEX + 1                                2037
2038  245         IYY = MAXO( 1 , MINO( IYY , 47 ) )                                      2038
2039  246   C                                                                             2039
2040  247         K = IYY + 2                                                             2040
2041  248         IYY = IYY                                                               2041
2042  249        . + INT( AMAX1( EMEO - EMEOX( K ) , 0.) / DYX( K ) )                     2042
2043  250        . - INT( AMAX1( EMEOX( K + 1 ) - EMEO , 0. ) / DYX( K ) )                2043
2044  251         IYY = MAXO( 1, MINO( IYY , 47 ) )                                       2044
2045  252   C                                                                             2045
2046  253         K1 = IYY + 2                                                            2046
2047  254         K2 = K1 + 1                                                             2047
2048  255         RT = ( EMEO - EMEOX( K1 ) ) / ( EMEOX( K2 ) - EMEOX( K1 ) )             2048
2049  256         T = TX( K1 ) + 100. * RT                                                2049
2050  257         CVM = CVMX( K1 ) + RT * ( CVMX( K2 ) - CVMX( K1 ) )                     2050
2051  258         ERS = 0.                                                                2051
2052  259   C                                                                             2052
2053  260   10    CONTINUE                                                                2053
2054  261         P = RGAS * T / VOL / GPERCC                                             2054
2055  262         RGAMM1 = CVM                                                            2055
2056  263   C                                                                             2056
2057  264         X = COVX / VOL / ( ( T + THETAX ) ** ALFAX )                            2057
2058  265         Z = X * EXP( BETAX * X )                                                2058
2059  266         X = 1. + BETAX * X                                                      2059
2060  267         RT = ALFAX * T / ( T + THETAX )                                         2060
2061  268         ERS = ERS + RT * Z * T                                                  2061
2062  269   C                                                                             2062
2063  270         IF ( ITER .EQ. NITER ) GO TO 20                                         2063
2064  271   C                                                                             2064
2065  272         CVM = CVM * XGX + SCVX                                                  2065
2066  273        *            + RT * Z * ( 2. - RT / ALFAX - RT * X )                     2066
2067  274         T = T - AMIN1( ERS / CVM , TLIMIT * T )                                 2067
2068  275   C                                                                             2068
2069  276         NITER = NITER + 1                                                       2069
2070  277   C                                                                             2070
2071  278         RT = 0.01 * T                                                           2071
2072  279         K1 = RT                                                                 2072
2073  280         K1 = MINO ( K1, 49 )                                                    2073
2074  281         K1 = MAXO ( K1, 3  )                                                    2074
2075  282         K2 = K1 + 1                                                             2075
2076  283         RT = RT - K1                                                            2076
2077  284         CVM = CVMX(K1) + RT * ( CVMX( K2 ) - CVMX( K1 ) )                       2077
2078  285         ERS = EMEOX( K1 ) + RT * ( EMEOX( K2 ) - EMEOX( K1 ) )                  2078
2079  286         ERS = ERS - EMEO                                                        2079
2080  287   C                                                                             2080
2081  288         GO TO 10                                                                2081
2082  289   C                                                                             2082
2083  290   20    CONTINUE                                                                2083
2084  291         P = P * ( 1. + Z )                                                      2084
2085  292         RGAMM1 = ( RGAMM1 +                                                     2085
2086  293        *           RT * Z * ( 2. - RT / ALFAX - RT * X ) ) / ( 1. + Z )         2086
2087  294         X = X * Z / ( 1. + Z )                                                  2087
2088  295         RGAMM1 = RGAMM1 / ( ( 1. - RT * X ) ** 2 + X * RGAMM1 )                 2088
2089  296         ERS = ERS / EMEO                                                        2089
```

```
2090    297          HYDV( IC , 7 ) = 1. / RGAMM1 + 1.                                  2090
2091    298          HYDV( IC , 5 ) = P                                                 2091
2092    299          END IF                                                             2092
2093    300          END DO                                                             2093
2094    301    C                                                                        2094
2095    302          ELSE                                                               2095
2096    303    C                                                                        2096
2097    304           DO IC = NC1 , NC2                                                 2097
2098    305           HYDV( IC , 5 ) = HYDV( IC , 8 ) * ( HYDV( IC , 7 ) - 1. )         2098
2099    306          END DO                                                             2099
2100    307          END IF                                                             2100
2101    308    C                                                                        2101
2102    309          NC1 = NC2 + 1                                                      2102
2103    310          NC2 = NC2 + NOFVEC( INC + 1 )                                      2103
2104    311     110   CONTINUE                                                         2104
2105    312    C                                                                        2105
2106    313           IF( NPRTCL . NE . 0 ) CALL KYDRFL                                 2106
2107    314           IJKNUM = IJKNUM + 1                                               2107
2108    315           WRITE(10,*) TT,(PR(KKJJ),KKJJ=1,NPRTCL)                           2108
2109    316     140   CONTINUE                                                         2109
2110    317    C                                                                        2110
2111    318           PMAX = -10000000.                                                 2111
2112    319           DO 415 IC = 1 , NC                                                2112
2113    320           IV1 = JC( 1 , IC )                                                2113
2114    321           IV2 = JC( 2 , IC )                                                2114
2115    322           IV3 = JC( 3 , IC )                                                2115
2116    323           IV4 = JC( 4 , IC )                                                2116
2117    324           HNUMM = HYDV( IC , 5 )                                            2117
2118    325           HNUMN = XC( 4 , IC )                                              2118
2119    326           HNUM( IV1 , 5 ) = HNUM( IV1 , 5 ) + HNUMM * HNUMN                 2119
2120    327           HNUM( IV1 , 1 ) = HNUM( IV1 , 1 ) + HNUMN                         2120
2121    328           HNUM( IV2 , 5 ) = HNUM( IV2 , 5 ) + HNUMM * HNUMN                 2121
2122    329           HNUM( IV2 , 1 ) = HNUM( IV2 , 1 ) + HNUMN                         2122
2123    330           HNUM( IV3 , 5 ) = HNUM( IV3 , 5 ) + HNUMM * HNUMN                 2123
2124    331           HNUM( IV3 , 1 ) = HNUM( IV3 , 1 ) + HNUMN                         2124
2125    332           HNUM( IV4 , 5 ) = HNUM( IV4 , 5 ) + HNUMM * HNUMN                 2125
2126    333           HNUM( IV4 , 1 ) = HNUM( IV4 , 1 ) + HNUMN                         2126
2127    334    415    CONTINUE                                                          2127
2128    335           DO IV = 1 , NV                                                    2128
2129    336           HNUM( IV , 5 ) = HNUM( IV , 5 ) / HNUM( IV , 1 )                  2129
2130    337           END DO                                                            2130
2131    338           DO IV = 1 , NV                                                    2131
2132    339           IF( HNUM( IV , 5 ) .GT. PMAX ) PMAX = HNUM( IV , 5 )              2132
2133    340           END DO                                                            2133
2134    341           PRINT * , PMAX                                                    2134
2135    342    C                                                                        2135
2136    343           ISNS = 0                                                          2136
2137    344           DO 300 IS = 1 , NS                                                2137
2138    345              IF(JS(9,IS).EQ.6.AND.XS(2,IS).LT.1.9649) THEN                  2138
2139    346              ISNS=ISNS+1                                                    2139
2140    347              ISURF(ISNS)=IS                                                 2140
2141    348              END IF                                                         2141
2142    349    300    CONTINUE                                                          2142
2143    350           print*,ISNS                                                       2143
2144    351    C                                                                        2144
2145    352    C       STEVE FORMAT                                                     2145
2146    353    C                                                                        2146
2147    354           DO 312 IV = 1 , NV                                                2147
2148    355           WRITE(17,1001) IV,(XV(KK,IV),KK=1,3)                              2148
2149    356    1001   FORMAT('n,',I5,',',2(F10.5,','),F10.5)                           2149
2150    357    312    CONTINUE                                                          2150
2151    358    C                                                                        2151
2152    359           DO 322 IS = 1 , ISNS                                              2152
2153    360              IK=ISURF(IS)                                                   2153
2154    361              WRITE(18,1002) IS,(JS(KK,IK),KK=1,3),JS(3,IK)                  2154
2155    362    1002   FORMAT('en,',4(I10,','),I10)                                     2155
2156    363    322    CONTINUE                                                          2156
2157    364    C                                                                        2157
2158    365           WRITE(19,1005) TT                                                 2158
2159    366    1005   FORMAT('time,',E13.5)                                             2159
2160    367           ITWO = 1                                                          2160
2161    368           IZERO = 0                                                         2161
2162    369           DO 342 IS = 1 , ISNS                                              2162
2163    370              IK=ISURF(IS)                                                   2163
```

```
2164    371          WRITE(19,1003) IS,ITWO,IZERO,HNUM(JS(1,IK),5),HNUM(JS(2,IK),5),
2165    372                                       HNUM(JS(3,IK),5),HNUM(JS(3,IK),5)
2166    373  1003    FORMAT('sfe,',2(I5,','),'pres,',I5,',',3(E12.5,','),E12.5)
2167    374  342     CONTINUE
2168    375  C
2169    376          WRITE(14,10101) 3*ISNS,ISNS,NDUMMY1,NDUMMY3,NDUMMY3
2170    377  10101   FORMAT(5I8)
2171    378  10102   FORMAT(I8,3E20.7)
2172    379  10103   FORMAT(2I8,A6,3I8)
2173    380  10104   FORMAT(I8,E20.7)
2174    381          CALL RYDRFL
2175    382          KKVV = 0
2176    383          DO 310 IV = 1 , ISNS
2177    384             IK=ISURF(IV)
2178    385             IV1 = JS(1,IK)
2179    386             IV2 = JS(2,IK)
2180    387             IV3 = JS(3,IK)
2181    388             XXV = XV(1,IV1)
2182    389             YYV = XV(2,IV1)
2183    390             ZZV = XV(3,IV1)
2184    391             XNN = -XN(IK)
2185    392             YNN = -YN(IK)
2186    393             ZNN = -ZN(IK)
2187    394             XXX = XXV + XNN * .001
2188    395             YYY = YYV + YNN * .001
2189    396             ZZZ = ZZV + ZNN * .001
2190    397             KKVV = KKVV + 1
2191    398             WRITE(14,10102) KKVV,XXX,YYY,ZZZ
2192    399             XXV = XV(1,IV2)
2193    400             YYV = XV(2,IV2)
2194    401             ZZV = XV(3,IV2)
2195    402             XXX = XXV + XNN * .001
2196    403             YYY = YYV + YNN * .001
2197    404             ZZZ = ZZV + ZNN * .001
2198    405             KKVV = KKVV + 1
2199    406             WRITE(14,10102) KKVV,XXX,YYY,ZZZ
2200    407             XXV = XV(1,IV3)
2201    408             YYV = XV(2,IV3)
2202    409             ZZV = XV(3,IV3)
2203    410             XXX = XXV + XNN * .001
2204    411             YYY = YYV + YNN * .001
2205    412             ZZZ = ZZV + ZNN * .001
2206    413             KKVV = KKVV + 1
2207    414             WRITE(14,10102) KKVV,XXX,YYY,ZZZ
2208    415  310     CONTINUE
2209    416          KKVV = 0
2210    417          DO 320 IS = 1 , ISNS
2211    418             IK=ISURF(IS)
2212    419             WRITE(14,10103) IS,IS,CTRI,KKVV+1,KKVV+2,KKVV+3
2213    420             KKVV = KKVV + 3
2214    421  320     CONTINUE
2215    422          WRITE(14,10101) VDATA
2216    423          WRITE(14,*) VLABEL
2217    424          KKVV = 0
2218    425          DO 430 IV = 1 , ISNS
2219    426             IK=ISURF(IV)
2220    427             PRR = PR(IK)
2221    428             WRITE(14,10104) KKVV+1,PRR
2222    429             WRITE(14,10104) KKVV+2,PRR
2223    430             WRITE(14,10104) KKVV+3,PRR
2224    431             KKVV = KKVV + 3
2225    432  430     CONTINUE
2226    433          ISNS = 0
2227    434          DO IS = 1 , NS
2228    435             IF(JS(9,IS).EQ.6) THEN
2229    436             XXS = XS(1,IS)
2230    437             YYS = XS(2,IS)
2231    438             ZZS = XS(3,IS)
2232    439             ISNS=ISNS+1
2233    440             ISURF(ISNS)=IS
2234    441             END IF
2235    442          END DO
2236    443          print*,ISNS
2237    444          WRITE(15,10101) 3*ISNS,ISNS,NDUMMY1,NDUMMY3,NDUMMY3
```

```
2238     445           KKVV = 0                                                  2238
2239     446           DO 410 IV = 1 , ISNS                                      2239
2240     447              IK=ISURF(IV)                                           2240
2241     448              IV1 = JS(1,IK)                                         2241
2242     449              IV2 = JS(2,IK)                                         2242
2243     450              IV3 = JS(3,IK)                                         2243
2244     451              XNN = -XN(IK)                                          2244
2245     452              YNN = -YN(IK)                                          2245
2246     453              ZNN = -ZN(IK)                                          2246
2247     454              XXV = XV(1,IV1)                                        2247
2248     455              YYV = XV(2,IV1)                                        2248
2249     456              ZZV = XV(3,IV1)                                        2249
2250     457              XXX = XXV + XNN * .001                                 2250
2251     458              YYY = YYV + YNN * .001                                 2251
2252     459              ZZZ = ZZV + ZNN * .001                                 2252
2253     460              KKVV = KKVV + 1                                        2253
2254     461              WRITE(15,10102) KKVV,XXX,YYY,ZZZ                       2254
2255     462              XXV = XV(1,IV2)                                        2255
2256     463              YYV = XV(2,IV2)                                        2256
2257     464              ZZV = XV(3,IV2)                                        2257
2258     465              XXX = XXV + XNN * .001                                 2258
2259     466              YYY = YYV + YNN * .001                                 2259
2260     467              ZZZ = ZZV + ZNN * .001                                 2260
2261     468              KKVV = KKVV + 1                                        2261
2262     469              WRITE(15,10102) KKVV,XXX,YYY,ZZZ                       2262
2263     470              XXV = XV(1,IV3)                                        2263
2264     471              YYV = XV(2,IV3)                                        2264
2265     472              ZZV = XV(3,IV3)                                        2265
2266     473              XXX = XXV + XNN * .001                                 2266
2267     474              YYY = YYV + YNN * .001                                 2267
2268     475              ZZZ = ZZV + ZNN * .001                                 2268
2269     476              KKVV = KKVV + 1                                        2269
2270     477              WRITE(15,10102) KKVV,XXX,YYY,ZZZ                       2270
2271     478  410      CONTINUE                                                  2271
2272     479           KKVV = 0                                                  2272
2273     480           DO 420 IS = 1 , ISNS                                      2273
2274     481              IK=ISURF(IS)                                           2274
2275     482              WRITE(15,10103) IS,IS,CTRI,KKVV+1,KKVV+2,KKVV+3        2275
2276     483              KKVV = KKVV + 3                                        2276
2277     484  420      CONTINUE                                                  2277
2278     485           WRITE(15,10101) VDATA                                     2278
2279     486           WRITE(15,*) VLABEL                                        2279
2280     487           KKVV = 0                                                  2280
2281     488           DO 330 IV = 1 , ISNS                                      2281
2282     489              IK=ISURF(IV)                                           2282
2283     490              PRR = PR(IK)                                           2283
2284     491              WRITE(15,10104) KKVV+1,PRR                             2284
2285     492              WRITE(15,10104) KKVV+2,PRR                             2285
2286     493              WRITE(15,10104) KKVV+3,PRR                             2286
2287     494              KKVV = KKVV + 3                                        2287
2288     495  330      CONTINUE                                                  2288
2289     496  C                                                                 2289
2290     497  C                                                                 2290
2291     498  C=================================================================2291
2292     499  C                                                                 2292
2293     500  C            I--------------------------------I                   2293
2294     501  C            I  OUTPUT FILE FOR RESTARTS      I                   2294
2295     502  C            I--------------------------------I                   2295
2296     503  C                                                                 2296
2297     504           IF( JT . EQ . 1 ) THEN                                    2297
2298     505           REWIND 8                                                  2298
2299     506           WRITE(9) NV,NE,NS,NC,NTIME                                2299
2300     507           WRITE(9) ((XV(IK,IV),IK=1,3),IV=1,NV)                     2300
2301     508           WRITE(9) ((JE(KK,IE),KK=1,2),IE=1,NE)                     2301
2302     509           WRITE(9) ((JS(KK,IS),KK=1,9),(XS(KI,IS),KI=1,5),          2302
2303     510        .             XN(IS),YN(IS),ZN(IS),XP(IS),YP(IS),ZP(IS),     2303
2304     511        .             XT(IS),YT(IS),ZT(IS),IS=1,NS)                  2304
2305     512           WRITE(9) ((XYZMDL(KI,IS),KI=1,4),IS=1,NS)                 2305
2306     513           WRITE(9) ((JC(KK,IC),KK=1,8),(XC(KI,IC),KI=1,4),IC=1,NC)  2306
2307     514           WRITE(9) ((RGRAD(IC,KI),UGRAD(IC,KI),VGRAD(IC,KI),        2307
2308     515        .             WGRAD(IC,KI),PGRAD(IC,KI),KI=1,3),IC=1,NC)     2308
2309     516           WRITE(9) SAREVG,                                          2309
2310     517        .           NVECE,NREME,NVECV,NREMV,NVECS,NREMS,NVECC,NREMC  2310
2311     518           WRITE(9) RIN,PIN,RINL,PINL,UVIN,UIN,VIN,WIN,TT            2311
```

```
2312  519          WRITE(9) NPRTCL                                          2312
2313  520          IF(NPRTCL.GT.0)                                          2313
2314  521        . WRITE(9) (IJKPRT(IK),IK=1,NPRTCL)                        2314
2315  522          END IF                                                   2315
2316  523          WRITE(9) ((HYDV(IC,IK),IK=1,8),IC=1,NC)                  2316
2317  524  C                                                                2317
2318  525          REWIND 88                                                2318
2319  526          WRITE(88) NV,NE,NS,NC,NTIME                              2319
2320  527          WRITE(88) ((XV(IK,IV),IK=1,3),IV=1,NV)                   2320
2321  528          WRITE(88) ((JE(KK,IE),KK=1,2),IE=1,NE)                   2321
2322  529          WRITE(88) ((JS(KK,IS),KK=1,9),(XS(KI,IS),KI=1,5),        2322
2323  530        .            XN(IS),YN(IS),ZN(IS),XP(IS),YP(IS),ZP(IS),    2323
2324  531        .            XT(IS),YT(IS),ZT(IS),IS=1,NS)                 2324
2325  532          WRITE(88) ((XYZMDL(KI,IS),KI=1,4),IS=1,NS)               2325
2326  533          WRITE(88) ((JC(KK,IC),KK=1,8),(XC(KI,IC),KI=1,4),IC=1,NC) 2326
2327  534          WRITE(88) ((RGRAD(IC,KI),UGRAD(IC,KI),VGRAD(IC,KI),      2327
2328  535        .            WGRAD(IC,KI),PGRAD(IC,KI),KI=1,3),IC=1,NC)    2328
2329  536          WRITE(88) SAREVG,                                        2329
2330  537        .           NVECE,NREME,NVECV,NREMV,NVECS,NREMS,NVECC,NREMC 2330
2331  538          WRITE(88) RIN,PIN,RINL,PINL,UVIN,UIN,VIN,WIN,TT          2331
2332  539          WRITE(88) NPRTCL                                         2332
2333  540          IF(NPRTCL.GT.0)                                          2333
2334  541        . WRITE(88) (IJKPRT(IK),IK=1,NPRTCL)                       2334
2335  542          WRITE(88) ((HYDV(IC,IK),IK=1,8),IC=1,NC)                 2335
2336  543  C                                                                2336
2337  544   120    CONTINUE                                                 2337
2338  545          REWIND 10                                                2338
2339  546          REWIND 26                                                2339
2340  547          WRITE(26,*) IJKNUM                                       2340
2341  548          DO KKJ = 1 , IJKNUM                                      2341
2342  549          READ (10,*) RO,(RRN(IK),IK=1,NPRTCL)                     2342
2343  550          WRITE (26,*) RO,(RRN(IK),IK=1,NPRTCL)                    2343
2344  551          END DO                                                   2344
2345  552  C                                                                2345
2346  553        RETURN                                                     2346
2347  554        END                                                        2347
2348  555  C                                                                2348
```



```
2349    1        SUBROUTINE GEOMTR                                         2349
2350    2  C                                                               2350
2351    3  C---------------------------------------------------------------I2351
2352    4  C                                                              I2352
2353    5  C      GEOMTR COMPUTE THE DUAL MESH AFTER INITIALIZATION THE GRID I2353
2354    6  C                                                              I2354
2355    7  C---------------------------------------------------------------I2355
2356    8  C                                                               2356
2357    9        include     'dmsh00.h'                                    2357
2358   10        include     'dhydm0.h'                                    2358
2359   11        include     'dphsm0.h'                                    2359
2360   12        include     'dmtrl0.h'                                    2360
2361   13  C                                                               2361
2362   14  C --- DEFINING BOUNDARY EDGES AND COMPUTING BAR CENTER OF TRIANGLES 2362
2363   15  C                                                               2363
2364   16        PRINT * , NE,NS                                           2364
2365   17        DO 110 IC = 1 , NC                                        2365
2366   18        SVOLM( IC ) = 1. / XC( 4 , IC )                           2366
2367   19   110  CONTINUE                                                  2367
2368   20  C                                                               2368
2369   21        DO 120 IS = 1 , NS                                        2369
2370   22  C                                                               2370
2371   23        ICL = JS( 7 , IS )                                        2371
2372   24        ICR = JS( 8 , IS )                                        2372
2373   25  C                                                               2373
2374   26        IV1 = JS( 1 , IS )                                        2374
2375   27        IV2 = JS( 2 , IS )                                        2375
2376   28        IV3 = JS( 3 , IS )                                        2376
2377   29  C                                                               2377
2378   30        X1 = XV( 1 , IV1 )                                        2378
2379   31        Y1 = XV( 2 , IV1 )                                        2379
2380   32        Z1 = XV( 3 , IV1 )                                        2380
2381   33  C                                                               2381
2382   34        A = XN( IS )                                              2382
```

```
2383      35          B = YN( IS )                                                  2383
2384      36          C = ZN( IS )                                                  2384
2385      37    C                                                                   2385
2386      38          D = - ( A * X1 + B * Y1 + C * Z1 )                            2386
2387      39    C                                                                   2387
2388      40          XCL = XC( 1 , ICL )                                           2388
2389      41          YCL = XC( 2 , ICL )                                           2389
2390      42          ZCL = XC( 3 , ICL )                                           2390
2391      43    C                                                                   2391
2392      44          DD = A * XCL + B * YCL + C * ZCL + D                          2392
2393      45    C                                                                   2393
2394      46          IATRB = JS( 9 , IS )                                          2394
2395      47          IF( IATRB . EQ . 0 ) THEN                                     2395
2396      48    C                                                                   2396
2397      49          XCR = XC( 1 , ICR )                                           2397
2398      50          YCR = XC( 2 , ICR )                                           2398
2399      51          ZCR = XC( 3 , ICR )                                           2399
2400      52    C                                                                   2400
2401      53          XX = XCR - XCL                                                2401
2402      54          YY = YCR - YCL                                                2402
2403      55          ZZ = ZCR - ZCL                                                2403
2404      56    C                                                                   2404
2405      57          DDD = A * XX + B * YY + C * ZZ                                2405
2406      58    C                                                                   2406
2407      59          XYZ = - DD / DDD                                              2407
2408      60          XYZMDL( 4 , IS ) = XYZ                                        2408
2409      61          XYZMDL( 1 , IS ) = XCL + XYZ * XX                             2409
2410      62          XYZMDL( 2 , IS ) = YCL + XYZ * YY                             2410
2411      63          XYZMDL( 3 , IS ) = ZCL + XYZ * ZZ                             2411
2412      64          XS( 5 , IS ) = SQRT( XX * XX + YY * YY + ZZ * ZZ )            2412
2413      65    C                                                                   2413
2414      66          ELSE                                                          2414
2415      67    C                                                                   2415
2416      68          XYZ = - DD                                                    2416
2417      69          XYZMDL( 1 , IS ) = XCL + XYZ * A                              2417
2418      70          XYZMDL( 2 , IS ) = YCL + XYZ * B                              2418
2419      71          XYZMDL( 3 , IS ) = ZCL + XYZ * C                              2419
2420      72          XS( 5 , IS ) = ABS( XYZ )                                     2420
2421      73          XYZMDL( 4 , IS ) = 1.                                         2421
2422      74    C                                                                   2422
2423      75          END IF                                                        2423
2424      76    C                                                                   2424
2425      77     120  CONTINUE                                                      2425
2426      78    C                                                                   2426
2427      79          RETURN                                                        2427
2428      80          END                                                           2428
2429      81    C                                                                   2429
2430      82              SUBROUTINE UPDATE                                         2430
2431      83    C                                                                   2431
2432      84    C-------------------------------------------------------------------I 2432
2433      85    C                                                                   I 2433
2434      86    C      UPDATE COMPUTE THE DUAL MESH AFTER INITIALIZATION THE GRID   I 2434
2435      87    C                                                                   I 2435
2436      88    C-------------------------------------------------------------------I 2436
2437      89    C                                                                   2437
2438      90          include     'dmsh00.h'                                        2438
2439      91          include     'dhydm0.h'                                        2439
2440      92          include     'dphsm0.h'                                        2440
2441      93          include     'dmtrl0.h'                                        2441
2442      94    C                                                                   2442
2443      95    C                                                                   2443
2444      96    C      READ IN VERTEX INFORMATION                                   2444
2445      97    C                                                                   2445
2446      98            READ (16,*) NV,NE,NC,NS                                   2446
2447      99            DO 1110 IK = 1 , NV                                       2447
2448     100            READ (16,*) IJ,XV(1,IK),XV(2,IK),XV(3,IK)                 2448
2449     101            XXX =XV(1,IK) + 34.5                                      2449
2450     102            YYY =XV(2,IK) - 65.75                                     2450
2451     103            ZZZ =XV(3,IK) + 11.5                                      2451
2452     104            XV(1,IK)=XXX*.0254                                        2452
2453     105            XV(2,IK)=YYY*.0254                                        2453
2454     106            XV(3,IK)=ZZZ*.0254                                        2454
2455     107    1110    CONTINUE                                                   2455
2456     108            PRINT * , NV                                              2456
```

```
2457     109   C
2458     110   C      READ IN EDGE INFORMATION ( EDGES OF TRIANGLES).
2459     111   C
2460     112            DO 1120 IK = 1 , NE
2461     113            READ (16,*) IJ,JE(1,IK),JE(2,IK)
2462     114   1120     CONTINUE
2463     115            PRINT * , NE
2464     116   C
2465     117   C      READ IN CELL (TETRAHIDRAL) INFORMATION.
2466     118   C
2467     119   C      CELL INFORMATION, FOR EACH CELL FOUR VERTICES
2468     120   C
2469     121            DO 1130 IK = 1 , NC
2470     122            READ (16,*) IJ,JC(1,IK),JC(2,IK),JC(3,IK),JC(4,IK)
2471     123   1130     CONTINUE
2472     124   C
2473     125            DO 1200 IK = 1 , NC
2474     126            IV1 = JC( 1 , IK )
2475     127            IV2 = JC( 2 , IK )
2476     128            IV3 = JC( 3 , IK )
2477     129            IV4 = JC( 4 , IK )
2478     130   C
2479     131   C      SIDE INFORMATION, FOR EACH CELL CENTROID OF CELL
2480     132   C
2481     133              XC( 1 , IK ) = ( XV( 1 , IV1 ) + XV( 1 , IV2 ) +
2482     134           .                   XV( 1 , IV3 ) + XV( 1 , IV4 ) ) * .25
2483     135              XC( 2 , IK ) = ( XV( 2 , IV1 ) + XV( 2 , IV2 ) +
2484     136           .                   XV( 2 , IV3 ) + XV( 2 , IV4 ) ) * .25
2485     137              XC( 3 , IK ) = ( XV( 3 , IV1 ) + XV( 3 , IV2 ) +
2486     138           .                   XV( 3 , IV3 ) + XV( 3 , IV4 ) ) * .25
2487     139   C
2488     140   C      SIDE INFORMATION, FOR EACH CELL VOLUME OF CELL
2489     141   C
2490     142            XPIJ = XV( 1 , IV2 ) - XV( 1 , IV1 )
2491     143            YPIJ = XV( 2 , IV2 ) - XV( 2 , IV1 )
2492     144            ZPIJ = XV( 3 , IV2 ) - XV( 3 , IV1 )
2493     145   C
2494     146            XPIK = XV( 1 , IV3 ) - XV( 1 , IV1 )
2495     147            YPIK = XV( 2 , IV3 ) - XV( 2 , IV1 )
2496     148            ZPIK = XV( 3 , IV3 ) - XV( 3 , IV1 )
2497     149   C
2498     150            XNIK = YPIJ * ZPIK - ZPIJ * YPIK
2499     151            YNIK = ZPIJ * XPIK - XPIJ * ZPIK
2500     152            ZNIK = XPIJ * YPIK - YPIJ * XPIK
2501     153   C
2502     154            XPIJ = XV( 1 , IV4 ) - XV( 1 , IV1 )
2503     155            YPIJ = XV( 2 , IV4 ) - XV( 2 , IV1 )
2504     156            ZPIJ = XV( 3 , IV4 ) - XV( 3 , IV1 )
2505     157   C
2506     158            VOL = ( XNIK * XPIJ + YNIK * YPIJ +
2507     159         .                        ZNIK * ZPIJ ) / 6.
2508     160            XC( 4 , IK ) = VOL
2509     161            IF( VOL . LT . 0. ) PRINT *,IK,VOL
2510     162   1200     CONTINUE
2511     163            PRINT * , NC
2512     164   C
2513     165   C      READ IN SIDE (TRIANGLE) INFORMATION.
2514     166   C
2515     167   C      SIDE INFORMATION, FOR EACH FACE THREE VERTICES
2516     168   C
2517     169            DO 1150 IK = 1 , NS
2518     170            READ (16,*) IJ,JS(1,IK),JS(2,IK),JS(3,IK)
2519     171   1150     CONTINUE
2520     172            PRINT * , NS,NC
2521     173   C
2522     174   C      SIDE INFORMATION, FOR EACH FACE THREE EDGES
2523     175   C
2524     176            DO 1160 IK = 1 , NS
2525     177            READ (16,*) IJ,JS(4,IK),JS(5,IK),JS(6,IK)
2526     178   1160     CONTINUE
2527     179            PRINT * , NS,NC,NV
2528     180   C
2529     181   C      CELL INFORMATION, FOR EACH CELL FOUR EDGES
2530     182   C
```

```
2531     183           DO 1140 IK = 1 , NC                                    2531
2532     184           READ (16,*) IJ,JC5,IDIR1,JC6,IDIR2,                    2532
2533     185          .                 JC7,IDIR3,JC8,IDIR4                   2533
2534     186           JC(5,IK) = IABS( JC5 )                                 2534
2535     187           JC(6,IK) = IABS( JC6 )                                 2535
2536     188           JC(7,IK) = IABS( JC7 )                                 2536
2537     189           JC(8,IK) = IABS( JC8 )                                 2537
2538     190  1140     CONTINUE                                               2538
2539     191           PRINT * , NS,NC,NV,NE                                  2539
2540     192  C                                                               2540
2541     193  C      SIDE INFORMATION, FOR EACH FACE LEFT AND RIGHT TETREHEDRA 2541
2542     194  C                                                               2542
2543     195           DO 1170 IK = 1 , NS                                    2543
2544     196           READ (16,*) IJ,JS(7,IK),JS(8,IK)                       2544
2545     197           JS( 9 , IK ) = 0                                       2545
2546     198  1170     CONTINUE                                               2546
2547     199           PRINT * , NC,NV,NE                                     2547
2548     200  C                                                               2548
2549     201  C      SIDE INFORMATION, FOR EACH FACE BOUNDARY CONDITION       2549
2550     202  C                                                               2550
2551     203  1180     CONTINUE                                               2551
2552     204           READ (16,*,END=1210) IJ,IDUMY,JS(9,IJ)                 2552
2553     205           GO TO 1180                                             2553
2554     206  1210     CONTINUE                                               2554
2555     207           PRINT * , NV,NE,NS,NC                                  2555
2556     208  C                                                               2556
2557     209           DO 1190 IK = 1 , NS                                    2557
2558     210           IV1 = JS( 1 , IK )                                     2558
2559     211           IV2 = JS( 2 , IK )                                     2559
2560     212           IV3 = JS( 3 , IK )                                     2560
2561     213  C                                                               2561
2562     214  C      SIDE INFORMATION, FOR EACH FACE TANGENTIAL VECTOR         2562
2563     215  C                                                               2563
2564     216             XP( IK ) = XV( 1 , IV2 ) - XV( 1 , IV1 )             2564
2565     217             YP( IK ) = XV( 2 , IV2 ) - XV( 2 , IV1 )             2565
2566     218             ZP( IK ) = XV( 3 , IV2 ) - XV( 3 , IV1 )             2566
2567     219             XPDUMY = XV( 1 , IV3 ) - XV( 1 , IV1 )               2567
2568     220             YPDUMY = XV( 2 , IV3 ) - XV( 2 , IV1 )               2568
2569     221             ZPDUMY = XV( 3 , IV3 ) - XV( 3 , IV1 )               2569
2570     222  C                                                               2570
2571     223  C      SIDE INFORMATION, FOR EACH FACE NORMAL UNIT VECTOR        2571
2572     224  C                                                               2572
2573     225             XN( IK ) = YP( IK ) * ZPDUMY - ZP( IK ) * YPDUMY     2573
2574     226             YN( IK ) = ZP( IK ) * XPDUMY - XP( IK ) * ZPDUMY     2574
2575     227             ZN( IK ) = XP( IK ) * YPDUMY - YP( IK ) * XPDUMY     2575
2576     228  C                                                               2576
2577     229  C      SIDE INFORMATION, FOR EACH FACE TANGENTIAL VECTOR         2577
2578     230  C                                                               2578
2579     231             XT( IK ) = - YP( IK ) * ZN( IK ) + ZP( IK ) * YN( IK ) 2579
2580     232             YT( IK ) = - ZP( IK ) * XN( IK ) + XP( IK ) * ZN( IK ) 2580
2581     233             ZT( IK ) = - XP( IK ) * YN( IK ) + YP( IK ) * XN( IK ) 2581
2582     234  C                                                               2582
2583     235             XYZDUM = XN(IK)*XN(IK) + YN(IK)*YN(IK) + ZN(IK)*ZN(IK) 2583
2584     236             IF(XYZDUM.EQ.0.) PRINT *,IK                          2584
2585     237             XYZDUM = 1. / SQRT( XYZDUM )                         2585
2586     238  C                                                               2586
2587     239  C      SIDE INFORMATION, FOR EACH FACE AREA OF FACE              2587
2588     240  C                                                               2588
2589     241             XS( 4 , IK ) = .5 / XYZDUM                           2589
2590     242  C                                                               2590
2591     243  C      SIDE INFORMATION, FOR EACH FACE CENTROID OF FACE          2591
2592     244  C                                                               2592
2593     245             XS( 1 , IK ) = ( XV( 1 , IV1 ) + XV( 1 , IV2 ) +     2593
2594     246          .                   XV( 1 , IV3 ) ) / 3.                2594
2595     247             XS( 2 , IK ) = ( XV( 2 , IV1 ) + XV( 2 , IV2 ) +     2595
2596     248          .                   XV( 2 , IV3 ) ) / 3.                2596
2597     249             XS( 3 , IK ) = ( XV( 3 , IV1 ) + XV( 3 , IV2 ) +     2597
2598     250          .                   XV( 3 , IV3 ) ) / 3.                2598
2599     251             XN( IK ) = XN( IK ) * XYZDUM                         2599
2600     252             YN( IK ) = YN( IK ) * XYZDUM                         2600
2601     253             ZN( IK ) = ZN( IK ) * XYZDUM                         2601
2602     254             XYZDUM = XP(IK)*XP(IK) + YP(IK)*YP(IK) + ZP(IK)*ZP(IK) 2602
2603     255             XYZDUM = 1. / SQRT( XYZDUM )                         2603
2604     256             XP( IK) = XP( IK ) * XYZDUM                          2604
```

```
2605     257            YP( IK) = YP( IK ) * XYZDUM                                    2605
2606     258            ZP( IK) = ZP( IK ) * XYZDUM                                    2606
2607     259            XYZDUM = XT(IK)*XT(IK) + YT(IK)*YT(IK) + ZT(IK)*ZT(IK)         2607
2608     260            XYZDUM = 1. / SQRT( XYZDUM )                                   2608
2609     261            XT( IK) = XT( IK ) * XYZDUM                                    2609
2610     262            YT( IK) = YT( IK ) * XYZDUM                                    2610
2611     263            ZT( IK) = ZT( IK ) * XYZDUM                                    2611
2612     264   1190     CONTINUE                                                       2612
2613     265            PRINT * , NS                                                   2613
2614     266   C                                                                       2614
2615     267          NVECV = NV / 128                                                 2615
2616     268          NREMV = NV - NVECV * 128                                         2616
2617     269          NVECE = NE / 128                                                 2617
2618     270          NREME = NE - NVECE * 128                                         2618
2619     271          NVECS = NS / 128                                                 2619
2620     272          NREMS = NS - NVECS * 128                                         2620
2621     273          NVECC = NC / 128                                                 2621
2622     274          NREMC = NC - NVECC * 128                                         2622
2623     275   C                                                                       2623
2624     276          DO 125 INV = 1 , NVECV                                           2624
2625     277          NOFVEV( INV ) = 128                                              2625
2626     278    125   CONTINUE                                                         2626
2627     279          NVEEV = NVECV                                                    2627
2628     280          IF( NREMV . GT . 0 ) THEN                                        2628
2629     281          NVEEV = NVECV + 1                                                2629
2630     282          NOFVEV( NVEEV ) = NREMV                                          2630
2631     283          END IF                                                           2631
2632     284   C                                                                       2632
2633     285          DO 105 INE = 1 , NVECE                                           2633
2634     286          NOFVEE( INE ) = 128                                              2634
2635     287    105   CONTINUE                                                         2635
2636     288          NVEEE = NVECE                                                    2636
2637     289          IF( NREME . GT . 0 ) THEN                                        2637
2638     290          NVEEE = NVECE + 1                                                2638
2639     291          NOFVEE( NVEEE ) = NREME                                          2639
2640     292          END IF                                                           2640
2641     293   C                                                                       2641
2642     294          DO 115 INS = 1 , NVECS                                           2642
2643     295          NOFVES( INS ) = 128                                              2643
2644     296    115   CONTINUE                                                         2644
2645     297          NVEES = NVECS                                                    2645
2646     298          IF( NREMS . GT . 0 ) THEN                                        2646
2647     299          NVEES = NVECS + 1                                                2647
2648     300          NOFVES( NVEES ) = NREMS                                          2648
2649     301          END IF                                                           2649
2650     302   C                                                                       2650
2651     303          DO 135 INC = 1 , NVECC                                           2651
2652     304          NOFVEC( INC ) = 128                                              2652
2653     305    135   CONTINUE                                                         2653
2654     306          NVEEC = NVECC                                                    2654
2655     307          IF( NREMC . GT . 0 ) THEN                                        2655
2656     308          NVEEC = NVECC + 1                                                2656
2657     309          NOFVEC( NVEEC ) = NREMC                                          2657
2658     310          END IF                                                           2658
2659     311   C                                                                       2659
2660     312           PRINT *,NV,NE,NS,NC                                            2660
2661     313           PRINT *,NVEEV,NVEEE,NVEES,NVEEC                                2661
2662     314           PRINT *,NREMV,NREME,NREMS,NREMC                                2662
2663     315   1001    FORMAT(4I7)                                                    2663
2664     316   1002    FORMAT(I7,3E20.12)                                             2664
2665     317   C                                                                       2665
2666     318          CALL GEOMTR                                                     2666
2667     319   C                                                                       2667
2668     320          RETURN                                                          2668
2669     321          END                                                             2669
2670     322   C                                                                       2670
```

```
      SUBROUTINE UPGRAD
C
C-----------------------------------------------------------------I
C                                                                 I
C      UPGRAD COMPUTE THE DUAL MESH AFTER ADDAPTING THE GRID      I
C                                                                 I
C-----------------------------------------------------------------I
C
      include     'dmsh00.h'
      include     'dhydm0.h'
      include     'dphsm0.h'
      include     'dmtrl0.h'
C
      REAL XELEFT(128),YELEFT(128),XERIGT(128),YERIGT(128)
C
C --- DEFINING BOUNDARY EDGES
C
        READ(8) NV,NE,NS,NC,NTINE
        READ(8) ((XV(IK,IV),IK=1,3),IV=1,NV)
        READ(8) ((JE(KK,IE),KK=1,2),IE=1,NE)
        READ(8) ((JS(KK,IS),KK=1,9),(XS(KI,IS),KI=1,5),
     .            XN(IS),YN(IS),ZN(IS),XP(IS),YP(IS),ZP(IS),
     .            XT(IS),YT(IS),ZT(IS),IS=1,NS)
        READ(8) ((XYZMDL(KI,IS),KI=1,4),IS=1,NS)
        READ(8) ((JC(KK,IC),KK=1,8),(XC(KI,IC),KI=1,4),IC=1,NC)
        READ(8) ((RGRAD(IC,KI),UGRAD(IC,KI),VGRAD(IC,KI),
     .            WGRAD(IC,KI),PGRAD(IC,KI),KI=1,3),IC=1,NC)
        READ(8) SAREVG,
     .          NVECE,NREME,NVECV,NREMV,NVECS,NREMS,NVECC,NREMC
         PRINT * , NE,NS
C
      DO 100 IC = 1 , NC
      SVOLM( IC ) = 1. / XC( 4 , IC )
  100 CONTINUE
C
      DO 105 INE = 1 , NVECE
      NOFVEE( INE ) = 128
  105 CONTINUE
      NVEEE = NVECE
      IF( NREME . GT . 0 ) THEN
      NVEEE = NVECE + 1
      NOFVEE( NVEEE ) = NREME
      END IF
C
      DO 115 INS = 1 , NVECS
      NOFVES( INS ) = 128
  115 CONTINUE
      NVEES = NVECS
      IF( NREMS . GT . 0 ) THEN
      NVEES = NVECS + 1
      NOFVES( NVEES ) = NREMS
      END IF
C
      DO 125 INV = 1 , NVECV
      NOFVEV( INV ) = 128
  125 CONTINUE
      NVEEV = NVECV
      IF( NREMV . GT . 0 ) THEN
      NVEEV = NVECV + 1
      NOFVEV( NVEEV ) = NREMV
      END IF
C
      DO 135 INC = 1 , NVECC
      NOFVEC( INC ) = 128
  135 CONTINUE
      NVEEC = NVECC
      IF( NREMC . GT . 0 ) THEN
      NVEEC = NVECC + 1
      NOFVEC( NVEEC ) = NREMC
      END IF
C
       PRINT *,NV,NE,NS,NC,NVECV,NREMV,NVECE,NREME,NVECS,NREMS,
     .                     NVECC,NREMC
C
```

```
2745     75         RETURN                                                    2745
2746     76         END                                                       2746
2747     77   C                                                               2747
```



```
2748      1         SUBROUTINE GRADNT                                         2748
2749      2   C                                                               2749
2750      3   C-----------------------------------------------------------I   2750
2751      4   C                                                           I   2751
2752      5   C      GRADNT COMPUTE THE GRADIENT FOR SECOND ORDER CALCULATION I   2752
2753      6   C                                                           I   2753
2754      7   C-----------------------------------------------------------I   2754
2755      8   C                                                               2755
2756      9         include     'dmsh00.h'                                    2756
2757     10         include     'dhydm0.h'                                    2757
2758     11         include     'dphsm0.h'                                    2758
2759     12         include     'dmtrl0.h'                                    2759
2760     13   C                                                               2760
2761     14         REAL RRMIDL(128),PPMIDL(128),UUMIDL(128),VVMIDL(128),     2761
2762     15        .     WWMIDL(128),AAMIDL(128)                             2762
2763     16         REAL RIGRAD(128),PIGRAD(128),UIGRAD(128),VIGRAD(128),     2763
2764     17        .     WIGRAD(128),AIGRAD(128)                             2764
2765     18         REAL RJGRAD(128),PJGRAD(128),UJGRAD(128),VJGRAD(128),     2765
2766     19        .     WJGRAD(128),AJGRAD(128)                             2766
2767     20         REAL RKGRAD(128),PKGRAD(128),UKGRAD(128),VKGRAD(128),     2767
2768     21        .     WKGRAD(128),AKGRAD(128)                             2768
2769     22         REAL RMAX(128),PMAX(128),UMAX(128),VMAX(128),WMAX(128),   2769
2770     23        .     AMAX(128)                                           2770
2771     24         REAL RMIN(128),PMIN(128),UMIN(128),VMIN(128),WMIN(128),   2771
2772     25        .     AMIN(128)                                           2772
2773     26         REAL ROR(4),UOR(4),VOR(4),WOR(4),POR(4),AOR(4)            2773
2774     27         REAL ROL(4),UOL(4),VOL(4),WOL(4),POL(4),AOL(4)            2774
2775     28   C                                                               2775
2776     29         DO 120 IH = 1 , 3                                         2776
2777     30   C                                                               2777
2778     31         DO 120 IC = 1 , NC                                        2778
2779     32   C                                                               2779
2780     33         RGRAD( IC , IH ) = 0.                                     2780
2781     34         UGRAD( IC , IH ) = 0.                                     2781
2782     35         VGRAD( IC , IH ) = 0.                                     2782
2783     36         WGRAD( IC , IH ) = 0.                                     2783
2784     37         PGRAD( IC , IH ) = 0.                                     2784
2785     38   C                                                               2785
2786     39    120  CONTINUE                                                  2786
2787     40   C                                                               2787
2788     41   C --- BEGIN LOOP OVER ALL EDGES IN THE DOMAIN ----------------- 2788
2789     42   C                                                               2789
2790     43         NS1 = 1                                                   2790
2791     44         NS2 = NOFVES( 1 )                                         2791
2792     45         DO 90 INS = 1 , NVEES                                     2792
2793     46   C                                                               2793
2794     47   C --- FETCH HYDRO QUANTITIES ---------------------------------- 2794
2795     48   C                                                               2795
2796     49         DO 105 IS = NS1 , NS2                                     2796
2797     50             KS = IS - NS1 + 1                                     2797
2798     51   C                                                               2798
2799     52          ICL = JS( 7 , IS )                                       2799
2800     53          ICR = JS( 8 , IS )                                       2800
2801     54   C                                                               2801
2802     55         IATRB = JS( 9 , IS )                                      2802
2803     56         IF( IATRB . EQ . 0 ) THEN                                 2803
2804     57   C                                                               2804
2805     58          XYZ = XYZMDL( 4 , IS )                                   2805
2806     59            RRMIDL( KS ) = HYDV( ICL , 1 ) + XYZ * ( HYDV( ICR , 1 ) -  2806
2807     60        .                                          HYDV( ICL , 1 ) )  2807
2808     61            UUMIDL( KS ) = HYDV( ICL , 2 ) + XYZ * ( HYDV( ICR , 2 ) -  2808
2809     62        .                                          HYDV( ICL , 2 ) )  2809
2810     63            VVMIDL( KS ) = HYDV( ICL , 3 ) + XYZ * ( HYDV( ICR , 3 ) -  2810
2811     64        .                                          HYDV( ICL , 3 ) )  2811
2812     65            WWMIDL( KS ) = HYDV( ICL , 4 ) + XYZ * ( HYDV( ICR , 4 ) -  2812
2813     66        .                                          HYDV( ICL , 4 ) )  2813
2814     67            PPMIDL( KS ) = HYDV( ICL , 5 ) + XYZ * ( HYDV( ICR , 5 ) -  2814
2815     68        .                                          HYDV( ICL , 5 ) )  2815
```

```
2816      69  C
2817      70        ELSE
2818      71  C
2819      72           RRMIDL( KS ) = HYDV( ICL , 1 )
2820      73           UUMIDL( KS ) = HYDV( ICL , 2 )
2821      74           VVMIDL( KS ) = HYDV( ICL , 3 )
2822      75           WWMIDL( KS ) = HYDV( ICL , 4 )
2823      76           PPMIDL( KS ) = HYDV( ICL , 5 )
2824      77  C
2825      78        END IF
2826      79  C
2827      80   105  CONTINUE
2828      81  C
2829      82        DO 110 IS = NS1 , NS2
2830      83           KS = IS - NS1 + 1
2831      84  C
2832      85           XEXN = XS( 4 , IS ) * XN( IS )
2833      86           XEYN = XS( 4 , IS ) * YN( IS )
2834      87           XEZN = XS( 4 , IS ) * ZN( IS )
2835      88  C
2836      89           RIGRAD( KS ) = RRMIDL( KS ) * XEXN
2837      90           UIGRAD( KS ) = UUMIDL( KS ) * XEXN
2838      91           VIGRAD( KS ) = VVMIDL( KS ) * XEXN
2839      92           WIGRAD( KS ) = WWMIDL( KS ) * XEXN
2840      93           PIGRAD( KS ) = PPMIDL( KS ) * XEXN
2841      94  C
2842      95           RJGRAD( KS ) = RRMIDL( KS ) * XEYN
2843      96           UJGRAD( KS ) = UUMIDL( KS ) * XEYN
2844      97           VJGRAD( KS ) = VVMIDL( KS ) * XEYN
2845      98           WJGRAD( KS ) = WWMIDL( KS ) * XEYN
2846      99           PJGRAD( KS ) = PPMIDL( KS ) * XEYN
2847     100  C
2848     101           RKGRAD( KS ) = RRMIDL( KS ) * XEZN
2849     102           UKGRAD( KS ) = UUMIDL( KS ) * XEZN
2850     103           VKGRAD( KS ) = VVMIDL( KS ) * XEZN
2851     104           WKGRAD( KS ) = WWMIDL( KS ) * XEZN
2852     105           PKGRAD( KS ) = PPMIDL( KS ) * XEZN
2853     106  C
2854     107   110  CONTINUE
2855     108  C
2856     109        DO 130 IS = NS1 , NS2
2857     110           KS = IS - NS1 + 1
2858     111  C
2859     112         ICL = JS( 7 , IS )
2860     113         ICR = JS( 8 , IS )
2861     114  C
2862     115        RGRAD( ICL , 1 ) = RGRAD( ICL , 1 ) + RIGRAD( KS )
2863     116        RGRAD( ICL , 2 ) = RGRAD( ICL , 2 ) + RJGRAD( KS )
2864     117        RGRAD( ICL , 3 ) = RGRAD( ICL , 3 ) + RKGRAD( KS )
2865     118        UGRAD( ICL , 1 ) = UGRAD( ICL , 1 ) + UIGRAD( KS )
2866     119        UGRAD( ICL , 2 ) = UGRAD( ICL , 2 ) + UJGRAD( KS )
2867     120        UGRAD( ICL , 3 ) = UGRAD( ICL , 3 ) + UKGRAD( KS )
2868     121        VGRAD( ICL , 1 ) = VGRAD( ICL , 1 ) + VIGRAD( KS )
2869     122        VGRAD( ICL , 2 ) = VGRAD( ICL , 2 ) + VJGRAD( KS )
2870     123        VGRAD( ICL , 3 ) = VGRAD( ICL , 3 ) + VKGRAD( KS )
2871     124        WGRAD( ICL , 1 ) = WGRAD( ICL , 1 ) + WIGRAD( KS )
2872     125        WGRAD( ICL , 2 ) = WGRAD( ICL , 2 ) + WJGRAD( KS )
2873     126        WGRAD( ICL , 3 ) = WGRAD( ICL , 3 ) + WKGRAD( KS )
2874     127        PGRAD( ICL , 1 ) = PGRAD( ICL , 1 ) + PIGRAD( KS )
2875     128        PGRAD( ICL , 2 ) = PGRAD( ICL , 2 ) + PJGRAD( KS )
2876     129        PGRAD( ICL , 3 ) = PGRAD( ICL , 3 ) + PKGRAD( KS )
2877     130  C
2878     131        IATRB = JS( 9 , IS )
2879     132        IF( IATRB . EQ . 0 ) THEN
2880     133  C
2881     134  C ... GRADIENT OF DENSITY ( U V W DIRECTION ) ......................
2882     135  C
2883     136        RGRAD( ICR , 1 ) = RGRAD( ICR , 1 ) - RIGRAD( KS )
2884     137        RGRAD( ICR , 2 ) = RGRAD( ICR , 2 ) - RJGRAD( KS )
2885     138        RGRAD( ICR , 3 ) = RGRAD( ICR , 3 ) - RKGRAD( KS )
2886     139  C
2887     140  C ... GRADIENT OF U VELOCITY ( U V W DIRECTION ). ..................
2888     141  C
2889     142        UGRAD( ICR , 1 ) = UGRAD( ICR , 1 ) - UIGRAD( KS )
```

```
2890     143         UGRAD( ICR , 2 ) = UGRAD( ICR , 2 ) - UJGRAD( KS )                2890
2891     144         UGRAD( ICR , 3 ) = UGRAD( ICR , 3 ) - UKGRAD( KS )                2891
2892     145   C                                                                       2892
2893     146   C ... GRADIENT OF V VELOCITY ( U V W DIRECTION ) .....                  2893
2894     147   C                                                                       2894
2895     148         VGRAD( ICR , 1 ) = VGRAD( ICR , 1 ) - VIGRAD( KS )                2895
2896     149         VGRAD( ICR , 2 ) = VGRAD( ICR , 2 ) - VJGRAD( KS )                2896
2897     150         VGRAD( ICR , 3 ) = VGRAD( ICR , 3 ) - VKGRAD( KS )                2897
2898     151   C                                                                       2898
2899     152   C ... GRADIENT OF W VELOCITY ( U V W DIRECTION ) .....                  2899
2900     153   C                                                                       2900
2901     154         WGRAD( ICR , 1 ) = WGRAD( ICR , 1 ) - WIGRAD( KS )                2901
2902     155         WGRAD( ICR , 2 ) = WGRAD( ICR , 2 ) - WJGRAD( KS )                2902
2903     156         WGRAD( ICR , 3 ) = WGRAD( ICR , 3 ) - WKGRAD( KS )                2903
2904     157   C                                                                       2904
2905     158   C ... GRADIENT OF PRESSURE ( U V W DIRECTION ) .....                    2905
2906     159   C                                                                       2906
2907     160         PGRAD( ICR , 1 ) = PGRAD( ICR , 1 ) - PIGRAD( KS )                2907
2908     161         PGRAD( ICR , 2 ) = PGRAD( ICR , 2 ) - PJGRAD( KS )                2908
2909     162         PGRAD( ICR , 3 ) = PGRAD( ICR , 3 ) - PKGRAD( KS )                2909
2910     163   C                                                                       2910
2911     164         END IF                                                            2911
2912     165   C                                                                       2912
2913     166    130  CONTINUE                                                        2913
2914     167   C                                                                       2914
2915     168         NS1 = NS2 + 1                                                     2915
2916     169         NS2 = NS2 + NOFVES( INS + 1 )                                     2916
2917     170    90   CONTINUE                                                        2917
2918     171   C                                                                       2918
2919     172         DO 140 IH = 1 , 3                                                 2919
2920     173   C                                                                       2920
2921     174         DO 140 IC = 1 , NC                                                2921
2922     175   C                                                                       2922
2923     176         RGRAD( IC , IH ) = RGRAD( IC , IH ) * SVOLM( IC )                 2923
2924     177         UGRAD( IC , IH ) = UGRAD( IC , IH ) * SVOLM( IC )                 2924
2925     178         VGRAD( IC , IH ) = VGRAD( IC , IH ) * SVOLM( IC )                 2925
2926     179         WGRAD( IC , IH ) = WGRAD( IC , IH ) * SVOLM( IC )                 2926
2927     180         PGRAD( IC , IH ) = PGRAD( IC , IH ) * SVOLM( IC )                 2927
2928     181   C                                                                       2928
2929     182    140  CONTINUE                                                        2929
2930     183   C                                                                       2930
2931     184         NC1 = 1                                                           2931
2932     185         NC2 = NOFVEC( 1 )                                                 2932
2933     186         DO 80 INC = 1 , NVEEC                                             2933
2934     187   C                                                                       2934
2935     188         DO 150 IC = NC1 , NC2                                             2935
2936     189            KC = IC - NC1 + 1                                              2936
2937     190   C                                                                       2937
2938     191          IS = JC( 5 , IC )                                                2938
2939     192   C                                                                       2939
2940     193          ICL = JS( 7 , IS )                                               2940
2941     194          ICR = JS( 8 , IS )                                               2941
2942     195   C                                                                       2942
2943     196          RROL = HYDV( ICL , 1 )                                           2943
2944     197          UUOL = HYDV( ICL , 2 )                                           2944
2945     198          VVOL = HYDV( ICL , 3 )                                           2945
2946     199          WWOL = HYDV( ICL , 4 )                                           2946
2947     200          PPOL = HYDV( ICL , 5 )                                           2947
2948     201   C                                                                       2948
2949     202         IATRB = JS( 9 , IS )                                              2949
2950     203         IF( IATRB . EQ . 0 ) THEN                                         2950
2951     204   C                                                                       2951
2952     205          RROR = HYDV( ICR , 1 )                                           2952
2953     206          UUOR = HYDV( ICR , 2 )                                           2953
2954     207          VVOR = HYDV( ICR , 3 )                                           2954
2955     208          WWOR = HYDV( ICR , 4 )                                           2955
2956     209          PPOR = HYDV( ICR , 5 )                                           2956
2957     210   C                                                                       2957
2958     211          ELSE                                                             2958
2959     212   C                                                                       2959
2960     213          RROR = RROL                                                      2960
2961     214          UUOR = UUOL                                                      2961
2962     215          VVOR = VVOL                                                      2962
2963     216          WWOR = WWOL                                                      2963
```

```
2964     217          PPOR = PPOL                                          2964
2965     218   C                                                           2965
2966     219          END IF                                               2966
2967     220   C                                                           2967
2968     221          ROL( 1 ) = RROL                                      2968
2969     222          UOL( 1 ) = UUOL                                      2969
2970     223          VOL( 1 ) = VVOL                                      2970
2971     224          WOL( 1 ) = WWOL                                      2971
2972     225          POL( 1 ) = PPOL                                      2972
2973     226   C                                                           2973
2974     227          ROR( 1 ) = RROR                                      2974
2975     228          UOR( 1 ) = UUOR                                      2975
2976     229          VOR( 1 ) = VVOR                                      2976
2977     230          WOR( 1 ) = WWOR                                      2977
2978     231          POR( 1 ) = PPOR                                      2978
2979     232   C                                                           2979
2980     233          IS = JC( 6 , IC )                                    2980
2981     234   C                                                           2981
2982     235          ICL = JS( 7 , IS )                                   2982
2983     236          ICR = JS( 8 , IS )                                   2983
2984     237   C                                                           2984
2985     238          RROL = HYDV( ICL , 1 )                               2985
2986     239          UUOL = HYDV( ICL , 2 )                               2986
2987     240          VVOL = HYDV( ICL , 3 )                               2987
2988     241          WWOL = HYDV( ICL , 4 )                               2988
2989     242          PPOL = HYDV( ICL , 5 )                               2989
2990     243   C                                                           2990
2991     244         IATRB = JS( 9 , IS )                                  2991
2992     245         IF( IATRB . EQ . 0 ) THEN                             2992
2993     246   C                                                           2993
2994     247          RROR = HYDV( ICR , 1 )                               2994
2995     248          UUOR = HYDV( ICR , 2 )                               2995
2996     249          VVOR = HYDV( ICR , 3 )                               2996
2997     250          WWOR = HYDV( ICR , 4 )                               2997
2998     251          PPOR = HYDV( ICR , 5 )                               2998
2999     252   C                                                           2999
3000     253          ELSE                                                 3000
3001     254   C                                                           3001
3002     255          RROR = RROL                                          3002
3003     256          UUOR = UUOL                                          3003
3004     257          VVOR = VVOL                                          3004
3005     258          WWOR = WWOL                                          3005
3006     259          PPOR = PPOL                                          3006
3007     260   C                                                           3007
3008     261          END IF                                               3008
3009     262   C                                                           3009
3010     263          ROL( 2 ) = RROL                                      3010
3011     264          UOL( 2 ) = UUOL                                      3011
3012     265          VOL( 2 ) = VVOL                                      3012
3013     266          WOL( 2 ) = WWOL                                      3013
3014     267          POL( 2 ) = PPOL                                      3014
3015     268   C                                                           3015
3016     269          ROR( 2 ) = RROR                                      3016
3017     270          UOR( 2 ) = UUOR                                      3017
3018     271          VOR( 2 ) = VVOR                                      3018
3019     272          WOR( 2 ) = WWOR                                      3019
3020     273          POR( 2 ) = PPOR                                      3020
3021     274   C                                                           3021
3022     275          IS = JC( 7 , IC )                                    3022
3023     276   C                                                           3023
3024     277          ICL = JS( 7 , IS )                                   3024
3025     278          ICR = JS( 8 , IS )                                   3025
3026     279   C                                                           3026
3027     280          RROL = HYDV( ICL , 1 )                               3027
3028     281          UUOL = HYDV( ICL , 2 )                               3028
3029     282          VVOL = HYDV( ICL , 3 )                               3029
3030     283          WWOL = HYDV( ICL , 4 )                               3030
3031     284          PPOL = HYDV( ICL , 5 )                               3031
3032     285   C                                                           3032
3033     286         IATRB = JS( 9 , IS )                                  3033
3034     287         IF( IATRB . EQ . 0 ) THEN                             3034
3035     288   C                                                           3035
3036     289          RROR = HYDV( ICR , 1 )                               3036
3037     290          UUOR = HYDV( ICR , 2 )                               3037
```

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3038     291          VVOR = HYDV( ICR , 3 )                                    3038
3039     292          WWOR = HYDV( ICR , 4 )                                    3039
3040     293          PPOR = HYDV( ICR , 5 )                                    3040
3041     294   C                                                                3041
3042     295          ELSE                                                      3042
3043     296   C                                                                3043
3044     297          RROR = RROL                                               3044
3045     298          UUOR = UUOL                                               3045
3046     299          VVOR = VVOL                                               3046
3047     300          WWOR = WWOL                                               3047
3048     301          PPOR = PPOL                                               3048
3049     302   C                                                                3049
3050     303          END IF                                                    3050
3051     304   C                                                                3051
3052     305          ROL( 3 ) = RROL                                           3052
3053     306          UOL( 3 ) = UUOL                                           3053
3054     307          VOL( 3 ) = VVOL                                           3054
3055     308          WOL( 3 ) = WWOL                                           3055
3056     309          POL( 3 ) = PPOL                                           3056
3057     310   C                                                                3057
3058     311          ROR( 3 ) = RROR                                           3058
3059     312          UOR( 3 ) = UUOR                                           3059
3060     313          VOR( 3 ) = VVOR                                           3060
3061     314          WOR( 3 ) = WWOR                                           3061
3062     315          POR( 3 ) = PPOR                                           3062
3063     316   C                                                                3063
3064     317          IS = JC( 8 , IC )                                         3064
3065     318   C                                                                3065
3066     319          ICL = JS( 7 , IS )                                        3066
3067     320          ICR = JS( 8 , IS )                                        3067
3068     321   C                                                                3068
3069     322          RROL = HYDV( ICL , 1 )                                    3069
3070     323          UUOL = HYDV( ICL , 2 )                                    3070
3071     324          VVOL = HYDV( ICL , 3 )                                    3071
3072     325          WWOL = HYDV( ICL , 4 )                                    3072
3073     326          PPOL = HYDV( ICL , 5 )                                    3073
3074     327   C                                                                3074
3075     328         IATRB = JS( 9 , IS )                                       3075
3076     329         IF( IATRB . EQ . 0 ) THEN                                  3076
3077     330   C                                                                3077
3078     331          RROR = HYDV( ICR , 1 )                                    3078
3079     332          UUOR = HYDV( ICR , 2 )                                    3079
3080     333          VVOR = HYDV( ICR , 3 )                                    3080
3081     334          WWOR = HYDV( ICR , 4 )                                    3081
3082     335          PPOR = HYDV( ICR , 5 )                                    3082
3083     336   C                                                                3083
3084     337          ELSE                                                      3084
3085     338   C                                                                3085
3086     339          RROR = RROL                                               3086
3087     340          UUOR = UUOL                                               3087
3088     341          VVOR = VVOL                                               3088
3089     342          WWOR = WWOL                                               3089
3090     343          PPOR = PPOL                                               3090
3091     344   C                                                                3091
3092     345          END IF                                                    3092
3093     346   C                                                                3093
3094     347          ROL( 4 ) = RROL                                           3094
3095     348          UOL( 4 ) = UUOL                                           3095
3096     349          VOL( 4 ) = VVOL                                           3096
3097     350          WOL( 4 ) = WWOL                                           3097
3098     351          POL( 4 ) = PPOL                                           3098
3099     352   C                                                                3099
3100     353          ROR( 4 ) = RROR                                           3100
3101     354          UOR( 4 ) = UUOR                                           3101
3102     355          VOR( 4 ) = VVOR                                           3102
3103     356          WOR( 4 ) = WWOR                                           3103
3104     357          POR( 4 ) = PPOR                                           3104
3105     358   C                                                                3105
3106     359          RMAX( KC ) = AMAX1( ROL( 1 ) , ROL( 2 ) , ROL( 3 ) , ROL( 4 ) ,  3106
3107     360         .                    ROR( 1 ) , ROR( 2 ) , ROR( 3 ) , ROR( 4 ) )  3107
3108     361          UMAX( KC ) = AMAX1( UOL( 1 ) , UOL( 2 ) , UOL( 3 ) , UOL( 4 ) ,  3108
3109     362         .                    UOR( 1 ) , UOR( 2 ) , UOR( 3 ) , UOR( 4 ) )  3109
3110     363          VMAX( KC ) = AMAX1( VOL( 1 ) , VOL( 2 ) , VOL( 3 ) , VOL( 4 ) ,  3110
3111     364         .                    VOR( 1 ) , VOR( 2 ) , VOR( 3 ) , VOR( 4 ) )  3111
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3112    365         WMAX( KC ) = AMAX1( WOL( 1 ) , WOL( 2 ) , WOL( 3 ) , WOL( 4 ) ,
3113    366        .                    WOR( 1 ) , WOR( 2 ) , WOR( 3 ) , WOR( 4 ) )
3114    367         PMAX( KC ) = AMAX1( POL( 1 ) , POL( 2 ) , POL( 3 ) , POL( 4 ) ,
3115    368        .                    POR( 1 ) , POR( 2 ) , POR( 3 ) , POR( 4 ) )
3116    369   C
3117    370         RMIN( KC ) = AMIN1( ROL( 1 ) , ROL( 2 ) , ROL( 3 ) , ROL( 4 ) ,
3118    371        .                    ROR( 1 ) , ROR( 2 ) , ROR( 3 ) , ROR( 4 ) )
3119    372         UMIN( KC ) = AMIN1( UOL( i ) , UOL( 2 ) , UOL( 3 ) , UOL( 4 ) ,
3120    373        .                    UOR( 1 ) , UOR( 2 ) , UOR( 3 ) , UOR( 4 ) )
3121    374         VMIN( KC ) = AMIN1( VOL( 1 ) , VOL( 2 ) , VOL( 3 ) , VOL( 4 ) ,
3122    375        .                    VOR( 1 ) , VOR( 2 ) , VOR( 3 ) , VOR( 4 ) )
3123    376         WMIN( KC ) = AMIN1( WOL( 1 ) , WOL( 2 ) , WOL( 3 ) , WOL( 4 ) ,
3124    377        .                    WOR( 1 ) , WOR( 2 ) , WOR( 3 ) , WOR( 4 ) )
3125    378         PMIN( KC ) = AMIN1( POL( 1 ) , POL( 2 ) , POL( 3 ) , POL( 4 ) ,
3126    379        .                    POR( 1 ) , POR( 2 ) , POR( 3 ) , POR( 4 ) )
3127    380   C
3128    381    150  CONTINUE
3129    382   C
3130    383         DO 180 IC = NC1 , NC2
3131    384            KC = IC - NC1 + 1
3132    385   C
3133    386            RRR( KC ) = RMAX( KC ) - HYDV( IC , 1 )
3134    387            RRL( KC ) = RMIN( KC ) - HYDV( IC , 1 )
3135    388            UUR( KC ) = UMAX( KC ) - HYDV( IC , 2 )
3136    389            UUL( KC ) = UMIN( KC ) - HYDV( IC , 2 )
3137    390            VVR( KC ) = VMAX( KC ) - HYDV( IC , 3 )
3138    391            VVL( KC ) = VMIN( KC ) - HYDV( IC , 3 )
3139    392            WWR( KC ) = WMAX( KC ) - HYDV( IC , 4 )
3140    393            WWL( KC ) = WMIN( KC ) - HYDV( IC , 4 )
3141    394            PPR( KC ) = PMAX( KC ) - HYDV( IC , 5 )
3142    395            PPL( KC ) = PMIN( KC ) - HYDV( IC , 5 )
3143    396   C
3144    397    180  CONTINUE
3145    398   C
3146    399         DO 170 IC = NC1 , NC2
3147    400            KC = IC - NC1 + 1
3148    401   C
3149    402          IS = JC( 5 , IC )
3150    403   C
3151    404          ICL = JS( 7 , IS )
3152    405          ICR = JS( 8 , IS )
3153    406   C
3154    407          XML = XYZMDL( 1 , IS ) - XC( 1 , ICL )
3155    408          YML = XYZMDL( 2 , IS ) - XC( 2 , ICL )
3156    409          ZML = XYZMDL( 3 , IS ) - XC( 3 , ICL )
3157    410   C
3158    411          RROL = 1.E-16 + RGRAD( ICL , 1 ) * XML +
3159    412        .                 RGRAD( ICL , 2 ) * YML + RGRAD( ICL , 3 ) * ZML
3160    413          UUOL = 1.E-16 + UGRAD( ICL , 1 ) * XML +
3161    414        .                 UGRAD( ICL , 2 ) * YML + UGRAD( ICL , 3 ) * ZML
3162    415          VVOL = 1.E-16 + VGRAD( ICL , 1 ) * XML +
3163    416        .                 VGRAD( ICL , 2 ) * YML + VGRAD( ICL , 3 ) * ZML
3164    417          WWOL = 1.E-16 + WGRAD( ICL , 1 ) * XML +
3165    418        .                 WGRAD( ICL , 2 ) * YML + WGRAD( ICL , 3 ) * ZML
3166    419          PPOL = 1.E-16 + PGRAD( ICL , 1 ) * XML +
3167    420        .                 PGRAD( ICL , 2 ) * YML + PGRAD( ICL , 3 ) * ZML
3168    421   C
3169    422         IATRB = JS( 9 , IS )
3170    423         IF( IATRB . EQ . 0 ) THEN
3171    424   C
3172    425          XMR = XYZMDL( 1 , IS ) - XC( 1 , ICR )
3173    426          YMR = XYZMDL( 2 , IS ) - XC( 2 , ICR )
3174    427          ZMR = XYZMDL( 3 , IS ) - XC( 3 , ICR )
3175    428   C
3176    429          RROR = 1.E-16 + RGRAD( ICR , 1 ) * XMR +
3177    430        .                 RGRAD( ICR , 2 ) * YMR + RGRAD( ICR , 3 ) * ZMR
3178    431          UUOR = 1.E-16 + UGRAD( ICR , 1 ) * XMR +
3179    432        .                 UGRAD( ICR , 2 ) * YMR + UGRAD( ICR , 3 ) * ZMR
3180    433          VVOR = 1.E-16 + VGRAD( ICR , 1 ) * XMR +
3181    434        .                 VGRAD( ICR , 2 ) * YMP + VGRAD( ICR , 3 ) * ZMR
3182    435          WWOR = 1.E-16 + WGRAD( ICR , 1 ) * XMR +
3183    436        .                 WGRAD( ICR , 2 ) * YMR + WGRAD( ICR , 3 ) * ZMR
3184    437          PPOR = 1.E-16 + PGRAD( ICR , 1 ) * XMR +
3185    438        .                 PGRAD( ICR , 2 ) * YMR + PGRAD( ICR , 3 ) * ZMR
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3186    439  C                                                                  3186
3187    440        ELSE                                                         3187
3188    441  C                                                                  3188
3189    442        RROR = RROL                                                  3189
3190    443        UUOR = UUOL                                                  3190
3191    444        VVOR = VVOL                                                  3191
3192    445        WWOR = WWOL                                                  3192
3193    446        PPOR = PPOL                                                  3193
3194    447  C                                                                  3194
3195    448        END IF                                                       3195
3196    449  C                                                                  3196
3197    450        ROL( 1 ) = 1. / RROL                                         3197
3198    451        UOL( 1 ) = 1. / UUOL                                         3198
3199    452        VOL( 1 ) = 1. / VVOL                                         3199
3200    453        WOL( 1 ) = 1. / WWOL                                         3200
3201    454        POL( 1 ) = 1. / PPOL                                         3201
3202    455  C                                                                  3202
3203    456        ROR( 1 ) = 1. / RROR                                         3203
3204    457        UOR( 1 ) = 1. / UUOR                                         3204
3205    458        VOR( 1 ) = 1. / VVOR                                         3205
3206    459        WOR( 1 ) = 1. / WWOR                                         3206
3207    460        POR( 1 ) = 1. / PPOR                                         3207
3208    461  C                                                                  3208
3209    462        IS = JC( 6 , IC )                                            3209
3210    463  C                                                                  3210
3211    464        ICL = JS( 7 , IS )                                           3211
3212    465        ICR = JS( 8 , IS )                                           3212
3213    466  C                                                                  3213
3214    467        XML = XYZMDL( 1 , IS ) - XC( 1 , ICL )                       3214
3215    468        YML = XYZMDL( 2 , IS ) - XC( 2 , ICL )                       3215
3216    469        ZML = XYZMDL( 3 , IS ) - XC( 3 , ICL )                       3216
3217    470  C                                                                  3217
3218    471        RROL = 1.E-16 + RGRAD( ICL , 1 ) * XML +                     3218
3219    472       .               RGRAD( ICL , 2 ) * YML + RGRAD( ICL , 3 ) * ZML 3219
3220    473        UUOL = 1.E-16 + UGRAD( ICL , 1 ) * XML +                     3220
3221    474       .               UGRAD( ICL , 2 ) * YML + UGRAD( ICL , 3 ) * ZML 3221
3222    475        VVOL = 1.E-16 + VGRAD( ICL , 1 ) * XML +                     3222
3223    476       .               VGRAD( ICL , 2 ) * YML + VGRAD( ICL , 3 ) * ZML 3223
3224    477        WWOL = 1.E-16 + WGRAD( ICL , 1 ) * XML +                     3224
3225    478       .               WGRAD( ICL , 2 ) * YML + WGRAD( ICL , 3 ) * ZML 3225
3226    479        PPOL = 1.E-16 + PGRAD( ICL , 1 ) * XML +                     3226
3227    480       .               PGRAD( ICL , 2 ) * YML + PGRAD( ICL , 3 ) * ZML 3227
3228    481  C                                                                  3228
3229    482       IATRB = JS( 9 , IS )                                         3229
3230    483       IF( IATRB . EQ . 0 ) THEN                                    3230
3231    484  C                                                                  3231
3232    485        XMR = XYZMDL( 1 , IS ) - XC( 1 , ICR )                       3232
3233    486        YMR = XYZMDL( 2 , IS ) - XC( 2 , ICR )                       3233
3234    487        ZMR = XYZMDL( 3 , IS ) - XC( 3 , ICR )                       3234
3235    488  C                                                                  3235
3236    489        RROR = 1.E-16 + RGRAD( ICR , 1 ) * XMR +                     3236
3237    490       .               RGRAD( ICR , 2 ) * YMR + RGRAD( ICR , 3 ) * ZMR 3237
3238    491        UUOR = 1.E-16 + UGRAD( ICR , 1 ) * XMR +                     3238
3239    492       .               UGRAD( ICR , 2 ) * YMR + UGRAD( ICR , 3 ) * ZMR 3239
3240    493        VVOR = 1.E-16 + VGRAD( ICR , 1 ) * XMR +                     3240
3241    494       .               VGRAD( ICR , 2 ) * YMR + VGRAD( ICR , 3 ) * ZMR 3241
3242    495        WWOR = 1.E-16 + WGRAD( ICR , 1 ) * XMR +                     3242
3243    496       .               WGRAD( ICR , 2 ) * YMR + WGRAD( ICR , 3 ) * ZMR 3243
3244    497        PPOR = 1.E-16 + PGRAD( ICR , 1 ) * XMR +                     3244
3245    498       .               PGRAD( ICR , 2 ) * YMR + PGRAD( ICR , 3 ) * ZMR 3245
3246    499  C                                                                  3246
3247    500        ELSE                                                         3247
3248    501  C                                                                  3248
3249    502        RROR = RROL                                                  3249
3250    503        UUOR = UUOL                                                  3250
3251    504        VVOR = VVOL                                                  3251
3252    505        WWOR = WWOL                                                  3252
3253    506        PPOR = PPOL                                                  3253
3254    507  C                                                                  3254
3255    508        END IF                                                       3255
3256    509  C                                                                  3256
3257    510        ROL( 2 ) = 1. / RROL                                         3257
3258    511        UOL( 2 ) = 1. / UUOL                                         3258
3259    512        VOL( 2 ) = 1. / VVOL                                         3259
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3260     513          WOL( 2 ) = 1. / WWOL                                                    3260
3261     514          POL( 2 ) = 1. / PPOL                                                    3261
3262     515    C                                                                             3262
3263     516          ROR( 2 ) = 1. / RROR                                                    3263
3264     517          UOR( 2 ) = 1. / UUOR                                                    3264
3265     518          VOR( 2 ) = 1. / VVOR                                                    3265
3266     519          WOR( 2 ) = 1. / WWOR                                                    3266
3267     520          POR( 2 ) = 1. / PPOR                                                    3267
3268     521    C                                                                             3268
3269     522          IS = JC( 7 , IC )                                                       3269
3270     523    C                                                                             3270
3271     524          ICL = JS( 7 , IS )                                                      3271
3272     525          ICR = JS( 8 , IS )                                                      3272
3273     526    C                                                                             3273
3274     527          XML = XYZMDL( 1 , IS ) - XC( 1 , ICL )                                  3274
3275     528          YML = XYZMDL( 2 , IS ) - XC( 2 , ICL )                                  3275
3276     529          ZML = XYZMDL( 3 , IS ) - XC( 3 , ICL )                                  3276
3277     530    C                                                                             3277
3278     531          RROL = 1.E-16 + RGRAD( ICL , 1 ) * XML +                                3278
3279     532         .               RGRAD( ICL , 2 ) * YML + RGRAD( ICL , 3 ) * ZML          3279
3280     533          UUOL = 1.E-16 + UGRAD( ICL , 1 ) * XML +                                3280
3281     534         .               UGRAD( ICL , 2 ) * YML + UGRAD( ICL , 3 ) * ZML          3281
3282     535          VVOL = 1.E-16 + VGRAD( ICL , 1 ) * XML +                                3282
3283     536         .               VGRAD( ICL , 2 ) * YML + VGRAD( ICL , 3 ) * ZML          3283
3284     537          WWOL = 1.E-16 + WGRAD( ICL , 1 ) * XML +                                3284
3285     538         .               WGRAD( ICL , 2 ) * YML + WGRAD( ICL , 3 ) * ZML          3285
3286     539          PPOL = 1.E-16 + PGRAD( ICL , 1 ) * XML +                                3286
3287     540         .               PGRAD( ICL , 2 ) * YML + PGRAD( ICL , 3 ) * ZML          3287
3288     541    C                                                                             3288
3289     542          IATRB = JS( 9 , IS )                                                    3289
3290     543          IF( IATRB . EQ . 0 ) THEN                                               3290
3291     544    C                                                                             3291
3292     545          XMR = XYZMDL( 1 , IS ) - XC( 1 , ICR )                                  3292
3293     546          YMR = XYZMDL( 2 , IS ) - XC( 2 , ICR )                                  3293
3294     547          ZMR = XYZMDL( 3 , IS ) - XC( 3 , ICR )                                  3294
3295     548    C                                                                             3295
3296     549          RROR = 1.E-16 + RGRAD( ICR , 1 ) * XMR +                                3296
3297     550         .               RGRAD( ICR , 2 ) * YMR + RGRAD( ICR , 3 ) * ZMR          3297
3298     551          UUOR = 1.E-16 + UGRAD( ICR , 1 ) * XMR +                                3298
3299     552         .               UGRAD( ICR , 2 ) * YMR + UGRAD( ICR , 3 ) * ZMR          3299
3300     553          VVOR = 1.E-16 + VGRAD( ICR , 1 ) * XMR +                                3300
3301     554         .               VGRAD( ICR , 2 ) * YMR + VGRAD( ICR , 3 ) * ZMR          3301
3302     555          WWOR = 1.E-16 + WGRAD( ICR , 1 ) * XMR +                                3302
3303     556         .               WGRAD( ICR , 2 ) * YMR + WGRAD( ICR , 3 ) * ZMR          3303
3304     557          PPOR = 1.E-16 + PGRAD( ICR , 1 ) * XMR +                                3304
3305     558         .               PGRAD( ICR , 2 ) * YMR + PGRAD( ICR , 3 ) * ZMR          3305
3306     559    C                                                                             3306
3307     560          ELSE                                                                    3307
3308     561    C                                                                             3308
3309     562          RROR = RROL                                                             3309
3310     563          UUOR = UUOL                                                             3310
3311     564          VVOR = VVOL                                                             3311
3312     565          WWOR = WWOL                                                             3312
3313     566          PPOR = PPOL                                                             3313
3314     567    C                                                                             3314
3315     568          END IF                                                                  3315
3316     569    C                                                                             3316
3317     570          ROL( 3 ) = 1. / RROL                                                    3317
3318     571          UOL( 3 ) = 1. / UUOL                                                    3318
3319     572          VOL( 3 ) = 1. / VVOL                                                    3319
3320     573          WOL( 3 ) = 1. / WWOL                                                    3320
3321     574          POL( 3 ) = 1. / PPOL                                                    3321
3322     575    C                                                                             3322
3323     576          ROR( 3 ) = 1. / RROR                                                    3323
3324     577          UOR( 3 ) = 1. / UUOR                                                    3324
3325     578          VOR( 3 ) = 1. / VVOR                                                    3325
3326     579          WOR( 3 ) = 1. / WWOR                                                    3326
3327     580          POR( 3 ) = 1. / PPOR                                                    3327
3328     581    C                                                                             3328
3329     582          IS = JC( 8 , IC )                                                       3329
3330     583    C                                                                             3330
3331     584          ICL = JS( 7 , IS )                                                      3331
3332     585          ICR = JS( 8 , IS )                                                      3332
3333     586    C                                                                             3333
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3334     587          XML = XYZMDL( 1 , IS ) - XC( 1 , ICL )                                3334
3335     588          YML = XYZMDL( 2 , IS ) - XC( 2 , ICL )                                3335
3336     589          ZML = XYZMDL( 3 , IS ) - XC( 3 , ICL )                                3336
3337     590    C                                                                           3337
3338     591          RROL = 1.E-16 + RGRAD( ICL , 1 ) * XML +                              3338
3339     592         .                RGRAD( ICL , 2 ) * YML + RGRAD( ICL , 3 ) * ZML     3339
3340     593          UUOL = 1.E-16 + UGRAD( ICL , 1 ) * XML +                              3340
3341     594         .                UGRAD( ICL , 2 ) * YML + UGRAD( ICL , 3 ) * ZML     3341
3342     595          VVOL = 1.E-16 + VGRAD( ICL , 1 ) * XML +                              3342
3343     596         .                VGRAD( ICL , 2 ) * YML + VGRAD( ICL , 3 ) * ZML     3343
3344     597          WWOL = 1.E-16 + WGRAD( ICL , 1 ) * XML +                              3344
3345     598         .                WGRAD( ICL , 2 ) * YML + WGRAD( ICL , 3 ) * ZML     3345
3346     599          PPOL = 1.E-16 + PGRAD( ICL , 1 ) * XML +                              3346
3347     600         .                PGRAD( ICL , 2 ) * YML + PGRAD( ICL , 3 ) * ZML     3347
3348     601    C                                                                           3348
3349     602          IATRB = JS( 9 , IS )                                                  3349
3350     603          IF( IATRB . EQ . 0 ) THEN                                             3350
3351     604    C                                                                           3351
3352     605          XMR = XYZMDL( 1 , IS ) - XC( 1 , ICR )                                3352
3353     606          YMR = XYZMDL( 2 , IS ) - XC( 2 , ICR )                                3353
3354     607          ZMR = XYZMDL( 3 , IS ) - XC( 3 , ICR )                                3354
3355     608    C                                                                           3355
3356     609          RROR = 1.E-16 + RGRAD( ICR , 1 ) * XMR +                              3356
3357     610         .                RGRAD( ICR , 2 ) * YMR + RGRAD( ICR , 3 ) * ZMR     3357
3358     611          UUOR = 1.E-16 + UGRAD( ICR , 1 ) * XMR +                              3358
3359     612         .                UGRAD( ICR , 2 ) * YMR + UGRAD( ICR , 3 ) * ZMR     3359
3360     613          VVOR = 1.E-16 + VGRAD( ICR , 1 ) * XMR +                              3360
3361     614         .                VGRAD( ICR , 2 ) * YMR + VGRAD( ICR , 3 ) * ZMR     3361
3362     615          WWOR = 1.E-16 + WGRAD( ICR , 1 ) * XMR +                              3362
3363     616         .                WGRAD( ICR , 2 ) * YMR + WGRAD( ICR , 3 ) * ZMR     3363
3364     617          PPOR = 1.E-16 + PGRAD( ICR , 1 ) * XMR +                              3364
3365     618         .                PGRAD( ICR , 2 ) * YMR + PGRAD( ICR , 3 ) * ZMR     3365
3366     619    C                                                                           3366
3367     620          ELSE                                                                  3367
3368     621    C                                                                           3368
3369     622          RROR = RROL                                                           3369
3370     623          UUOR = UUOL                                                           3370
3371     624          VVOR = VVOL                                                           3371
3372     625          WWOR = WWOL                                                           3372
3373     626          PPOR = PPOL                                                           3373
3374     627    C                                                                           3374
3375     628          END IF                                                                3375
3376     629    C                                                                           3376
3377     630          ROL( 4 ) = 1. / RROL                                                  3377
3378     631          UOL( 4 ) = 1. / UUOL                                                  3378
3379     632          VOL( 4 ) = 1. / VVOL                                                  3379
3380     633          WOL( 4 ) = 1. / WWOL                                                  3380
3381     634          POL( 4 ) = 1. / PPOL                                                  3381
3382     635    C                                                                           3382
3383     636          ROR( 4 ) = 1. / RROR                                                  3383
3384     637          UOR( 4 ) = 1. / UUOR                                                  3384
3385     638          VOR( 4 ) = 1. / VVOR                                                  3385
3386     639          WOR( 4 ) = 1. / WWOR                                                  3386
3387     640          POR( 4 ) = 1. / PPOR                                                  3387
3388     641    C                                                                           3388
3389     642          ISNR = SIGN( 1. , ROR( 1 ) )                                          3389
3390     643          ISNL = SIGN( 1. , ROL( 1 ) )                                          3390
3391     644    C                                                                           3391
3392     645          TEMPR = ( 1 + ISNR ) * RRR( KC ) +                                    3392
3393     646         .        ( 1 - ISNR ) * RRL( KC )                                     3393
3394     647          RUVPR1 = 0.5 * TEMPR * ROR( 1 )                                       3394
3395     648    C                                                                           3395
3396     649          TEMPL = ( 1 + ISNL ) * RRR( KC ) +                                    3396
3397     650         .        ( 1 - ISNL ) * RRL( KC )                                     3397
3398     651          RUVPL1 = 0.5 * TEMPL * ROL( 1 )                                       3398
3399     652    C                                                                           3399
3400     653          ISNR = SIGN( 1. , ROR( 2 ) )                                          3400
3401     654          ISNL = SIGN( 1. , ROL( 2 ) )                                          3401
3402     655    C                                                                           3402
3403     656          TEMPR = ( 1 + ISNR ) * RRR( KC ) +                                    3403
3404     657         .        ( 1 - ISNR ) * RRL( KC )                                     3404
3405     658          RUVPR2 = 0.5 * TEMPR * ROR( 2 )                                       3405
3406     659    C                                                                           3406
3407     660          TEMPL = ( 1 + ISNL ) * RRR( KC ) +                                    3407
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3408     661         .         ( 1 - ISNL ) * RRL( KC )                                  3408
3409     662           RUVPL2 = 0.5 * TEMPL * ROL( 2 )                                 3409
3410     663   C                                                                         3410
3411     664           ISNR = SIGN( 1. , ROR( 3 ) )                                    3411
3412     665           ISNL = SIGN( 1. , ROL( 3 ) )                                    3412
3413     666   C                                                                         3413
3414     667           TEMPR = ( 1 + ISNR ) * RRR( KC ) +                              3414
3415     668         .         ( 1 - ISNR ) * RRL( KC )                                  3415
3416     669           RUVPR3 = 0.5 * TEMPR * ROR( 3 )                                 3416
3417     670   C                                                                         3417
3418     671           TEMPL = ( 1 + ISNL ) * RRR( KC ) +                              3418
3419     672         .         ( 1 - ISNL ) * RRL( KC )                                  3419
3420     673           RUVPL3 = 0.5 * TEMPL * ROL( 3 )                                 3420
3421     674   C                                                                         3421
3422     675           ISNR = SIGN( 1. , ROR( 4 ) )                                    3422
3423     676           ISNL = SIGN( 1. , ROL( 4 ) )                                    3423
3424     677   C                                                                         3424
3425     678           TEMPR = ( 1 + ISNR ) * RRR( KC ) +                              3425
3426     679         .         ( 1 - ISNR ) * RRL( KC )                                  3426
3427     680           RUVPR4 = 0.5 * TEMPR * ROR( 4 )                                 3427
3428     681   C                                                                         3428
3429     682           TEMPL = ( 1 + ISNL ) * RRR( KC ) +                              3429
3430     683         .         ( 1 - ISNL ) * RRL( KC )                                  3430
3431     684           RUVPL4 = 0.5 * TEMPL * ROL( 4 )                                 3431
3432     685   C                                                                         3432
3433     686           RMIN( KC ) = AMIN1( 1. , RUVPR1 , RUVPL1 , RUVPR2 , RUVPL2 ,    3433
3434     687         .                           RUVPR3 , RUVPL3 , RUVPR4 , RUVPL4 )   3434
3435     688   C                                                                         3435
3436     689           ISNR = SIGN( 1. , UOR( 1 ) )                                    3436
3437     690           ISNL = SIGN( 1. , UOL( 1 ) )                                    3437
3438     691   C                                                                         3438
3439     692           TEMPR = ( 1 + ISNR ) * UUR( KC ) +                              3439
3440     693         .         ( 1 - ISNR ) * UUL( KC )                                  3440
3441     694           RUVPR1 = 0.5 * TEMPR * UOR( 1 )                                 3441
3442     695   C                                                                         3442
3443     696           TEMPL = ( 1 + ISNL ) * UUR( KC ) +                              3443
3444     697         .         ( 1 - ISNL ) * UUL( KC )                                  3444
3445     698           RUVPL1 = 0.5 * TEMPL * UOL( 1 )                                 3445
3446     699   C                                                                         3446
3447     700           ISNR = SIGN( 1. , UOR( 2 ) )                                    3447
3448     701           ISNL = SIGN( 1. , UOL( 2 ) )                                    3448
3449     702   C                                                                         3449
3450     703           TEMPR = ( 1 + ISNR ) * UUR( KC ) +                              3450
3451     704         .         ( 1 - ISNR ) * UUL( KC )                                  3451
3452     705           RUVPR2 = 0.5 * TEMPR * UOR( 2 )                                 3452
3453     706   C                                                                         3453
3454     707           TEMPL = ( 1 + ISNL ) * UUR( KC ) +                              3454
3455     708         .         ( 1 - ISNL ) * UUL( KC )                                  3455
3456     709           RUVPL2 = 0.5 * TEMPL * UOL( 2 )                                 3456
3457     710   C                                                                         3457
3458     711           ISNR = SIGN( 1. , UOR( 3 ) )                                    3458
3459     712           ISNL = SIGN( 1. , UOL( 3 ) )                                    3459
3460     713   C                                                                         3460
3461     714           TEMPR = ( 1 + ISNR ) * UUR( KC ) +                              3461
3462     715         .         ( 1 - ISNR ) * UUL( KC )                                  3462
3463     716           RUVPR3 = 0.5 * TEMPR * UOR( 3 )                                 3463
3464     717   C                                                                         3464
3465     718           TEMPL = ( 1 + ISNL ) * UUR( KC ) +                              3465
3466     719         .         ( 1 - ISNL ) * UUL( KC )                                  3466
3467     720           RUVPL3 = 0.5 * TEMPL * UOL( 3 )                                 3467
3468     721   C                                                                         3468
3469     722           ISNR = SIGN( 1. , UOR( 4 ) )                                    3469
3470     723           ISNL = SIGN( 1. , UOL( 4 ) )                                    3470
3471     724   C                                                                         3471
3472     725           TEMPR = ( 1 + ISNR ) * UUR( KC ) +                              3472
3473     726         .         ( 1 - ISNR ) * UUL( KC )                                  3473
3474     727           RUVPR4 = 0.5 * TEMPR * UOR( 4 )                                 3474
3475     728   C                                                                         3475
3476     729           TEMPL = ( 1 + ISNL ) * UUR( KC ) +                              3476
3477     730         .         ( 1 - ISNL ) * UUL( KC )                                  3477
3478     731           RUVPL4 = 0.5 * TEMPL * UOL( 4 )                                 3478
3479     732   C                                                                         3479
3480     733           UMIN( KC ) = AMIN1( 1. , RUVPR1 , RUVPL1 , RUVPR2 , RUVPL2 ,    3480
3481     734         .                           RUVPR3 , RUVPL3 , RUVPR4 , RUVPL4 )   3481
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3482    735  C                                                                3482
3483    736         ISNR = SIGN( 1. , VOR( 1 ) )                              3483
3484    737         ISNL = SIGN( 1. , VOL( 1 ) )                              3484
3485    738  C                                                                3485
3486    739         TEMPR = ( 1 + ISNR ) * VVR( KC ) +                        3486
3487    740        .        ( 1 - ISNR ) * VVL( KC )                          3487
3488    741         RUVPR1 = 0.5 * TEMPR * VOR( 1 )                           3488
3489    742  C                                                                3489
3490    743         TEMPL = ( 1 + ISNL ) * VVR( KC ) +                        3490
3491    744        .        ( 1 - ISNL ) * VVL( KC )                          3491
3492    745         RUVPL1 = 0.5 * TEMPL * VOL( 1 )                           3492
3493    746  C                                                                3493
3494    747         ISNR = SIGN( 1. , VOR( 2 ) )                              3494
3495    748         ISNL = SIGN( 1. , VOL( 2 ) )                              3495
3496    749  C                                                                3496
3497    750         TEMPR = ( 1 + ISNR ) * VVR( KC ) +                        3497
3498    751        .        ( 1 - ISNR ) * VVL( KC )                          3498
3499    752         RUVPR2 = 0.5 * TEMPR * VOR( 2 )                           3499
3500    753  C                                                                3500
3501    754         TEMPL = ( 1 + ISNL ) * VVR( KC ) +                        3501
3502    755        .        ( 1 - ISNL ) * VVL( KC )                          3502
3503    756         RUVPL2 = 0.5 * TEMPL * VOL( 2 )                           3503
3504    757  C                                                                3504
3505    758         ISNR = SIGN( 1. , VOR( 3 ) )                              3505
3506    759         ISNL = SIGN( 1. , VOL( 3 ) )                              3506
3507    760  C                                                                3507
3508    761         TEMPR = ( 1 + ISNR ) * VVR( KC ) +                        3508
3509    762        .        ( 1 - ISNR ) * VVL( KC )                          3509
3510    763         RUVPR3 = 0.5 * TEMPR * VOR( 3 )                           3510
3511    764  C                                                                3511
3512    765         TEMPL = ( 1 + ISNL ) * VVR( KC ) +                        3512
3513    766        .        ( 1 - ISNL ) * VVL( KC )                          3513
3514    767         RUVPL3 = 0.5 * TEMPL * VOL( 3 )                           3514
3515    768  C                                                                3515
3516    769         ISNR = SIGN( 1. , VOR( 4 ) )                              3516
3517    770         ISNL = SIGN( 1. , VOL( 4 ) )                              3517
3518    771  C                                                                3518
3519    772         TEMPR = ( 1 + ISNR ) * VVR( KC ) +                        3519
3520    773        .        ( 1 - ISNR ) * VVL( KC )                          3520
3521    774         RUVPR4 = 0.5 * TEMPR * VOR( 4 )                           3521
3522    775  C                                                                3522
3523    776         TEMPL = ( 1 + ISNL ) * VVR( KC ) +                        3523
3524    777        .        ( 1 - ISNL ) * VVL( KC )                          3524
3525    778         RUVPL4 = 0.5 * TEMPL * VOL( 4 )                           3525
3526    779  C                                                                3526
3527    780         VMIN( KC ) = AMIN1( 1. , RUVPR1 , RUVPL1 , RUVPR2 , RUVPL2 ,3527
3528    781        .                           RUVPR3 , RUVPL3 , RUVPR4 , RUVPL4 )3528
3529    782  C                                                                3529
3530    783         ISNR = SIGN( 1. , WOR( 1 ) )                              3530
3531    784         ISNL = SIGN( 1. , WOL( 1 ) )                              3531
3532    785  C                                                                3532
3533    786         TEMPR = ( 1 + ISNR ) * WWR( KC ) +                        3533
3534    787        .        ( 1 - ISNR ) * WWL( KC )                          3534
3535    788         RUVPR1 = 0.5 * TEMPR * WOR( 1 )                           3535
3536    789  C                                                                3536
3537    790         TEMPL = ( 1 + ISNL ) * WWR( KC ) +                        3537
3538    791        .        ( 1 - ISNL ) * WWL( KC )                          3538
3539    792         RUVPL1 = 0.5 * TEMPL * WOL( 1 )                           3539
3540    793  C                                                                3540
3541    794         ISNR = SIGN( 1. , WOR( 2 ) )                              3541
3542    795         ISNL = SIGN( 1. , WOL( 2 ) )                              3542
3543    796  C                                                                3543
3544    797         TEMPR = ( 1 + ISNR ) * WWR( KC ) +                        3544
3545    798        .        ( 1 - ISNR ) * WWL( KC )                          3545
3546    799         RUVPR2 = 0.5 * TEMPR * WOR( 2 )                           3546
3547    800  C                                                                3547
3548    801         TEMPL = ( 1 + ISNL ) * WWR( KC ) +                        3548
3549    802        .        ( 1 - ISNL ) * WWL( KC )                          3549
3550    803         RUVPL2 = 0.5 * TEMPL * WOL( 2 )                           3550
3551    804  C                                                                3551
3552    805         ISNR = SIGN( 1. , WOR( 3 ) )                              3552
3553    806         ISNL = SIGN( 1. , WOL( 3 ) )                              3553
3554    807  C                                                                3554
3555    808         TEMPR = ( 1 + ISNR ) * WWR( KC ) +                        3555
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3556     809          .         ( 1 - ISNR ) * WWL( KC )                                    3556
3557     810            RUVPR3 = 0.5 * TEMPR * WOR( 3 )                                   3557
3558     811    C                                                                          3558
3559     812            TEMPL = ( 1 + ISNL ) * WWR( KC ) +                                 3559
3560     813          .         ( 1 - ISNL ) * WWL( KC )                                    3560
3561     814            RUVPL3 = 0.5 * TEMPL * WOL( 3 )                                   3561
3562     815    C                                                                          3562
3563     816            ISNR = SIGN( 1. , WOR( 4 ) )                                      3563
3564     817            ISNL = SIGN( 1. , WOL( 4 ) )                                      3564
3565     818    C                                                                          3565
3566     819            TEMPR = ( 1 + ISNR ) * WWR( KC ) +                                3566
3567     820          .         ( 1 - ISNR ) * WWL( KC )                                    3567
3568     821            RUVPR4 = 0.5 * TEMPR * WOR( 4 )                                   3568
3569     822    C                                                                          3569
3570     823            TEMPL = ( 1 + ISNL ) * WWR( KC ) +                                3570
3571     824          .         ( 1 - ISNL ) * WWL( KC )                                    3571
3572     825            RUVPL4 = 0.5 * TEMPL * WOL( 4 )                                   3572
3573     826    C                                                                          3573
3574     827            WMIN( KC ) = AMIN1( 1. , RUVPR1 , RUVPL1 , RUVPR2 , RUVPL2 ,      3574
3575     828          .                     RUVPR3 , RUVPL3 , RUVPR4 , RUVPL4 )          3575
3576     829    C                                                                          3576
3577     830            ISNR = SIGN( 1. , POR( 1 ) )                                      3577
3578     831            ISNL = SIGN( 1. , POL( 1 ) )                                      3578
3579     832    C                                                                          3579
3580     833            TEMPR = ( 1 + ISNR ) * PPR( KC ) +                                3580
3581     834          .         ( 1 - ISNR ) * PPL( KC )                                    3581
3582     835            RUVPR1 = 0.5 * TEMPR * POR( 1 )                                   3582
3583     836    C                                                                          3583
3584     837            TEMPL = ( 1 + ISNL ) * PPR( KC ) +                                3584
3585     838          .         ( 1 - ISNL ) * PPL( KC )                                    3585
3586     839            RUVPL1 = 0.5 * TEMPL * POL( 1 )                                   3586
3587     840    C                                                                          3587
3588     841            ISNR = SIGN( 1. , POR( 2 ) )                                      3588
3589     842            ISNL = SIGN( 1. , POL( 2 ) )                                      3589
3590     843    C                                                                          3590
3591     844            TEMPR = ( 1 + ISNR ) * PPR( KC ) +                                3591
3592     845          .         ( 1 - ISNR ) * PPL( KC )                                    3592
3593     846            RUVPR2 = 0.5 * TEMPR * POR( 2 )                                   3593
3594     847    C                                                                          3594
3595     848            TEMPL = ( 1 + ISNL ) * PPR( KC ) +                                3595
3596     849          .         ( 1 - ISNL ) * PPL( KC )                                    3596
3597     850            RUVPL2 = 0.5 * TEMPL * POL( 2 )                                   3597
3598     851    C                                                                          3598
3599     852            ISNR = SIGN( 1. , POR( 3 ) )                                      3599
3600     853            ISNL = SIGN( 1. , POL( 3 ) )                                      3600
3601     854    C                                                                          3601
3602     855            TEMPR = ( 1 + ISNR ) * PPR( KC ) +                                3602
3603     856          .         ( 1 - ISNR ) * PPL( KC )                                    3603
3604     857            RUVPR3 = 0.5 * TEMPR * POR( 3 )                                   3604
3605     858    C                                                                          3605
3606     859            TEMPL = ( 1 + ISNL ) * PPR( KC ) +                                3606
3607     860          .         ( 1 - ISNL ) * PPL( KC )                                    3607
3608     861            RUVPL3 = 0.5 * TEMPL * POL( 3 )                                   3608
3609     862    C                                                                          3609
3610     863            ISNR = SIGN( 1. , POR( 4 ) )                                      3610
3611     864            ISNL = SIGN( 1. , POL( 4 ) )                                      3611
3612     865    C                                                                          3612
3613     866            TEMPR = ( 1 + ISNR ) * PPR( KC ) +                                3613
3614     867          .         ( 1 - ISNR ) * PPL( KC )                                    3614
3615     868            RUVPR4 = 0.5 * TEMPR * POR( 4 )                                   3615
3616     869    C                                                                          3616
3617     870            TEMPL = ( 1 + ISNL ) * PPR( KC ) +                                3617
3618     871          .         ( 1 - ISNL ) * PPL( KC )                                    3618
3619     872            RUVPL4 = 0.5 * TEMPL * POL( 4 )                                   3619
3620     873    C                                                                          3620
3621     874            PMIN( KC ) = AMIN1( 1. , RUVPR1 , RUVPL1 , RUVPR2 , RUVPL2 ,      3621
3622     875          .                     RUVPR3 , RUVPL3 , RUVPR4 , RUVPL4 )          3622
3623     876    C                                                                          3623
3624     877     170    CONTINUE                                                          3624
3625     878    C                                                                          3625
3626     879          DO 330 IH = 1 , 3                                                   3626
3627     880    C                                                                          3627
3628     881          DO 330 IC = NC1 , NC2                                               3628
3629     882             KC = IC - NC1 + 1                                                3629
```

```
3630     883   C                                                              3630
3631     884         RGRAD( IC , IH ) = RGRAD( IC , IH ) * RMIN( KC )         3631
3632     885         UGRAD( IC , IH ) = UGRAD( IC , IH ) * UMIN( KC )         3632
3633     886         VGRAD( IC , IH ) = VGRAD( IC , IH ) * VMIN( KC )         3633
3634     887         WGRAD( IC , IH ) = WGRAD( IC , IH ) * WMIN( KC )         3634
3635     888         PGRAD( IC , IH ) = PGRAD( IC , IH ) * PMIN( KC )         3635
3636     889   C                                                              3636
3637     890    330  CONTINUE                                                 3637
3638     891   C                                                              3638
3639     892       NC1 = NC2 + 1                                              3639
3640     893       NC2 = NC2 + NOFVEC( INC + 1 )                              3640
3641     894    80   CONTINUE                                                 3641
3642     895   C                                                              3642
3643     896       CALL FCHART                                                3643
3644     897   C                                                              3644
3645     898       RETURN                                                     3645
3646     899       END                                                        3646
3647     900   C                                                              3647
```



```
3648       1       SUBROUTINE FIRST                                          3648
3649       2   C                                                             3649
3650       3   C-------------------------------------------------------------I3650
3651       4   C                                                             I3651
3652       5   C      FIRST IS TO BY PASS GRADIENT AND CHARACTERSTIC COMPUTATION I3652
3653       6   C                                                             I3653
3654       7   C-------------------------------------------------------------I3654
3655       8   C                                                             3655
3656       9       include     'dmsh00.h'                                    3656
3657      10       include     'dhydm0.h'                                    3657
3658      11       include     'dphsm0.h'                                    3658
3659      12       include     'dmtrl0.h'                                    3659
3660      13   C                                                             3660
3661      14       DO 110 IS = 1 , NS                                        3661
3662      15   C                                                             3662
3663      16        ICL = JS( 7 , IS )                                       3663
3664      17        ICR = JS( 8 , IS )                                       3664
3665      18   C                                                             3665
3666      19        RL( IS ) = HYDV( ICL , 1 )                               3666
3667      20        UL( IS ) = HYDV( ICL , 2 ) * XN( IS ) +                  3667
3668      21     .             HYDV( ICL , 3 ) * YN( IS ) +                  3668
3669      22     .             HYDV( ICL , 4 ) * ZN( IS )                    3669
3670      23        VL( IS ) = HYDV( ICL , 2 ) * XP( IS ) +                  3670
3671      24     .             HYDV( ICL , 3 ) * YP( IS ) +                  3671
3672      25     .             HYDV( ICL , 4 ) * ZP( IS )                    3672
3673      26        WL( IS ) = HYDV( ICL , 2 ) * XT( IS ) +                  3673
3674      27     .             HYDV( ICL , 3 ) * YT( IS ) +                  3674
3675      28     .             HYDV( ICL , 4 ) * ZT( IS )                    3675
3676      29        PL( IS ) = HYDV( ICL , 5 )                               3676
3677      30        AL( IS ) = HYDV( ICL , 6 )                               3677
3678      31        GL( IS ) = HYDV( ICL , 7 )                               3678
3679      32        EL( IS ) = HYDV( ICL , 8 )                               3679
3680      33   C                                                             3680
3681      34        IATRB = JS( 9 , IS )                                     3681
3682      35        IF( IATRB . EQ . 0 ) THEN                                3682
3683      36   C                                                             3683
3684      37        RR( IS ) = HYDV( ICR , 1 )                               3684
3685      38        UR( IS ) = HYDV( ICR , 2 ) * XN( IS ) +                  3685
3686      39     .             HYDV( ICR , 3 ) * YN( IS ) +                  3686
3687      40     .             HYDV( ICR , 4 ) * ZN( IS )                    3687
3688      41        VR( IS ) = HYDV( ICR , 2 ) * XP( IS ) +                  3688
3689      42     .             HYDV( ICR , 3 ) * YP( IS ) +                  3689
3690      43     .             HYDV( ICR , 4 ) * ZP( IS )                    3690
3691      44        WR( IS ) = HYDV( ICR , 2 ) * XT( IS ) +                  3691
3692      45     .             HYDV( ICR , 3 ) * YT( IS ) +                  3692
3693      46     .             HYDV( ICR , 4 ) * ZT( IS )                    3693
3694      47        PR( IS ) = HYDV( ICR , 5 )                               3694
3695      48        AR( IS ) = HYDV( ICR , 6 )                               3695
3696      49        GR( IS ) = HYDV( ICR , 7 )                               3696
3697      50        ER( IS ) = HYDV( ICR , 8 )                               3697
3698      51   C                                                             3698
3699      52       ELSE                                                      3699
3700      53   C                                                             3700
```

```
3701      54          IF( IATRB . EQ . 8 ) THEN                                                3701
3702      55    C                                                                              3702
3703      56           RR( IS ) = RIN                                                          3703
3704      57           UR( IS ) = UIN * XN( IS ) + VIN * YN( IS ) + WIN * ZN( IS )             3704
3705      58           VR( IS ) = UIN * XP( IS ) + VIN * YP( IS ) + WIN * ZP( IS )             3705
3706      59           WR( IS ) = UIN * XT( IS ) + VIN * YT( IS ) + WIN * ZT( IS )             3706
3707      60           PR( IS ) = PIN                                                          3707
3708      61           AR( IS ) = AL( IS )                                                     3708
3709      62           GR( IS ) = GL( IS )                                                     3709
3710      63           ER( IS ) = EL( IS )                                                     3710
3711      64    C                                                                              3711
3712      65          END IF                                                                   3712
3713      66    C                                                                              3713
3714      67          IF( IATRB . EQ . 7 ) THEN                                                3714
3715      68    C                                                                              3715
3716      69             RR( IS ) = RL( IS )                                                   3716
3717      70             UR( IS ) = UL( IS )                                                   3717
3718      71             VR( IS ) = VL( IS )                                                   3718
3719      72             WR( IS ) = WL( IS )                                                   3719
3720      73             PR( IS ) = PL( IS )                                                   3720
3721      74             AR( IS ) = AL( IS )                                                   3721
3722      75             GR( IS ) = GL( IS )                                                   3722
3723      76             ER( IS ) = EL( IS )                                                   3723
3724      77    C                                                                              3724
3725      78          END IF                                                                   3725
3726      79    C                                                                              3726
3727      80          IF( IATRB . EQ . 6 ) THEN                                                3727
3728      81    C                                                                              3728
3729      82             RR( IS ) = RL( IS )                                                   3729
3730      83             UR( IS ) = - UL( IS )                                                 3730
3731      84             VR( IS ) = VL( IS )                                                   3731
3732      85             WR( IS ) = WL( IS )                                                   3732
3733      86             PR( IS ) = PL( IS )                                                   3733
3734      87             AR( IS ) = AL( IS )                                                   3734
3735      88             GR( IS ) = GL( IS )                                                   3735
3736      89             ER( IS ) = EL( IS )                                                   3736
3737      90    C                                                                              3737
3738      91          END IF                                                                   3738
3739      92    C                                                                              3739
3740      93          END IF                                                                   3740
3741      94    C                                                                              3741
3742      95     110  CONTINUE                                                                3742
3743      96    C                                                                              3743
3744      97          RETURN                                                                   3744
3745      98          END                                                                      3745
3746      99    C                                                                              3746
```

```
      1         SUBROUTINE FCHART
      2   C
      3   C-----------------------------------------------------------------I
      4   C                                                                 I
      5   C      CHARCT INTRODUCE CORRECTION FOR SECOND ORDER CALCULATION   I
      6   C                                                                 I
      7   C-----------------------------------------------------------------I
      8   C
      9         include     'dmsh00.h'
     10         include     'dhydm0.h'
     11         include     'dphsm0.h'
     12         include     'dmtrl0.h'
     13   C
     14         REAL ZZLEFT(128),ZOLEFT(128),ZPLEFT(128),ZMLEFT(128)
     15         REAL ZZRIGT(128),ZORIGT(128),ZPRIGT(128),ZMRIGT(128)
     16         REAL UPLEFT(128),UMLEFT(128),URLEFT(128)
     17         REAL UPRIGT(128),UMRIGT(128),URRIGT(128)
     18         REAL UVLEFT(128),UVRIGT(128),CNLEFT(128),CNRIGT(128)
     19         REAL RLEFTT(128),ULEFTT(128),VLEFTT(128),PLEFTT(128),
    20     .     ALEFTT(128)
     21         REAL RRIGHT(128),URIGHT(128),VRIGHT(128),PRIGHT(128),
    22     .     ARIGHT(128)
     23   C
     24         NS1 = 1
     25         NS2 = NOFVES( 1 )
     26         DO 90 INS = 1 , NVEES
     27   C
     28         DO 110 IS = NS1 , NS2
     29            KS = IS - NS1 + 1
     30   C
     31          ICL = JS( 7 , IS )
     32          ICR = JS( 8 , IS )
     33   C
     34          GL( IS ) = HYDV( ICL , 7 )
     35          CNLFTS = GL( IS )  * HYDV( ICL , 5 ) / HYDV( ICL , 1 )
     36          CNLFT = SQRT( CNLFTS )
     37   C
     38         IATRB = JS( 9 , IS )
     39         IF( IATRB . EQ . 0 ) THEN
     40   C
     41          XYZ = 1. / XS( 5 , IS )
     42            XXN = ( XC( 1 , ICR ) - XC( 1 , ICL ) ) * XYZ
     43            YYN = ( XC( 2 , ICR ) - XC( 2 , ICL ) ) * XYZ
     44            ZZN = ( XC( 3 , ICR ) - XC( 3 , ICL ) ) * XYZ
     45   C
     46            UVLFT = HYDV( ICL , 2 ) * XXN +
    47     .              HYDV( ICL , 3 ) * YYN +
    48     .              HYDV( ICL , 4 ) * ZZN
     49   C
     50          GR( IS ) = HYDV( ICR , 7 )
     51          CNRGTS = GR( IS ) * HYDV( ICR , 5 ) / HYDV( ICR , 1 )
     52          CNRGT = SQRT( CNRGTS )
     53   C
     54            UVRGT = HYDV( ICR , 2 ) * XXN +
    55     .              HYDV( ICR , 3 ) * YYN +
    56     .              HYDV( ICR , 4 ) * ZZN
     57   C
     58          ELSE
     59   C
     60          CNRGT = CNLFT
     61   C
     62          XYZ = 1. / XS( 5 , IS )
     63            XXN = ( XYZMDL( 1 , IS ) - XC( 1 , ICL ) ) * XYZ
     64            YYN = ( XYZMDL( 2 , IS ) - XC( 2 , ICL ) ) * XYZ
     65            ZZN = ( XYZMDL( 3 , IS ) - XC( 3 , ICL ) ) * XYZ
     66   C
     67            UVLFT = HYDV( ICL , 2 ) * XXN +
    68     .              HYDV( ICL , 3 ) * YYN +
    69     .              HYDV( ICL , 4 ) * ZZN
     70   C
     71            UVRGT = UVLFT
     72            GR( IS ) = GL( IS )
     73   C
     74          END IF
```

```
3821      75  C                                                                  3821
3822      76            CNLEFT( KS ) = CNLFT                                    3822
3823      77            CNRIGT( KS ) = CNRGT                                    3823
3824      78  C                                                                  3824
3825      79            UVLEFT( KS ) = UVLFT                                    3825
3826      80            UVRIGT( KS ) = UVRGT                                    3826
3827      81  C                                                                  3827
3828      82   110  CONTINUE                                                     3828
3829      83  C                                                                  3829
3830      84         DO 130 KS = 1 , NOFVES( INS )                             3830
3831      85  C                                                                  3831
3832      86         ZZLEFT( KS ) =   .5 * ( UVLEFT( KS ) + CNLEFT( KS ) ) * DTT 3832
3833      87         ZZRIGT( KS ) = - .5 * ( UVRIGT( KS ) - CNRIGT( KS ) ) * DTT 3833
3834      88  C                                                                  3834
3835      89   130  CONTINUE                                                     3835
3836      90  C                                                                  3836
3837      91  C  CHARACTERISTICS LOCATIONS                                       3837
3838      92  C                                                                  3838
3839      93         DO 140 KS = 1 , NOFVES( INS )                             3839
3840      94  C                                                                  3840
3841      95         IF( ZZLEFT( KS ) . LT . 0. ) ZZLEFT( KS ) = 0.            3841
3842      96         IF( ZZRIGT( KS ) . LT . 0. ) ZZRIGT( KS ) = 0.            3842
3843      97  C                                                                  3843
3844      98   140  CONTINUE                                                     3844
3845      99  C                                                                  3845
3846     100         DO 150 KS = 1 , NOFVES( INS )                             3846
3847     101  C                                                                  3847
3848     102         ZOLEFT( KS ) =   .5 * UVLEFT( KS ) * DTT                  3848
3849     103         ZORIGT( KS ) = - .5 * UVRIGT( KS ) * DTT                  3849
3850     104         ZPLEFT( KS ) =   .5 * ( UVLEFT( KS ) + CNLEFT( KS ) ) * DTT 3850
3851     105         ZPRIGT( KS ) = - .5 * ( UVRIGT( KS ) + CNRIGT( KS ) ) * DTT 3851
3852     106         ZMLEFT( KS ) =   .5 * ( UVLEFT( KS ) - CNLEFT( KS ) ) * DTT 3852
3853     107         ZMRIGT( KS ) = - .5 * ( UVRIGT( KS ) - CNRIGT( KS ) ) * DTT 3853
3854     108  C                                                                  3854
3855     109   150  CONTINUE                                                     3855
3856     110  C                                                                  3856
3857     111  C  FIRST GUESS LEFT AND RIGHT VARIABLES, LINEAR INTERPOLATON       3857
3858     112  C                                                                  3858
3859     113         DO 160 IS = NS1 , NS2                                     3859
3860     114             KS = IS - NS1 + 1                                     3860
3861     115  C                                                                  3861
3862     116          ICL = JS( 7 , IS )                                        3862
3863     117          ICR = JS( 8 , IS )                                        3863
3864     118  C                                                                  3864
3865     119         IATRB = JS( 9 , IS )                                      3865
3866     120         IF( IATRB . EQ . 0 ) THEN                                 3866
3867     121  C                                                                  3867
3868     122          XYZ = 1. / XS( 5 , IS )                                   3868
3869     123            XXN = ( XC( 1 , ICR ) - XC( 1 , ICL ) ) * XYZ           3869
3870     124            YYN = ( XC( 2 , ICR ) - XC( 2 , ICL ) ) * XYZ           3870
3871     125            ZZN = ( XC( 3 , ICR ) - XC( 3 , ICL ) ) * XYZ           3871
3872     126  C                                                                  3872
3873     127            XXL = ( XYZMDL( 1 , IS ) - XC( 1 , ICL ) )              3873
3874     128            YYL = ( XYZMDL( 2 , IS ) - XC( 2 , ICL ) )              3874
3875     129            ZZL = ( XYZMDL( 3 , IS ) - XC( 3 , ICL ) )              3875
3876     130  C                                                                  3876
3877     131         XX = XXL - ZZLEFT( KS ) * XXN                             3877
3878     132         YY = YYL - ZZLEFT( KS ) * YYN                             3878
3879     133         ZZ = ZZL - ZZLEFT( KS ) * ZZN                             3879
3880     134  C                                                                  3880
3881     135          HRRL =  HYDV( ICL , 1 ) + RGRAD( ICL , 1 ) * XX +         3881
3882     136        .   RGRAD( ICL , 2 ) * YY + RGRAD( ICL , 3 ) * ZZ           3882
3883     137          HUUL =  HYDV( ICL , 2 ) + UGRAD( ICL , 1 ) * XX +         3883
3884     138        .   UGRAD( ICL , 2 ) * YY + UGRAD( ICL , 3 ) * ZZ           3884
3885     139          HVVL =  HYDV( ICL , 3 ) + VGRAD( ICL , 1 ) * XX +         3885
3886     140        .   VGRAD( ICL , 2 ) * YY + VGRAD( ICL , 3 ) * ZZ           3886
3887     141          HWWL =  HYDV( ICL , 4 ) + WGRAD( ICL , 1 ) * XX +         3887
3888     142        .   WGRAD( ICL , 2 ) * YY + WGRAD( ICL , 3 ) * ZZ           3888
3889     143          HPPL =  HYDV( ICL , 5 ) + PGRAD( ICL , 1 ) * XX +         3889
3890     144        .   PGRAD( ICL , 2 ) * YY + PGRAD( ICL , 3 ) * ZZ           3890
3891     145  C                                                                  3891
3892     146          GMTLFT = GL( IS ) * HRRL * HPPL                           3892
3893     147          SQGMTL = SQRT( GMTLFT )                                   3893
3894     148  C                                                                  3894
```

```
3895  149        XX = ( ZPLEFT( KS ) - ZZLEFT( KS ) ) * XXN                        3895
3896  150        YY = ( ZPLEFT( KS ) - ZZLEFT( KS ) ) * YYN                        3896
3897  151        ZZ = ( ZPLEFT( KS ) - ZZLEFT( KS ) ) * ZZN                        3897
3898  152        UUU = UGRAD( ICL , 1 ) * XX + UGRAD( ICL , 2 ) * YY +             3898
3899  153       .      UGRAD( ICL , 3 ) * ZZ                                      3899
3900  154        PPP = PGRAD( ICL , 1 ) * XX + PGRAD( ICL , 2 ) * YY +             3900
3901  155       .      PGRAD( ICL , 3 ) * ZZ                                      3901
3902  156        UPLFT = - .5 * ( UUU + PPP / SQGMTL ) / SQGMTL                    3902
3903  157  C                                                                       3903
3904  158        XX = ( ZMLEFT( KS ) - ZZLEFT( KS ) ) * XXN                        3904
3905  159        YY = ( ZMLEFT( KS ) - ZZLEFT( KS ) ) * YYN                        3905
3906  160        ZZ = ( ZMLEFT( KS ) - ZZLEFT( KS ) ) * ZZN                        3906
3907  161        UUU = UGRAD( ICL , 1 ) * XX + UGRAD( ICL , 2 ) * YY +             3907
3908  162       .      UGRAD( ICL , 3 ) * ZZ                                      3908
3909  163        PPP = PGRAD( ICL , 1 ) * XX + PGRAD( ICL , 2 ) * YY +             3909
3910  164       .      PGRAD( ICL , 3 ) * ZZ                                      3910
3911  165        UMLFT =   .5 * ( UUU - PPP / SQGMTL ) / SQGMTL                    3911
3912  166  C                                                                       3912
3913  167        XX = ( ZOLEFT( KS ) - ZZLEFT( KS ) ) * XXN                        3913
3914  168        YY = ( ZOLEFT( KS ) - ZZLEFT( KS ) ) * YYN                        3914
3915  169        ZZ = ( ZOLEFT( KS ) - ZZLEFT( KS ) ) * ZZN                        3915
3916  170        PPP = PGRAD( ICL , 1 ) * XX + PGRAD( ICL , 2 ) * YY +             3916
3917  171       .      PGRAD( ICL , 3 ) * ZZ                                      3917
3918  172  C                                                                       3918
3919  173        XX = XXL - ZOLEFT( KS ) * XXN                                     3919
3920  174        YY = YYL - ZOLEFT( KS ) * YYN                                     3920
3921  175        ZZ = ZZL - ZOLEFT( KS ) * ZZN                                     3921
3922  176  C                                                                       3922
3923  177        RRRR = HYDV( ICL , 1 ) + RGRAD( ICL , 1 ) * XX +                  3923
3924  178       .                         RGRAD( ICL , 2 ) * YY + RGRAD( ICL , 3 ) * ZZ   3924
3925  179        URLFT = PPP / GMTLFT + 1. / HRRL - 1. / RRRR                      3925
3926  180  C                                                                       3926
3927  181           XXR = ( XYZMDL( 1 , IS ) - XC( 1 , ICR ) )                     3927
3928  182           YYR = ( XYZMDL( 2 , IS ) - XC( 2 , ICR ) )                     3928
3929  183           ZZR = ( XYZMDL( 3 , IS ) - XC( 3 , ICR ) )                     3929
3930  184  C                                                                       3930
3931  185        XX = XXR + ZZRIGT( KS ) * XXN                                     3931
3932  186        YY = YYR + ZZRIGT( KS ) * YYN                                     3932
3933  187        ZZ = ZZR + ZZRIGT( KS ) * ZZN                                     3933
3934  188  C                                                                       3934
3935  189         HRRR =  HYDV( ICR , 1 ) + RGRAD( ICR , 1 ) * XX +               3935
3936  190       .   RGRAD( ICR , 2 ) * YY + RGRAD( ICR , 3 ) * ZZ                 3936
3937  191         HUUR =  HYDV( ICR , 2 ) + UGRAD( ICR , 1 ) * XX +               3937
3938  192       .   UGRAD( ICR , 2 ) * YY + UGRAD( ICR , 3 ) * ZZ                 3938
3939  193         HVVR =  HYDV( ICR , 3 ) + VGRAD( ICR , 1 ) * XX +               3939
3940  194       .   VGRAD( ICR , 2 ) * YY + VGRAD( ICR , 3 ) * ZZ                 3940
3941  195         HWWR =  HYDV( ICR , 4 ) + WGRAD( ICR , 1 ) * XX +               3941
3942  196       .   WGRAD( ICR , 2 ) * YY + WGRAD( ICR , 3 ) * ZZ                 3942
3943  197         HPPR =  HYDV( ICR , 5 ) + PGRAD( ICR , 1 ) * XX +               3943
3944  198       .   PGRAD( ICR , 2 ) * YY + PGRAD( ICR , 3 ) * ZZ                 3944
3945  199  C                                                                       3945
3946  200         GMTRGT = GR( IS ) * HRRR * HPPR                                 3946
3947  201         SQGMTR = SQRT( GMTRGT )                                         3947
3948  202  C                                                                       3948
3949  203        XX = ( ZZRIGT( KS ) - ZPRIGT( KS ) ) * XXN                        3949
3950  204        YY = ( ZZRIGT( KS ) - ZPRIGT( KS ) ) * YYN                        3950
3951  205        ZZ = ( ZZRIGT( KS ) - ZPRIGT( KS ) ) * ZZN                        3951
3952  206        UUU = UGRAD( ICR , 1 ) * XX + UGRAD( ICR , 2 ) * YY +             3952
3953  207       .      UGRAD( ICR , 3 ) * ZZ                                      3953
3954  208        PPP = PGRAD( ICR , 1 ) * XX + PGRAD( ICR , 2 ) * YY +             3954
3955  209       .      PGRAD( ICR , 3 ) * ZZ                                      3955
3956  210        UPRGT = - .5 * ( UUU + PPP / SQGMTR ) / SQGMTR                    3956
3957  211  C                                                                       3957
3958  212        XX = ( ZZRIGT( KS ) - ZMRIGT( KS ) ) * XXN                        3958
3959  213        YY = ( ZZRIGT( KS ) - ZMRIGT( KS ) ) * YYN                        3959
3960  214        ZZ = ( ZZRIGT( KS ) - ZMRIGT( KS ) ) * ZZN                        3960
3961  215        UUU = UGRAD( ICR , 1 ) * XX + UGRAD( ICR , 2 ) * YY +             3961
3962  216       .      UGRAD( ICR , 3 ) * ZZ                                      3962
3963  217        PPP = PGRAD( ICR , 1 ) * XX + PGRAD( ICR , 2 ) * YY +             3963
3964  218       .      PGRAD( ICR , 3 ) * ZZ                                      3964
3965  219        UMRGT =   .5 * ( UUU - PPP / SQGMTR ) / SQGMTR                    3965
3966  220  C                                                                       3966
3967  221        XX = ( ZZRIGT( KS ) - ZORIGT( KS ) ) * XXN                        3967
3968  222        YY = ( ZZRIGT( KS ) - ZORIGT( KS ) ) * YYN                        3968
```

```
3969     223         ZZ = ( ZZRIGT( KS ) - ZORIGT( KS ) ) * ZZN                                3969
3970     224         PPP = PGRAD( ICR , 1 ) * XX + PGRAD( ICR , 2 ) * YY +                     3970
3971     225        .      PGRAD( ICR , 3 ) * ZZ                                              3971
3972     226   C                                                                               3972
3973     227         XX = XXR + ZORIGT( KS ) * XXN                                             3973
3974     228         YY = YYR + ZORIGT( KS ) * YYN                                             3974
3975     229         ZZ = ZZR + ZORIGT( KS ) * ZZN                                             3975
3976     230   C                                                                               3976
3977     231         RRRR = HYDV( ICR , 1 ) + RGRAD( ICR , 1 ) * XX +                          3977
3978     232        .                   RGRAD( ICR , 2 ) * YY + RGRAD( ICR , 3 ) * ZZ        3978
3979     233         URRGT = PPP / GMTRGT + 1. / HRRR - 1. / RRRR                              3979
3980     234   C                                                                               3980
3981     235         ELSE                                                                      3981
3982     236   C                                                                               3982
3983     237          XYZ = 1. / XS( 5 , IS )                                                  3983
3984     238            XXN = ( XYZMDL( 1 , IS ) - XC( 1 , ICL ) ) * XYZ                       3984
3985     239            YYN = ( XYZMDL( 2 , IS ) - XC( 2 , ICL ) ) * XYZ                       3985
3986     240            ZZN = ( XYZMDL( 3 , IS ) - XC( 3 , ICL ) ) * XYZ                       3986
3987     241   C                                                                               3987
3988     242            XXL = ( XYZMDL( 1 , IS ) - XC( 1 , ICL ) )                             3988
3989     243            YYL = ( XYZMDL( 2 , IS ) - XC( 2 , ICL ) )                             3989
3990     244            ZZL = ( XYZMDL( 3 , IS ) - XC( 3 , ICL ) )                             3990
3991     245   C                                                                               3991
3992     246         XX = XXL - ZZLEFT( KS ) * XXN                                             3992
3993     247         YY = YYL - ZZLEFT( KS ) * YYN                                             3993
3994     248         ZZ = ZZL - ZZLEFT( KS ) * ZZN                                             3994
3995     249   C                                                                               3995
3996     250          HRRL =  HYDV( ICL , 1 ) + RGRAD( ICL , 1 ) * XX +                        3996
3997     251        .   RGRAD( ICL , 2 ) * YY + RGRAD( ICL , 3 ) * ZZ                          3997
3998     252          HUUL =  HYDV( ICL , 2 ) + UGRAD( ICL , 1 ) * XX +                        3998
3999     253        .   UGRAD( ICL , 2 ) * YY + UGRAD( ICL , 3 ) * ZZ                          3999
4000     254          HVVL =  HYDV( ICL , 3 ) + VGRAD( ICL , 1 ) * XX +                        4000
4001     255        .   VGRAD( ICL , 2 ) * YY + VGRAD( ICL , 3 ) * ZZ                          4001
4002     256          HWWL =  HYDV( ICL , 4 ) + WGRAD( ICL , 1 ) * XX +                        4002
4003     257        .   WGRAD( ICL , 2 ) * YY + WGRAD( ICL , 3 ) * ZZ                          4003
4004     258          HPPL =  HYDV( ICL , 5 ) + PGRAD( ICL , 1 ) * XX +                        4004
4005     259        .   PGRAD( ICL , 2 ) * YY + PGRAD( ICL , 3 ) * ZZ                          4005
4006     260   C                                                                               4006
4007     261          GMTLFT = GL( IS ) * HRRL * HPPL                                          4007
4008     262          SQGMTL = SQRT( GMTLFT )                                                  4008
4009     263   C                                                                               4009
4010     264         XX = ( ZPLEFT( KS ) - ZZLEFT( KS ) ) * XXN                                4010
4011     265         YY = ( ZPLEFT( KS ) - ZZLEFT( KS ) ) * YYN                                4011
4012     266         ZZ = ( ZPLEFT( KS ) - ZZLEFT( KS ) ) * ZZN                                4012
4013     267         UUU = UGRAD( ICL , 1 ) * XX + UGRAD( ICL , 2 ) * YY +                     4013
4014     268        .      UGRAD( ICL , 3 ) * ZZ                                              4014
4015     269         PPP = PGRAD( ICL , 1 ) * XX + PGRAD( ICL , 2 ) * YY +                     4015
4016     270        .      PGRAD( ICL , 3 ) * ZZ                                              4016
4017     271         UPLFT = - .5 * ( UUU + PPP / SQGMTL ) / SQGMTL                            4017
4018     272   C                                                                               4018
4019     273         XX = ( ZMLEFT( KS ) - ZZLEFT( KS ) ) * XXN                                4019
4020     274         YY = ( ZMLEFT( KS ) - ZZLEFT( KS ) ) * YYN                                4020
4021     275         ZZ = ( ZMLEFT( KS ) - ZZLEFT( KS ) ) * ZZN                                4021
4022     276         UUU = UGRAD( ICL , 1 ) * XX + UGRAD( ICL , 2 ) * YY +                     4022
4023     277        .      UGRAD( ICL , 3 ) * ZZ                                              4023
4024     278         PPP = PGRAD( ICL , 1 ) * XX + PGRAD( ICL , 2 ) * YY +                     4024
4025     279        .      PGRAD( ICL , 3 ) * ZZ                                              4025
4026     280         UMLFT =   .5 * ( UUU - PPP / SQGMTL ) / SQGMTL                            4026
4027     281   C                                                                               4027
4028     282         XX = ( ZOLEFT( KS ) - ZZLEFT( KS ) ) * XXN                                4028
4029     283         YY = ( ZOLEFT( KS ) - ZZLEFT( KS ) ) * YYN                                4029
4030     284         ZZ = ( ZOLEFT( KS ) - ZZLEFT( KS ) ) * ZZN                                4030
4031     285         PPP = PGRAD( ICL , 1 ) * XX + PGRAD( ICL , 2 ) * YY +                     4031
4032     286        .      PGRAD( ICL , 3 ) * ZZ                                              4032
4033     287   C                                                                               4033
4034     288         XX = XXL - ZOLEFT( KS ) * XXN                                             4034
4035     289         YY = YYL - ZOLEFT( KS ) * YYN                                             4035
4036     290         ZZ = ZZL - ZOLEFT( KS ) * ZZN                                             4036
4037     291   C                                                                               4037
4038     292         RRRR = HYDV( ICL , 1 ) + RGRAD( ICL , 1 ) * XX +                          4038
4039     293        .                   RGRAD( ICL , 2 ) * YY + RGRAD( ICL , 3 ) * ZZ        4039
4040     294         URLFT = PPP / GMTLFT + 1. / HRRL - 1. / RRRR                              4040
4041     295   C                                                                               4041
4042     296          HRRR =  HRRL                                                             4042
```

```
4043     297          HUUR =  HUUL                                                    4043
4044     298          HVVR =  HVVL                                                    4044
4045     299          HWWR =  HWWL                                                    4045
4046     300          HPPR =  HPPL                                                    4046
4047     301   C                                                                      4047
4048     302          GMTRGT = GMTLFT                                                 4048
4049     303          SQGMTR = SQGMTL                                                 4049
4050     304   C                                                                      4050
4051     305         UPRGT = UPLFT                                                    4051
4052     306         UMRGT = UMLFT                                                    4052
4053     307         URRGT = URLFT                                                    4053
4054     308   C                                                                      4054
4055     309         END IF                                                           4055
4056     310   C                                                                      4056
4057     311         RRL( KS ) = HRRL                                                 4057
4058     312         UUL( KS ) = HUUL                                                 4058
4059     313         VVL( KS ) = HVVL                                                 4059
4060     314         WWL( KS ) = HWWL                                                 4060
4061     315         PPL( KS ) = HPPL                                                 4061
4062     316   C                                                                      4062
4063     317         RRR( KS ) = HRRR                                                 4063
4064     318         UUR( KS ) = HUUR                                                 4064
4065     319         VVR( KS ) = HVVR                                                 4065
4066     320         WWR( KS ) = HWWR                                                 4066
4067     321         PPR( KS ) = HPPR                                                 4067
4068     322   C                                                                      4068
4069     323         UPLEFT( KS ) = UPLFT                                             4069
4070     324         UMLEFT( KS ) = UMLFT                                             4070
4071     325         URLEFT( KS ) = URLFT                                             4071
4072     326   C                                                                      4072
4073     327         UPRIGT( KS ) = UPRGT                                             4073
4074     328         UMRIGT( KS ) = UMRGT                                             4074
4075     329         URRIGT( KS ) = URRGT                                             4075
4076     330   C                                                                      4076
4077     331    160  CONTINUE                                                        4077
4078     332   C                                                                      4078
4079     333   C  CORRECTION OF THE FIRST GUESS                                       4079
4080     334   C                                                                      4080
4081     335         DO 170 KS = 1 , NOFVES( INS )                                    4081
4082     336   C                                                                      4082
4083     337         IF( UVLEFT( KS ) + CNLEFT( KS ) . LE . 0. ) UPLEFT( KS ) = 0.    4083
4084     338         IF( UVLEFT( KS ) - CNLEFT( KS ) . LE . 0. ) UMLEFT( KS ) = 0.    4084
4085     339         IF( UVLEFT( KS ) .                LE . 0. ) URLEFT( KS ) = 0.    4085
4086     340   C                                                                      4086
4087     341         IF( UVRIGT( KS ) + CNRIGT( KS ) . GE . 0. ) UPRIGT( KS ) = 0.    4087
4088     342         IF( UVRIGT( KS ) - CNRIGT( KS ) . GE . 0. ) UMRIGT( KS ) = 0.    4088
4089     343         IF( UVRIGT( KS ) .                GE . 0. ) URRIGT( KS ) = 0.    4089
4090     344   C                                                                      4090
4091     345    170  CONTINUE                                                        4091
4092     346   C                                                                      4092
4093     347   C  FINAL VALUES FOR RIGHT AND LEFT STATES                              4093
4094     348   C                                                                      4094
4095     349         DO 180 KS = 1 , NOFVES( INS )                                    4095
4096     350            IS = KS + NS1 - 1                                             4096
4097     351   C                                                                      4097
4098     352          GMTLFT = GL( IS ) * RRL( KS ) * PPL( KS )                       4098
4099     353          SQGMTL = SQRT( GMTLFT )                                         4099
4100     354   C                                                                      4100
4101     355          GMTRGT = GR( IS ) * RRR( KS ) * PPR( KS )                       4101
4102     356          SQGMTR = SQRT( GMTRGT )                                         4102
4103     357   C                                                                      4103
4104     358          RRL( KS ) = 1. / ( 1. / RRL( KS ) - ( UPLEFT( KS ) +            4104
4105     359        .                              UMLEFT( KS ) + URLEFT( KS ) ) )    4105
4106     360          UUL( KS ) = UUL( KS ) + SQGMTL * ( UPLEFT( KS ) -               4106
4107     361        .                                    UMLEFT( KS ) )             4107
4108     362          VVL( KS ) = VVL( KS ) + SQGMTL * ( UPLEFT( KS ) -               4108
4109     363        .                                    UMLEFT( KS ) )             4109
4110     364          WWL( KS ) = WWL( KS ) + SQGMTL * ( UPLEFT( KS ) -               4110
4111     365        .                                    UMLEFT( KS ) )             4111
4112     366          PPL( KS ) = PPL( KS ) + GMTLFT * ( UPLEFT( KS ) +               4112
4113     367        .                                    UMLEFT( KS ) )             4113
4114     368   C                                                                      4114
4115     369          RRR( KS ) = 1. / ( 1. / RRR( KS ) - ( UPRIGT( KS ) +            4115
4116     370        .                             UMRIGT( KS ) + URRIGT( KS ) ) )    4116
```

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4117     371          UUR( KS ) = UUR( KS ) + SQGMTR * ( UPRIGT( KS ) -                4117
4118     372         .                                   UMRIGT( KS ) )               4118
4119     373          VVR( KS ) = VVR( KS ) + SQGMTR * ( UPRIGT( KS ) -                4119
4120     374         .                                   UMRIGT( KS ) )               4120
4121     375          WWR( KS ) = WWR( KS ) + SQGMTR * ( UPRIGT( KS ) -                4121
4122     376         .                                   UMRIGT( KS ) )               4122
4123     377          PPR( KS ) = PPR( KS ) + GMTRGT * ( UPRIGT( KS ) +                4123
4124     378         .                                   UMRIGT( KS ) )               4124
4125     379    C                                                                      4125
4126     380     180  CONTINUE                                                        4126
4127     381    C                                                                      4127
4128     382          DO 200 IS = NS1 , NS2                                          4128
4129     383             KS = IS - NS1 + 1                                           4129
4130     384    C                                                                      4130
4131     385          ICL = JS( 7 , IS )                                             4131
4132     386          ICR = JS( 8 , IS )                                             4132
4133     387    C                                                                      4133
4134     388          RL( IS ) = RRL( KS )                                           4134
4135     389          UL( IS ) = UUL( KS ) * XN( IS ) +                              4135
4136     390         .           VVL( KS ) * YN( IS ) +                              4136
4137     391         .           WWL( KS ) * ZN( IS )                                4137
4138     392          VL( IS ) = UUL( KS ) * XP( IS ) +                              4138
4139     393         .           VVL( KS ) * YP( IS ) +                              4139
4140     394         .           WWL( KS ) * ZP( IS )                                4140
4141     395          WL( IS ) = UUL( KS ) * XT( IS ) +                              4141
4142     396         .           VVL( KS ) * YT( IS ) +                              4142
4143     397         .           WWL( KS ) * ZT( IS )                                4143
4144     398          PL( IS ) = PPL( KS )                                           4144
4145     399          AL( IS ) = HYDV( ICL , 6 )                                     4145
4146     400          GL( IS ) = HYDV( ICL , 7 )                                     4146
4147     401          EL( IS ) = HYDV( ICL , 8 )                                     4147
4148     402    C                                                                      4148
4149     403          IATRB = JS( 9 , IS )                                           4149
4150     404          IF( IATRB . EQ . 0 ) THEN                                      4150
4151     405    C                                                                      4151
4152     406          RR( IS ) = RRR( KS )                                           4152
4153     407          UR( IS ) = UUR( KS ) * XN( IS ) +                              4153
4154     408         .           VVR( KS ) * YN( IS ) +                              4154
4155     409         .           WWR( KS ) * ZN( IS )                                4155
4156     410          VR( IS ) = UUR( KS ) * XP( IS ) +                              4156
4157     411         .           VVR( KS ) * YP( IS ) +                              4157
4158     412         .           WWR( KS ) * ZP( IS )                                4158
4159     413          WR( IS ) = UUR( KS ) * XT( IS ) +                              4159
4160     414         .           VVR( KS ) * YT( IS ) +                              4160
4161     415         .           WWR( KS ) * ZT( IS )                                4161
4162     416          PR( IS ) = PPR( KS )                                           4162
4163     417          AR( IS ) = HYDV( ICR , 6 )                                     4163
4164     418          GR( IS ) = HYDV( ICR , 7 )                                     4164
4165     419          ER( IS ) = HYDV( ICR , 8 )                                     4165
4166     420    C                                                                      4166
4167     421          ELSE                                                           4167
4168     422    C                                                                      4168
4169     423          IF( IATRB . EQ . 8 ) THEN                                      4169
4170     424    C                                                                      4170
4171     425          RR( IS ) = RIN                                                 4171
4172     426          UR( IS ) = UIN * XN( IS ) + VIN * YN( IS ) + WIN * ZN( IS )    4172
4173     427          VR( IS ) = UIN * XP( IS ) + VIN * YP( IS ) + WIN * ZP( IS )    4173
4174     428          WR( IS ) = UIN * XT( IS ) + VIN * YT( IS ) + WIN * ZT( IS )    4174
4175     429          PR( IS ) = PIN                                                 4175
4176     430          AR( IS ) = AL( IS )                                            4176
4177     431          GR( IS ) = GL( IS )                                            4177
4178     432          ER( IS ) = EL( IS )                                            4178
4179     433    C                                                                      4179
4180     434          END IF                                                         4180
4181     435    C                                                                      4181
4182     436          IF( IATRB . EQ . 7 ) THEN                                      4182
4183     437    C                                                                      4183
4184     438            RR( IS ) = RL( IS )                                          4184
4185     439            UR( IS ) = UL( IS )                                          4185
4186     440            VR( IS ) = VL( IS )                                          4186
4187     441            WR( IS ) = WL( IS )                                          4187
4188     442            PR( IS ) = PL( IS )                                          4188
4189     443            AR( IS ) = AL( IS )                                          4189
4190     444            GR( IS ) = GL( IS )                                          4190
```

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4191    445            ER( IS ) = EL( IS )                                    4191
4192    446    C                                                              4192
4193    447          END IF                                                   4193
4194    448    C                                                              4194
4195    449          IF( IATRB . EQ . 6 ) THEN                                4195
4196    450    C                                                              4196
4197    451            RR( IS ) = RL( IS )                                    4197
4198    452            UR( IS ) = - UL( IS )                                  4198
4199    453            VR( IS ) = VL( IS )                                    4199
4200    454            WR( IS ) = WL( IS )                                    4200
4201    455            PR( IS ) = PL( IS )                                    4201
4202    456            AR( IS ) = AL( IS )                                    4202
4203    457            GR( IS ) = GL( IS )                                    4203
4204    458            ER( IS ) = EL( IS )                                    4204
4205    459    C                                                              4205
4206    460          END IF                                                   4206
4207    461    C                                                              4207
4208    462          END IF                                                   4208
4209    463    C                                                              4209
4210    464     200  CONTINUE                                                 4210
4211    465    C                                                              4211
4212    466          NS1 = NS2 + 1                                            4212
4213    467          NS2 = NS2 + NOFVES( INS + 1 )                            4213
4214    468     90   CONTINUE                                                 4214
4215    469    C                                                              4215
4216    470          RETURN                                                   4216
4217    471          END                                                      4217
```



```
4218      1          SUBROUTINE EOS1 (RRR,EEE,N,GAMMA)                      4218
4219      2    C                                                            4219
4220      3    C     AIR IS ASSUMED TO BE CALORICALLY IMPERFECT, THERMALLY PERFECT.  4220
4221      4    C     THEREFORE, INCLUDE IMPERFECTIONS VIA A VARIABLE GAMMA DEPENDENT 4221
4222      5    C     ON DENSITY AND INTERNAL ENERGY.  THIS ROUTINE PERFORMS A TABLE  4222
4223      6    C     LOOK UP FOR GAMMA.                                       4223
4224      7    C                                                              4224
4225      8    C     INPUT VARIBLE DEFINITIONS.                               4225
4226      9    C     RRR = MASS DENSITY                                       4226
4227     10    C     EEE = INTERNAL ENERGY PER UNIT VOLUME                    4227
4228     11    C           (CONVERTED FOR INTERNAL *CALL TO ENERGY PER UNIT MASS)  4228
4229     12    C     N   = NUMBER OF ENTRIES IN ARRAYS RRR & EEE              4229
4230     13    C                                                              4230
4231     14          PARAMETER (M = 64)                                       4231
4232     15    C                                                              4232
4233     16          DIMENSION RRR(N), EEE(N), GAMMA(N)                       4233
4234     17          DIMENSION T11(M), T12(M), T21(M), T22(M), RHO(M), E(M)   4234
4235     18          DIMENSION OMP(M), Q(M), I(M), J(M)                       4235
4236     19          DIMENSION G1(168),G2(112),G3(112),G4(112),G5(112),       4236
4237     20         !          G6(112),G7(112),GF(840)                        4237
4238     21    C                                                              4238
4239     22    C     NOTE:  THE TABLE LOOK UP TREATS ARRAY GF AS THOUGH IT    4239
4240     23    C     WERE DIMENSIONED (8,105).                                4240
4241     24    C                                                              4241
4242     25          EQUIVALENCE (G1(1),GF(  1)), (G2(1),GF(169)), (G3(1),GF(281)),  4242
4243     26         !            (G4(1),GF(393)), (G5(1),GF(505)), (G6(1),GF(617)),  4243
4244     27         !            (G7(1),GF(729))                              4244
4245     28    C                                                              4245
4246     29          DATA XL16E  /2.772588722239774483568908181041479110717773437 5/  4246
4247     30    C-------------------------------------------------------------- --  4247
4248     31    C     G = GAMMA - 1.0 IS STORED FOR 32 BIT WORD MACHINES IN POWERS OF  4248
4249     32    C     16 ACROSS FOR MASS DENSITY VARIATION AND INTERMEDIATE VALUES  4249
4250     33    C     1 - 16 FOR POWERS OF 16 VERTICALLY WHICH REPRESENT THE INTERNAL  4250
4251     34    C     ENERGY VARIATION.                                        4251
4252     35    C                                                              4252
4253     36    C     16**(7)  .GE. RHO .GE. 16**(-6)                          4253
4254     37    C     16**(15) .GE.  E  .GE. 16**(8)                           4254
4255     38    C-------------------------------------------------------------  4255
4256     39          DATA G1 /8*.4222,8*.4152,8*.4110,8*.4081,8*.4058,8*.4040,  4256
4257     40         !         8*.4024,8*.4011,8*.3998,8*.3988,8*.3978,8*.3969,  4257
4258     41         !         8*.3961,8*.3953,8*.3935,8*.3918,                  4258
4259     42         !        .3723,.3715,.3707,.3699,.3690,.3680,.3663,.3637,   4259
4260     43         !        .3555,.3538,.3522,.3502,.3476,.3430,.3344,.3238,   4260
4261     44         !        .3370,.3370,.3370,.3364,.3347,.3277,.3099,.2885,   4261
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4262   45      !       .3257,.3227,.3201,.3134,.3062,.3014,.2884,.2591,                4262
4263   46      !       .3166,.3110,.3063,.2946,.2831,.2783,.2677,.2358/                4263
4264   47       DATA G2/.3111,.3006,.2940,.2787,.2635,.2588,.2502,.2236,               4264
4265   48      !       .3075,.2906,.2810,.2665,.2466,.2418,.2350,.2131,                4265
4266   49      !       .3043,.2819,.2695,.2554,.2317,.2269,.2216,.2038,                4266
4267   50      !       .2929,.2740,.2593,.2455,.2206,.2136,.2097,.1955,                4267
4268   51      !       .2840,.2672,.2500,.2366,.2166,.2015,.1988,.1879,                4268
4269   52      !       .2764,.2611,.2429,.2285,.2125,.1890,.1890,.1811,                4269
4270   53      !       .2714,.2555,.2384,.2210,.2079,.1818,.1799,.1747,                4270
4271   54      !       .2669,.2514,.2343,.2141,.2037,.1822,.1709,.1689,                4271
4272   55      !       .2624,.2473,.2304,.2096,.1998,.1828,.1684,.1639,                4272
4273   56      !       .2596,.2446,.2268,.2087,.1961,.1834,.1673,.1601,                4273
4274   57      !       .2401,.2191,.1972,.1775,.1592,.1444,.1358,.1203,                4274
4275   58      !       .2002,.1960,.1749,.1536,.1376,.1252,.1107,.1044,                4275
4276   59      !       .1911,.1829,.1633,.1420,.1266,.1101,.1012,.0933,                4276
4277   60      !       .1950,.1781,.1566,.1415,.1241,.1118,.1009,.0948/                4277
4278   61       DATA G3/.2001,.1789,.1594,.1443,.1306,.1189,.1095,.1013,               4278
4279   62      !       .2040,.1826,.1657,.1494,.1338,.1177,.1081,.0980,                4279
4280   63      !       .2034,.1854,.1683,.1497,.1322,.1169,.1051,.0946,                4280
4281   64      !       .1969,.1855,.1685,.1487,.1304,.1149,.1024,.0916,                4281
4282   65      !       .1899,.1837,.1677,.1475,.1287,.1126,.1002,.0900,                4282
4283   66      !       .1841,.1817,.1667,.1464,.1272,.1109,.0983,.0888,                4283
4284   67      !       .1800,.1800,.1659,.1455,.1262,.1097,.0965,.0878,                4284
4285   68      !       .1779,.1787,.1657,.1450,.1254,.1087,.0949,.0868,                4285
4286   69      !       .1773,.1778,.1656,.1447,.1250,.1080,.0939,.0859,                4286
4287   70      !       .1783,.1778,.1658,.1448,.1248,.1076,.0933,.0851,                4287
4288   71      !       .1808,.1781,.1667,.1451,.1248,.1074,.0930,.0843,                4288
4289   72      !       .2134,.2040,.1978,.1782,.1565,.1368,.1206,.1074,                4289
4290   73      !       .2210,.2072,.1957,.1739,.1516,.1312,.1137,.1000,                4290
4291   74      !       .2245,.2109,.1989,.1772,.1563,.1390,.1247,.1133/                4291
4292   75       DATA G4/.2299,.2132,.2017,.1795,.1579,.1384,.1221,.1090,               4292
4293   76      !       .2350,.2157,.2023,.1798,.1575,.1370,.1197,.1057,                4293
4294   77      !       .2397,.2194,.2034,.1796,.1572,.1372,.1205,.1070,                4294
4295   78      !       .2452,.2227,.2050,.1805,.1576,.1379,.1236,.1118,                4295
4296   79      !       .2510,.2256,.2069,.1814,.1581,.1383,.1231,.1103,                4296
4297   80      !       .2560,.2282,.2091,.1822,.1585,.1385,.1226,.1083,                4297
4298   81      !       .2605,.2312,.2111,.1829,.1588,.1386,.1222,.1070,                4298
4299   82      !       .2677,.2358,.2129,.1836,.1592,.1386,.1218,.1071,                4299
4300   83      !       .2759,.2403,.2145,.1857,.1598,.1389,.1219,.1078,                4300
4301   84      !       .2834,.2445,.2160,.1878,.1603,.1394,.1223,.1084,                4301
4302   85      !       .2905,.2484,.2175,.1898,.1613,.1399,.1226,.1090,                4302
4303   86      !       .2963,.2531,.2199,.1918,.1625,.1407,.1230,.1096,                4303
4304   87      !       .4323,.3582,.3109,.2889,.2803,.2706,.2410,.2224,                4304
4305   88      !       .4610,.4026,.3624,.3212,.2926,.2551,.2375,.2015/                4305
4306   89       DATA G5/.4199,.3837,.3401,.2979,.2623,.2318,.2108,.1854,               4306
4307   90      !       .3924,.3642,.3194,.2760,.2427,.2157,.1902,.1721,                4307
4308   91      !       .3794,.3479,.3025,.2673,.2311,.2019,.1842,.1613,                4308
4309   92      !       .3674,.3448,.2961,.2593,.2255,.1994,.1785,.1594,                4309
4310   93      !       .3573,.3443,.2910,.2517,.2293,.2006,.1843,.1679,                4310
4311   94      !       .3661,.3438,.2935,.2597,.2336,.2225,.2143,.2116,                4311
4312   95      !       .3674,.3435,.3080,.2728,.2606,.2577,.2573,.2573,                4312
4313   96      !       .3685,.3453,.3210,.3014,.2942,.2933,.2932,.2932,                4313
4314   97      !       .3814,.3612,.3341,.3276,.3257,.3253,.3252,.3252,                4314
4315   98      !       .3903,.3752,.3570,.3522,.3513,.3510,.3506,.3496,                4315
4316   99      !       .4012,.3899,.3782,.3751,.3743,.3741,.3734,.3713,                4316
4317  100      !       .4155,.4057,.3956,.3930,.3920,.3913,.3907,.3890,                4317
4318  101      !       .4290,.4205,.4118,.4092,.4077,.4065,.4059,.4047,                4318
4319  102      !       .5411,.5385,.5359,.5353,.5351,.5350,.5350,.5350/                4319
4320  103       DATA G6/.5823,.5812,.5801,.5797,.5796,.5797,.5797,.5797,               4320
4321  104      !       .6096,.6090,.6085,.6082,.6082,.6083,.6083,.6083,                4321
4322  105      !       .6308,.6306,.6305,.6303,.6303,.6305,.6305,.6305,                4322
4323  106      !       .6481,.6483,.6485,.6483,.6484,.6486,.6487,.6487,                4323
4324  107      !       .6627,.6632,.6637,.6636,.6637,.6640,.6640,.6640,                4324
4325  108      !       .6754,.6761,.6769,.6768,.6770,.6773,.6773,.6773,                4325
4326  109      !       .6866,.6875,.6885,.6884,.6886,.6890,.6890,.6890,                4326
4327  110      !       .6966,.6977,.6989,.6989,.6991,.6995,.6995,.6995,                4327
4328  111      !       .7056,.7070,.7083,.7083,.7085,.7090,.7090,.7090,                4328
4329  112      !       .7139,.7154,.7169,.7169,.7172,.7176,.7177,.7177,                4329
4330  113      !       .7214,.7231,.7248,.7248,.7251,.7256,.7256,.7256,                4330
4331  114      !       .7285,.7303,.7321,.7321,.7325,.7330,.7330,.7330,                4331
4332  115      !       .7350,.7370,.7390,.7390,.7393,.7398,.7399,.7399,                4332
4333  116      !       .7411,.7432,.7453,.7454,.7457,.7463,.7463,.7463/                4333
4334  117       DATA G7/.8069,.8103,.8138,.8139,.8145,.8152,.8153,.8153,               4334
4335  118      !       .8454,.8496,.8538,.8540,.8547,.8556,.8557,.8557,                4335
```

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     119      !       .8727,.8774,.8822,.8825,.8832,.8842,.8843,.8843,
     120      !       .8938,.8990,.9042,.9046,.9054,.9064,.9065,.9065,
     121      !       .9111,.9166,.9222,.9226,.9235,.9246,.9247,.9247,
     122      !       .9258,.9316,.9374,.9379,.9387,.9399,.9400,.9400,
     123      !       .9384,.9445,.9506,.9511,.9520,.9532,.9533,.9533,
     124      !       .9496,.9559,.9622,.9627,.9637,.9649,.9650,.9650,
     125      !       .9596,.9661,.9727,.9731,.9741,.9754,.9755,.9755,
     126      !       .9686,.9753,.9821,.9826,.9836,.9849,.9850,.9850,
     127      !       .9769,.9837,.9906,.9912,.9922,.9936,.9937,.9937,
     128      !       .9845,.9915,.9986,.9991,.9999,.9999,.9999,.9999,
     129      !       .9915,.9987,.9999,.9999,.9999,.9999,.9999,.9999,
     130      !       .9981,.9999,.9999,.9999,.9999,.9999,.9999,.9999/
     131   C-------------------------------------------------------------
     132   C     REAL AIR EOS, TABLE LOOKUP ON GILMORE DATA.  (NO TEMP. MODEL)
     133   C     TO AVOID COSTLY LOGARITHMIC FUNCTIONS THE TABLE "G" IS STORED IN A
     134   C     FORM SO THAT THE HEXADECIMAL WORD STRUCTURE OF A 32 BIT MACHINE
     135   C     MAY BE EXPLOITED.
     136   C     THIS LOGIC MAY BE TRANSFERED TO OTHER MACHINES BY RECALCULATING
     137   C     THE TABLE "G" APPROPRIATE TO THE WORD ARCITECTURE OF THAT MACHINE.
     138   C     MACHINE DEPENDENT FUNCTIONS AND KEY NUMBERS MUST ALSO BE CHANGED.
     139   C-------------------------------------------------------------
     140         RL16E = 1./XL16E
     141         IST = 0
     142         NR  = N
     143   C
     144     10  CONTINUE
     145         NST = MIN0(NR,M)
     146   C
     147         DO 20 IRE=1,NST
     148         RHO(IRE) = .774413*RRR(IST+IRE)
     149         E(IRE) = AMAX1(3.e8,10000.*EEE(IST+IRE)/RRR(IST+IRE))
     150   C
     151   C     CALCULATE MASS DENSITY VARIATION INDEX "I".
     152   C
     153         TEM = ALOG(RHO(IRE))*RL16E + 500.0
     154         I(IRE)   = AINT(TEM)
     155         OMP(IRE) = TEM - FLOAT(I(IRE))
     156         I(IRE)   = 502 - I(IRE)
     157         I(IRE)   = MAX0(I(IRE),1)
     158   C
     159   C     CALCULATE INTERNAL ENERGY VARIATION INDEX "J".
     160   C
     161         TEM = ALOG(E(IRE))*RL16E
     162         JCY = AINT(TEM)
     163         TEM = TEM - FLOAT(JCY)
     164         TEM = EXP(XL16E*TEM)
     165         JCY = JCY - 7
     166         JS  = AINT(TEM)
     167         Q(IRE)   = TEM - FLOAT(JS)
     168         J(IRE)   = JS + 15*JCY
     169         J(IRE)   = MIN0(J(IRE),104)
     170         J(IRE)   = I(IRE) + 8*J(IRE)
     171         I(IRE)   = J(IRE) - 8
     172     20  CONTINUE
     173   C
     174         DO 30 IRE=1,NST
     175         T11(IRE) = GF(I(IRE))
     176         T21(IRE) = GF(I(IRE)+1)
     177         T12(IRE) = GF(J(IRE))
     178         T22(IRE) = GF(J(IRE)+1)
     179     30  CONTINUE
     180   C
     181   C     CALCULATE GAMMA BY LINEAR INTERPOLATION.
     182   C
     183         DO 40 IRE=1,NST
     184         T12(IRE) = T12(IRE) - T11(IRE)
     185         T22(IRE) = T22(IRE) - T21(IRE)
     186         GAMMA(IST+IRE) =       OMP(IRE) *(T11(IRE) + Q(IRE)*T12(IRE))
     187        !               + (1. - OMP(IRE))*(T21(IRE) + Q(IRE)*T22(IRE))
     188        !               +  1.
     189     40  CONTINUE
     190   C
     191         NR  = NR - NST
     192         IST = IST + NST
```

```
4410    193         IF(NR.GT.0) GO TO 10                                    4410
4411    194   C                                                             4411
4412    195         RETURN                                                  4412
4413    196         END                                                     4413
4414    197   C                                                             4414
```



```
4415      1         SUBROUTINE MATRLA                                       4415
4416      2   C                                                             4416
4417      3   C     READS MATERIAL PROPERTIES                               4417
4418      4   C     EVALUATES MATERIAL RELATED CONTANTS                     4418
4419      5   C                                                             4419
4420      6         include     'dmtr10.h'                                  4420
4421      7         CHARACTER*8   PRODCT(15), PHASE(15), GG, SS, VV, NASAP  4421
4422      8         REAL        X(15), KVOL(15), M(15), RHOS(15), CVS(15)   4422
4423      9         REAL        CF(7,2), CV(0:5,2)                          4423
4424     10   C                                                             4424
4425     11         DATA        KVOL/15*0./                                 4425
4426     12         DATA        GG/'G'/, SS/'S'/, VV/'VVVV'/                4426
4427     13         DATA        CV/12*0./                                   4427
4428     14         DATA PRODCT/'O2','N2',13*'VVVV    '/                    4428
4429     15         DATA PHASE/2*'G',13*'       '/                        4429
4430     16   C                                                             4430
4431     17   C      DATA PRODCT/'H2O','H2','CO2','CO','NH3','CH4','N2','Cs'4431
4432     18   C     1      ,7*'VVVV    '/                                   4432
4433     19   C      DATA PHASE/7*'G','S',7*'       '/                     4433
4434     20   C                                                             4434
4435     21         ALFAA=.5                                                4435
4436     22         BETAA=.09585                                            4436
4437     23         THETAA=400.                                             4437
4438     24         CAPPAA=12.685                                           4438
4439     25         NNASA=100                                               4439
4440     26         X(1)=21.                                                4440
4441     27         X(2)=79.                                                4441
4442     28         KVOL(1)=350.                                            4442
4443     29         KVOL(2)=380.                                            4443
4444     30         M(1)=32.                                                4444
4445     31         M(2)=28.016                                             4445
4446     32         CVS(1)=0.                                               4446
4447     33         CVS(2)=0.                                               4447
4448     34         RHOS(1)=0.                                              4448
4449     35         RHOS(2)=0.                                              4449
4450     36         NS = 0                                                  4450
4451     37         NG = 0                                                  4451
4452     38   C                                                             4452
4453     39         TMS = 0.                                                4453
4454     40         COVA = 0.                                               4454
4455     41         GML = 0.                                                4455
4456     42         SML = 0.                                                4456
4457     43         SV = 0.                                                 4457
4458     44         SCVA = 0.                                               4458
4459     45   C                                                             4459
4460     46          REWIND 4                                               4460
4461     47         DO 110 I = 1, 15                                        4461
4462     48         IF ( PRODCT(I) .EQ. VV ) GO TO 10                       4462
4463     49         NS = I                                                  4463
4464     50   C                                                             4464
4465     51         IF ( PHASE(I) .EQ. GG ) THEN                            4465
4466     52         NG = NG + 1                                             4466
4467     53         GML = GML + X(I)                                        4467
4468     54         TMS = TMS + X(I)*M(I)                                   4468
4469     55         COVA = COVA + X(I)*KVOL(I)                              4469
4470     56   C                                                             4470
4471     57         ELSE IF ( PHASE(I) .EQ. SS ) THEN                       4471
4472     58         PHASE(I) = VV                                           4472
4473     59         SML = SML + X(I)                                        4473
4474     60         TMS = TMS + X(I)*M(I)                                   4474
4475     61         SCVA = SCVA + X(I)*CVS(I)                               4475
4476     62         SV = SV + X(I)*M(I)/RHOS(I)                             4476
4477     63   C                                                             4477
4478     64         ELSE                                                    4478
4479     65         STOP ' PRODUCTS EITHER SOLID, S, OR GAS, G'             4479
4480     66   C                                                             4480
```

```
4481      67          END IF                                                    4481
4482      68    110   CONTINUE                                                  4482
4483      69    C                                                               4483
4484      70    10    IF ( NS .LT. 1 ) STOP ' NO PRODUCTS ?'                    4484
4485      71    C                                                               4485
4486      72          COVA = COVA * CAPPAA / GML                                4486
4487      73          FSA = TMS/AMAX1(SV,1.E-15)                                4487
4488      74          TML = GML + SML                                           4488
4489      75          XGA = GML/TML                                             4489
4490      76          SCVA = SCVA/TML                                           4490
4491      77          WMA = TMS/TML                                             4491
4492      78    C                                                               4492
4493      79          DO 130 INASA = 1, NNASA                                   4493
4494      80          IF ( NG .EQ. 0 ) GO TO 20                                 4494
4495      81    1     READ (4,1001) NASAP, ID                                   4495
4496      82    1001  FORMAT(A8,71X,I1)                                        4496
4497      83          IF ( ID .NE. 1 ) GO TO 1                                  4497
4498      84    C                                                               4498
4499      85          DO 120 I = 1, NS                                          4499
4500      86            IF ( NASAP .EQ. PRODCT(I) .AND. PHASE(I) .EQ. GG ) THEN 4500
4501      87            PHASE(I) = VV                                           4501
4502      88            NG = NG - 1                                             4502
4503      89            READ (4,1002) ((CF(K,KK),K=1,7),KK=1,2)                 4503
4504      90    1002    FORMAT(5E15.8)                                          4504
4505      91    C                                                               4505
4506      92              CF(1,1) = CF(1,1) - 1.                                4506
4507      93              CF(1,2) = CF(1,2) - 1.                                4507
4508      94              DO 115 K = 0, 5                                       4508
4509      95              CV(K,1) = CV(K,1) + (X(I)/GML)*CF(K+1,1)              4509
4510      96    115       CV(K,2) = CV(K,2) + (X(I)/GML)*CF(K+1,2)              4510
4511      97    C                                                               4511
4512      98            END IF                                                  4512
4513      99    120   CONTINUE                                                  4513
4514     100    C                                                               4514
4515     101    130   CONTINUE                                                  4515
4516     102    C                                                               4516
4517     103    20    DO 140 I = 1, NS                                          4517
4518     104          IF ( PHASE(I) .NE. VV ) STOP ' SPECIES NOT FOUND IN NASA' 4518
4519     105    140   CONTINUE                                                  4519
4520     106    C                                                               4520
4521     107          DO 150 I = 3, 50                                          4521
4522     108    150   TA(I) = FLOAT(100*I)                                      4522
4523     109    C                                                               4523
4524     110          CALL PSM ( CV(0,2),4, TA(3),8,  CVMA(3)  )                4524
4525     111          CALL PSM ( CV(0,1),4, TA(11),40, CVMA(11) )               4525
4526     112    C                                                               4526
4527     113          DO 155 K = 1, 4                                           4527
4528     114          CV(K,1) = CV(K,1)/FLOAT(K+1)                              4528
4529     115    155   CV(K,2) = CV(K,2)/FLOAT(K+1)                              4529
4530     116    C                                                               4530
4531     117          CALL PSM ( CV(0,2),4, TA(3),8,  EMEOA(3)  )               4531
4532     118          CALL PSM ( CV(0,1),4, TA(11),40, EMEOA(11) )              4532
4533     119    C                                                               4533
4534     120          DO 160 I = 3, 10                                          4534
4535     121    160   EMEOA(I) = TA(I)*EMEOA(I)                                 4535
4536     122          DO 161 I = 11, 50                                         4536
4537     123    161   EMEOA(I) = TA(I)*EMEOA(I)                                 4537
4538     124    C                                                               4538
4539     125          DO 180 I = 3, 50                                          4539
4540     126    180   EMEOA(I) = EMEOA(I)*XGA + TA(I)*SCVA                      4540
4541     127    C                                                               4541
4542     128          CALL BILD (EMEOA,48,RANGEA,DYA)                           4542
4543     129    C                                                               4543
4544     130          RETURN                                                    4544
4545     131          END                                                       4545
```

```
4546      1          SUBROUTINE PSM (A,NPOL, T,N, SMM)                    4546
4547      2    C                                                          4547
4548      3          REAL     A(0:NPOL), T(N), SMM(N)                   4548
4549      4    C                                                          4549
4550      5          DO 10 J = 1, N                                       4550
4551      6    10    SMM(J) = A(NPOL)                                     4551
4552      7    C                                                          4552
4553      8          DO 20 K = NPOL-1, 0, -1                              4553
4554      9    C                                                          4554
4555     10            DO 15 J = 1, N                                     4555
4556     11    15      SMM(J) = SMM(J) * T(J) + A(K)                      4556
4557     12    C                                                          4557
4558     13    20    CONTINUE                                             4558
4559     14    C                                                          4559
4560     15          RETURN                                               4560
4561     16          END                                                  4561
4562     17    C                                                          4562
```



```
4563      1          SUBROUTINE BILD(Y,N,RANGE,DY)                        4563
4564      2    C                                                          4564
4565      3          REAL Y(N),RANGE,DY(200)                              4565
4566      4          IF( N .GT. 201 ) STOP ' ONLY 201 POINTS ALLOWED '    4566
4567      5    C                                                          4567
4568      6          RANGE = (Y(N+2) - Y(3)) / (N-1)                      4568
4569      7          DO 10 I = 1 , N-1                                    4569
4570      8          DY(I+2) = Y(I+3) - Y(I+2)                            4570
4571      9     10   CONTINUE                                             4571
4572     10    C                                                          4572
4573     11          RETURN                                               4573
4574     12          END                                                  4574
```



```
4575      1          SUBROUTINE MATRLX                                    4575
4576      2    C                                                          4576
4577      3    C     READS MATERIAL PROPERTIES                            4577
4578      4    C     EVALUATES MATERIAL RELATED CONTANTS                  4578
4579      5    C                                                          4579
4580      6          include     'dmtr10.h'                               4580
4581      7          CHARACTER*8   PRODCT(15), PHASE(15), GG, SS, VV, NASAP 4581
4582      8          REAL        X(15), KVOL(15), M(15), RHOS(15), CVS(15) 4582
4583      9          REAL        CF(7,2), CV(0:5,2)                       4583
4584     10    C                                                          4584
4585     11          DATA        KVOL/15*0./                              4585
4586     12          DATA        GG/'G'/, SS/'S'/, VV/'VVVV'/             4586
4587     13          DATA        CV/12*0./                                4587
4588     14    C                                                          4588
4589     15          DATA PRODCT/'H2O','CO2','CO','N2','Cs',10*'VVVV    '/ 4589
4590     16          DATA PHASE/4*'G','S',10*'       '/                   4590
4591     17    C                                                          4591
4592     18          ALFAX=.5                                             4592
4593     19          BETAX=.09585                                         4593
4594     20          THETAX=400.                                          4594
4595     21          CAPPAX=12.685                                        4595
4596     22          NNASA=100                                            4596
4597     23          X(1)=2.5                                             4597
4598     24          X(2)=1.66                                            4598
4599     25          X(3)=.188                                            4599
4600     26          X(4)=1.5                                             4600
4601     27          X(5)=5.15                                            4601
4602     28          KVOL(1)=250.                                         4602
4603     29          KVOL(2)=600.                                         4603
4604     30          KVOL(3)=390.                                         4604
4605     31          KVOL(4)=380.                                         4605
4606     32          KVOL(5)=0.                                           4606
4607     33          M(1)=18.                                             4607
4608     34          M(2)=44.                                             4608
4609     35          M(3)=28.                                             4609
4610     36          M(4)=28.                                             4610
4611     37          M(5)=12.                                             4611
4612     38          CVS(5)=1.1                                           4612
4613     39          RHOS(5)=2.6                                          4613
```

```
4614      40          NS = 0                                                4614
4615      41          NG = 0                                                4615
4616      42    C                                                           4616
4617      43          TMS = 0.                                              4617
4618      44          COVX = 0.                                             4618
4619      45          GML = 0.                                              4619
4620      46          SML = 0.                                              4620
4621      47          SV = 0.                                               4621
4622      48          SCVX = 0.                                             4622
4623      49    C                                                           4623
4624      50          REWIND 4                                              4624
4625      51          DO 110 I = 1, 15                                      4625
4626      52          IF ( PRODCT(I) .EQ. VV ) GO TO 10                     4626
4627      53          NS = I                                                4627
4628      54    C                                                           4628
4629      55          IF ( PHASE(I) .EQ. GG ) THEN                          4629
4630      56          NG = NG + 1                                           4630
4631      57          GML = GML + X(I)                                      4631
4632      58          TMS = TMS + X(I)*M(I)                                 4632
4633      59          COVX = COVX + X(I)*KVOL(I)                            4633
4634      60    C                                                           4634
4635      61          ELSE IF ( PHASE(I) .EQ. SS ) THEN                     4635
4636      62          PHASE(I) = VV                                         4636
4637      63          SML = SML + X(I)                                      4637
4638      64          TMS = TMS + X(I)*M(I)                                 4638
4639      65          SCVX = SCVX + X(I)*CVS(I)                             4639
4640      66          SV = SV + X(I)*M(I)/RHOS(I)                           4640
4641      67    C                                                           4641
4642      68          ELSE                                                  4642
4643      69          STOP ' PRODUCTS EITHER SOLID, S, OR GAS, G'           4643
4644      70    C                                                           4644
4645      71          END IF                                                4645
4646      72    110   CONTINUE                                              4646
4647      73    C                                                           4647
4648      74    10    IF ( NS .LT. 1 ) STOP ' NO PRODUCTS ?'                4648
4649      75    C                                                           4649
4650      76          COVX = COVX * CAPPAX / GML                            4650
4651      77          FSX = TMS/AMAX1(SV,1.E-15)                            4651
4652      78          TML = GML + SML                                       4652
4653      79          XGX = GML/TML                                         4653
4654      80          SCVX = SCVX / TML                                     4654
4655      81          WMX = TMS/TML                                         4655
4656      82    C                                                           4656
4657      83          DO 130 INASA = 1, NNASA                               4657
4658      84          IF ( NG .EQ. 0 ) GO TO 20                             4658
4659      85    1     READ (4,1001) NASAP, ID                               4659
4660      86    1001  FORMAT(A8,71X,I1)                                     4660
4661      87          IF ( ID .NE. 1 ) GO TO 1                              4661
4662      88    C                                                           4662
4663      89          DO 120 I = 1, NS                                      4663
4664      90            IF ( NASAP .EQ. PRODCT(I) .AND. PHASE(I) .EQ. GG ) THEN 4664
4665      91            PHASE(I) = VV                                       4665
4666      92            NG = NG - 1                                         4666
4667      93            READ (4,1002) ((CF(K,KK),K=1,7),KK=1,2)             4667
4668      94    1002    FORMAT(5E15.8)                                      4668
4669      95    C                                                           4669
4670      96              CF(1,1) = CF(1,1) - 1.                            4670
4671      97              CF(1,2) = CF(1,2) - 1.                            4671
4672      98              DO 115 K = 0, 5                                   4672
4673      99              CV(K,1) = CV(K,1) + (X(I)/GML)*CF(K+1,1)          4673
4674     100    115      CV(K,2) = CV(K,2) + (X(I)/GML)*CF(K+1,2)          4674
4675     101    C                                                           4675
4676     102            END IF                                              4676
4677     103    120   CONTINUE                                              4677
4678     104    C                                                           4678
4679     105    130   CONTINUE                                              4679
4680     106    C                                                           4680
4681     107    20    DO 140 I = 1, NS                                      4681
4682     108          IF ( PHASE(I) .NE. VV ) STOP ' SPECIES NOT FOUND IN NASA' 4682
4683     109    140   CONTINUE                                              4683
4684     110    C                                                           4684
4685     111          DO 150 I = 3, 50                                      4685
4686     112    150   TX(I) = FLOAT(100*I)                                  4686
4687     113    C                                                           4687
```

```
4688     114          CALL PSM ( CV(0,2),4, TX(3),8,  CVMX(3)  )
4689     115          CALL PSM ( CV(0,1),4, TX(11),40, CVMX(11) )
4690     116    C
4691     117          DO 155 K = 1, 4
4692     118          CV(K,1) = CV(K,1)/FLOAT(K+1)
4693     119    155   CV(K,2) = CV(K,2)/FLOAT(K+1)
4694     120    C
4695     121          CALL PSM ( CV(0,2),4, TX(3),8,  EMEOX(3)  )
4696     122          CALL PSM ( CV(0,1),4, TX(11),40, EMEOX(11) )
4697     123    C
4698     124          DO 160 I = 3, 10
4699     125    160   EMEOX(I) = TX(I)*EMEOX(I)
4700     126          DO 161 I = 11, 50
4701     127    161   EMEOX(I) = TX(I)*EMEOX(I)
4702     128    C
4703     129          DO 180 I = 3, 50
4704     130    180   EMEOX(I) = EMEOX(I)*XGX + TX(I)*SCVX
4705     131    C
4706     132          CALL BILD (EMEOX,48,RANGEX,DYX)
4707     133    C
4708     134          RETURN
4709     135          END
```



```
4710       1          SUBROUTINE VOLMTETC ( I1, I2, I3, X, Y, Z , VOLUMT )
4711       2    C
4712       3    C-------------------------------------------------------------------I
4713       4    C                                                                   I
4714       5    C       VOLMTETC FINDS THE VOLUME OF THE TETRAHEDRON DEFINED BY THE I
4715       6    C       GRID VERTICES I1, I2, I3, AND THE POINT (X, Y, Z).          I
4716       7    C       THE CODE ASSUMES THAT THE AREAL VECTOR OF THE BASE TRIANGLE I
4717       8    C       FORMED BY I1, I2 AND I3 POINTS IN THE DIRECTION OF (X, Y, Z): I
4718       9    C       BY THE RIGHT HAND RULE, IF I1, I2 AND I3 ARE ARRANGED       I
4719      10    C       COUNTER-CLOCKWISE AS VIEWED FROM ABOVE THE PLANE OF THE     I
4720      11    C       TRIANGLE, (X, Y, Z) ALSO LIES ABOVE THE PLANE).  BUT NOTE --  I
4721      12    C                                                                   I
4722      13    C               THE VOLUME RETURNED IS A SIGNED QUANTITY - IE.      I
4723      14    C               IF THE VERTICES ARE NOT ORDERED BY THE RIGHT        I
4724      15    C               HAND RULE THE VOLUME WILL BE NEGATIVE.              I
4725      16    C                                                                   I
4726      17    C                                                                   I
4727      18    C       DECEMBER, 1991: M. FRITTS, FRITTS%MCL.SAINET@CCC.NERSC.GOV, I
4728      19    C                                (301) 266-0992                     I
4729      20    C                                                                   I
4730      21    C-------------------------------------------------------------------I
4731      22    C
4732      23    C===================================================================
4733      24    C
4734      25          DOUBLE PRECISION R21X,R21Y,R21Z,R31X,R31Y,R31Z,R41X,R41Y,R41Z
4735      26          DOUBLE PRECISION VOLUMT,X,Y,Z
4736      27    C
4737      28    C
4738      29          include     'dmsh00.h'
4739      30    C
4740      31    C===================================================================
4741      32    C
4742      33    C --- FIND THE VOLUME OF THE TETRAHEDRON.-----------------------------
4743      34    C
4744      35           R21X = XV(1,I2) - XV(1,I1)
4745      36           R21Y = XV(2,I2) - XV(2,I1)
4746      37           R21Z = XV(3,I2) - XV(3,I1)
4747      38           R31X = XV(1,I3) - XV(1,I1)
4748      39           R31Y = XV(2,I3) - XV(2,I1)
4749      40           R31Z = XV(3,I3) - XV(3,I1)
4750      41           R41X = X        - XV(1,I1)
4751      42           R41Y = Y        - XV(2,I1)
4752      43           R41Z = Z        - XV(3,I1)
4753      44    C
4754      45           VOLUMT  = ( R41X*( R21Y*R31Z - R21Z*R31Y ) -
4755      46         1             R41Y*( R21X*R31Z - R21Z*R31X ) +
4756      47         2             R41Z*( R21X*R31Y - R21Y*R31X )   )/6.D0
4757      48    C
4758      49    C
```

```
4759      50   C       ------                                          4759
4760      51           RETURN                                          4760
4761      52   C       ------                                          4761
4762      53   C                                                       4762
4763      54   C     ---                                               4763
4764      55           END                                             4764
4765      56   C                                                       4765
```

#	routine	page
1	AUGUST	1
2	HYDRFL	13
3	HYDRMN	18
4	GEOMTR	25
5	UPDATE	29
6	UPGRAD	30

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1	AUGUST	1
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```
      PROGRAM AUGUST
C=====================================================================
C
C       The AUGUST Code
C
C                       - Adaptive
C                       - Unstructured
C                       - Godunov
C                       - Upwind
C                       - Second order
C                       - Triangular
C
C                       The geometry structure comes from BERMUDA
C                       The solver is based on FUGGS
C
C
C       Version:   2.00      june 17, 1991
C
C       Authors:   Itzhak Lottati    (703)749-8648
C                  Shmuel Eidelman   (703)448-6491
C                  Adam Drobot       (703)734-5840
C
C                  Science Applications International Corporation
C                  Applied Physics Operation
C                  1710 Goodridge Drive
C                  McLean, Virginia 22102
C
C=====================================================================
C
C
C-----------------------------------------------------------------I
C                                                                 I
C     BERMUDA IS A MULTIDIMENSIONAL CODE WHICH IS BASED ON THE    I
C           USE OF TRIANGULAR GRIDS AS THE FUNDAMENTAL MESH       I
C           FOR FIELD LIKE QUANTITIES.  THE CODE REQUIRES         I
C           THAT ALL QUANTITIES ARE BASED AT THE BARICENTER       I
C           OF SIDES/TRIANGLES.                                   I
C                                                                 I
C           THE QUIP IS THAT THOSE WHO WORK ON BERMUDA            I
C           TRIANGLES ARE NEVER HEARD FROM AGAIN.                 I
C                                                                 I
C           THE BASIC MODULES IN BERMUDA INCLUDE:                 I
C                                                                 I
C                 A HYDRODYNAMICS CODE                          I
C                       .BASED ON A FIRST ORDER GODUNOV         I
C                        METHOD OR A SECOND ORDER GODUNOV       I
C                        WITH MESH ADAPTATION.                  I
C                                                                 I
C-----------------------------------------------------------------I
C
C     GRID SETUP TABLES AND THEIR MEANING:
C
C     ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C     +                                                          +
C     +   LIST OF VERTICES                                       +
C     +                                                          +
C     +       IV          - VERTEX INDEX                       +
C     +       JV(1,IV)    - S STATUS OF THE POINT              +
C     +                     S=0 FREE POINT WHICH MAY BE        +
C     +                         DELETED/MOVED                  +
C     +                     S=1 POINT RESTRICTED TO A SURFACE  +
C     +                     S=2 POINT RESTRICTED TO A LINE     +
C     +                     S=3 POINT WHICH IS FIXED AND MAY   +
C     +                         NOT BE REMOVED                 +
C     +       JV(2,IV)    - INDEX OF A LINE WHICH INCLUDE THE  +
C     +                     POINT                              +
C     +                     NEGATIVE MEANS THE POINT IS ON A   +
C     +                     BOUNDARY LINE                      +
C     +       XV(1,IV)    - X POSITION OF VERTEX               +
C     +       XV(2,IV)    - Y POSITION OF VERTEX               +
C     +                                                          +
C     ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C
```

```
C     +-------------------------------------------------------------+
C     +                                                             +
C     +   LIST OF EDGES                                            +
C     +                                                             +
C     +        IE          - EDGE INDEX                           +
C     +        JE(1,IE)    - INDEX OF LOWER EDGE VERTEX           +
C     +        JE(2,IE)    - INDEX OF UPPER EDGE VERTEX           +
C     +                                                             +
C     +   FOR TWO DIMENSIONAL PROBLEMS                            +
C     +                                                             +
C     +        JE(3,IE)    - INDEX OF LEFT  SIDE                  +
C     +        JE(4,IE)    - INDEX OF RIGHT SIDE                  +
C     +                                                             +
C     +        IF JE(3-4,IE) IS NEGATIVE THIS INDICATES THAT THE  +
C     +                      EDGE LIES ALONG A BOUNDARY.            +
C     +                                                             +
C     +        JE(5,IE)    - INDEX DEFINING BOUNDARY CONDITION    +
C     +                      0 - ORDINARY EDGE INTERIOR             +
C     +                      6 - WALL V-PERPENDICULAR=0             +
C     +                      7 - SUPERSONIC OUTFLOW                 +
C     +                      8 - INFLOW BOUNDARY                    +
C     +                                                             +
C     +        XE(1,IE)    - LENGTH OF EDGE                       +
C     +        XE(2,IE)    - DISTANCE BETWEEN ADJOINING SIDE      +
C     +                      POINTS.                                +
C     +                                                             +
C     +-------------------------------------------------------------+
C
C     +-------------------------------------------------------------+
C     +                                                             +
C     +   LIST OF SIDES                                            +
C     +                                                             +
C     +        IS          - SIDE INDEX                           +
C     +        JS(1,IS)    - INDEX OF FIRST  VERTEX               +
C     +        JS(2,IS)    - INDEX OF SECOND VERTEX               +
C     +        JS(3,IS)    - INDEX OF THIRD  VERTEX               +
C     +                                                             +
C     +        THE VERTICES RUN AROUND THE SIDE IN ORDER          +
C     +        COUNTER-CLOCKWISE FASHION                          +
C     +                                                             +
C     +        JS(4,IS)    - INDEX OF THE FIRST  EDGE             +
C     +        JS(5,IS)    - INDEX OF THE SECOND EDGE             +
C     +        JS(6,IS)    - INDEX OF THE THIRD  EDGE             +
C     +                                                             +
C     +        THE EDGES ARE ARRANGED IN COUNTER-iCLOCKWISE       +
C     +        FASHION. EDGE ONE RUNS FROM VERTEX-ONE TO          +
C     +        VERTEX-TWO ETC.. THE SIGN OF JS(4-6,IS) INDICATES  +
C     +        IF EDGE DATA IS STORED THE SAME WAY. IF IT IS      +
C     +        JS>0 AND IT IS REVERSED JS<0                       +
C     +                                                             +
C     +        XS(1,IS)     - X POSITION OF SIDE POINT            +
C     +        XS(2,IS)     - Y POSITION OF SIDE POINT            +
C     +        XS(3,IS)     - AREA OF SIDE                        +
C     +                                                             +
C     +                                                             +
C     +-------------------------------------------------------------+
C
C=====================================================================
C
C --- DEFINITION FOR ALL HYDRODYNAMIC QUANTITIES  ------------------
C
C-------------------------------------------------------------I
C                                                             I
C    USE OF PARAMETERS:                                       I
C                                                             I
C        MHQ     - MAXIMUM NUMBER OF HYDRO QUANTITIES.        I
C                                                             I
C                                                             I
C-------------------------------------------------------------I
C
C=====================================================================
C
      include     'cmsh00.h'
      include     'chyd00.h'
```

```
      include     'cint00.h'
      include     'cphs10.h'
      include     'cphs20.h'
C
C-----------------------------------------------------------------------
C
      NAMELIST /DATA/ ICOND,ICONP,ITRIGR,IOPTN,
     .                XMCHIN,RIN,PIN,ALFA,HRGG,IHRN,NTIME,MDUMP,NDUMP,
     .                KDUMP,IOSPCL,IOPLFT,IOPRCN,IOPORD,IOPBYN,IAXSYM,
     .                IOPEOS,MPRTCL,IOPINT,IOPADD,IOPDEL,AREADD,AREDEL,
     .                IWINDW,ISTATC
C
C-----------------------------------------------------------------------
C
C
C     --- MEANING OF NAMELIST VARIABLES:                                I
C                                                                       I
C     ICOND = 0 READ INPUT GRID FOR A NEW RUN                           I
C           = 1 READ THE GRID FROM PREVIOUS RUN                         I
C     ICONP = 0 PRIMITIVE VARIABLES SET TO ZERO                         I
C           = 1 VARIABLES READ FROM PREVIOUS RUN                        I
C     ITRIGR = 0 USING THE INPUT GRID AS THE INITIAL GRID               I
C            = 1 THE INPUT GRID TRIPLED BY ADDING AN EXTRA VERTEX IN    I
C                EACH TRIANGLE                                          I
C     IOPTN = 1 SOLUTION FOR STEADY STATE,                              I
C           = 2 SOLUTION FOR TRANSIENT PHENOMENA                        I
C                                                                       I
C     XMCHIN = FOR TRANSIENT SHOCK CALCULATIONS(IOPTN=2)THIS VARIABLE   I
C              IS USED TO SPECIFY THE UPSTREAM MACH NUMBER               I
C                                                                       I
C              RIN = THE AMBIENT DENSITY IN THE CHAMBER                 I
C                                                                       I
C              PIN = THE AMBIENT PRESSURE IN THE CHAMBER                I
C                                                                       I
C              APPLYING NORMAL SHOCK WAVES RELATIONS FOR AN ADIABATIC   I
C              FLOW RELATION STATIC-PRESSURE RATIO ACROSS THE SHOCK      I
C              AS WELL AS THE DENSITY RATIO AND MACH NUMBER RATIO        I
C              ARE COMPUTED TO SET CORRECTLY THE CONDITION AT THE        I
C              INLET EDGES( EDGE BOUNDARY 8 ) OF THE COMPUTATIONAL       I
C              DOMAIN                                                    I
C                                                                       I
C              FOR STEADY STATE SHOCK CALCULATIONS(IOPTN=1)THIS IS THE   I
C              INFLOW MACH NUMBER. ALL DOMAIN VELOCITIES ARE THEN        I
C              INITIALIZED WITH THIS VALUE.                              I
C                                                                       I
C              RIN = THE AMBIENT DENSITY AT INFINITY                    I
C                                                                       I
C              PIN = THE AMBIENT PRESSURE AT INFINITY                   I
C                                                                       I
C              ALL COMPUTATIONAL DOMAIN ARE THEN INITIALIZED WITH       I
C              THOSE VALUES.                                             I
C                                                                       I
C     ALFA  = THE DIRECTION OF INFLOW IN DEGREES RELATIVE TO A RIGHT    I
C             HAND COORDINATE SYSTEM. ALFA=0 MEANS FLOW FROM LEFT TO    I
C             RIGHT. ALFA=90 MEANS FROM BOTTOM TO TOP. ALFA=-90 OR 270  I
C             MEANS FLOW FROM TOP TO BOTTOM ETC.                        I
C     HRGG  = INITIAL GAMMA IN THE EQUATION OF STATE                    I
C             THE CODE RUNS USING THE AIR EQUATION AS A BASELINE AND    I
C             SHOULD BE MODIFIED IF SOMETHING ELSE IS DESIRED.          I
C     IHRN  = NUMBER OF ITERATIONS IN THE RIEMANN SOLVER TO FIND THE    I
C             DIAPHRAGM SOLUTION.(3 to 4 SHOULD BE USED AND INCREASED   I
C             ONLY FOR HIGH MACH NUMBER CASES).                         I
C                                                                       I
C     NTIME = NUMBER OF REPEATS FOR THE INTEGRATION/REFINEMENT/         I
C             COARSENING SEQUENCE                                       I
C             AN OUTPUT DUMP IS DONE EVERY SEQUENCE REPEAT.             I
C     MDUMP = NUMBER OF OUTERMOST LOOP ITERATIONS IN THE CALCULATION    I
C             WHERE COARSENING OF THE GRID IS PERFORMED EVERY SEQUENCE  I
C             REPEAT.                                                   I
C     NDUMP = NUMBER OF OUTER LOOP ITERATIONS IN THE CALCULATION WHERE  I
C             REFINING IS DONE EVERY SEQUENCE REPEAT WITHOUT COARSENINGI
C     KDUMP = NUMBER OF ITERATIONS PERFORMED WITH NO REFINEMENT OR      I
C             COARSENING. IT IS THE INNER LOOP OF THE CALCULATION.      I
C             IF KDUMP=0 IS READ IN, KDUMP WILL BE SET BY THE           I
```

```
C             CODE AUTOMATICALLY ACCORDING TO THE VARIABLE AREADD.
C
C        +--------------------  o NTIME - DUMPING DATA
C        I
C        I    +---------------  o MDUMP - COARSENING
C        I    I
C        I    I    +----------  o NDUMP - REFINENEMENT
C        I    I    I
C        I    I    I   +------  o KDUMP - INTEGRATION
C        I    I    I   I
C        I    I    I   I
C        I    I    I   +------  o ..... INNER LOOP
C        I    I    I
C        I    I    +----------  o ..... OUTER LOOP
C        I    I
C        I    +---------------  o ..... OUTERMOST LOOP
C        I
C        +--------------------  o ..... DUMPING LOOP
C
C     IOSPCL = 0 NOT USING REDEFNITION OF POINTS ON THE BOUNDARY
C            = 1 USING REDEFENITION OF POINTS ON THE BOUNDARY
C     IOPLFT = 0 THE COMPUTATION OF LIFT DRAG AND MOMENT TURNED OFF
C            = 1 THE COMPUTATION OF LIFT DRAG AND MOMENT TURNED ON
C     IOPRCN = 0 A GLOBAL SWAPING ( RECONNECTION ) PROCEDURE IS OFF
C            = 1 A GLOBAL SWAPING ( RECONNECTION ) PROCEDURE IS ON
C     IOPORD = 1 THE CODE WILL RUN FIRST ORDER GODUNOV METHOD
C            = 2 THE CODE WILL RUN SECOND ORDER GODUNOV METHOD
C     IOPBYN = 0 NO BUOYANCY EFFECT ARE COMPUTED
C            = 1 BUOYANCY EFFECT IN THE Y DIRECTION ARE COMPUTED
C     IAXSYM = 0 THE CODE WILL RUN IN A PURE TWO DIMENSIONAL MODE
C            = 1 THE CODE WILL RUN IN AN AXI SYMMETRICAL MODE (X AXIS)
C            = 2 THE CODE WILL RUN IN AN AXI SYMMETRICAL MODE (Y AXIS)
C     IOPEOS = 0 THE CODE WILL RUN WITH CONSTANT GAMA
C            = 1 THE CODE WILL RUN WITH VARIABLE GAMA USING EQUATION
C                OF STATE FOR AIR
C
C     MPRTCL = 0 NO PARTICLE TRACING
C            = 1 THE CODE WILL TRACE PARTICLES
C     IOPINT = 0 NOT REFINING INITIALY THE EDGE BOUNDARY NO 8
C            = 1 REFINING INITIALY THE EDGE BOUNDARY NO 8
C     IOPADD = 0 THE REFINEMENT PROCEDURE IS TURNED OFF
C            = 1 THE REFINEMENT PROCEDURE IS TURNED ON
C     IOPDEL = 0 THE COARSENING PROCEDURE IS TURNED OFF
C            = 1 THE COARSENING PROCEDURE IS TURNED ON
C     AREADD = SPECIFY THE MINIMUM VALUE THAT A TRIANGLE SHOULD HAVE
C              AFTER REFINEMENT AS A FRACTION OF AVERAGE TRIANGLE AREA
C     AREDEL = SPECIFY THE MAXIMUM VALUE THAT A TRIANGLE SHOULD HAVE
C              AFTER COARSENING AS A FRACTION OF AVERAGE TRIANGLE AREA
C
C     IWINDW = 0 NO RESTRICTION ON THE REGION FOR REFINING THE GRID
C            = 1 SETTING A WINDOW FOR REFINING THE GRID
C     ISTATC = 0 THE ADAPTATION WILL BE DONE ON A MOVING WAVE
C            = 1 THE ADAPTATION WILL BE DONE ON A STEADY STATE
C                CONDITION
C
C-----------------------------------------------------------------------
C
      CHARACTER*15 ZHEADER,MNAME,MVNAME
      CHARACTER*1  FILLCH
      INTEGER NUMQUADS
C
C --- OPEN ALL FILES FOR THIS RUN ----------------------------------------
C
      OPEN( 4,FILE='naca4' ,FORM='UNFORMATTED')
      OPEN(88,FILE='naca82',FORM='UNFORMATTED')
      OPEN( 8,FILE='naca2' ,FORM='UNFORMATTED')
      OPEN( 9,FILE='naca3' ,FORM='UNFORMATTED')
      OPEN( 2,FILE='data.d',FORM='FORMATTED')
      OPEN(16,FILE='wedge45.zon',STATUS='OLD')
      OPEN(18,FILE='nacaa' ,FORM='UNFORMATTED')
C
C=======================================================================
C
C --- DEFAULT VALUES FOR INPUT DATA  -------------------------------------
```

```
296   296  C                                                                296
297   297        THIRD = 1. / 3.                                            297
298   298  C                                                                298
299   299        ICOND = 0                                                  299
300   300        ICONP = 0                                                  300
301   301        ITRIGR = 0                                                 301
302   302        IOPTN = 1                                                  302
303   303  C                                                                303
304   304        XMCHIN = 25.                                               304
305   305        RIN = 1.                                                   305
306   306        PIN = 1.                                                   306
307   307  C                                                                307
308   308        ALFA = 0.                                                  308
309   309        HRGG = 1.4                                                 309
310   310        IHRN = 4                                                   310
311   311        NTIME = 1                                                  311
312   312        MDUMP = 80                                                 312
313   313        NDUMP = 1                                                  313
314   314        KDUMP = 0                                                  314
315   315        IOSPCL = 0                                                 315
316   316        IOPLFT = 0                                                 316
317   317        IOPRCN = 0                                                 317
318   318        IOPORD = 2                                                 318
319   319        IOPBYN = 0                                                 319
320   320        IAXSYM = 0                                                 320
321   321        IOPEOS = 0                                                 321
322   322  C                                                                322
323   323        MPRTCL = 0                                                 323
324   324        IOPINT = 0                                                 324
325   325        IOPADD = 0                                                 325
326   326        IOPDEL = 0                                                 326
327   327        AREADD = 0.005                                             327
328   328        AREDEL = 1.                                                328
329   329        IWINDW = 0                                                 329
330   330        ISTATC = 0                                                 330
331   331  C                                                                331
332   332  C --- READ THE INPUT DATA ----------------------------------------332
333   333  C                                                                333
334   334        READ (2,DATA)                                              334
335   335  C                                                                335
336   336  C --- PRINTOUT THE RUN PARAMETERS --------------------------------336
337   337  C                                                                337
338   338          PRINT 101,    ICOND,ICONP,ITRIGR,IOPTN,                  338
339   339       .                XMCHIN,RIN,PIN,ALFA,HRGG,IHRN,NTIME,MDUMP,NDUMP,  339
340   340       .                KDUMP,IOSPCL,IOPLFT,IOPRCN,IOPORD,IOPBYN,IAXSYM,  340
341   341       .                IOPEOS,MPRTCL,IOPINT,IOPADD,IOPDEL,AREADD,AREDEL,  341
342   342       .                IWINDW,ISTATC                              342
343   343  C                                                                343
344   344  C --- SET RUN CONDITIONS AND PRINTOUT TO CONSOLE -----------------344
345   345  C                                                                345
346   346        XREADD = 1. / AREADD                                       346
347   347        NAREAD = ALOG( XREADD ) / ALOG( 3. ) + 1                   347
348   348        IF( NAREAD . LT . 3 ) NAREAD = 3                           348
349   349        IF( NAREAD . GT . 5 ) NAREAD = 5                           349
350   350        IF( ISTATC . EQ . 1 ) NAREAD = 3                           350
351   351        PRINT*,AREADD,AREDEL,NAREAD                                351
352   352        PRINT * ,ICOND,ICONP                                       352
353   353  C                                                                353
354   354        NPT = 0                                                    354
355   355        IJKINT = 3                                                 355
356   356        IF( ICOND . EQ . 0 ) THEN                                  356
357   357        DO 122 IS = 1 , MSM                                        357
358   358        KSDELT( IS ) = 0                                           358
359   359  122   CONTINUE                                                   359
360   360        END IF                                                     360
361   361        HYDMOM( 1 ) = 0.                                           361
362   362        HYDMOM( 2 ) = 0.                                           362
363   363        HYDMOM( 4 ) = 0.                                           363
364   364  C                                                                364
365   365        DO 124 IK = 1 , MBP                                        365
366   366        GAMAG( IK ) = HRGG                                         366
367   367   124  CONTINUE                                                   367
368   368  C                                                                368
369   369  C=================================================================369
```

```
370   370   C                                                                370
371   371   C --- READ IN THE MESH DATA ---------------------------------------- 371
372   372   C                                                                372
373   373   C(1)>>>>>                                                        373
374   374         IF( ICOND . EQ . 0 ) THEN                                  374
375   375         IF( ICONP . EQ . 1 ) CALL UPGRAD                           375
376   376   C                                                                376
377   377   C------------------------------------------------------------------ 377
378   378   C A "SMART" FORMAT MESH FILE IS READ. THE FILE IS SELECTED BY THE  378
379   379   C NORMAL MACINTOSH FILE DIALOG BECAUSE OF THE '*' IN PLACE OF THE  379
380   380   C FILE NAME. VERTICES OF EACH TRIANGLE ARE FORMED FROM THE INPUT.   380
381   381   C------------------------------------------------------------------ 381
382   382         READ (16,900) ZHEADER                                        382
383   383   900   FORMAT(A15)                                                  383
384   384         IF (ZHEADER .NE. 'SMaRT-Z-T-(003)') THEN                     384
385   385   C---------------------- THIS ROUTINE CANNOT READ ANY OTHER INPUT    385
386   386         PRINT *, 'MESH FILE IS NOT THE CORRECT KIND OR VERSION'      386
387   387         CALL EXIT                                                    387
388   388         ENDIF                                                        388
389   389         READ (16,910) FILLCH,NV,NVMK                                 389
390   390         PRINT *,NV,NVMK                                              390
391   391         READ (16,910) FILLCH,NE,NEMK                                 391
392   392         PRINT *,NE,NEMK                                              392
393   393         READ (16,910) FILLCH,NS                                      393
394   394         PRINT *,NS                                                   394
395   395         READ (16,910) FILLCH,NUMQUADS                                395
396   396         PRINT *,NUMQUADS                                             396
397   397   910   FORMAT(A1,2I7)                                               397
398   398         READ (16,920) FILLCH,NZMK,NSMK,NNMK                          398
399   399         PRINT *,NZMK,NSMK,NNMK                                       399
400   400   920   FORMAT(A1,1X,3I3)                                            400
401   401         IF (NV .GT. MVM) THEN                                        401
402   402   C------------------------- CHECK NODE (I.E., VERTEX) STORAGE SIZE   402
403   403         PRINT 1020,NV,MVM,NVMK                                       403
404   404   1010  FORMAT(1X,'TOO MANY NODES. ',I9,', MAX = ',I5)              404
405   405         CALL EXIT                                                    405
406   406         ENDIF                                                        406
407   407         IF (NE .GT. MEM) THEN                                        407
408   408   C--------------------------- CHECK SIDE (I.E., EDGE) STORAGE SIZE   408
409   409         PRINT 1020,NE,MEM,NEMK                                       409
410   410   1020  FORMAT(1X,'TOO MANY SIDES. ',I9,', MAX = ',I5)              410
411   411         CALL EXIT                                                    411
412   412         ENDIF                                                        412
413   413         IF (NS .GT. MSM) THEN                                        413
414   414   C---------------- CHECK ZONE (I.E., SIDE OR TRIANGLE) STORAGE SIZE  414
415   415         PRINT 1030,NS,MSM                                            415
416   416   1030  FORMAT(1X,'TOO MANY ZONES. ',I9,', MAX = ',I5)              416
417   417         CALL EXIT                                                    417
418   418         ENDIF                                                        418
419   419         IF (NUMQUADS .GT. 0) THEN                                    419
420   420   C------------------------- CHECK FOR QUADRILATERALS IN THE INPUT    420
421   421         PRINT 1040                                                   421
422   422   1040  FORMAT(1X,'NO QUADRILATERALS ARE ALLOWED.')                  422
423   423         CALL EXIT                                                    423
424   424         ENDIF                                                        424
425   425   C------------------ READ MARKER DEFINITIONS                       425
426   426   C                   THE FOLLOWING JUST READS THE VARIABLES WITHOUT STORING 426
427   427   C                   THEM INTO PERMANENT ARRAYS, EFFECTIVELY JUST READING 427
428   428   C                   PAST THE MARKER DEFINTION INFORMATION.       428
429   429         DO 21 NZM = 1,NZMK                                           429
430   430         READ (16,1050) NMN,MNAME,NVAL                                430
431   431         DO 20 NZMV = 1,NVAL                                          431
432   432         READ (16,1050) NMV,MVNAME                                    432
433   433   20    CONTINUE                                                     433
434   434   21    CONTINUE                                                     434
435   435   1050  FORMAT(3X,I2,1X,A15,1X,I2)                                  435
436   436         DO 31 NZM = 1,NSMK                                           436
437   437         READ (16,1050) NMN,MNAME,NVAL                                437
438   438         DO 30 NSMV = 1,NVAL                                          438
439   439         READ (16,1050) NMV,MVNAME                                    439
440   440   30    CONTINUE                                                     440
441   441   31    CONTINUE                                                     441
442   442         DO 41 NZM = 1,NNMK                                           442
443   443         READ (16,1050) NMN,MNAME,NVAL                                443
```

```
      DO 40 NNMV = 1,NVAL
      READ (16,1050) NMV,MVNAME
40    CONTINUE
41    CONTINUE
C------------------ READ IN VERTEX INFORMATION
      DO 51 IV = 1 , NV
      IS = IV
      READ (16,1210) IK,XV(1,IS),XV(2,IS)
      JV(1,IV) = 0
C     INITIALIZE ANY VERTEX MARKER STORAGE, I.E. JV(*,IV)
51    CONTINUE
      PRINT 1060,NV
1060  FORMAT(I5,' NODES (VERTICES) READ IN.')
1210  FORMAT(I7,E15.9,1X,E15.9)
      IF (NVMK .GT. 0) THEN
C------------------ READ IN VERTEX MARKER INFORMATION
      DO 55 IV = 1,NVMK
      READ (16,*) IXV,MV1,MV2,MV3,MV4
      JV(1,IXV) = MV1
C          STORE THESE MARKERS IN JV(*, IXV) AS DESIRED
55    CONTINUE
      PRINT 1070,NVMK
1070  FORMAT(I5,' NODE (VERTEX) MARKERS READ IN.')
      ENDIF
C------------------ READ IN EDGE INFORMATION ( EDGES OF TRIANGLES).
      DO 60 IE = 1 , NE
      IS = IE
      READ (16,*) IJ,JE(1,IS),JE(2,IS),JE(3,IS),JE(4,IS)
C     INITIALIZE ANY MARKER STORAGE.
      JE(5,IE) = 0
60    CONTINUE
      PRINT 1080,NE
1080  FORMAT(I5,' SIDES (EDGES) READ IN.')
      IF (NEMK .GT. 0) THEN
C------------------ READ IN EDGE MARKER INFORMATION
      DO 65 IV = 1,NEMK
      READ (16,*) IXE,MV1,MV2,MV3,MV4
      JE(5,IXE) = MV1
65    CONTINUE
      PRINT 1090,NEMK
1090  FORMAT(I5,' SIDE (EDGE) MARKERS READ IN.')
      ENDIF
C------------------ READ IN SIDE (TRIANGLE) INFORMATION.
      DO 81 IS = 1 , NS
      IE = IS
      READ (16,1100) IJ, MV1,MV2,MV3,MV4,
     .               IV1,ID1,IV2,ID2,IV3,ID3
1100  FORMAT (I7,4I3,3(I7,I2))
      JS(4,IE) = IV1 * ID1
      JS(5,IE) = IV2 * ID2
      JS(6,IE) = IV3 * ID3
C      JS(7,IE) = MV1
C
C     STORE THESE MARKERS IN JS(*, IS) AS DESIRED
C
81    CONTINUE
      PRINT 1110,NS
1110  FORMAT(I5,' ZONES (SIDES) READ IN.')
      CLOSE (16)
C------------------ FORM VERTEX INDICES FOR EACH SIDE (TRIANGLE).
      DO 85 IS = 1 , NS
      DO 85  J = 1 , 3
      IE = JS( J + 3 , IS )
      IEABS = IABS( IE )
      IF ( IE . GT . 0 ) THEN
      JS( J , IS ) = JE( 1 , IEABS )
      ELSE
      JS( J , IS ) = JE( 2 , IEABS )
      END IF
85    CONTINUE
C
C-----------------------------------------------------------------------
C
      IF(IOSPCL.EQ.1)THEN
```

```
518     518   C                                                                      518
519     519   C --- SPECIAL CASE FOR HALF CIRCLE  BOUNDARY DATA ---------------------  519
520     520   C                                                                      520
521     521         DO 382 IE = 1 , NE                                               521
522     522         IJE5 = JE( 5 , IE )                                              522
523     523         IF( IJE5 . EQ . 6 ) THEN                                         523
524     524   C                                                                      524
525     525         IV1 = JE( 1 , IE )                                               525
526     526         IV2 = JE( 2 , IE )                                               526
527     527   C                                                                      527
528     528         XXS1 = XV( 1 , IV1 )                                             528
529     529         YYS1 = XV( 2 , IV1 )                                             529
530     530         XXS2 = XV( 1 , IV2 )                                             530
531     531         YYS2 = XV( 2 , IV2 )                                             531
532     532         DXX = XXS1 - 1.50                                                532
533     533         ANGL = 1.570796327                                               533
534     534         IF( DXX . NE . 0 ) ANGL = ATAN2( YYS1 , DXX )                    534
535     535         XV( 1 , IV1 ) = COS( ANGL ) + 1.5                                535
536     536         XV( 2 , IV1 ) = SIN( ANGL )                                      536
537     537         DXX = XXS2 - 1.50                                                537
538     538         ANGL = 1.570796327                                               538
539     539         IF( DXX . NE . 0 ) ANGL = ATAN2( YYS2 , DXX )                    539
540     540         XV( 1 , IV2 ) = COS( ANGL ) + 1.5                                540
541     541         XV( 2 , IV2 ) = SIN( ANGL )                                      541
542     542   C      XXS = XV( 1 , IV1 ) * 1.008930411364                            542
543     543   C      YYS = .6 * ( .2969 * SQRT( XXS ) - .126 * XXS -                 543
544     544   C     .             .3516 * XXS * XXS + .2843 * XXS * XXS * XXS -      544
545     545   C     .             .1015 * XXS * XXS * XXS * XXS )                    545
546     546   C      XV( 2 , IV1 ) = SIGN( 1. , XV( 2 , IV1 ) ) * YYS                546
547     547   C      IF( XXS . GT . .3 . AND . XXS . LT . .7 ) JV( 1 , IV1 ) = 0     547
548     548   C                                                                      548
549     549   C      XXS = XV( 1 , IV2 ) * 1.008930411364                            549
550     550   C      YYS = .6 * ( .2969 * SQRT( XXS ) - .126 * XXS -                 550
551     551   C     .             .3516 * XXS * XXS + .2843 * XXS * XXS * XXS -      551
552     552   C     .             .1015 * XXS * XXS * XXS * XXS )                    552
553     553   C      XV( 2 , IV2 ) = SIGN( 1. , XV( 2 , IV2 ) ) * YYS                553
554     554   C      IF( XXS . GT . .3 . AND . XXS . LT . .7 ) JV( 1 , IV2 ) = 0     554
555     555   C      IF( XE( 1 , IE ).GT. .2 ) CALL DISECT ( IE , IDONE , IJKINT )   555
556     556         END IF                                                           556
557     557   382   CONTINUE                                                         557
558     558         END IF                                                           558
559     559   C                                                                      559
560     560   C=====================================================================560
561     561   C                                                                      561
562     562   C                                                                      562
563     563   C --- CALCULATE GRID QUANTITIES THROUGH GEOMTR ------------------------ 563
564     564   C                                                                      564
565     565         CALL UPDATE                                                      565
566     566   C                                                                      566
567     567   C=====================================================================567
568     568   C                                                                      568
569     569   C --- REFINE THE INITIAL GRID BY A FACTOR OF THREE IF CALLED FOR ------- 569
570     570   C                                                                      570
571     571   C>>>>>>                                                                571
572     572         IF( ITRIGR . EQ . 1 ) THEN                                       572
573     573         NSS = NS                                                         573
574     574         DO 110 IS = 1 , NSS                                              574
575     575           CALL VERCEN( IS )                                              575
576     576   110   CONTINUE                                                         576
577     577         NEE = NE                                                         577
578     578         DO 120 IE = 1 , NEE                                              578
579     579           IF( JE( 5 , IE ) . NE . 0 ) THEN                               579
580     580             CALL DISECT ( IE , IDONE , IJKINT )                          580
581     581           ENDIF                                                          581
582     582   120   CONTINUE                                                         582
583     583         DO 130 IK = 1 , 3                                                583
584     584         PRINT*,NV,NE,NS,IK                                               584
585     585           DO 130 IE = 1 , NE                                             585
586     586             CALL RECNC( IE , IDONE , ITL , ITR , JA , JB , JC , JD )     586
587     587             CALL RECNC( JA , JADONE , ITL , ITR , JAA , JAB , JAC , JAD ) 587
588     588             CALL RECNC( JB , JBDONE , ITL , ITR , JBA , JBB , JBC , JBD ) 588
589     589             CALL RECNC( JC , JCDONE , ITL , ITR , JCA , JCB , JCC , JCD ) 589
590     590             CALL RECNC( JD , JDDONE , ITL , ITR , JDA , JDB , JDC , JDD ) 590
591     591   130   CONTINUE                                                         591
```

```
      END IF
C<<<<<<
C
C=======================================================================
C
C --- FIND AVERAGE TRIANGLE AREA ----------------------------------------
C
      SAREMN = 1000000.
      SAREMX = 0.
      SAREVG = 0.
      DO 105 IS = 1 , NS
       AREASS = XS( 3 , IS )
       SAREMX = AMAX1( SAREMX , AREASS )
       SAREMN = AMIN1( SAREMN , AREASS )
       SAREVG = SAREVG + AREASS
 105  CONTINUE
      AVGARE = SAREVG
      SAREVG = SAREVG / NS
      FMINVG = SAREVG * AREADD
      SAREMN = SAREMN / SAREVG
      SAREMX = SAREMX / SAREVG
      PRINT*,SAREVG,SAREMX,SAREMN
C
C --- DO INITIAL REFINEMENT FOR ALL INFLOW BOUNDARIES DEFINED ----------
C     BY EDGES THAT CONTAIN BOUNDARY CONDITION 8(INFLOW)
C
      IF(IOPINT.EQ.1)THEN
      NOFDIV = 2
      CALL INTPTN( AREADD , NOFDIV , 1 , LTRIG )
      NOFDIV = 2
      CALL DYYPTN( AREADD , NOFDIV , 1 , LTRIG )
      NOFDIV = 2
      CALL INTPTN( AREADD , NOFDIV , 2 , LTRIG )
      NOFDIV = 2
      CALL DYYPTN( AREADD , NOFDIV , 2 , LTRIG )
      NOFDIV = 2
      CALL INTPTN( AREADD , NOFDIV , 3 , LTRIG )
      NOFDIV = 2
      CALL DYYPTN( AREADD , NOFDIV , 3 , LTRIG )
C
      PRINT*,NV,NE,NS
      ENDIF
C
C=======================================================================
C
C --- FOR ICOND>0 READ IN PREVIOUS RUN'S DATA ---------------------------
C
C(1)----
      ELSE
        CALL UPGRAD
C       CALL GEOMTR
       IF( ICONP . EQ . 0 ) THEN
        READ (88) RIN,PIN,RINL,PINL,UVIN,UIN,VIN,TT,
     .                  HYDMOM(1),HYDMOM(2),HYDMOM(4)
        PRINT *, RIN,PIN,UVIN,UIN,VIN,TT
        READ (88) ((HYDV(IS,IK),IK=1,5),IS=1,NS)
        READ (88) ((HYDVVV(IV,IK),IK=1,5),IV=1,NV)
        READ (88) IJKINT,(KSDELT(IS),IS=1,NS)
         IF( MPRTCL . EQ . 1 )
     .     READ (88) NPT,((XPRTCL(IK,IPT),IK=1,2),IPT=1,NPT),
     .                                    (IJKPRT(IPT),IPT=1,NPT)
      ENDIF
      ENDIF
C(1)<<<<
C
C --- INITIALIZATION OF THE PROBLEM -------------------------------------
C
      SARERV = 1. / SAREVG
      SARESQ = SQRT( SAREVG )
      FMINVG = SAREVG * AREADD
      HRSM = 1.E-8
      HRGP = HRGG + 1.
      HRGM = HRGG - 1.
      CF   = HRGP / ( 2. * HRGG )
```

```
      C
            JDUMP = 9
            IF(KDUMP.EQ.0)THEN
            KDUMP = JDUMP
            ENDIF
      C
            TT = 0.
      C
            PIRAD = ATAN( 1. ) / 45.
            ALPHA = ALFA * PIRAD
            PRINT *,ALFA,PIRAD,ALPHA
            PRINT *,XMCHIN,PIN,RIN
      C
            COSS = COS( ALPHA )
            SINN = SIN( ALPHA )
            TANN = TAN( ALPHA )
      C
      C=====================================================================
      C
      C --- SET THE INITIAL VALUE FOR PRIMITIVE VARIABLES --------------------
      C
      C(2)>>>>
            IF( IOPTN . EQ . 1 ) THEN
            UVIN = XMCHIN * SQRT( HRGG * PIN / RIN )
            UIN = UVIN * COSS
            VIN = UVIN * SINN
            RIN = 1.
            PIN = 1.
      C
            DO 150 IS = 1 , NS
            HYDV( IS , 1 ) = RIN
            HYDV( IS , 2 ) = 0.
            HYDV( IS , 3 ) = 0.
            HYDV( IS , 4 ) = PIN
            HYDV( IS , 5 ) = HRGG
            XSS = XS( 1 , IS )
            IF( XSS . LT . .0 ) THEN
            HYDV( IS , 1 ) = .125 * RIN
            HYDV( IS , 4 ) = .100 * PIN
            END IF
      150   CONTINUE
      C
            DO 176 IV = 1 , NV
            HYDVVV( IV , 1 ) = RIN
            HYDVVV( IV , 2 ) = 0.
            HYDVVV( IV , 3 ) = 0.
            HYDVVV( IV , 4 ) = PIN / HRGM
            HYDVVV( IV , 5 ) = HRGG
            XSS = XV( 1 , IV )
            IF( XSS . LT . -.0 ) THEN
            HYDVVV( IV , 1 ) = RIN
            HYDVVV( IV , 4 ) = PIN / HRGM
            END IF
      176   CONTINUE
      C(2)----
            ELSE
      C
            XMSQR = XMCHIN * XMCHIN
            IF( ICOND . EQ . 1 . AND . ICONP . EQ . 0 ) THEN
            ELSE
            PINL = PIN
            RINL = RIN
            RINRTO = ( HRGG + 1. ) * XMSQR /
           .         ( ( HRGG - 1. ) * XMSQR + 2. )
            PINRTO = ( 2. * HRGG * XMSQR - ( HRGG - 1. ) ) /
           .                               ( HRGG + 1. )
            PIN = PINRTO * PINL
            RIN = RINRTO * RINL
            YMCHIN = SQRT( ( ( HRGG - 1. ) * XMSQR + 2. ) /
           .               ( 2. * HRGG * XMSQR - ( HRGG - 1. ) ) )
            PRINT*,HRGG,RIN,PIN,YMCHIN
            PRINT*,HRGG,RINL,PINL,XMCHIN
            UVIN = XMCHIN * SQRT( HRGG * PINL / RINL ) -
           .       YMCHIN * SQRT( HRGG * PIN / RIN )
```

```
      END IF
      DO 175 IV = 1 , NV
      HYDVVV( IV , 1 ) = RINL
      HYDVVV( IV , 2 ) = 0.
      HYDVVV( IV , 3 ) = 0.
      HYDVVV( IV , 4 ) = PINL / HRGM
      HYDVVV( IV , 5 ) = HRGG
      XSS = XV( 1 , IV )
      IF( XSS . LT . -.0 ) THEN
      HYDVVV( IV , 1 ) = RIN
      HYDVVV( IV , 2 ) = UVIN * RIN
      HYDVVV( IV , 4 ) = PIN / HRGM + .5 * RIN * UVIN * UVIN
      END IF
175   CONTINUE
      DO 170 IS = 1 , NS
      HYDV( IS , 1 ) = RINL
      HYDV( IS , 2 ) = 0.
      HYDV( IS , 3 ) = 0.
      HYDV( IS , 4 ) = PINL
      HYDV( IS , 5 ) = HRGG
      XSS = XS( 1 , IS )
      IF( XSS . LT . -.0 ) THEN
      HYDV( IS , 1 ) = RIN
      HYDV( IS , 2 ) = UVIN
      HYDV( IS , 4 ) = PIN
      END IF
170   CONTINUE
C
      IF( IOPEOS . EQ . 1 ) THEN
      HRGGN = HRGG
      HRGGL = HRGG
      RINRTO = ( HRGGN + 1. ) * XMSQR /
     .         ( ( HRGGN - 1. ) * XMSQR + 2. )
      PINRTO = ( 2. * HRGGN * XMSQR - ( HRGGN - 1. ) ) /
     .                                ( HRGGN + 1. )
      PIN = PINRTO * PINL
      RIN = RINRTO * RINL
      TTNN = PIN / ( HRGGN - 1. )
      RRNN = RIN
      TTNL = PINL / ( HRGGL - 1. )
      RRNL = RINL
      DO 1122 KI = 1 , 9
         CALL EOS( RRNN , TTNN , 1 , HRGGN )
         CALL EOS( RRNL , TTNL , 1 , HRGGL )
      RINRTO = ( HRGGN + 1. ) * XMSQR /
     .         ( ( HRGGN - 1. ) * XMSQR + 2. )
      PINRTO = ( 2. * HRGGN * XMSQR - ( HRGGN - 1. ) ) /
     .                                ( HRGGN + 1. )
      RIN = RINRTO * RINL
      PIN = PINRTO * PINL
      TTNN = PIN / ( HRGGN - 1. )
      RRNN = RIN
      TTNL = PINL / ( HRGGL - 1. )
      RRNL = RINL
      YMCHIN = SQRT( ( ( HRGGN - 1. ) * XMSQR + 2. ) /
     .                 ( 2. * HRGGN * XMSQR - ( HRGGN - 1. ) ) )
      PRINT*,HRGGN,RIN,PIN,YMCHIN
      PRINT*,HRGGL,RINL,PINL,XMCHIN
1122  CONTINUE
      UVIN = XMCHIN * SQRT( HRGGL * PINL / RINL ) -
     .       YMCHIN * SQRT( HRGGN * PIN / RIN )
      DO 172 IS = 1 , NS
      HYDV( IS , 5 ) = HRGGL
172   CONTINUE
      END IF
      UIN = UVIN * COSS
      VIN = UVIN * SINN
C
      ENDIF
C(2)<<<<
C
      IF( MPRTCL . EQ . 1 ) THEN
        IKXY = 0
        DO 190 IKX = 1 , 30
```

```
      DO 190 IKY = 1 , 15
      IKXY = IKXY + 1
      XPRTCL( 1 , IKXY ) = ( IKX - 1 ) * .1 + .05
      XPRTCL( 2 , IKXY ) = ( IKY - 1 ) * .1 + .05
190   CONTINUE
      NPT = IKXY
      PRINT *, NPT
      CALL PRLCTN
      PRINT *, NPT
     ENDIF
C
C=======================================================================
C
C --- READ INPUT DATA FROM THE PREVIOUS RUN -----------------------------
C
      PRINT * ,ICOND,ICONP
      IF( ICONP . EQ . 1 ) THEN
        READ (88) RIN,PIN,RINL,PINL,UVIN,UIN,VIN,TT,
     .            HYDMOM(1),HYDMOM(2),HYDMOM(4)
        PRINT *, RIN,PIN,UVIN,UIN,VIN,TT
        READ (88) ((HYDV(IS,IK),IK=1,5),IS=1,NS)
        READ (88) ((HYDVVV(IV,IK),IK=1,5),IV=1,NV)
        READ (88) IJKINT,(KSDELT(IS),IS=1,NS)
         IF( MPRTCL . EQ . 1 )
     .     READ (88) NPT,((XPRTCL(IK,IPT),IK=1,2),IPT=1,NPT),
     .                                    (IJKPRT(IPT),IPT=1,NPT)
      ENDIF
C
C=======================================================================
C
C --- PERFORM THE ACTUAL CALCULATION ------------------------------------
C
      CALL HYDRMN
C
C=======================================================================
C
C --- EXIT POINT FROM PROGRAM -------------------------------------------
C
C     --------
      STOP 777
C     --------
C
C --- FORMATS -----------------------------------------------------------
C
101   FORMAT(1H ,'ICOND=',I2,5X,'ICONP=',I2,5X,'ITRIGR=',I2,5X,
     .           'IOPTN=',I2,/,1X,
     .           'XMCHIN=',F13.6,5X,'RIN=',F13.6,5X,'PIN=',F13.6,/,1X,
     .           'ALFA=',F13.6,5X,'HRGG=',F13.6,5X,'IHRN=',I2,5X,/,1X,
     .           'NTIME=',I2,5X,'MDUMP=',I5,5X,'NDUMP=',I5,5X,/,1X
     .           'KDUMP=',I5,5X,'IOSPCL=',I2,5X,'IOPLFT=',I2,5X,/,1X,
     .           'IOPRCN=',I2,5X,'IOPORD=',I2,5X,'IOPBYN=',I2,5X,/,1X
     .           'IAXSYM=',I2,5X,'IOPEOS=',I2,5X,'MPRTCL=',I6,5X,/,1X,
     .           'IOPINT=',I2,5X,'IOPADD=',I2,5X,'IOPDEL=',I2,5X,/,1X,
     .           'AREADD=',F13.6,5X,'AREDEL=',F13.6,5X,/,1X,
     .           'IWINDW=',I2,5X,'ISTATC=',I2)
C
C     ---
      END
```

```
      SUBROUTINE HYDRFL
C
C-----------------------------------------------------------------I
C                                                                 I
C     HYDRFL IS A 2 DIMENSIONAL RIEMANN SOLVER THAT COMPUTES THE  I
C           FLUXES ACROSS NORMAL INTERFACES FOR UPDATING  SIDE   I
C           OR TRIANGLE BASED QUANTITIES.                         I
C                                                                 I
C-----------------------------------------------------------------I
C
      include     'cmsh00.h'
      include     'chyd00.h'
      include     'cint00.h'
      include     'cphs10.h'
      include     'cphs20.h'
C
C=================================================================
C
      REAL DELP(MBP),WSOP(MBP),WSOM(MBP),WSOO(MBP),
     .     RSTAR(MBP),CSTAR(MBP),PMAX(MBP),PMIN(MBP)
      REAL RRIGHT(MBP),URIGHT(MBP),VRIGHT(MBP),PRIGHT(MBP)
      REAL RLEFTT(MBP),ULEFTT(MBP),VLEFTT(MBP),PLEFTT(MBP)
C
C=================================================================
C
C
C --- BEGIN LOOP OVER ALL EDGES IN THE DOMAIN -------------------
C
      DO 280 IH = 1 , 4
      DO 280 IS = 1 , NS
      HYDFLX( IS , IH ) = 0.
 280  CONTINUE
C
      NE1 = 1
      NE2 = NOFVEE( 1 )
      DO 110 INE = 1 , NVEEE
C
C --- FETCH HYDRO QUANTITIES ------------------------------------
C     FOR LEFT AND RIGHT SIDE OF THE INTERFACE ON WHICH THE
C     RIEMANN PROBLEM IS SOLVED
C
      DO 120 IE = NE1 , NE2
          KE = IE - NE1 + 1
C
          RRR( KE ) = RR( IE )
          UUR( KE ) = UR( IE )
          VVR( KE ) = VR( IE )
          PPR( KE ) = PR( IE )
C
          RRL( KE ) = RL( IE )
          UUL( KE ) = UL( IE )
          VVL( KE ) = VL( IE )
          PPL( KE ) = PL( IE )
 120  CONTINUE
C
C --- ASSIGN GAMA A VALUE ---------------------------------------
C
      DO 130 KE = 1 , NOFVEE( INE )
         IE = KE + NE1 - 1
         ISL = JE( 3 , IE )
         ISR = JE( 4 , IE )
         GAMAL( KE ) = HYDV( ISL , 5 )
         IF( ISR . NE . 0 ) THEN
           GAMAR( KE ) = HYDV( ISR , 5 )
         ELSE
           GAMAR( KE ) = GAMAL( KE )
         END IF
C
C --- THIS SECTION OF CODE SOLVES FOR "PSTAR" AND "USTAR" IN ----------
C     THE RIEMANN PROBLEM USING NEWTON'S METHOD.
C
          WLEFT( KE ) = SQRT( GAMAL( KE ) * PPL( KE ) * RRL( KE ) )
          WRIGT( KE ) = SQRT( GAMAR( KE ) * PPR( KE ) * RRR( KE ) )
C
```

```
946      75            WLESQ( KE ) = WLEFT( KE ) * WLEFT( KE )
947      76            WRISQ( KE ) = WRIGT( KE ) * WRIGT( KE )
948      77      C
949      78            PMIN( KE ) = AMIN1( PPL( KE ) , PPR( KE ) )
950      79            PSML( KE ) = HRSM * PMIN( KE )
951      80      C
952      81      C --- FORM THE STARTING GUESS FOR THE SOLUTION ------------------------
953      82      C
954      83            PSTAR( KE ) = ( WLEFT( KE ) * PPR( KE ) +
955      84           .                WRIGT( KE ) * PPL( KE ) -
956      85           .                WLEFT( KE ) * WRIGT( KE ) *
957      86           .              ( UUR( KE ) - UUL( KE ) ) ) /
958      87           .              ( WLEFT( KE ) + WRIGT( KE ) )
959      88            PSTAR( KE ) = AMAX1( PSTAR( KE ) , PSML( KE ) )
960      89       130  CONTINUE
961      90      C
962      91            DO 140 I = 1 , IHRN
963      92      C
964      93      C --- BEGIN THE NEWTON ITERATION -------------------------------------
965      94      C
966      95            DO 150 KE = 1 , NOFVEE( INE )
967      96      C
968      97              CF = ( GAMAL( KE ) + 1 . ) / GAMAL( KE ) * .5
969      98              WLEFS( KE ) = ( 1. + CF * ( PSTAR( KE ) /
970      99           .                            PPL( KE ) - 1. ) ) * WLESQ( KE )
971     100              WLEFT( KE ) = SQRT( WLEFS( KE ) )
972     101              ZLEFT( KE ) = 2. * WLEFT( KE ) * WLEFS( KE ) /
973     102           .                ( WLESQ( KE ) + WLEFS( KE ) )
974     103              USTL( KE )  = UUL( KE ) -
975     104           .              ( PSTAR( KE ) - PPL( KE ) ) / WLEFT( KE )
976     105       150  CONTINUE
977     106      C
978     107            DO 152 KE = 1 , NOFVEE( INE )
979     108      C
980     109              CF = ( GAMAR( KE ) + 1 . ) / GAMAR( KE ) * .5
981     110              WRIFS( KE ) = ( 1. + CF * ( PSTAR( KE ) /
982     111           .                            PPR( KE ) - 1. ) ) * WRISQ( KE )
983     112              WRIGT( KE ) = SQRT( WRIFS( KE ) )
984     113              ZRIGT( KE ) = 2. * WRIGT( KE ) * WRIFS( KE ) /
985     114           .                ( WRISQ( KE ) + WRIFS( KE ) )
986     115              USTR( KE )  = UUR( KE ) +
987     116           .              ( PSTAR( KE ) - PPR( KE ) ) / WRIGT( KE )
988     117       152  CONTINUE
989     118      C
990     119            DO 160 KE = 1 , NOFVEE( INE )
991     120              DPST( KE )  = ZLEFT( KE ) * ZRIGT( KE ) *
992     121           .                ( USTR( KE ) - USTL( KE ) ) /
993     122           .                ( ZLEFT( KE ) + ZRIGT( KE ) )
994     123              PSTAR( KE ) = PSTAR( KE ) - DPST( KE )
995     124              PSTAR( KE ) = AMAX1( PSTAR( KE ) , PSML( KE ) )
996     125       160    CONTINUE
997     126       140    CONTINUE
998     127      C
999     128      C --- FORM FINAL SOLUTIONS -------------------------------------------
1000    129      C
1001    130            DO 170 KE = 1 , NOFVEE( INE )
1002    131      C
1003    132              CF = ( GAMAL( KE ) + 1. ) / GAMAL( KE ) * .5
1004    133              WLEFT( KE ) = SQRT( WLESQ( KE ) * ( 1. +
1005    134           .                CF * ( PSTAR( KE ) / PPL( KE ) - 1. ) ) )
1006    135       170  CONTINUE
1007    136      C
1008    137            DO 172 KE = 1 , NOFVEE( INE )
1009    138      C
1010    139              CF = ( GAMAR( KE ) + 1. ) / GAMAR( KE ) * .5
1011    140              WRIGT( KE ) = SQRT( WRISQ( KE ) * ( 1. +
1012    141           .                CF * ( PSTAR( KE ) / PPR( KE ) - 1. ) ) )
1013    142       172  CONTINUE
1014    143      C
1015    144            DO 180 KE = 1 , NOFVEE( INE )
1016    145              USTAR( KE ) = ( PPL( KE ) - PPR( KE ) +
1017    146           .                  WLEFT( KE ) * UUL( KE ) +
1018    147           .                  WRIGT( KE ) * UUR( KE ) ) /
1019    148           .                ( WLEFT( KE ) + WRIGT( KE ) )
```

```
1020     149    180  CONTINUE                                                        1020
1021     150  C                                                                     1021
1022     151  C --- BEGIN PROCEDURE TO OBTAIN FLUXES FROM REIMANN FORMALISM ----------1022
1023     152  C                                                                     1023
1024     153        DO 190 KE = 1 , NOFVEE( INE )                                   1024
1025     154           IF( USTAR( KE ) . LE . 0.0 ) THEN                            1025
1026     155  C                                                                     1026
1027     156             RO( KE ) = RRR( KE )                                       1027
1028     157             PO( KE ) = PPR( KE )                                       1028
1029     158             UO( KE ) = UUR( KE )                                       1029
1030     159             CO( KE ) = SQRT( GAMAR( KE ) * PPR( KE ) / RRR( KE ) )     1030
1031     160             WO( KE ) = WRIGT( KE )                                     1031
1032     161             ISN( KE ) = 1                                              1032
1033     162  C                                                                     1033
1034     163             VGDNV( KE ) = VVR( KE )                                    1034
1035     164  C                                                                     1035
1036     165           ELSE                                                         1036
1037     166  C                                                                     1037
1038     167             RO( KE ) = RRL( KE )                                       1038
1039     168             PO( KE ) = PPL( KE )                                       1039
1040     169             UO( KE ) = UUL( KE )                                       1040
1041     170             CO( KE ) = SQRT( GAMAL( KE ) * PPL( KE ) / RRL( KE ) )     1041
1042     171             WO( KE ) = WLEFT( KE )                                     1042
1043     172             ISN( KE ) = - 1                                            1043
1044     173  C                                                                     1044
1045     174             VGDNV( KE ) = VVL( KE )                                    1045
1046     175           END IF                                                       1046
1047     176    190  CONTINUE                                                      1047
1048     177  C                                                                     1048
1049     178        DO 200 KE = 1 , NOFVEE( INE )                                   1049
1050     179           DELP( KE ) = PSTAR( KE ) - PO( KE )                          1050
1051     180           WSOP( KE ) = ISN( KE ) * UO( KE ) + WO( KE ) / RO( KE )      1051
1052     181           WSOM( KE ) = ISN( KE ) * UO( KE ) + CO( KE )                 1052
1053     182    200   CONTINUE                                                      1053
1054     183  C                                                                     1054
1055     184        DO 210 KE = 1 , NOFVEE( INE )                                   1055
1056     185          IF( DELP( KE ) . GT . 0. ) THEN                              1056
1057     186            WSOO( KE ) = WSOP( KE )                                    1057
1058     187          ELSE                                                         1058
1059     188            WSOO( KE ) = WSOM( KE )                                    1059
1060     189          END IF                                                       1060
1061     190    210  CONTINUE                                                      1061
1062     191  C                                                                     1062
1063     192  C --- USE OUTER STATE SOLUTION ----------------------------------------1063
1064     193  C                                                                     1064
1065     194        DO 220 KE = 1 , NOFVEE( INE )                                   1065
1066     195           PGDNV( KE ) = PO( KE )                                       1066
1067     196           UGDNV( KE ) = UO( KE )                                       1067
1068     197           CGDNV( KE ) = CO( KE )                                       1068
1069     198           RGDNV( KE ) = RO( KE )                                       1069
1070     199    220  CONTINUE                                                      1070
1071     200  C                                                                     1071
1072     201  C --- COMPUTE STARRED VALUES ------------------------------------------1072
1073     202  C                                                                     1073
1074     203        DO 230 KE = 1 , NOFVEE( INE )                                   1074
1075     204           IE = KE + NE1 - 1                                            1075
1076     205           ISL = JE( 3 , IE )                                           1076
1077     206           ISR = JE( 4 , IE )                                           1077
1078     207           IF( ISR . NE . 0 ) THEN                                      1078
1079     208           GAMAG( KE ) = .5 * ( HYDV( ISL , 5 ) + HYDV( ISR , 5 ) )     1079
1080     209           ELSE                                                         1080
1081     210           GAMAG( KE ) = HYDV( ISL , 5 )                                1081
1082     211           END IF                                                       1082
1083     212  C                                                                     1083
1084     213             RSTAR( KE ) = 1. / ( 1. / RO( KE ) - DELP( KE ) /          1084
1085     214          .                       ( WO( KE ) * WO( KE ) ) )             1085
1086     215  C                                                                     1086
1087     216             CSTAR( KE ) = SQRT( GAMAG( KE ) * PSTAR( KE ) / RSTAR( KE ) )1087
1088     217             WSOM( KE )  = ISN( KE ) * USTAR( KE ) + CSTAR( KE )       1088
1089     218    230  CONTINUE                                                      1089
1090     219  C                                                                     1090
1091     220        DO 240 KE = 1 , NOFVEE( INE )                                   1091
1092     221          IF( DELP( KE ) . GT . 0. ) THEN                              1092
1093     222            SPIN( KE ) = WSOP( KE )                                    1093
```

```
1094     223           ELSE                                                    1094
1095     224             SPIN( KE ) = WSOM( KE )                               1095
1096     225           END IF                                                  1096
1097     226    240  CONTINUE                                                  1097
1098     227   C                                                               1098
1099     228         DO 250 KE = 1 , NOFVEE( INE )                             1099
1100     229   C                                                               1100
1101     230         IF( WSOO( KE ) . GE . 0. ) THEN                           1101
1102     231             IF( SPIN( KE ) . GE . 0. ) THEN                       1102
1103     232   C                                                               1103
1104     233   C --- USE THE STARRED STATE RESULTS ----------------------------1104
1105     234   C                                                               1105
1106     235                             RGDNV( KE ) = RSTAR( KE )             1106
1107     236                             UGDNV( KE ) = USTAR( KE )             1107
1108     237                             CGDNV( KE ) = CSTAR( KE )             1108
1109     238                             PGDNV( KE ) = PSTAR( KE )             1109
1110     239             ELSE                                                  1110
1111     240   C                                                               1111
1112     241   C --- EVALUATE THE INSIDE RAREFACTION WAVE ---------------------1112
1113     242   C                                                               1113
1114     243             HRGG = GAMAG( KE )                                    1114
1115     244             HRGM = GAMAG( KE ) - 1.                               1115
1116     245             HRGP = GAMAG( KE ) + 1.                               1116
1117     246             CGDNV( KE ) = ( CSTAR( KE ) * 2. -                    1117
1118     247        .                    ISN( KE ) * USTAR( KE ) * HRGM ) / HRGP 1118
1119     248             UGDNV( KE ) = - ISN( KE ) * CGDNV( KE )               1119
1120     249             RGDNV( KE ) = ( CGDNV( KE ) / CO( KE ) ) **           1120
1121     250        .                  ( 2. / HRGM ) * RO( KE )               1121
1122     251             PGDNV( KE ) = CGDNV( KE ) * CGDNV( KE ) * RGDNV( KE ) / HRGG 1122
1123     252   C                                                               1123
1124     253             END IF                                                1124
1125     254   C                                                               1125
1126     255         END IF                                                    1126
1127     256    250  CONTINUE                                                 1127
1128     257   C                                                               1128
1129     258             DO 142 IE = NE1 , NE2                                 1129
1130     259             KE = IE - NE1 + 1                                     1130
1131     260   C                                                               1131
1132     261             RRR( KE ) = XN( IE )                                  1132
1133     262             UUR( KE ) = YN( IE )                                  1133
1134     263             VVR( KE ) = XXN( IE )                                 1134
1135     264             PPR( KE ) = YYN( IE )                                 1135
1136     265             PPL( KE ) = XE( 2 , IE )                              1136
1137     266             RRL( KE ) = XE( 1 , IE )                              1137
1138     267             UUL( KE ) = XYMIDL( IE )                              1138
1139     268   C                                                               1139
1140     269    142  CONTINUE                                                 1140
1141     270   C                                                               1141
1142     271   C --- SEARCH FOR MINIMUM VALUE OF TIMESTEP ...DTT... -----------1142
1143     272   C                                                               1143
1144     273         DO 260 KE = 1 , NOFVEE( INE )                             1144
1145     274         CTT = SQRT( GAMAG( KE ) * PGDNV( KE ) / RGDNV( KE ) )     1145
1146     275         VEL = UGDNV( KE )                                         1146
1147     276   C                                                               1147
1148     277         PROJCT = RRR( KE ) * VVR( KE ) + UUR( KE ) * PPR( KE )    1148
1149     278         DTU = PPL( KE ) * ABS( PROJCT ) / ( CTT + ABS( VEL ) )    1149
1150     279         DT1 = DTU * UUL( KE )                                     1150
1151     280         DT2 = DTU - DT1                                           1151
1152     281         DTT = AMIN1( DTT , DT1 , DT2 )                            1152
1153     282    260  CONTINUE                                                 1153
1154     283   C                                                               1154
1155     284   C --- NOW FIND THE FLUXES AT EACH INTERFACE --------------------1155
1156     285   C                                                               1156
1157     286         DO 270 KE = 1 , NOFVEE( INE )                             1157
1158     287             HRGG = GAMAG( KE )                                    1158
1159     288             HRGM = GAMAG( KE ) - 1.                               1159
1160     289             HRGP = GAMAG( KE ) + 1.                               1160
1161     290   C                                                               1161
1162     291   C ... FLUX FOR DENSITY ..........................................1162
1163     292   C                                                               1163
1164     293         RO( KE ) = RGDNV( KE ) * UGDNV( KE )                      1164
1165     294   C                                                               1165
1166     295   C ... FLUX FOR MOMENTUM DENSITY .................................1166
1167     296   C                                                               1167
```

```
1168    297         UO( KE ) = PGDNV( KE ) * RRR( KE ) +                          1168
1169    298        .              RO( KE ) * ( UGDNV( KE ) * RRR( KE ) -         1169
1170    299        .                           VGDNV( KE ) * UUR( KE ) )         1170
1171    300         WO( KE ) = PGDNV( KE ) * UUR( KE ) +                          1171
1172    301        .              RO( KE ) * ( UGDNV( KE ) * UUR( KE ) +         1172
1173    302        .                           VGDNV( KE ) * RRR( KE ) )         1173
1174    303   C                                                                  1174
1175    304   C ... FLUX FOR ENERGY DENSITY ..........................................1175
1176    305   C                                                                  1176
1177    306         PO( KE ) = UGDNV( KE ) * ( PGDNV( KE ) * HRGG / HRGM +        1177
1178    307        .      .5 * RGDNV( KE ) * ( UGDNV( KE ) * UGDNV( KE ) +       1178
1179    308        .                           VGDNV( KE ) * VGDNV( KE ) ) )     1179
1180    309   C                                                                  1180
1181    310    270  CONTINUE                                                     1181
1182    311   C                                                                  1182
1183    312   C --- COLLECT INTERFACE FLUXES FOR EACH TRIANGLE ----------------------1183
1184    313   C                                                                  1184
1185    314         DO 290 IE = NE1 , NE2                                        1185
1186    315          KE = IE - NE1 + 1                                           1186
1187    316   C                                                                  1187
1188    317          ISL = JE( 3 , IE )                                          1188
1189    318          ISR = JE( 4 , IE )                                          1189
1190    319   C                                                                  1190
1191    320          DFLUX = RRL( KE )                                           1191
1192    321   C                                                                  1192
1193    322         IF( JE( 5 , IE ) . EQ . 0 ) THEN                             1193
1194    323   C                                                                  1194
1195    324   C ... FLUX FOR DENSITY ..................................................1195
1196    325   C                                                                  1196
1197    326         HYDFLX( ISL , 1 ) = HYDFLX( ISL , 1 ) + DFLUX * RO( KE )     1197
1198    327         HYDFLX( ISR , 1 ) = HYDFLX( ISR , 1 ) - DFLUX * RO( KE )     1198
1199    328   C                                                                  1199
1200    329   C ... FLUX FOR MOMENTUM DENSITY ( U DIRECTION ) ..........................1200
1201    330   C                                                                  1201
1202    331         HYDFLX( ISL , 2 ) = HYDFLX( ISL , 2 ) + DFLUX * UO( KE )     1202
1203    332         HYDFLX( ISR , 2 ) = HYDFLX( ISR , 2 ) - DFLUX * UO( KE )     1203
1204    333   C                                                                  1204
1205    334   C ... FLUX FOR MOMENTUM DENSITY ( V DIRECTION ) ..........................1205
1206    335   C                                                                  1206
1207    336         HYDFLX( ISL , 3 ) = HYDFLX( ISL , 3 ) + DFLUX * WO( KE )     1207
1208    337         HYDFLX( ISR , 3 ) = HYDFLX( ISR , 3 ) - DFLUX * WO( KE )     1208
1209    338   C                                                                  1209
1210    339   C ... FLUX FOR ENERGY DENSITY ...........................................1210
1211    340   C                                                                  1211
1212    341         HYDFLX( ISL , 4 ) = HYDFLX( ISL , 4 ) + DFLUX * PO( KE )     1212
1213    342         HYDFLX( ISR , 4 ) = HYDFLX( ISR , 4 ) - DFLUX * PO( KE )     1213
1214    343   C                                                                  1214
1215    344         ELSE                                                         1215
1216    345   C                                                                  1216
1217    346   C ... FLUX FOR DENSITY ..................................................1217
1218    347   C                                                                  1218
1219    348         HYDFLX( ISL , 1 ) = HYDFLX( ISL , 1 ) + DFLUX * RO( KE )     1219
1220    349   C                                                                  1220
1221    350   C ... FLUX FOR MOMENTUM DENSITY ( U DIRECTION ) ..........................1221
1222    351   C                                                                  1222
1223    352         HYDFLX( ISL , 2 ) = HYDFLX( ISL , 2 ) + DFLUX * UO( KE )     1223
1224    353   C                                                                  1224
1225    354   C ... FLUX FOR MOMENTUM DENSITY ( V DIRECTION ) ..........................1225
1226    355   C                                                                  1226
1227    356         HYDFLX( ISL , 3 ) = HYDFLX( ISL , 3 ) + DFLUX * WO( KE )     1227
1228    357   C                                                                  1228
1229    358   C ... FLUX FOR ENERGY DENSITY ...........................................1229
1230    359   C                                                                  1230
1231    360         HYDFLX( ISL , 4 ) = HYDFLX( ISL , 4 ) + DFLUX * PO( KE )     1231
1232    361   C                                                                  1232
1233    362         END IF                                                       1233
1234    363    290  CONTINUE                                                     1234
1235    364   C                                                                  1235
1236    365         NE1 = NE2 + 1                                                1236
1237    366         NE2 = NE2 + NOFVEE( INE + 1 )                                1237
1238    367    110  CONTINUE                                                     1238
1239    368   C                                                                  1239
1240    369   C==================================================================1240
1241    370   C                                                                  1241
```

```
1242   371   C --- EXIT POINT FROM SUBROUTINE ----------------------------------------
1243   372   C
1244   373   C     ------
1245   374         RETURN
1246   375   C     ------
1247   376   C
1248   377   C     ---
1249   378         END
```



```
1250     1         SUBROUTINE HYDRMN
1251     2   C
1252     3   C-------------------------------------------------------------I
1253     4   C                                                             I
1254     5   C      HYDRMN IS THE MAIN SUBROUTINE FOR THE UNSTRUCTURED GRID I
1255     6   C             HYDRODYNAMIC SOLVER. THIS SUBROUTINE OBTAINS THE I
1256     7   C             EDGE BASED FLUXES FOR EACH TRIANGLE/SIDE FROM   I
1257     8   C             SUBROUTINE --- HYDRFL --- . IT ALSO CONTROLS    I
1258     9   C             THE REFINEMENT AND COARSENING OF THE GRID.      I
1259    10   C             THE SUBROUTINE GENERATES THE OUTPUT THAT IS USED I
1260    11   C             FOR POST-PROCESSING.                            I
1261    12   C                                                             I
1262    13   C                                                             I
1263    14   C-------------------------------------------------------------I
1264    15   C
1265    16         include     'cmsh00.h'
1266    17         include     'chyd00.h'
1267    18         include     'cint00.h'
1268    19         include     'cphs10.h'
1269    20         include     'cphs20.h'
1270    21   C
1271    22   C=================================================================
1272    23   C
1273    24         REAL RRN(MBP),URN(MBP),VRN(MBP),EPN(MBP),XSAR(MBP),
1274    25        .     TTN(MBP),XYRAD(MBP)
1275    26         INTEGER IEDIST(2)
1276    27   C
1277    28   C=================================================================
1278    29   C
1279    30         CFL = 0.90
1280    31   C
1281    32   C --- SET SPECIFIC TIME FOR A DUMP ---------------------------------
1282    33   C
1283    34         TLIMIT=30.
1284    35         FLATDR = .9
1285    36         LDUMP = KDUMP
1286    37         IF( IJKINT . EQ . 3 ) THEN
1287    38         LDUMP = 6
1288    39         IF( LDUMP . LT . KDUMP ) LDUMP = KDUMP
1289    40         END IF
1290    41   C
1291    42         DO 120 JT  = 1 , NTIME
1292    43         DO 130 IT  = 1 , MDUMP
1293    44   C
1294    45         DO 140 ITT = 1 , NDUMP
1295    46         IJKKJI = ( JT - 1 ) * NDUMP * MDUMP + ( IT - 1 ) * NDUMP + ITT
1296    47         IJKIJK = IJKINT + IJKKJI
1297    48   C
1298    49         DO 142 IKT = 1 , LDUMP
1299    50   C
1300    51   C --- SELECT ORDER OF INTEGRATION ----------------------------------
1301    52   C
1302    53         IF(IOPORD.EQ.1)THEN
1303    54            CALL FIRST
1304    55         ELSEIF(IOPORD.EQ.2)THEN
1305    56            CALL GRADNG
1306    57         ENDIF
1307    58   C
1308    59   C --- SET TIMESTEP TO HIGH VALUE IT WILL BE CALCULATED PROPERLY --------
1309    60   C     IN THE FLUX SUBROUTINE
1310    61   C
1311    62         DTT = 1.E24
1312    63   C
```

```
      C --- FIND THE FLUXES ------------------------------------------------
      C
            CALL HYDRFL
      C
            DTT = DTT * CFL
            TT = TT + DTT
            PRINT *,JT,IT,ITT,IKT,DTT,TT,NS
      C
      C --- INITIALIZE THE VERTEX BASED QUANTITIES NEEDED FOR COARSENING AND -
      C     FOR REFINEMENT, AND FOR POST-PROCESSING
      C
             DO 210 IV = 1 , NV
             PR( IV ) = 0.
             DO 210 IR = 1 , MHQ
             HYDVVV( IV , IR ) = 0.
      210    CONTINUE
      C
            NS1 = 1
            NS2 = NOFVES( 1 )
            DO 110 INS = 1 , NVEES
      C
            DO 150 IS = NS1 , NS2
                KS = IS - NS1 + 1
                RRR( KS ) = HYDV( IS , 1 )
                UUR( KS ) = HYDV( IS , 2 )
                VVR( KS ) = HYDV( IS , 3 )
                PPR( KS ) = HYDV( IS , 4 )
      C
                RRL( KS ) = HYDFLX( IS , 1 )
                UUL( KS ) = HYDFLX( IS , 2 )
                VVL( KS ) = HYDFLX( IS , 3 )
                PPL( KS ) = HYDFLX( IS , 4 )
      C
                XSAR( KS ) = SAREA( IS )
      150    CONTINUE
      C
            DO 170 KS = 1 , NOFVES( INS )
               IS = KS + NS1 - 1
              GAMAG( KS ) = HYOV( IS , 5 )
              HRGM = GAMAG( KS ) - 1.
      C
            RRN( KS ) = RRR( KS )
            URN( KS ) = RRR( KS ) * UUR( KS )
            VRN( KS ) = RRR( KS ) * VVR( KS )
            EPN( KS ) = PPR( KS ) / HRGM + .5 * RRR( KS ) *
           .                       ( UUR( KS ) * UUR( KS ) +
           .                         VVR( KS ) * VVR( KS ) )
      170    CONTINUE
      C
      c=====================================================================
      C
      C --- COMPUTING THE SOURCE TERM ASSOCIATED WITH AXI-SYMMETRIC CASE -----
      C
                XYDUMY = 1. / 6.283185307
                DO 188 KS = 1 , NOFVES( INS )
                XYRAD( KS ) = XYDUMY
      188       CONTINUE
      C
      C --- Y-AXIS IS AXIS OF SYMMETRY ----------------------------------------
      C
                IF( IAXSYM . EQ . 2 )THEN
                DO 180 KS = 1 , NOFVES( INS )
                IS = KS + NS1 - 1
                XS2S = XS( 1 , IS )
                XYRAD( KS ) = XS2S
                IF( XS2S . GT . .0005 ) THEN
                  DTA = DTT * UUR( KS ) / XS2S
                  RRN( KS ) = RRN( KS ) * ( 1. - DTA )
                  URN( KS ) = URN( KS ) * ( 1. - DTA )
                  VRN( KS ) = VRN( KS ) * ( 1. - DTA )
                  EPN( KS ) = EPN( KS ) * ( 1. - DTA ) - PPR( KS ) * DTA
                END IF
      180       CONTINUE
      C
```

```
C --- X-AXIS IS AXIS OF SYMMETRY ------------------------------------
C
          ELSEIF( IAXSYM . EQ . 1 )THEN
          DO 182 KS = 1 , NOFVES( INS )
          IS = KS + NS1 - 1
          XS2S = XS( 2 , IS )
          XYRAD( KS ) = XS2S
          IF( XS2S . GT . .0005 ) THEN
            DTA = DTT * VVR( KS ) / XS2S
            RRN( KS ) = RRN( KS ) * ( 1. - DTA )
            URN( KS ) = URN( KS ) * ( 1. - DTA )
            VRN( KS ) = VRN( KS ) * ( 1. - DTA )
            EPN( KS ) = EPN( KS ) * ( 1. - DTA ) - PPR( KS ) * DTA
          END IF
182    CONTINUE
        ENDIF
C
C --- COMPUTE THE EFFECT OF THE BOUYANCY(GRAVITY) TERM ----------------
C
        GRAVTY = 9.81
C
        IF( IOPBYN . EQ . 2 )THEN
          DO 184 KS = 1 , NOFVES( INS )
          DTA = DTT * RRR( KS ) * GRAVTY
            VRN( KS ) = VRN( KS ) - DTA
            EPN( KS ) = EPN( KS ) - DTA * VVR( KS )
184     CONTINUE
C
        ELSEIF( IOPBYN . EQ . 1 )THEN
          DO 186 KS = 1 , NOFVES( INS )
          DTA = DTT * RRR( KS ) * GRAVTY
            URN( KS ) = URN( KS ) - DTA
            EPN( KS ) = EPN( KS ) - DTA * UUR( KS )
186     CONTINUE
        END IF
C
C=====================================================================
C
C --- UPDATE THE HYDRODYNAMIC QUANTITIES ------------------------------
C     STORING THE FLUXES FOR THE REFINEMENT/COARSENING STEPS
C
        DO 190 KS = 1 , NOFVES( INS )
        IS = KS + NS1 - 1
        DTA = DTT * XSAR( KS )
C
        RRLL = RRL( KS )
        UULL = UUL( KS )
        VVLL = VVL( KS )
        RRN( KS ) = RRN( KS ) - RRLL * DTA
        URN( KS ) = URN( KS ) - UULL * DTA
        VRN( KS ) = VRN( KS ) - VVLL * DTA
C
        PPLL = PPL( KS )
        HYDFLX( IS , 4 ) = ABS( PPLL ) / EPN( KS ) * DTA
        EPN( KS ) = EPN( KS ) - PPLL * DTA
C
190    CONTINUE
C
        DO 202 IS = NS1 , NS2
        KS = IS - NS1 + 1
        ENERGY = 1. / RRN( KS ) * ( URN( KS ) * URN( KS ) +
     .                              VRN( KS ) * VRN( KS ) )
        TTN( KS ) = EPN( KS ) - .5 * ENERGY
        HYDFLX( IS , 1 ) = ENERGY / TTN( KS )
        HYDFLX( IS , 2 ) = RRN( KS )
C
202    CONTINUE
C --- EQUATION OF STATE FOR AIR ---------------------------------------
C
        IF( IOPEOS . EQ . 1 )THEN
          CALL EOS( RRN , TTN , NOFVES( INS ) , GAMAG )
        ELSE
        ENDIF
C
```

```
1461     212   C --- ACCUMULATE VALUES AT THE VERTICES FOR ADAPTATION AND ALSO --------
1462     213   C     FOR POST-PROCESSING
1463     214   C
1464     215             DO 220 KS = 1 , NOFVES( INS )
1465     216             IS = KS + NS1 - 1
1466     217   C
1467     218             IV1 = JS( 1 , IS )
1468     219             IV2 = JS( 2 , IS )
1469     220             IV3 = JS( 3 , IS )
1470     221   C
1471     222             VOLUME = 6.283185307 * XYRAD( KS )
1472     223   C
1473     224             XYAREA = XS( 3 , IS ) * VOLUME
1474     225             XYFDR = XYAREA * RRN( KS )
1475     226             XYFDU = XYAREA * URN( KS )
1476     227             XYFDV = XYAREA * VRN( KS )
1477     228             XYFDP = XYAREA * EPN( KS )
1478     229             XYFDG = XYAREA * GAMAG( KS )
1479     230   C
1480     231             HYDVVV( IV1 , 1 ) = HYDVVV( IV1 , 1 ) + XYFDR
1481     232             HYDVVV( IV1 , 2 ) = HYDVVV( IV1 , 2 ) + XYFDU
1482     233             HYDVVV( IV1 , 3 ) = HYDVVV( IV1 , 3 ) + XYFDV
1483     234             HYDVVV( IV1 , 4 ) = HYDVVV( IV1 , 4 ) + XYFDP
1484     235             HYDVVV( IV1 , 5 ) = HYDVVV( IV1 , 5 ) + XYFDG
1485     236             PR( IV1 ) = PR( IV1 ) + XYAREA
1486     237   C
1487     238             HYDVVV( IV2 , 1 ) = HYDVVV( IV2 , 1 ) + XYFDR
1488     239             HYDVVV( IV2 , 2 ) = HYDVVV( IV2 , 2 ) + XYFDU
1489     240             HYDVVV( IV2 , 3 ) = HYDVVV( IV2 , 3 ) + XYFDV
1490     241             HYDVVV( IV2 , 4 ) = HYDVVV( IV2 , 4 ) + XYFDP
1491     242             HYDVVV( IV2 , 5 ) = HYDVVV( IV2 , 5 ) + XYFDG
1492     243             PR( IV2 ) = PR( IV2 ) + XYAREA
1493     244   C
1494     245             HYDVVV( IV3 , 1 ) = HYDVVV( IV3 , 1 ) + XYFDR
1495     246             HYDVVV( IV3 , 2 ) = HYDVVV( IV3 , 2 ) + XYFDU
1496     247             HYDVVV( IV3 , 3 ) = HYDVVV( IV3 , 3 ) + XYFDV
1497     248             HYDVVV( IV3 , 4 ) = HYDVVV( IV3 , 4 ) + XYFDP
1498     249             HYDVVV( IV3 , 5 ) = HYDVVV( IV3 , 5 ) + XYFDG
1499     250             PR( IV3 ) = PR( IV3 ) + XYAREA
1500     251   C
1501     252             IENUMR = 0
1502     253             IE1 = IABS( JS( 4 , IS ) )
1503     254             IJE5 = JE( 5 , IE1 )
1504     255             IF( IJE5 . NE . 0 ) THEN
1505     256             IENUMR = IENUMR + 1
1506     257             IEDIST( IENUMR ) = IE1
1507     258             END IF
1508     259             IE2 = IABS( JS( 5 , IS ) )
1509     260             IJE5 = JE( 5 , IE2 )
1510     261             IF( IJE5 . NE . 0 ) THEN
1511     262             IENUMR = IENUMR + 1
1512     263             IEDIST( IENUMR ) = IE2
1513     264             END IF
1514     265             IE3 = IABS( JS( 6 , IS ) )
1515     266             IJE5 = JE( 5 , IE3 )
1516     267             IF( IJE5 . NE . 0 ) THEN
1517     268             IENUMR = IENUMR + 1
1518     269             IEDIST( IENUMR ) = IE3
1519     270             END IF
1520     271   C
1521     272             IF( IENUMR . NE . 0 ) THEN
1522     273             DO 322 IK = 1 , IENUMR
1523     274             IEK = IEDIST( IENUMR )
1524     275             IJE55 = JE( 5 , IEK )
1525     276             RRNN = RRN( KS )
1526     277             URNN = URN( KS )
1527     278             VRNN = VRN( KS )
1528     279             EPNN = EPN( KS )
1529     280   C          IF( IJE55 . EQ . 6 . OR . IJE55 . EQ . 5 ) THEN
1530     281   C          UUVV =   - ( URN( KS ) * XN( IEK ) +
1531     282   C     .                 VRN( KS ) * YN( IEK ) )
1532     283   C          VVUU =     - URN( KS ) * YN( IEK ) +
1533     284   C     .                 VRN( KS ) * XN( IEK )
1534     285   C          URNN = UUVV * XN( IEK ) - VVUU * YN( IEK )
```

```
1535  286  C         VRNN = UUVV * YN( IEK ) + VVUU * XN( IEK )                    1535
1536  287  C         ELSE IF( IJE55 . EQ . 8 ) THEN                                1536
1537  288  C         RRNN = RIN                                                    1537
1538  289  C         URNN = RIN * UIN                                              1538
1539  290  C         VRNN = RIN * VIN                                              1539
1540  291  C         EPNN = PIN / HRGM + .5 * RIN * UVIN * UVIN                    1540
1541  292  C         END IF                                                        1541
1542  293  C                                                                       1542
1543  294           XYFDR = XYAREA * RRNN                                         1543
1544  295           XYFDU = XYAREA * URNN                                         1544
1545  296           XYFDV = XYAREA * VRNN                                         1545
1546  297           XYFDP = XYAREA * EPNN                                         1546
1547  298           XYFDG = XYAREA * GAMAG( KS )                                  1547
1548  299  C                                                                       1548
1549  300           IV1 = JE( 1 , IEK )                                           1549
1550  301           IV2 = JE( 2 , IEK )                                           1550
1551  302           HYDVVV( IV1 , 1 ) = HYDVVV( IV1 , 1 ) + XYFDR                 1551
1552  303           HYDVVV( IV1 , 2 ) = HYDVVV( IV1 , 2 ) + XYFDU                 1552
1553  304           HYDVVV( IV1 , 3 ) = HYDVVV( IV1 , 3 ) + XYFDV                 1553
1554  305           HYDVVV( IV1 , 4 ) = HYDVVV( IV1 , 4 ) + XYFDP                 1554
1555  306           HYDVVV( IV1 , 5 ) = HYDVVV( IV1 , 5 ) + XYFDG                 1555
1556  307           PR( IV1 ) = PR( IV1 ) + XYAREA                                1556
1557  308  C                                                                       1557
1558  309           HYDVVV( IV2 , 1 ) = HYDVVV( IV2 , 1 ) + XYFDR                 1558
1559  310           HYDVVV( IV2 , 2 ) = HYDVVV( IV2 , 2 ) + XYFDU                 1559
1560  311           HYDVVV( IV2 , 3 ) = HYDVVV( IV2 , 3 ) + XYFDV                 1560
1561  312           HYDVVV( IV2 , 4 ) = HYDVVV( IV2 , 4 ) + XYFDP                 1561
1562  313           HYDVVV( IV2 , 5 ) = HYDVVV( IV2 , 5 ) + XYFDG                 1562
1563  314           PR( IV2 ) = PR( IV2 ) + XYAREA                                1563
1564  315  322      CONTINUE                                                      1564
1565  316           END IF                                                        1565
1566  317  C                                                                       1566
1567  318  220      CONTINUE                                                      1567
1568  319  C                                                                       1568
1569  320  C --- CONSTRUCT NONCONSERVED HYDRODYNAMIC QUATITIES ------------------ 1569
1570  321  C                                                                       1570
1571  322       DO 195 IS = NS1 , NS2                                            1571
1572  323       KS = IS - NS1 + 1                                                1572
1573  324       HDUM          = 1. / RRN( KS )                                   1573
1574  325       HYDV( IS , 1 ) = RRN( KS )                                       1574
1575  326       HYDV( IS , 2 ) = URN( KS ) * HDUM                                1575
1576  327       HYDV( IS , 3 ) = VRN( KS ) * HDUM                                1576
1577  328       HYDV( IS , 5 ) = GAMAG( KS )                                     1577
1578  329       HYDV( IS , 4 ) = TTN( KS ) * ( HYDV( IS , 5 ) - 1. )             1578
1579  330   195 CONTINUE                                                         1579
1580  331  C                                                                       1580
1581  332       NS1 = NS2 + 1                                                    1581
1582  333       NS2 = NS2 + NOFVES( INS + 1 )                                    1582
1583  334  110  CONTINUE                                                         1583
1584  335  C                                                                       1584
1585  336  C --- END OF LOOP OVER TRIANGLES ------------------------------------ 1585
1586  337  C                                                                       1586
1587  338  C=================================================================== 1587
1588  339  C                                                                       1588
1589  340  C --- CALL FOR PARTICLE TRACERS ------------------------------------- 1589
1590  341  C                                                                       1590
1591  342       IF( MPRTCL . EQ . 1 )THEN                                        1591
1592  343  C                                                                       1592
1593  344         CALL PRPTHC                                                    1593
1594  345  C                                                                       1594
1595  346       ENDIF                                                            1595
1596  347  C                                                                       1596
1597  348  C --- END OF INNER LOOP OVER ... KDUMP ... ---------------------------- 1597
1598  349  C                                                                       1598
1599  350  C=================================================================== 1599
1600  351  C                                                                       1600
1601  352  C --- NORMALIZE CONSERVATIVE  VERTEX BASED QUANTITIES ----------------- 1601
1602  353  C                                                                       1602
1603  354       DO 230 IV = 1 , NV                                               1603
1604  355       VAREA = 1. / PR( IV )                                            1604
1605  356       DO 230 IR = 1 , MHQ                                              1605
1606  357       HYDVVV( IV , IR ) = HYDVVV( IV , IR ) * VAREA                    1606
1607  358  230  CONTINUE                                                         1607
1608  359  C                                                                       1608
```

```
1609     360   142    CONTINUE                                                        1609
1610     361   C --- WRITE THE DUMP FILE DATA FOR POST-PROCESSING ----------------- 1610
1611     362   C                                                                     1611
1612     363         IF( IT . EQ . MDUMP . AND . ITT . EQ . NDUMP ) THEN             1612
1613     364           WRITE (9) NV,NE,NS,NPT,NTIME                                  1613
1614     365           WRITE (9) ((XV(IK,IV),IK=1,2),IV=1,NV)                        1614
1615     366           WRITE (9) (JV(2,IV),IV=1,NV)                                  1615
1616     367           WRITE (9) ((JE(KK,IE),KK=1,5),IE=1,NE)                        1616
1617     368           WRITE (9) ((JS(KK,IS),KK=1,6),IS=1,NS)                        1617
1618     369           WRITE (9) ((XS(KK,IS),KK=1,2),IS=1,NS)                        1618
1619     370           WRITE (9) RIN,PIN,UVIN,UIN,VIN,TT,IOPLFT                      1619
1620     371           WRITE (9) ((HYDV(IS,IK),IK=1,5),IS=1,NS)                      1620
1621     372   C                                                                     1621
1622     373   C --- WRITE OUT PARTICLE TRACER DATA ----------------------------------1622
1623     374   C                                                                     1623
1624     375           IF( MPRTCL . EQ . 1 )THEN                                     1624
1625     376             WRITE (9) ((XPRTCL(IK,IPT),IK=1,2),IPT=1,NPT),              1625
1626     377        .                ((WPRTCL(IK,IPT),IK=1,2),IPT=1,NPT)           1626
1627     378           ENDIF                                                         1627
1628     379   C                                                                     1628
1629     380   C --- PRINT CONSOLE MESSAGE AT END OF LOOP ----------------------------1629
1630     381   C                                                                     1630
1631     382           PRINT * , JT,NV,NE,NS                                         1631
1632     383   C                                                                     1632
1633     384         END IF                                                          1633
1634     385   C                                                                     1634
1635     386   C=====================================================================1635
1636     387   C                                                                     1636
1637     388   C             I--------------------------------I                      1637
1638     389   C             I  REFINEMENT/ADDITION OF POINTS  I                     1638
1639     390   C             I--------------------------------I                      1639
1640     391   C                                                                     1640
1641     392   C                                                                     1641
1642     393   C --- CALCULATE THE GRADIENT OF THE MACH NUMBER FOR STEADY STATE ------1642
1643     394   C     ADAPTIVE STEP AND GENERATE THE QUANTITIES ON WHICH WE ADAPT.     1643
1644     395   C                                                                     1644
1645     396   C --- ADAPTATION TO STATIC QUANTITIES BASED ON GRADIENTS OF ------------1645
1646     397   C     MACH NUMBER, PRESSURE, AND DENSITY. OVERRIDES                   1646
1647     398   C     ADAPTATION ON DYNAMIC FLUXES OF ENERGY AND DENSITY              1647
1648     399   C                                                                     1648
1649     400         IF( ISTATC . EQ . 1 ) THEN                                      1649
1650     401         CALL GRDFLX                                                     1650
1651     402         DO 240 IS = 1 , NS                                              1651
1652     403         HYDFLX( IS , 1 ) = ABS( PL( IS ) ) + ABS( PR( IS ) )            1652
1653     404         HYDFLX( IS , 2 ) = ABS( RL( IS ) ) + ABS( RR( IS ) )            1653
1654     405         HYDFLX( IS , 4 ) = ABS( VL( IS ) ) + ABS( VR( IS ) )            1654
1655     406   240   CONTINUE                                                        1655
1656     407   C                                                                     1656
1657     408         ELSE                                                            1657
1658     409   C                                                                     1658
1659     410         CALL GRDENG                                                     1659
1660     411         DO 242 IS = 1 , NS                                              1660
1661     412         HYDFLX( IS , 1 ) = ( UL( IS ) * UL( IS ) + UR( IS ) * UR( IS ) ) /1661
1662     413        .                   ( HYDFLX( IS , 1 ) + 1.E-12 )              1662
1663     414         HYDFLX( IS , 2 ) = ( RL( IS ) * RL( IS ) + RR( IS ) * RR( IS ) ) /1663
1664     415        .                   ( HYDFLX( IS , 2 ) + 1.E-12 )              1664
1665     416         HYDFLX( IS , 4 ) = ( VL( IS ) * VL( IS ) + VR( IS ) * VR( IS ) ) /1665
1666     417        .                   ( HYDFLX( IS , 4 ) + 1.E-12 )              1666
1667     418   242   CONTINUE                                                        1667
1668     419         END IF                                                          1668
1669     420   C                                                                     1669
1670     421         DYDMOM = HYDFLX( 1 , 4 )                                        1670
1671     422         DO 250 IS = 1 , NS                                              1671
1672     423         DYDMOM = AMAX1( DYDMOM , HYDFLX( IS , 4 ) )                     1672
1673     424   250   CONTINUE                                                        1673
1674     425         HYDMOM( 4 ) = .5 * ( DYDMOM + HYDMOM( 4 ) )                     1674
1675     426         PRINT*,HYDMOM( 4 )                                              1675
1676     427   C                                                                     1676
1677     428         DYDMOM = HYDFLX( 1 , 2 )                                        1677
1678     429         DO 260 IS = 1 , NS                                              1678
1679     430         DYDMOM = AMAX1( DYDMOM , HYDFLX( IS , 2 ) )                     1679
1680     431   260   CONTINUE                                                        1680
1681     432         HYDMOM( 2 ) = .5 * ( DYDMOM + HYDMOM( 2 ) )                     1681
1682     433         PRINT*,HYDMOM( 2 )                                              1682
```

```
1683     434   C                                                                      1683
1684     435         DYDMOM = HYDFLX( 1 , 1 )                                         1684
1685     436         DO 270 IS = 1 , NS                                               1685
1686     437         DYDMOM = AMAX1( DYDMOM , HYDFLX( IS , 1 ) )                      1686
1687     438   270   CONTINUE                                                         1687
1688     439         HYDMOM( 1 ) = .5 * ( DYDMOM + HYDMOM( 1 ) )                      1688
1689     440         PRINT*,HYDMOM( 1 )                                               1689
1690     441   C                                                                      1690
1691     442   C --- REFINEMENT STEP DONE HERE ----------------------------------------1691
1692     443   C                                                                      1692
1693     444         IF(IOPADD.EQ.1) THEN                                             1693
1694     445           NOFDIV = 4                                                     1694
1695     446           CALL DYNPTN( AREADD , NOFDIV , IJKIJK , LTRIG )                1695
1696     447           NOFDIV = 2                                                     1696
1697     448           CALL DYYPTN( AREADD , NOFDIV , IJKIJK , LTRIG )                1697
1698     449           NOFDIV = 1                                                     1698
1699     450           CALL DYYPTN( AREADD , NOFDIV , IJKIJK , LTRIG )                1699
1700     451           CALL DYYPTN( AREADD , NOFDIV , IJKIJK , LTRIG )                1700
1701     452   C                                                                      1701
1702     453           PRINT*,NV,NE,NS                                                1702
1703     454         ENDIF                                                            1703
1704     455    140  CONTINUE                                                         1704
1705     456   C                                                                      1705
1706     457   C --- END OF OUTER LOOP DEFINED BY ...NDUMP... -------------------------1706
1707     458   C                                                                      1707
1708     459   C=======================================================================1708
1709     460   C                                                                      1709
1710     461   C            I---------------------------------I                       1710
1711     462   C            I  COARSENING/DELETION OF POINTS  I                       1711
1712     463   C            I---------------------------------I                       1712
1713     464   C                                                                      1713
1714     465   C                                                                      1714
1715     466          IF(IOPDEL.EQ.1)THEN                                             1715
1716     467             IF( IJKIJK . GT . 19 ) CALL DELPTNT( AREDEL , IJKIJK )       1716
1717     468           PRINT*,NV,NE,NS                                                1717
1718     469          ENDIF                                                           1718
1719     470    130   CONTINUE                                                        1719
1720     471   C                                                                      1720
1721     472   C --- END OF OUTERMOST LOOP DEFINED BY ...MDUMP... ---------------------1721
1722     473   C                                                                      1722
1723     474   C=======================================================================1723
1724     475   C                                                                      1724
1725     476   C            I---------------------------------I                       1725
1726     477   C            I  DIAGNOSTIC FOR LIFT/DRAG       I                       1726
1727     478   C            I---------------------------------I                       1727
1728     479   C                                                                      1728
1729     480         IF(IOPLFT.EQ.1)THEN                                              1729
1730     481           CALL LIFTDR                                                    1730
1731     482         ENDIF                                                            1731
1732     483   C                                                                      1732
1733     484   C=======================================================================1733
1734     485   C                                                                      1734
1735     486   C            I---------------------------------I                       1735
1736     487   C            I  OUTPUT FILE FOR RESTARTS       I                       1736
1737     488   C            I---------------------------------I                       1737
1738     489   C                                                                      1738
1739     490   C                                                                      1739
1740     491          REWIND 88                                                       1740
1741     492          ITERAT = ITERAT + 1                                             1741
1742     493          WRITE (88) NV,NVMK,NE,NEMK,NS,NSMK,ITERAT                       1742
1743     494          WRITE (88) ((JV(KK,IV),KK=1,2),(XV(IK,IV),IK=1,2),IV=1,NV)      1743
1744     495          WRITE (88) ((JE(KK,IE),KK=1,5),(XE(KI,IE),KI=1,2),IE=1,NE)      1744
1745     496          WRITE (88) (XN(IE),YN(IE),XXN(IE),YYN(IE),IE=1,NE)              1745
1746     497          WRITE (88) ((JS(KK,IS),KK=1,6),(XS(KI,IS),KI=1,3),IS=1,NS)      1746
1747     498          WRITE (88) (XMIDL(IE),YMIDL(IE),XYMIDL(IE),IE=1,NE)             1747
1748     499          WRITE (88) SAREVG,NVECE,NREME,NVECV,NREMV,NVECS,NREMS           1748
1749     500          WRITE (88) RIN,PIN,RINL,PINL,UVIN,UIN,VIN,TT,                   1749
1750     501         .             HYDMOM(1),HYDMOM(2),HYDMOM(4)                      1750
1751     502          WRITE (88) ((HYDV(IS,IK),IK=1,5),IS=1,NS)                       1751
1752     503          WRITE (88) ((HYDVVV(IV,IK),IK=1,5),IV=1,NV)                     1752
1753     504          WRITE (88) IJKIJK,(KSDELT(IS),IS=1,NS)                          1753
1754     505           IF( MPRTCL . EQ . 1 )                                          1754
1755     506         . WRITE (88) NPT,((XPRTCL(IK,IPT),IK=1,2),IPT=1,NPT),           1755
1756     507         .                           (IJKPRT(IPT),IPT=1,NPT)             1756
```

```
      REWIND 8
      WRITE (8) NV,NVMK,NE,NEMK,NS,NSMK,ITERAT
      WRITE (8) ((JV(KK,IV),KK=1,2),(XV(IK,IV),IK=1,2),IV=1,NV)
      WRITE (8) ((JE(KK,IE),KK=1,5),(XE(KI,IE),KI=1,2),IE=1,NE)
      WRITE (8) (XN(IE),YN(IE),XXN(IE),YYN(IE),IE=1,NE)
      WRITE (8) ((JS(KK,IS),KK=1,6),(XS(KI,IS),KI=1,3),IS=1,NS)
      WRITE (8) (XMIDL(IE),YMIDL(IE),XYMIDL(IE),IE=1,NE)
      WRITE (8) SAREVG,NVECE,NREME,NVECV,NREMV,NVECS,NREMS
      WRITE (8) RIN,PIN,RINL,PINL,UVIN,UIN,VIN,TT,
     .            HYDMOM(1),HYDMOM(2),HYDMOM(4)
      WRITE (8) ((HYDV(IS,IK),IK=1,5),IS=1,NS)
      WRITE (8) ((HYDVVV(IV,IK),IK=1,5),IV=1,NV)
      WRITE (8) IJKIJK,(KSDELT(IS),IS=1,NS)
       IF( MPRTCL . EQ . 1 )
     . WRITE (8) NPT,((XPRTCL(IK,IPT),IK=1,2),IPT=1,NPT),
     .                                (IJKPRT(IPT),IPT=1,NPT)
C
 120  CONTINUE
C
C --- END MAIN SEQUENCE LOOP DEFINED BY ...NTIME...----------------------
C
C=======================================================================
C
C --- EXIT POINT FROM SUBROUTINE -----------------------------------------
C
C     ------
      RETURN
C     ------
C
C --- FORMATS ------------------------------------------------------------
C
C     ---
      END
```



```
      SUBROUTINE GEOMTR
C
C-----------------------------------------------------------------I
C                                                                 I
C     GEOMTR COMPUTE GEOMETRICAL PARAMETERS TO COMPLETE THE GRID  I
C           DEFINITION NEEDED BY THE CODE.                        I
C                                                                 I
C                                                                 I
C-----------------------------------------------------------------I
C
      include     'cmsh00.h'
      include     'chyd00.h'
      include     'cint00.h'
      include     'cphs10.h'
      include     'cphs20.h'
C
C=======================================================================
C
      REAL XELEFT(MBP),YELEFT(MBP),XERIGT(MBP),YERIGT(MBP)
C
C=======================================================================
C
C
C --- MAKE SURE THAT THE DOMAIN IS ALWAYS TO THE LEFT OF BOUNDARY ------
C     EDGES BY ORIENTING THEM CORRECTLY.
C
      DO 105 IE = 1 , NE
        IJE5 = JE( 5 , IE )
        IF( IJE5 . NE . 0 ) THEN
          ISR = JE( 4 , IE )
          IF( ISR . NE . 0 ) THEN
            IV2 = JE( 1 , IE )
            IV1 = JE( 2 , IE )
            JE( 1 , IE ) = IV1
            JE( 2 , IE ) = IV2
            JE( 3 , IE ) = ISR
            JE( 4 , IE ) = 0
```

```
1828      38              DO 106 IR = 1 , 3                                       1828
1829      39              JEE = IABS( JS( IR + 3 , ISR ) )                        1829
1830      40              IF( JEE . EQ . IE ) JS( IR + 3 , ISR ) = IE             1830
1831      41    106       CONTINUE                                                1831
1832      42            ENDIF                                                     1832
1833      43          ENDIF                                                       1833
1834      44    105   CONTINUE                                                    1834
1835      45    C                                                                 1835
1836      46    C --- FIND UNIT VECTORS NORMAL TO THE EDGES ----------------------1836
1837      47    C     AND EDGE CROSSING OF LINE BETWEEN TRIANGLE BARICENTERS      1837
1838      48    C     AND ALSO TRIANGLE AREAS.                                    1838
1839      49    C                                                                 1839
1840      50          NE1 = 1                                                     1840
1841      51          NE2 = NOFVEE( 1 )                                           1841
1842      52          DO 110 INE = 1 , NVEEE                                      1842
1843      53          DO 140 IE = NE1 , NE2                                       1843
1844      54            KE = IE - NE1 + 1                                         1844
1845      55            IV1 = JE( 1 , IE )                                        1845
1846      56            IV2 = JE( 2 , IE )                                        1846
1847      57            ISL = JE( 3 , IE )                                        1847
1848      58            ISR = JE( 4 , IE )                                        1848
1849      59    C                                                                 1849
1850      60    C --- FIND UNIT VECTOR NORMAL TO AN EDGE -------------------------1850
1851      61    C     STORED IN XN(IE),YN(IE)                                     1851
1852      62    C                                                                 1852
1853      63            DXD = XV( 1 , IV2 ) - XV( 1 , IV1 )                       1853
1854      64            DYD = XV( 2 , IV2 ) - XV( 2 , IV1 )                       1854
1855      65            XE( 1 , IE ) = SQRT( DXD * DXD + DYD * DYD )              1855
1856      66            XEY = 1. / XE( 1 , IE )                                   1856
1857      67            XD = DXD * XEY                                            1857
1858      68            YD = DYD * XEY                                            1858
1859      69    C                                                                 1859
1860      70            XN( IE ) =   YD                                           1860
1861      71            YN( IE ) = - XD                                           1861
1862      72    C                                                                 1862
1863      73            IJE5 = JE( 5 , IE )                                       1863
1864      74    C                                                                 1864
1865      75    C=======-----------------------------------------------------------1865
1866      76    C                                                                 1866
1867      77    C --- BOUNDARY TRIANGLES ----------------------------------------1867
1868      78    C                                                                 1868
1869      79            IF( IJE5 . NE . 0 ) THEN                                  1869
1870      80            IV3 = JS( 1 , ISL )                                       1870
1871      81            IF( IV3 . EQ . IV1 . OR . IV3 . EQ . IV2 ) IV3 = JS( 2 , ISL )  1871
1872      82            IF( IV3 . EQ . IV1 . OR . IV3 . EQ . IV2 ) IV3 = JS( 3 , ISL )  1872
1873      83            XELEFT( KE ) = ( XV( 1 , IV3 ) + XV( 1 , IV2 ) +          1873
1874      84           .                                 XV( 1 , IV1 ) ) * THIRD  1874
1875      85            YELEFT( KE ) = ( XV( 2 , IV3 ) + XV( 2 , IV2 ) +          1875
1876      86           .                                 XV( 2 , IV1 ) ) * THIRD  1876
1877      87    C                                                                 1877
1878      88            AA = XV( 1 , IV2 ) - XV( 1 , IV1 )                        1878
1879      89            BB = XV( 2 , IV2 ) - XV( 2 , IV1 )                        1879
1880      90            CC = XELEFT( KE ) - XV( 1 , IV1 )                         1880
1881      91            DD = YELEFT( KE ) - XV( 2 , IV1 )                         1881
1882      92            EE = ( AA * CC + BB * DD ) * XEY * XEY                    1882
1883      93            XERIGT( KE ) = XV( 1 , IV1 ) + AA * EE                    1883
1884      94            YERIGT( KE ) = XV( 2 , IV1 ) + BB * EE                    1884
1885      95    C                                                                 1885
1886      96            DXD = XERIGT( KE ) - XELEFT( KE )                         1886
1887      97            DYD = YERIGT( KE ) - YELEFT( KE )                         1887
1888      98            XE( 2 , IE ) = SQRT( DXD * DXD + DYD * DYD )              1888
1889      99    C                                                                 1889
1890     100    C --- UNIT VECTOR FROM LEFT TO RIGHT BARI-CENTER AT INTERFACE ----1890
1891     101    C     STORED IN XXN(IE),YYN(IE)                                   1891
1892     102    C                                                                 1892
1893     103            XY = 1. / XE( 2 , IE )                                    1893
1894     104            XXN( IE ) = DXD * XY                                      1894
1895     105            YYN( IE ) = DYD * XY                                      1895
1896     106    C                                                                 1896
1897     107    C --- LENGTH OF LINE BETWEEN BARI-CENTERS ------------------------1897
1898     108    C     STORED IN XE(2,IE)                                          1898
1899     109    C                                                                 1899
1900     110            XE( 2 , IE ) = 2. * XE( 2 , IE )                          1900
1901     111    C                                                                 1901
```

```
1902     112   C --- COORDINATES OF BARI-CENTERS FOR EACH TRIANGLE --------------------
1903     113   C     STORED IN XS(1,IS),XS(2,IS)
1904     114   C
1905     115         XS( 1 , ISL ) = XELEFT( KE )
1906     116         XS( 2 , ISL ) = YELEFT( KE )
1907     117   C
1908     118   C --- INTERSECTION POINT ON INTERFACE FOR LINE CONNECTING BARI-CENTERS -
1909     119   C     STORED IN XMIDL(IE),YMIDL(IE) AND FRACTION OF LENGHT BETWEEN
1910     120   C     LEFT BARI-CENTER TO INTERSECTION POINT IN XYMIDL(IE).
1911     121   C
1912     122         XYMIDL( IE ) = .5
1913     123         XMIDL( IE ) = XERIGT( KE )
1914     124         YMIDL( IE ) = YERIGT( KE )
1915     125   C
1916     126   C-------------------------------------------------------------------------
1917     127   C
1918     128   C
1919     129   C --- REGULAR TRIANGLES ----------------------------------------------------
1920     130   C
1921     131         ELSE
1922     132         IV3 = JS( 1 , ISL )
1923     133         IF( IV3 . EQ . IV1 . OR . IV3 . EQ . IV2 ) IV3 = JS( 2 , ISL )
1924     134         IF( IV3 . EQ . IV1 . OR . IV3 . EQ . IV2 ) IV3 = JS( 3 , ISL )
1925     135         XELEFT( KE ) = ( XV( 1 , IV3 ) + XV( 1 , IV2 ) +
1926     136        .                                 XV( 1 , IV1 ) ) * THIRD
1927     137         YELEFT( KE ) = ( XV( 2 , IV3 ) + XV( 2 , IV2 ) +
1928     138        .                                 XV( 2 , IV1 ) ) * THIRD
1929     139   C
1930     140         IV3 = JS( 1 , ISR )
1931     141         IF( IV3 . EQ . IV1 . OR . IV3 . EQ . IV2 ) IV3 = JS( 2 , ISR )
1932     142         IF( IV3 . EQ . IV1 . OR . IV3 . EQ . IV2 ) IV3 = JS( 3 , ISR )
1933     143         XERIGT( KE ) = ( XV( 1 , IV3 ) + XV( 1 , IV2 ) +
1934     144        .                                 XV( 1 , IV1 ) ) * THIRD
1935     145         YERIGT( KE ) = ( XV( 2 , IV3 ) + XV( 2 , IV2 ) +
1936     146        .                                 XV( 2 , IV1 ) ) * THIRD
1937     147   C
1938     148          DXD = XERIGT( KE ) - XELEFT( KE )
1939     149          DYD = YERIGT( KE ) - YELEFT( KE )
1940     150   C
1941     151   C --- LENGTH OF LINE BETWEEN BARI-CENTERS ----------------------------
1942     152   C     STORED IN XE(2,IE)
1943     153   C
1944     154          XE( 2 , IE ) = SQRT( DXD * DXD + DYD * DYD )
1945     155   C
1946     156   C --- UNIT VECTOR FROM LEFT TO RIGHT BARI-CENTER AT INTERFACE ----------
1947     157   C     STORED IN XXN(IE),YYN(IE)
1948     158   C
1949     159          XY = 1. / XE( 2 , IE )
1950     160          XXN( IE ) = DXD * XY
1951     161          YYN( IE ) = DYD * XY
1952     162   C
1953     163   C --- COORDINATES OF BARI-CENTERS FOR EACH TRIANGLE --------------------
1954     164   C     STORED IN XS(1,IS),XS(2,IS)
1955     165   C
1956     166         XS( 1 , ISL ) = XELEFT( KE )
1957     167         XS( 2 , ISL ) = YELEFT( KE )
1958     168         XS( 1 , ISR ) = XERIGT( KE )
1959     169         XS( 2 , ISR ) = YERIGT( KE )
1960     170   C
1961     171         AA = XV( 1 , IV2 ) - XV( 1 , IV1 )
1962     172         BB = XV( 2 , IV2 ) - XV( 2 , IV1 )
1963     173         CC = XELEFT( KE ) - XERIGT( KE )
1964     174         DD = YELEFT( KE ) - YERIGT( KE )
1965     175         ACA = XERIGT( KE ) - XV( 1 , IV1 )
1966     176         DBD = YERIGT( KE ) - XV( 2 , IV1 )
1967     177         EE = ( ACA * DD - DBD * CC ) / ( AA * DD - BB * CC )
1968     178   C
1969     179   C --- INTERSECTION POINT ON INTERFACE FOR LINE CONNECTING BARI-CENTERS -
1970     180   C     STORED IN XMIDL(IE),YMIDL(IE) AND FRACTION OF LENGHT BETWEEN
1971     181   C     LEFT BARI-CENTER TO INTERSECTION POINT IN XYMIDL(IE).
1972     182   C
1973     183         XMIDL( IE ) = XV( 1 , IV1 ) + AA * EE
1974     184         YMIDL( IE ) = XV( 2 , IV1 ) + BB * EE
1975     185   C
```

```
1976    186          XEMID = XMIDL( IE ) - XELEFT( KE )                                1976
1977    187          YEMID = YMIDL( IE ) - YELEFT( KE )                                1977
1978    188    C                                                                       1978
1979    189          XYMIDL( IE ) = SQRT( XEMID * XEMID + YEMID * YEMID ) * XY         1979
1980    190    C                                                                       1980
1981    191          ENDIF                                                             1981
1982    192     140  CONTINUE                                                          1982
1983    193    C                                                                       1983
1984    194          NE1 = NE2 + 1                                                     1984
1985    195          NE2 = NE2 + NOFVEE( INE + 1 )                                     1985
1986    196     110  CONTINUE                                                          1986
1987    197    C                                                                       1987
1988    198    C --- CALCULATE AREA OF TRIANGLES ------------------------------------ 1988
1989    199    C                                                                       1989
1990    200          DO 150 IS = 1 , NS                                                1990
1991    201          IV1 = JS( 1 , IS )                                                1991
1992    202          IV2 = JS( 2 , IS )                                                1992
1993    203          IV3 = JS( 3 , IS )                                                1993
1994    204          DX  = XV( 1 , IV2 ) - XV( 1 , IV1 )                               1994
1995    205          DXX = XV( 1 , IV3 ) - XV( 1 , IV1 )                               1995
1996    206          DY  = XV( 2 , IV2 ) - XV( 2 , IV1 )                               1996
1997    207          DYY = XV( 2 , IV3 ) - XV( 2 , IV1 )                               1997
1998    208          XS( 3 , IS ) = .5 * ( DX * DYY - DXX * DY )                       1998
1999    209     150  CONTINUE                                                          1999
2000    210    C                                                                       2000
2001    211          PRINT * , NE,NS                                                   2001
2002    212    C                                                                       2002
2003    213    C --- FIND AN EDGE ASSOCIATED WITH A VERTEX -------------------------- 2003
2004    214    C     THE VALUE WILL BE NEGATIVE IF ON THE BOUNDARY                     2004
2005    215    C                                                                       2005
2006    216          DO 180 IV = 1 , NV                                                2006
2007    217          JV( 2 , IV ) = 0                                                  2007
2008    218     180  CONTINUE                                                          2008
2009    219    C                                                                       2009
2010    220          DO 160 IE = 1 , NE                                                2010
2011    221          IV1 = JE( 1 , IE )                                                2011
2012    222          IJE5 = JE( 5 , IE )                                               2012
2013    223          IF( IJE5 . NE . 0 ) THEN                                          2013
2014    224          JV( 2 , IV1 ) = - IE                                              2014
2015    225          END IF                                                            2015
2016    226     160  CONTINUE                                                          2016
2017    227    C                                                                       2017
2018    228          DO 170 IE = 1 , NE                                                2018
2019    229    C                                                                       2019
2020    230          IV1 = JE( 1 , IE )                                                2020
2021    231          IV2 = JE( 2 , IE )                                                2021
2022    232    C                                                                       2022
2023    233          IF( JV( 2 , IV1 ) . EQ . 0 ) THEN                                 2023
2024    234          JV( 2 , IV1 ) = IE                                                2024
2025    235          END IF                                                            2025
2026    236    C                                                                       2026
2027    237          IF( JV( 2 , IV2 ) . EQ . 0 ) THEN                                 2027
2028    238          JV( 2 , IV2 ) = IE                                                2028
2029    239          END IF                                                            2029
2030    240    C                                                                       2030
2031    241     170  CONTINUE                                                          2031
2032    242    C                                                                       2032
2033    243          DO 190 IS = 1 , NS                                                2033
2034    244          SAREA( IS ) = 1. / XS( 3 , IS )                                   2034
2035    245     190  CONTINUE                                                          2035
2036    246    C                                                                       2036
2037    247    C======================================================================= 2037
2038    248    C                                                                       2038
2039    249    C --- OPTION FOR GLOBAL RECONNECTION --------------------------------- 2039
2040    250    C                                                                       2040
2041    251          IF(IOPRCN.EQ.1)THEN                                               2041
2042    252          DO 200 IE = 1 , NE                                                2042
2043    253          CALL RECNC( IE , IDONE , ITL , ITR , JA , JB , JC , JD )          2043
2044    254          CALL RECNC( JA , JADONE , ITL , ITR , JAA , JAB , JAC , JAD )     2044
2045    255          CALL RECNC( JB , JBDONE , ITL , ITR , JBA , JBB , JBC , JBD )     2045
2046    256          CALL RECNC( JC , JCDONE , ITL , ITR , JCA , JCB , JCC , JCD )     2046
2047    257          CALL RECNC( JD , JDDONE , ITL , ITR , JDA , JDB , JDC , JDD )     2047
2048    258     200  CONTINUE                                                          2048
2049    259          ENDIF                                                             2049
```

```
2050    260  C                                                                2050
2051    261  C=================================================================2051
2052    262  C                                                                2052
2053    263  C --- EXIT POINT FROM SUBROUTINE ---------------------------------2053
2054    264  C                                                                2054
2055    265  C     ------                                                     2055
2056    266        RETURN                                                     2056
2057    267  C     ------                                                     2057
2058    268  C                                                                2058
2059    269  C     ---                                                        2059
2060    270        END                                                        2060
```



```
2061      1        SUBROUTINE UPDATE                                          2061
2062      2  C                                                                2062
2063      3  C-----------------------------------------------------------------I2063
2064      4  C                                                                 I2064
2065      5  C      UPDATE BUFFERS IN A BLOCK OF NODES,EDGES, AND CELLS TO     I2065
2066      6  C      CONSTRUCT THE NEW GEOMETRY FOR THE MESH.                   I2066
2067      7  C      THE BLOCKING SIZE IS DETERMINED BY PARAMETER ...MBL...     I2067
2068      8  C                                                                 I2068
2069      9  C-----------------------------------------------------------------I2069
2070     10  C                                                                2070
2071     11  C=================================================================2071
2072     12  C                                                                2072
2073     13        include     'cmsh00.h'                                     2073
2074     14        include     'chyd00.h'                                     2074
2075     15        include     'cint00.h'                                     2075
2076     16        include     'cphs10.h'                                     2076
2077     17        include     'cphs20.h'                                     2077
2078     18  C                                                                2078
2079     19  C=================================================================2079
2080     20  C                                                                2080
2081     21  C --- BREAK UP THE VERTEX, EDGE, AND TRIANGLE DATA INTO BLOCKS ---2081
2082     22  C                                                                2082
2083     23        NVECE = NE / MBL                                           2083
2084     24        NREME = NE - NVECE * MBL                                   2084
2085     25        NVECS = NS / MBL                                           2085
2086     26        NREMS = NS - NVECS * MBL                                   2086
2087     27        NVECV = NV / MBL                                           2087
2088     28        NREMV = NV - NVECV * MBL                                   2088
2089     29          PRINT *,NV,NE,NS,NVECE,NREME,NVECV,NREMV,NVECS,NREMS     2089
2090     30  C                                                                2090
2091     31        DO 105 INE = 1 , NVECE                                     2091
2092     32        NOFVEE( INE ) = MBL                                        2092
2093     33   105  CONTINUE                                                   2093
2094     34        NVEEE = NVECE                                              2094
2095     35        IF( NREME . GT . 0 ) THEN                                  2095
2096     36        NVEEE = NVECE + 1                                          2096
2097     37        NOFVEE( NVEEE ) = NREME                                    2097
2098     38        END IF                                                     2098
2099     39  C                                                                2099
2100     40        DO 115 INS = 1 , NVECS                                     2100
2101     41        NOFVES( INS ) = MBL                                        2101
2102     42   115  CONTINUE                                                   2102
2103     43        NVEES = NVECS                                              2103
2104     44        IF( NREMS . GT . 0 ) THEN                                  2104
2105     45        NVEES = NVECS + 1                                          2105
2106     46        NOFVES( NVEES ) = NREMS                                    2106
2107     47        END IF                                                     2107
2108     48  C                                                                2108
2109     49        DO 125 INV = 1 , NVECV                                     2109
2110     50        NOFVEV( INV ) = MBL                                        2110
2111     51   125  CONTINUE                                                   2111
2112     52        NVEEV = NVECV                                              2112
2113     53        IF( NREMV . GT . 0 ) THEN                                  2113
2114     54        NVEEV = NVECV + 1                                          2114
2115     55        NOFVEV( NVEEV ) = NREMV                                    2115
2116     56        END IF                                                     2116
2117     57  C                                                                2117
2118     58  C --- CALL TO THE GEOMETRY DEFINITION SUBROUTINE -----------------2118
2119     59  C                                                                2119
2120     60        CALL GEOMTR                                                2120
```

```
2121      61   C                                                                 2121
2122      62   C=================================================================2122
2123      63   C                                                                 2123
2124      64   C --- EXIT POINT FROM SUBROUTINE ---------------------------------2124
2125      65   C                                                                 2125
2126      66   C     ------                                                      2126
2127      67         RETURN                                                      2127
2128      68   C     ------                                                      2128
2129      69   C                                                                 2129
2130      70   C     ---                                                         2130
2131      71         END                                                         2131
```



```
2132       1         SUBROUTINE UPGRAD                                          2132
2133       2   C                                                                2133
2134       3   C-----------------------------------------------------------------I2134
2135       4   C                                                                 I2135
2136       5   C      UPGRAD READS THE RESTART FILE FROM A PREVIOUS RUN          I2136
2137       6   C      AND BREAKS THE DATA INTO BLOCKS AS DEFINED BY THE          I2137
2138       7   C      PARAMETER ...MBL...                                        I2138
2139       8   C                                                                 I2139
2140       9   C-----------------------------------------------------------------I2140
2141      10   C                                                                2141
2142      11         include     'cmsh00.h'                                     2142
2143      12         include     'chyd00.h'                                     2143
2144      13         include     'cint00.h'                                     2144
2145      14         include     'cphs10.h'                                     2145
2146      15         include     'cphs20.h'                                     2146
2147      16   C                                                                2147
2148      17   C=================================================================2148
2149      18   C                                                                2149
2150      19   C      MVM MAX NUMBER OF VERTICES  (POINTS)                      2150
2151      20   C      MEM MAX NUMBER OF EDGES     (INTERFACES)                  2151
2152      21   C      MSM MAX NUMBER OF SIDES     (TRIANGLES)                   2152
2153      22   C                                                                2153
2154      23   C=================================================================2154
2155      24   C                                                                2155
2156      25   C                                                                2156
2157      26         READ (88) NV,NVMK,NE,NEMK,NS,NSMK,ITERAT                   2157
2158      27   C                                                                2158
2159      28   C --- READ IN VERTEX INFORMATION ---------------------------------2159
2160      29   C                                                                2160
2161      30           READ (88) ((JV(IK,IV),IK=1,2),(XV(IK,IV),IK=1,2),IV=1,NV)2161
2162      31   C                                                                2162
2163      32   C --- READ IN EDGE INFORMATION ( EDGES OF TRIANGLES).------------2163
2164      33   C                                                                2164
2165      34           READ (88) ((JE(KK,IE),KK=1,5),(XE(KI,IE),KI=1,2),IE=1,NE)2165
2166      35           READ (88) (XN(IE),YN(IE),XXN(IE),YYN(IE),IE=1,NE)       2166
2167      36   C                                                                2167
2168      37   C --- READ IN SIDE (TRIANGLE) INFORMATION.------------------------2168
2169      38   C                                                                2169
2170      39            READ (88) ((JS(KK,IS),KK=1,6),(XS(KI,IS),KI=1,3),IS=1,NS)2170
2171      40            READ (88) (XMIDL(IE),YMIDL(IE),XYMIDL(IE),IE=1,NE)     2171
2172      41            READ (88) SAREVG,NVECE,NREME,NVECV,NREMV,NVECS,NREMS    2172
2173      42   C                                                                2173
2174      43   C --- PRINT PROMT TO CONSOLE -------------------------------------2174
2175      44   C                                                                2175
2176      45            PRINT * , NE,NS                                        2176
2177      46   C                                                                2177
2178      47   C --- DEFINE INVERSE AREA OF TRIANGLES ---------------------------2178
2179      48   C                                                                2179
2180      49         DO 100 IS = 1 , NS                                         2180
2181      50         SAREA( IS ) = 1. / XS( 3 , IS )                            2181
2182      51    100  CONTINUE                                                   2182
2183      52   C                                                                2183
2184      53   C --- BREAKUP THE DATA STRUCTURE INTO BLOCKS ----------------------2184
2185      54   C                                                                2185
2186      55         DO 105 INE = 1 , NVECE                                     2186
2187      56         NOFVEE( INE ) = MBL                                        2187
2188      57    105  CONTINUE                                                   2188
2189      58         NVEEE = NVECE                                              2189
2190      59         IF( NREME . GT . 0 ) THEN                                  2190
2191      60         NVEEE = NVECE + 1                                          2191
```

```
2192      61          NOFVEE( NVEEE ) = NREME                                    2192
2193      62          END IF                                                     2193
2194      63    C                                                                2194
2195      64          DO 115 INS = 1 , NVECS                                     2195
2196      65          NOFVES( INS ) = MBL                                        2196
2197      66     115  CONTINUE                                                   2197
2198      67          NVEES = NVECS                                              2198
2199      68          IF( NREMS . GT . 0 ) THEN                                  2199
2200      69          NVEES = NVECS + 1                                          2200
2201      70          NOFVES( NVEES ) = NREMS                                    2201
2202      71          END IF                                                     2202
2203      72    C                                                                2203
2204      73          DO 125 INV = 1 , NVECV                                     2204
2205      74          NOFVEV( INV ) = MBL                                        2205
2206      75     125  CONTINUE                                                   2206
2207      76          NVEEV = NVECV                                              2207
2208      77          IF( NREMV . GT . 0 ) THEN                                  2208
2209      78          NVEEV = NVECV + 1                                          2209
2210      79          NOFVEV( NVEEV ) = NREMV                                    2210
2211      80          END IF                                                     2211
2212      81    C                                                                2212
2213      82    C --- PRINTOUT THE VERTEX,EDGE, AND TRIANGLE BLOCK DATA ---------- 2213
2214      83    C                                                                2214
2215      84           PRINT *,NV,NE,NS,NVECE,NREME,NVECV,NREMV,NVECS,NREMS      2215
2216      85    C                                                                2216
2217      86    C================================================================ 2217
2218      87    C                                                                2218
2219      88    C --- EXIT POINT FROM SUBROUTINE ---------------------------------- 2219
2220      89    C                                                                2220
2221      90    C     ------                                                     2221
2222      91          RETURN                                                     2222
2223      92    C     ------                                                     2223
2224      93    C                                                                2224
2225      94    C     ---                                                        2225
2226      95          END                                                        2226
```

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```
      SUBROUTINE GRDFLX
C
C-----------------------------------------------------------------I
C                                                                 I
C      GRAFLX COMPUTE THE GRADIENT FOR ERROR INDICATOR            I
C            CALCULATION FOR STEADY STATE                         I
C                                                                 I
C-----------------------------------------------------------------I
C
      include     'cmsh00.h'
      include     'chyd00.h'
      include     'cint00.h'
      include     'cphs10.h'
      include     'cphs20.h'
C
C=================================================================
C
      REAL AA(3,3),BB(3,4),B(3),INDX(3),ATEMP(3,3,3),BTEMP(3,4,3)
      REAL AA0(3,3),BB0(3,4)
C
C=================================================================
C
C
C
C --- BEGIN LOOP OVER ALL CELLS IN THE DOMAIN -------------------------
C
      NS1 = 1
      NS2 = NOFVES( 1 )
      DO 90 INS = 1 , NVEES
C
C --- FETCH HYDRO QUANTITIES ------------------------------------------
C
      DO 105 IS = NS1 , NS2
         KS = IS - NS1 + 1
C
       XSM = XS( 1 , IS )
       YSM = XS( 2 , IS )
       XSM2 = XSM * XSM
       YSM2 = YSM * YSM
       XYSM = XSM * YSM
C
       AA0( 1 , 1 ) = 1.0
       AA0( 1 , 2 ) = XSM
       AA0( 1 , 3 ) = YSM
C
       AA0( 2 , 1 ) = XSM
       AA0( 2 , 2 ) = XSM2
       AA0( 2 , 3 ) = XYSM
C
       AA0( 3 , 1 ) = YSM
       AA0( 3 , 2 ) = XYSM
       AA0( 3 , 3 ) = YSM2
C
       BB1 = HYDV( IS , 4 )
       BB2 = SQRT ( ( HYDV( IS , 2 ) *  HYDV( IS , 2 ) +
     .                HYDV( IS , 3 ) *  HYDV( IS , 3 ) ) *
     .      HYDV( IS , 1 ) /  HYDV( IS , 4 ) / HYDV( IS , 5 ) )
C
       BB1X = BB1 * XSM
       BB2X = BB2 * XSM
C
       BB1Y = BB1 * YSM
       BB2Y = BB2 * YSM
C
       BB0( 1 , 1 ) = BB1
       BB0( 1 , 2 ) = BB2
C
       BB0( 2 , 1 ) = BB1X
       BB0( 2 , 2 ) = BB2X
C
       BB0( 3 , 1 ) = BB1Y
       BB0( 3 , 2 ) = BB2Y
C
       DO 115 IK = 1 , 3
```

```
      IE = JS( IK + 3 , IS )
      IF( IE . GT . 0 ) THEN
      ISS = JE( 4 , IE )
      ELSE
      ISS = JE( 3 , -IE )
      END IF
C
      IF( ISS . NE . 0 ) THEN
      XSS = XS( 1 , ISS )
      YSS = XS( 2 , ISS )
C
      HYDVP = HYDV( ISS , 4 )
      HYDVR = SQRT ( ( HYDV( ISS , 2 ) *  HYDV( ISS , 2 ) +
     .                 HYDV( ISS , 3 ) *  HYDV( ISS , 3 ) ) *
     .        HYDV( ISS , 1 ) /  HYDV( ISS , 4 ) / HYDV( ISS , 5 ) )
C
      ELSE
C
      IE = IABS( IE )
      XSS = 2. * XMIDL( IE ) - XSM
      YSS = 2. * YMIDL( IE ) - YSM
C
      HYDVP = BB1
      HYDVR = BB2
      IJE5 = JE( 5 , IE )
      IF( IJE5 . EQ . 8 ) THEN
      HYDVP =   PIN
      HYDVR =   SQRT( UVIN * UVIN * RIN / PIN / HRGG )
      END IF
C
      END IF
C
      XSS2 = XSS * XSS
      YSS2 = YSS * YSS
      XYSS = XSS * YSS
C
      ATEMP( 1 , 1 , IK ) = 1.0
      ATEMP( 1 , 2 , IK ) = XSS
      ATEMP( 1 , 3 , IK ) = YSS
C
      ATEMP( 2 , 1 , IK ) = XSS
      ATEMP( 2 , 2 , IK ) = XSS2
      ATEMP( 2 , 3 , IK ) = XYSS
C
      ATEMP( 3 , 1 , IK ) = YSS
      ATEMP( 3 , 2 , IK ) = XYSS
      ATEMP( 3 , 3 , IK ) = YSS2
C
      BTEMP( 1 , 1 , IK ) = HYDVP
      BTEMP( 1 , 2 , IK ) = HYDVR
C
      BTEMP( 2 , 1 , IK ) = HYDVP * XSS
      BTEMP( 2 , 2 , IK ) = HYDVR * XSS
C
      BTEMP( 3 , 1 , IK ) = HYDVP * YSS
      BTEMP( 3 , 2 , IK ) = HYDVR * YSS
C
  115 CONTINUE
C
      AA( 1 , 1 ) =   AA0( 1 , 1 )     + ATEMP( 1 , 1 , 1 ) +
     .              ATEMP( 1 , 1 , 2 ) + ATEMP( 1 , 1 , 3 )
      AA( 1 , 2 ) =   AA0( 1 , 2 )     + ATEMP( 1 , 2 , 1 ) +
     .              ATEMP( 1 , 2 , 2 ) + ATEMP( 1 , 2 , 3 )
      AA( 1 , 3 ) =   AA0( 1 , 3 )     + ATEMP( 1 , 3 , 1 ) +
     .              ATEMP( 1 , 3 , 2 ) + ATEMP( 1 , 3 , 3 )
C
      AA( 2 , 1 ) =   AA0( 2 , 1 )     + ATEMP( 2 , 1 , 1 ) +
     .              ATEMP( 2 , 1 , 2 ) + ATEMP( 2 , 1 , 3 )
      AA( 2 , 2 ) =   AA0( 2 , 2 )     + ATEMP( 2 , 2 , 1 ) +
     .              ATEMP( 2 , 2 , 2 ) + ATEMP( 2 , 2 , 3 )
      AA( 2 , 3 ) =   AA0( 2 , 3 )     + ATEMP( 2 , 3 , 1 ) +
     .              ATEMP( 2 , 3 , 2 ) + ATEMP( 2 , 3 , 3 )
C
      AA( 3 , 1 ) =   AA0( 3 , 1 )     + ATEMP( 3 , 1 , 1 ) +
```

```
148     148          .                ATEMP( 3 , 1 , 2 ) + ATEMP( 3 , 1 , 3 )                148
149     149            AA( 3 , 2 ) =   AA0( 3 , 2 )     + ATEMP( 3 , 2 , 1 ) +              149
150     150          .                ATEMP( 3 , 2 , 2 ) + ATEMP( 3 , 2 , 3 )                150
151     151            AA( 3 , 3 ) =   AA0( 3 , 3 )     + ATEMP( 3 , 3 , 1 ) +              151
152     152          .                ATEMP( 3 , 3 , 2 ) + ATEMP( 3 , 3 , 3 )                152
153     153     C                                                                            153
154     154            BB( 1 , 1 ) =   BB0( 1 , 1 )     + BTEMP( 1 , 1 , 1 ) +              154
155     155          .                BTEMP( 1 , 1 , 2 ) + BTEMP( 1 , 1 , 3 )                155
156     156            BB( 1 , 2 ) =   BB0( 1 , 2 )     + BTEMP( 1 , 2 , 1 ) +              156
157     157          .                BTEMP( 1 , 2 , 2 ) + BTEMP( 1 , 2 , 3 )                157
158     158     C                                                                            158
159     159            BB( 2 , 1 ) =   BB0( 2 , 1 )     + BTEMP( 2 , 1 , 1 ) +              159
160     160          .                BTEMP( 2 , 1 , 2 ) + BTEMP( 2 , 1 , 3 )                160
161     161            BB( 2 , 2 ) =   BB0( 2 , 2 )     + BTEMP( 2 , 2 , 1 ) +              161
162     162          .                BTEMP( 2 , 2 , 2 ) + BTEMP( 2 , 2 , 3 )                162
163     163     C                                                                            163
164     164            BB( 3 , 1 ) =   BB0( 3 , 1 )     + BTEMP( 3 , 1 , 1 ) +              164
165     165          .                BTEMP( 3 , 1 , 2 ) + BTEMP( 3 , 1 , 3 )                165
166     166            BB( 3 , 2 ) =   BB0( 3 , 2 )     + BTEMP( 3 , 2 , 1 ) +              166
167     167          .                BTEMP( 3 , 2 , 2 ) + BTEMP( 3 , 2 , 3 )                167
168     168     C                                                                            168
169     169            DETERM = AA( 1 , 1 ) * ( AA( 2 , 2 ) * AA( 3 , 3 ) -                169
170     170          .                          AA( 3 , 2 ) * AA( 2 , 3 ) ) +               170
171     171          .          AA( 2 , 1 ) * ( AA( 3 , 2 ) * AA( 1 , 3 ) -                171
172     172          .                          AA( 1 , 2 ) * AA( 3 , 3 ) ) +               172
173     173          .          AA( 3 , 1 ) * ( AA( 1 , 2 ) * AA( 2 , 3 ) -                173
174     174          .                          AA( 2 , 2 ) * AA( 1 , 3 ) )                 174
175     175     C                                                                            175
176     176            DTRMIN = 1. / DETERM                                                 176
177     177     C                                                                            177
178     178            AAA1 = AA( 2 , 3 ) * AA( 3 , 1 ) - AA( 2 , 1 ) * AA( 3 , 3 )        178
179     179            AAA2 = AA( 3 , 3 ) * AA( 1 , 1 ) - AA( 3 , 1 ) * AA( 1 , 3 )        179
180     180            AAA3 = AA( 1 , 3 ) * AA( 2 , 1 ) - AA( 1 , 1 ) * AA( 2 , 3 )        180
181     181     C                                                                            181
182     182            AAA4 = AA( 2 , 1 ) * AA( 3 , 2 ) - AA( 3 , 1 ) * AA( 2 , 2 )        182
183     183            AAA5 = AA( 3 , 1 ) * AA( 1 , 2 ) - AA( 1 , 1 ) * AA( 3 , 2 )        183
184     184            AAA6 = AA( 1 , 1 ) * AA( 2 , 2 ) - AA( 2 , 1 ) * AA( 1 , 2 )        184
185     185     C                                                                            185
186     186            PL( IS ) = DTRMIN * ( BB( 1 , 1 ) * AAA1 +                           186
187     187          .                       BB( 2 , 1 ) * AAA2 +                           187
188     188          .                       BB( 3 , 1 ) * AAA3 )                           188
189     189     C                                                                            189
190     190            PR( IS ) = DTRMIN * ( BB( 1 , 1 ) * AAA4 +                           190
191     191          .                       BB( 2 , 1 ) * AAA5 +                           191
192     192          .                       BB( 3 , 1 ) * AAA6 )                           192
193     193     C                                                                            193
194     194            RL( IS ) = DTRMIN * ( BB( 1 , 2 ) * AAA1 +                           194
195     195          .                       BB( 2 , 2 ) * AAA2 +                           195
196     196          .                       BB( 3 , 2 ) * AAA3 )                           196
197     197     C                                                                            197
198     198            RR( IS ) = DTRMIN * ( BB( 1 , 2 ) * AAA4 +                           198
199     199          .                       BB( 2 , 2 ) * AAA5 +                           199
200     200          .                       BB( 3 , 2 ) * AAA6 )                           200
201     201     C                                                                            201
202     202      105  CONTINUE                                                             202
203     203     C                                                                            203
204     204            NS1 = NS2 + 1                                                        204
205     205            NS2 = NS2 + NOFVES( INS + 1 )                                        205
206     206      90    CONTINUE                                                             206
207     207     C                                                                            207
208     208     C=============================================================================208
209     209     C                                                                            209
210     210     C --- EXIT POINT FROM SUBROUTINE ------------------------------------------ 210
211     211     C                                                                            211
212     212     C     ------                                                                 212
213     213           RETURN                                                                 213
214     214     C     ------                                                                 214
215     215     C                                                                            215
216     216     C     ---                                                                    216
217     217           END                                                                    217
```

```
      SUBROUTINE GRDENG
C
C-----------------------------------------------------------------------I
C                                                                       I
C      GRAENG COMPUTE THE GRADIENT FOR SECOND ORDER CALCULATION         I
C                                                                       I
C-----------------------------------------------------------------------I
C
      include     'cmsh00.h'
      include     'chyd00.h'
      include     'cint00.h'
      include     'cphs10.h'
      include     'cphs20.h'
C
C=======================================================================
C
      REAL RRMIDL(MBP),PPMIDL(MBP),UUMIDL(MBP),VVMIDL(MBP)
      REAL RIGRAD(MBP),PIGRAD(MBP),UIGRAD(MBP),VIGRAD(MBP)
      REAL RJGRAD(MBP),PJGRAD(MBP),UJGRAD(MBP),VJGRAD(MBP)
      REAL AA(3,3),BB(3,4),B(3),INDX(3),ATEMP(3,3,3),BTEMP(3,4,3)
      REAL AA0(3,3),BB0(3,4)
C
C=======================================================================
C
C --- BEGIN LOOP OVER ALL CELLS IN THE DOMAIN -------------------------
C
      NS1 = 1
      NS2 = NOFVES( 1 )
      DO 90 INS = 1 , NVEES
C
C --- FETCH HYDRO QUANTITIES ------------------------------------------
C
      DO 105 IS = NS1 , NS2
C
       XSM = XS( 1 , IS )
       YSM = XS( 2 , IS )
       XSM2 = XSM * XSM
       YSM2 = YSM * YSM
       XYSM = XSM * YSM
C
       AA0( 1 , 1 ) = 1.0
       AA0( 1 , 2 ) = XSM
       AA0( 1 , 3 ) = YSM
C
       AA0( 2 , 1 ) = XSM
       AA0( 2 , 2 ) = XSM2
       AA0( 2 , 3 ) = XYSM
C
       AA0( 3 , 1 ) = YSM
       AA0( 3 , 2 ) = XYSM
       AA0( 3 , 3 ) = YSM2
C
       BB1 = HYDFLX( IS , 1 )
       BB2 = HYDFLX( IS , 2 )
       BB3 = HYDFLX( IS , 4 )
C
       BB1X = BB1 * XSM
       BB2X = BB2 * XSM
       BB3X = BB3 * XSM
C
       BB1Y = BB1 * YSM
       BB2Y = BB2 * YSM
       BB3Y = BB3 * YSM
C
       BB0( 1 , 1 ) = BB1
       BB0( 1 , 2 ) = BB2
       BB0( 1 , 3 ) = BB3
C
       BB0( 2 , 1 ) = BB1X
       BB0( 2 , 2 ) = BB2X
       BB0( 2 , 3 ) = BB3X
C
       BB0( 3 , 1 ) = BB1Y
       BB0( 3 , 2 ) = BB2Y
```

```
292     75          BB0( 3 , 3 ) = BB3Y                                                                  292
293     76    C                                                                                          293
294     77          DO 115 IK = 1 , 3                                                                    294
295     78          IE = JS( IK + 3 , IS )                                                               295
296     79          IF( IE . GT . 0 ) THEN                                                               296
297     80          ISS = JE( 4 , IE )                                                                   297
298     81          ELSE                                                                                 298
299     82          ISS = JE( 3 , - IE )                                                                 299
300     83          END IF                                                                               300
301     84    C                                                                                          301
302     85          IF( ISS . NE . 0 ) THEN                                                              302
303     86          XSS = XS( 1 , ISS )                                                                  303
304     87          YSS = XS( 2 , ISS )                                                                  304
305     88    C                                                                                          305
306     89          HYDVR = HYDFLX( ISS , 1 )                                                            306
307     90          HYDVU = HYDFLX( ISS , 2 )                                                            307
308     91          HYDVV = HYDFLX( ISS , 4 )                                                            308
309     92    C                                                                                          309
310     93          ELSE                                                                                 310
311     94    C                                                                                          311
312     95          IE = IABS( IE )                                                                      312
313     96          HYDVR = BB1                                                                          313
314     97          HYDVU = BB2                                                                          314
315     98          HYDVV = BB3                                                                          315
316     99    C                                                                                          316
317    100          XSS = 2. * XMIDL( IE ) - XSM                                                         317
318    101          YSS = 2. * YMIDL( IE ) - YSM                                                         318
319    102    C                                                                                          319
320    103          END IF                                                                               320
321    104    C                                                                                          321
322    105          XSS2 = XSS * XSS                                                                     322
323    106          YSS2 = YSS * YSS                                                                     323
324    107          XYSS = XSS * YSS                                                                     324
325    108    C                                                                                          325
326    109          ATEMP( 1 , 1 , IK ) = 1.0                                                            326
327    110          ATEMP( 1 , 2 , IK ) = XSS                                                            327
328    111          ATEMP( 1 , 3 , IK ) = YSS                                                            328
329    112    C                                                                                          329
330    113          ATEMP( 2 , 1 , IK ) = XSS                                                            330
331    114          ATEMP( 2 , 2 , IK ) = XSS2                                                           331
332    115          ATEMP( 2 , 3 , IK ) = XYSS                                                           332
333    116    C                                                                                          333
334    117          ATEMP( 3 , 1 , IK ) = YSS                                                            334
335    118          ATEMP( 3 , 2 , IK ) = XYSS                                                           335
336    119          ATEMP( 3 , 3 , IK ) = YSS2                                                           336
337    120    C                                                                                          337
338    121          BTEMP( 1 , 1 , IK ) = HYDVR                                                          338
339    122          BTEMP( 1 , 2 , IK ) = HYDVU                                                          339
340    123          BTEMP( 1 , 3 , IK ) = HYDVV                                                          340
341    124    C                                                                                          341
342    125          BTEMP( 2 , 1 , IK ) = HYDVR * XSS                                                    342
343    126          BTEMP( 2 , 2 , IK ) = HYDVU * XSS                                                    343
344    127          BTEMP( 2 , 3 , IK ) = HYDVV * XSS                                                    344
345    128    C                                                                                          345
346    129          BTEMP( 3 , 1 , IK ) = HYDVR * YSS                                                    346
347    130          BTEMP( 3 , 2 , IK ) = HYDVU * YSS                                                    347
348    131          BTEMP( 3 , 3 , IK ) = HYDVV * YSS                                                    348
349    132    C                                                                                          349
350    133     115  CONTINUE                                                                            350
351    134    C                                                                                          351
352    135          AA( 1 , 1 ) =   AA0( 1 , 1 )     + ATEMP( 1 , 1 , 1 ) +                              352
353    136         .                AtEMP( 1 , 1 , 2 ) + ATEMP( 1 , 1 , 3 )                             353
354    137          AA( 1 , 2 ) =   AA0( 1 , 2 )     + ATEMP( 1 , 2 , 1 ) +                              354
355    138         .                ATEMP( 1 , 2 , 2 ) + ATEMP( 1 , 2 , 3 )                             355
356    139          AA( 1 , 3 ) =   AA0( 1 , 3 )     + ATEMP( 1 , 3 , 1 ) +                              356
357    140         .                ATEMP( 1 , 3 , 2 ) + ATEMP( 1 , 3 , 3 )                             357
358    141    C                                                                                          358
359    142          AA( 2 , 1 ) =   AA0( 2 , 1 )     + ATEMP( 2 , 1 , 1 ) +                              359
360    143         .                ATEMP( 2 , 1 , 2 ) + ATEMP( 2 , 1 , 3 )                             360
361    144          AA( 2 , 2 ) =   AA0( 2 , 2 )     + ATEMP( 2 , 2 , 1 ) +                              361
362    145         .                ATEMP( 2 , 2 , 2 ) + ATEMP( 2 , 2 , 3 )                             362
363    146          AA( 2 , 3 ) =   AA0( 2 , 3 )     + ATEMP( 2 , 3 , 1 ) +                              363
364    147         .                ATEMP( 2 , 3 , 2 ) + ATEMP( 2 , 3 , 3 )                             364
365    148    C                                                                                          365
```

```
      AA( 3 , 1 ) =  AA0( 3 , 1 )    + ATEMP( 3 , 1 , 1 ) +
     .               ATEMP( 3 , 1 , 2 ) + ATEMP( 3 , 1 , 3 )
      AA( 3 , 2 ) =  AA0( 3 , 2 )    + ATEMP( 3 , 2 , 1 ) +
     .               ATEMP( 3 , 2 , 2 ) + ATEMP( 3 , 2 , 3 )
      AA( 3 , 3 ) =  AA0( 3 , 3 )    + ATEMP( 3 , 3 , 1 ) +
     .               ATEMP( 3 , 3 , 2 ) + ATEMP( 3 , 3 , 3 )
C
      BB( 1 , 1 ) =  BB0( 1 , 1 )    + BTEMP( 1 , 1 , 1 ) +
     .               BTEMP( 1 , 1 , 2 ) + BTEMP( 1 , 1 , 3 )
      BB( 1 , 2 ) =  BB0( 1 , 2 )    + BTEMP( 1 , 2 , 1 ) +
     .               BTEMP( 1 , 2 , 2 ) + BTEMP( 1 , 2 , 3 )
      BB( 1 , 3 ) =  BB0( 1 , 3 )    + BTEMP( 1 , 3 , 1 ) +
     .               BTEMP( 1 , 3 , 2 ) + BTEMP( 1 , 3 , 3 )
C
      BB( 2 , 1 ) =  BB0( 2 , 1 )    + BTEMP( 2 , 1 , 1 ) +
     .               BTEMP( 2 , 1 , 2 ) + BTEMP( 2 , 1 , 3 )
      BB( 2 , 2 ) =  BB0( 2 , 2 )    + BTEMP( 2 , 2 , 1 ) +
     .               BTEMP( 2 , 2 , 2 ) + BTEMP( 2 , 2 , 3 )
      BB( 2 , 3 ) =  BB0( 2 , 3 )    + BTEMP( 2 , 3 , 1 ) +
     .               BTEMP( 2 , 3 , 2 ) + BTEMP( 2 , 3 , 3 )
C
      BB( 3 , 1 ) =  BB0( 3 , 1 )    + BTEMP( 3 , 1 , 1 ) +
     .               BTEMP( 3 , 1 , 2 ) + BTEMP( 3 , 1 , 3 )
      BB( 3 , 2 ) =  BB0( 3 , 2 )    + BTEMP( 3 , 2 , 1 ) +
     .               BTEMP( 3 , 2 , 2 ) + BTEMP( 3 , 2 , 3 )
      BB( 3 , 3 ) =  BB0( 3 , 3 )    + BTEMP( 3 , 3 , 1 ) +
     .               BTEMP( 3 , 3 , 2 ) + BTEMP( 3 , 3 , 3 )
C
      DETERM = AA( 1 , 1 ) * ( AA( 2 , 2 ) * AA( 3 , 3 ) -
     .                         AA( 3 , 2 ) * AA( 2 , 3 ) ) +
     .         AA( 2 , 1 ) * ( AA( 1 , 3 ) * AA( 3 , 2 ) -
     .                         AA( 3 , 3 ) * AA( 1 , 2 ) ) +
     .         AA( 3 , 1 ) * ( AA( 1 , 2 ) * AA( 2 , 3 ) -
     .                         AA( 2 , 2 ) * AA( 1 , 3 ) )
C
      DTRMIN = 1. / DETERM
C
      AAA1 = AA( 2 , 3 ) * AA( 3 , 1 ) - AA( 2 , 1 ) * AA( 3 , 3 )
      AAA2 = AA( 3 , 3 ) * AA( 1 , 1 ) - AA( 3 , 1 ) * AA( 1 , 3 )
      AAA3 = AA( 1 , 3 ) * AA( 2 , 1 ) - AA( 1 , 1 ) * AA( 2 , 3 )
C
      AAA4 = AA( 2 , 1 ) * AA( 3 , 2 ) - AA( 3 , 1 ) * AA( 2 , 2 )
      AAA5 = AA( 3 , 1 ) * AA( 1 , 2 ) - AA( 1 , 1 ) * AA( 3 , 2 )
      AAA6 = AA( 1 , 1 ) * AA( 2 , 2 ) - AA( 2 , 1 ) * AA( 1 , 2 )
C
      RR( IS ) = DTRMIN * ( BB( 1 , 1 ) * AAA1 +
     .                      BB( 2 , 1 ) * AAA2 +
     .                      BB( 3 , 1 ) * AAA3 )
C
      RL( IS ) = DTRMIN * ( BB( 1 , 1 ) * AAA4 +
     .                      BB( 2 , 1 ) * AAA5 +
     .                      BB( 3 , 1 ) * AAA6 )
C
      UR( IS ) = DTRMIN * ( BB( 1 , 2 ) * AAA1 +
     .                      BB( 2 , 2 ) * AAA2 +
     .                      BB( 3 , 2 ) * AAA3 )
C
      UL( IS ) = DTRMIN * ( BB( 1 , 2 ) * AAA4 +
     .                      BB( 2 , 2 ) * AAA5 +
     .                      BB( 3 , 2 ) * AAA6 )
C
      VR( IS ) = DTRMIN * ( BB( 1 , 3 ) * AAA1 +
     .                      BB( 2 , 3 ) * AAA2 +
     .                      BB( 3 , 3 ) * AAA3 )
C
      VL( IS ) = DTRMIN * ( BB( 1 , 3 ) * AAA4 +
     .                      BB( 2 , 3 ) * AAA5 +
     .                      BB( 3 , 3 ) * AAA6 )
C
  105 CONTINUE
C
      NS1 = NS2 + 1
      NS2 = NS2 + NOFVES( INS + 1 )
   90 CONTINUE
```

```
440   223   C                                                                      440
441   224   C=======================================================================441
442   225   C                                                                      442
443   226   C --- EXIT POINT FROM SUBROUTINE ------------------------------------- 443
444   227   C                                                                      444
445   228   C     ------                                                           445
446   229         RETURN                                                           446
447   230   C     ------                                                           447
448   231   C                                                                      448
449   232   C     ---                                                              449
450   233         END                                                              450
```



```
451     1         SUBROUTINE GRADNL                                                451
452     2   C                                                                      452
453     3   C----------------------------------------------------------------------I453
454     4   C                                                                      I454
455     5   C      GRADNL COMPUTE THE GRADIENT FOR SECOND ORDER CALCULATION        I455
456     6   C             SEARCH FOR ALL TRIANGLES SUROUNDING THE TARGET           I456
457     7   C             CELL FOR COMPUTING THE GRADIENT APPLYING LEAST           I457
458     8   C             SQUARE TECHNIQUE                                         I458
459     9   C                                                                      I459
460    10   C----------------------------------------------------------------------I460
461    11   C                                                                      461
462    12         include     'cmsh00.h'                                           462
463    13         include     'chyd00.h'                                           463
464    14         include     'cint00.h'                                           464
465    15         include     'cphs10.h'                                           465
466    16         include     'cphs20.h'                                           466
467    17   C                                                                      467
468    18   C=======================================================================468
469    19   C                                                                      469
470    20         REAL RRMIDL(MBP),PPMIDL(MBP),UUMIDL(MBP),VVMIDL(MBP)             470
471    21         REAL RIGRAD(MBP),PIGRAD(MBP),UIGRAD(MBP),VIGRAD(MBP)             471
472    22         REAL RJGRAD(MBP),PJGRAD(MBP),UJGRAD(MBP),VJGRAD(MBP)             472
473    23         REAL RMAX(MBP),PMAX(MBP),UMAX(MBP),VMAX(MBP)                     473
474    24         REAL RMIN(MBP),PMIN(MBP),UMIN(MBP),VMIN(MBP)                     474
475    25         REAL RLEFTT(MBP),ULEFTT(MBP),VLEFTT(MBP),PLEFTT(MBP)             475
476    26         REAL RRIGHT(MBP),URIGHT(MBP),VRIGHT(MBP),PRIGHT(MBP)             476
477    27         REAL ROR(3),UOR(3),VOR(3),POR(3)                                 477
478    28         REAL ROL(3),UOL(3),VOL(3),POL(3)                                 478
479    29         REAL AA(3,3),BB(3,4),B(3),INDX(3),ATEMP(3,3),BTEMP(3,4)          479
480    30   C                                                                      480
481    31   C=======================================================================481
482    32   C                                                                      482
483    33   C --- BEGIN LOOP OVER ALL CELLS IN THE DOMAIN ------------------------ 483
484    34   C                                                                      484
485    35         NS1 = 1                                                          485
486    36         NS2 = NOFVES( 1 )                                                486
487    37         DO 90 INS = 1 , NVEES                                            487
488    38   C                                                                      488
489    39   C --- FETCH HYDRO QUANTITIES ----------------------------------------- 489
490    40   C                                                                      490
491    41         DO 105 IS = NS1 , NS2                                            491
492    42   C                                                                      492
493    43          JJCOLR = 0                                                      493
494    44   C                                                                      494
495    45          DO 115 IK = 1 , 3                                               495
496    46          IVV = JS( IK , IS )                                             496
497    47          IEE = JV( 2 , IVV )                                             497
498    48   C                                                                      498
499    49          IF( IEE . GT . 0 ) THEN                                         499
500    50   C                                                                      500
501    51          IV1 = JE( 1 , IEE )                                             501
502    52          IF( IV1 . EQ . IVV ) THEN                                       502
503    53          ISI = JE( 3 , IEE )                                             503
504    54          ELSE                                                            504
505    55          ISI = JE( 4 , IEE )                                             505
506    56          END IF                                                          506
507    57          ISS = ISI                                                       507
508    58          IE = IEE                                                        508
509    59   C                                                                      509
510    60   150    CONTINUE                                                        510
```

```
      C
            JJCOLR = JJCOLR + 1
            IICOLR( JJCOLR ) = ISS
      C
            DO 160 IR = 1 , 3
            JR = MOD( IR , 3 ) + 1
            IEA = IABS( JS( JR + 3 , ISS ) )
            IF( IEA . EQ . IE ) THEN
            JJR = MOD( JR + 1 , 3 ) + 4
            IER = IABS( JS( JJR , ISS ) )
      C
            IV1 = JE( 1 , IER )
            IF( IV1 . EQ . IVV ) THEN
            ISR = JE( 3 , IER )
            ELSE
            ISR = JE( 4 , IER )
            END IF
            END IF
      C
      160   CONTINUE
      C
            IF( ISR . NE . ISI ) THEN
            ISS = ISR
            IE = IER
            GO TO 150
            END IF
      C
            ELSE
      C
            IEE = - IEE
            IV1 = JE( 1 , IEE )
            IF( IV1 . EQ . IVV ) THEN
            ISI = JE( 3 , IEE )
            ELSE
            ISI = JE( 4 , IEE )
            END IF
            ISS = ISI
            ISI = 0
            IE = IEE
      C
      170   CONTINUE
      C
            JJCOLR = JJCOLR + 1
            IICOLR( JJCOLR ) = ISS
      C
            DO 180 IR = 1 , 3
            JR = MOD( IR , 3 ) + 1
            IEA = IABS( JS( JR + 3 , ISS ) )
            IF( IEA . EQ . IE ) THEN
            JJR = MOD( JR + 1 , 3 ) + 4
            IER = IABS( JS( JJR , ISS ) )
      C
            IV1 = JE( 1 , IER )
            IF( IV1 . EQ . IVV ) THEN
            ISR = JE( 3 , IER )
            ELSE
            ISR = JE( 4 , IER )
            END IF
            END IF
      C
      180   CONTINUE
      C
            IF( ISR . NE . ISI ) THEN
            ISS = ISR
            IE = IER
            GO TO 170
            END IF
      C
            END IF
      115   CONTINUE
      C
            ATEMP( 1 , 1 ) = 0.
            ATEMP( 1 , 2 ) = 0.
            ATEMP( 1 , 3 ) = 0.
```

```
585     135   C
586     136         ATEMP( 2 , 1 ) = 0.
587     137         ATEMP( 2 , 2 ) = 0.
588     138         ATEMP( 2 , 3 ) = 0.
589     139   C
590     140         ATEMP( 3 , 1 ) = 0.
591     141         ATEMP( 3 , 2 ) = 0.
592     142         ATEMP( 3 , 3 ) = 0.
593     143   C
594     144         BTEMP( 1 , 1 ) = 0.
595     145         BTEMP( 1 , 2 ) = 0.
596     146         BTEMP( 1 , 3 ) = 0.
597     147         BTEMP( 1 , 4 ) = 0.
598     148   C
599     149         BTEMP( 2 , 1 ) = 0.
600     150         BTEMP( 2 , 2 ) = 0.
601     151         BTEMP( 2 , 3 ) = 0.
602     152         BTEMP( 2 , 4 ) = 0.
603     153   C
604     154         BTEMP( 3 , 1 ) = 0.
605     155         BTEMP( 3 , 2 ) = 0.
606     156         BTEMP( 3 , 3 ) = 0.
607     157         BTEMP( 3 , 4 ) = 0.
608     158   C
609     159         DO 225 KK = 2 , JJCOLR
610     160         ISS = IICOLR( KK )
611     161         IF( ISS . NE . 0 ) THEN
612     162         XSS = XS( 1 , ISS )
613     163         YSS = XS( 2 , ISS )
614     164   C
615     165         HYDVR = HYDV( ISS , 1 )
616     166         HYDVU = HYDV( ISS , 2 )
617     167         HYDVV = HYDV( ISS , 3 )
618     168         HYDVP = HYDV( ISS , 4 )
619     169   C
620     170         XSS2 = XSS * XSS
621     171         YSS2 = YSS * YSS
622     172         XYSS = XSS * YSS
623     173   C
624     174         ATEMP( 1 , 1 ) = ATEMP( 1 , 1 ) + 1.0
625     175         ATEMP( 1 , 2 ) = ATEMP( 1 , 2 ) + XSS
626     176         ATEMP( 1 , 3 ) = ATEMP( 1 , 3 ) + YSS
627     177   C
628     178         ATEMP( 2 , 1 ) = ATEMP( 2 , 1 ) + XSS
629     179         ATEMP( 2 , 2 ) = ATEMP( 2 , 2 ) + XSS2
630     180         ATEMP( 2 , 3 ) = ATEMP( 2 , 3 ) + XYSS
631     181   C
632     182         ATEMP( 3 , 1 ) = ATEMP( 3 , 1 ) + YSS
633     183         ATEMP( 3 , 2 ) = ATEMP( 3 , 2 ) + XYSS
634     184         ATEMP( 3 , 3 ) = ATEMP( 3 , 3 ) + YSS2
635     185   C
636     186         BTEMP( 1 , 1 ) = BTEMP( 1 , 1 ) + HYDVR
637     187         BTEMP( 1 , 2 ) = BTEMP( 1 , 2 ) + HYDVU
638     188         BTEMP( 1 , 3 ) = BTEMP( 1 , 3 ) + HYDVV
639     189         BTEMP( 1 , 4 ) = BTEMP( 1 , 4 ) + HYDVP
640     190   C
641     191         BTEMP( 2 , 1 ) = BTEMP( 2 , 1 ) + HYDVR * XSS
642     192         BTEMP( 2 , 2 ) = BTEMP( 2 , 2 ) + HYDVU * XSS
643     193         BTEMP( 2 , 3 ) = BTEMP( 2 , 3 ) + HYDVV * XSS
644     194         BTEMP( 2 , 4 ) = BTEMP( 2 , 4 ) + HYDVP * XSS
645     195   C
646     196         BTEMP( 3 , 1 ) = BTEMP( 3 , 1 ) + HYDVR * YSS
647     197         BTEMP( 3 , 2 ) = BTEMP( 3 , 2 ) + HYDVU * YSS
648     198         BTEMP( 3 , 3 ) = BTEMP( 3 , 3 ) + HYDVV * YSS
649     199         BTEMP( 3 , 4 ) = BTEMP( 3 , 4 ) + HYDVP * YSS
650     200   C
651     201         END IF
652     202   C
653     203   225   CONTINUE
654     204   C
655     205         AA( 1 , 1 ) =   ATEMP( 1 , 1 )
656     206         AA( 1 , 2 ) =   ATEMP( 1 , 2 )
657     207         AA( 1 , 3 ) =   ATEMP( 1 , 3 )
658     208   C
```

```
      AA( 2 , 1 ) =   ATEMP( 2 , 1 )
      AA( 2 , 2 ) =   ATEMP( 2 , 2 )
      AA( 2 , 3 ) =   ATEMP( 2 , 3 )
C
      AA( 3 , 1 ) =   ATEMP( 3 , 1 )
      AA( 3 , 2 ) =   ATEMP( 3 , 2 )
      AA( 3 , 3 ) =   ATEMP( 3 , 3 )
C
      BB( 1 , 1 ) =   BTEMP( 1 , 1 )
      BB( 1 , 2 ) =   BTEMP( 1 , 2 )
      BB( 1 , 3 ) =   BTEMP( 1 , 3 )
      BB( 1 , 4 ) =   BTEMP( 1 , 4 )
C
      BB( 2 , 1 ) =   BTEMP( 2 , 1 )
      BB( 2 , 2 ) =   BTEMP( 2 , 2 )
      BB( 2 , 3 ) =   BTEMP( 2 , 3 )
      BB( 2 , 4 ) =   BTEMP( 2 , 4 )
C
      BB( 3 , 1 ) =   BTEMP( 3 , 1 )
      BB( 3 , 2 ) =   BTEMP( 3 , 2 )
      BB( 3 , 3 ) =   BTEMP( 3 , 3 )
      BB( 3 , 4 ) =   BTEMP( 3 , 4 )
C
      DETERM = AA( 1 , 1 ) * ( AA( 2 , 2 ) * AA( 3 , 3 ) -
     .                         AA( 3 , 2 ) * AA( 2 , 3 ) ) +
     .         AA( 2 , 1 ) * ( AA( 1 , 3 ) * AA( 3 , 2 ) -
     .                         AA( 3 , 3 ) * AA( 1 , 2 ) ) +
     .         AA( 3 , 1 ) * ( AA( 1 , 2 ) * AA( 2 , 3 ) -
     .                         AA( 2 , 2 ) * AA( 1 , 3 ) )
C
      DTRMIN = 1. / DETERM
C
      AAA1 = AA( 2 , 3 ) * AA( 3 , 1 ) - AA( 2 , 1 ) * AA( 3 , 3 )
      AAA2 = AA( 3 , 3 ) * AA( 1 , 1 ) - AA( 3 , 1 ) * AA( 1 , 3 )
      AAA3 = AA( 1 , 3 ) * AA( 2 , 1 ) - AA( 1 , 1 ) * AA( 2 , 3 )
C
      AAA4 = AA( 2 , 1 ) * AA( 3 , 2 ) - AA( 3 , 1 ) * AA( 2 , 2 )
      AAA5 = AA( 3 , 1 ) * AA( 1 , 2 ) - AA( 1 , 1 ) * AA( 3 , 2 )
      AAA6 = AA( 1 , 1 ) * AA( 2 , 2 ) - AA( 2 , 1 ) * AA( 1 , 2 )
C
      RGRAD( IS , 1 ) = DTRMIN * ( BB( 1 , 1 ) * AAA1 +
     .                             BB( 2 , 1 ) * AAA2 +
     .                             BB( 3 , 1 ) * AAA3 )
C
      RGRAD( IS , 2 ) = DTRMIN * ( BB( 1 , 1 ) * AAA4 +
     .                             BB( 2 , 1 ) * AAA5 +
     .                             BB( 3 , 1 ) * AAA6 )
C
      UGRAD( IS , 1 ) = DTRMIN * ( BB( 1 , 2 ) * AAA1 +
     .                             BB( 2 , 2 ) * AAA2 +
     .                             BB( 3 , 2 ) * AAA3 )
C
      UGRAD( IS , 2 ) = DTRMIN * ( BB( 1 , 2 ) * AAA4 +
     .                             BB( 2 , 2 ) * AAA5 +
     .                             BB( 3 , 2 ) * AAA6 )
C
      VGRAD( IS , 1 ) = DTRMIN * ( BB( 1 , 3 ) * AAA1 +
     .                             BB( 2 , 3 ) * AAA2 +
     .                             BB( 3 , 3 ) * AAA3 )
C
      VGRAD( IS , 2 ) = DTRMIN * ( BB( 1 , 3 ) * AAA4 +
     .                             BB( 2 , 3 ) * AAA5 +
     .                             BB( 3 , 3 ) * AAA6 )
C
      PGRAD( IS , 1 ) = DTRMIN * ( BB( 1 , 4 ) * AAA1 +
     .                             BB( 2 , 4 ) * AAA2 +
     .                             BB( 3 , 4 ) * AAA3 )
C
      PGRAD( IS , 2 ) = DTRMIN * ( BB( 1 , 4 ) * AAA4 +
     .                             BB( 2 , 4 ) * AAA5 +
     .                             BB( 3 , 4 ) * AAA6 )
C
  105 CONTINUE
C
```

```
      NS1 = NS2 + 1
      NS2 = NS2 + NOFVES( INS + 1 )
   90 CONTINUE
C
C=======================================================================
C
C --- CALL THE MONOTONICITY LIMITER ------------------------------
C
      CALL MONOTN
C
C=======================================================================
C
C
C --- EXIT POINT FROM SUBROUTINE ---------------------------------------
C
C     ------
      RETURN
C     ------
C
C     ---
      END
```



```
      SUBROUTINE GRADNT
C
C-----------------------------------------------------------------I
C                                                                 I
C     GRADNT COMPUTE THE GRADIENT FOR SECOND ORDER CALCULATION    I
C            USE THE INFORMATION IN THE THREE NEIGHBOURING        I
C            TRIANGLES THAT HAVE COMMON EDGES TO COMPUTE          I
C            GRADIENT APPLYING LEAST SQUARE TECHNIQUE             I
C                                                                 I
C-----------------------------------------------------------------I
C
      include     'cmsh00.h'
      include     'chyd00.h'
      include     'cint00.h'
      include     'cphs10.h'
      include     'cphs20.h'
C
C=======================================================================
C
      REAL RRMIDL(MBP),PPMIDL(MBP),UUMIDL(MBP),VVMIDL(MBP)
      REAL RIGRAD(MBP),PIGRAD(MBP),UIGRAD(MBP),VIGRAD(MBP)
      REAL RJGRAD(MBP),PJGRAD(MBP),UJGRAD(MBP),VJGRAD(MBP)
      REAL RMAX(MBP),PMAX(MBP),UMAX(MBP),VMAX(MBP)
      REAL RMIN(MBP),PMIN(MBP),UMIN(MBP),VMIN(MBP)
      REAL RLEFTT(MBP),ULEFTT(MBP),VLEFTT(MBP),PLEFTT(MBP)
      REAL RRIGHT(MBP),URIGHT(MBP),VRIGHT(MBP),PRIGHT(MBP)
      REAL ROR(3),UOR(3),VOR(3),POR(3)
      REAL ROL(3),UOL(3),VOL(3),POL(3)
      REAL AA(3,3),BB(3,4),B(3),INDX(3),ATEMP(3,3,3),BTEMP(3,4,3)
      REAL AA0(3,3),BB0(3,4)
C
C=======================================================================
C
C --- BEGIN LOOP OVER ALL CELLS IN THE DOMAIN --------------------------
C
      NS1 = 1
      NS2 = NOFVES( 1 )
      DO 90 INS = 1 , NVEES
C
C --- FETCH HYDRO QUANTITIES -------------------------------------------
C
      DO 105 IS = NS1 , NS2
C
       XSM = XS( 1 , IS )
       YSM = XS( 2 , IS )
       XSM2 = XSM * XSM
       YSM2 = YSM * YSM
       XYSM = XSM * YSM
C
       AA0( 1 , 1 ) = 1.0
```

```
804      51          AA0( 1 , 2 ) = XSM                                      804
805      52          AA0( 1 , 3 ) = YSM                                      805
806      53    C                                                             806
807      54          AA0( 2 , 1 ) = XSM                                      807
808      55          AA0( 2 , 2 ) = XSM2                                     808
809      56          AA0( 2 , 3 ) = XYSM                                     809
810      57    C                                                             810
811      58          AA0( 3 , 1 ) = YSM                                      811
812      59          AA0( 3 , 2 ) = XYSM                                     812
813      60          AA0( 3 , 3 ) = YSM2                                     813
814      61    C                                                             814
815      62          BB1 = HYDV( IS , 1 )                                    815
816      63          BB2 = HYDV( IS , 2 )                                    816
817      64          BB3 = HYDV( IS , 3 )                                    817
818      65          BB4 = HYDV( IS , 4 )                                    818
819      66    C                                                             819
820      67          BB1X = BB1 * XSM                                        820
821      68          BB2X = BB2 * XSM                                        821
822      69          BB3X = BB3 * XSM                                        822
823      70          BB4X = BB4 * XSM                                        823
824      71    C                                                             824
825      72          BB1Y = BB1 * YSM                                        825
826      73          BB2Y = BB2 * YSM                                        826
827      74          BB3Y = BB3 * YSM                                        827
828      75          BB4Y = BB4 * YSM                                        828
829      76    C                                                             829
830      77          BB0( 1 , 1 ) = BB1                                      830
831      78          BB0( 1 , 2 ) = BB2                                      831
832      79          BB0( 1 , 3 ) = BB3                                      832
833      80          BB0( 1 , 4 ) = BB4                                      833
834      81    C                                                             834
835      82          BB0( 2 , 1 ) = BB1X                                     835
836      83          BB0( 2 , 2 ) = BB2X                                     836
837      84          BB0( 2 , 3 ) = BB3X                                     837
838      85          BB0( 2 , 4 ) = BB4X                                     838
839      86    C                                                             839
840      87          BB0( 3 , 1 ) = BB1Y                                     840
841      88          BB0( 3 , 2 ) = BB2Y                                     841
842      89          BB0( 3 , 3 ) = BB3Y                                     842
843      90          BB0( 3 , 4 ) = BB4Y                                     843
844      91    C                                                             844
845      92          DO 115 IK = 1 , 3                                       845
846      93          IE = JS( IK + 3 , IS )                                  846
847      94          IF( IE . GT . 0 ) THEN                                  847
848      95          ISS = JE( 4 , IE )                                      848
849      96          ELSE                                                    849
850      97          ISS = JE( 3 , - IE )                                    850
851      98          END IF                                                  851
852      99    C                                                             852
853     100          IF( ISS . NE . 0 ) THEN                                 853
854     101          XSS = XS( 1 , ISS )                                     854
855     102          YSS = XS( 2 , ISS )                                     855
856     103    C                                                             856
857     104          HYDVR = HYDV( ISS , 1 )                                 857
858     105          HYDVU = HYDV( ISS , 2 )                                 858
859     106          HYDVV = HYDV( ISS , 3 )                                 859
860     107          HYDVP = HYDV( ISS , 4 )                                 860
861     108    C                                                             861
862     109          ELSE                                                    862
863     110    C                                                             863
864     111          IE = IABS( IE )                                         864
865     112          HYDVR = BB1                                             865
866     113          HYDVU = BB2                                             866
867     114          HYDVV = BB3                                             867
868     115          HYDVP = BB4                                             868
869     116    C                                                             869
870     117          XSS = 2. * XMIDL( IE ) - XSM                            870
871     118          YSS = 2. * YMIDL( IE ) - YSM                            871
872     119    C                                                             872
873     120    C      IJE5 = JE( 5 , IE )                                     873
874     121    C      IF( IJE5 . EQ . 6 . OR . IJE5 . EQ . 5 ) THEN           874
875     122    C      UUVV =   - ( BB2 * XN( IE ) + BB3 * YN( IE ) )          875
876     123    C      VVUU =     - BB2 * YN( IE ) + BB3 * XN( IE )            876
877     124    C      HYDVU = UUVV * XN( IE ) - VVUU * YN( IE )               877
```

```
878     125   C       HYDVV = UUVV * YN( IE ) + VVUU * XN( IE )
879     126   C
880     127   C       ELSEIF( IJE5 . EQ . 8 ) THEN
881     128   C       HYDVR =   RIN
882     129   C       HYDVU =   UIN
883     130   C       HYDVV =   VIN
884     131   C       HYDVP =   PIN
885     132   C
886     133   C       END IF
887     134           END IF
888     135   C
889     136           XSS2 = XSS * XSS
890     137           YSS2 = YSS * YSS
891     138           XYSS = XSS * YSS
892     139   C
893     140           ATEMP( 1 , 1 , IK ) = 1.0
894     141           ATEMP( 1 , 2 , IK ) = XSS
895     142           ATEMP( 1 , 3 , IK ) = YSS
896     143   C
897     144           ATEMP( 2 , 1 , IK ) = XSS
898     145           ATEMP( 2 , 2 , IK ) = XSS2
899     146           ATEMP( 2 , 3 , IK ) = XYSS
900     147   C
901     148           ATEMP( 3 , 1 , IK ) = YSS
902     149           ATEMP( 3 , 2 , IK ) = XYSS
903     150           ATEMP( 3 , 3 , IK ) = YSS2
904     151   C
905     152           BTEMP( 1 , 1 , IK ) = HYDVR
906     153           BTEMP( 1 , 2 , IK ) = HYDVU
907     154           BTEMP( 1 , 3 , IK ) = HYDVV
908     155           BTEMP( 1 , 4 , IK ) = HYDVP
909     156   C
910     157           BTEMP( 2 , 1 , IK ) = HYDVR * XSS
911     158           BTEMP( 2 , 2 , IK ) = HYDVU * XSS
912     159           BTEMP( 2 , 3 , IK ) = HYDVV * XSS
913     160           BTEMP( 2 , 4 , IK ) = HYDVP * XSS
914     161   C
915     162           BTEMP( 3 , 1 , IK ) = HYDVR * YSS
916     163           BTEMP( 3 , 2 , IK ) = HYDVU * YSS
917     164           BTEMP( 3 , 3 , IK ) = HYDVV * YSS
918     165           BTEMP( 3 , 4 , IK ) = HYDVP * YSS
919     166   C
920     167    115  CONTINUE
921     168   C
922     169           AA( 1 , 1 ) = AA0( 1 , 1 ) * 3.  + ATEMP( 1 , 1 , 1 ) +
923     170          .                  ATEMP( 1 , 1 , 2 ) + ATEMP( 1 , 1 , 3 )
924     171           AA( 1 , 2 ) = AA0( 1 , 2 ) * 3.  + ATEMP( 1 , 2 , 1 ) +
925     172          .                  ATEMP( 1 , 2 , 2 ) + ATEMP( 1 , 2 , 3 )
926     173           AA( 1 , 3 ) = AA0( 1 , 3 ) * 3.  + ATEMP( 1 , 3 , 1 ) +
927     174          .                  ATEMP( 1 , 3 , 2 ) + ATEMP( 1 , 3 , 3 )
928     175   C
929     176           AA( 2 , 1 ) = AA0( 2 , 1 ) * 3.  + ATEMP( 2 , 1 , 1 ) +
930     177          .                  ATEMP( 2 , 1 , 2 ) + ATEMP( 2 , 1 , 3 )
931     178           AA( 2 , 2 ) = AA0( 2 , 2 ) * 3.  + ATEMP( 2 , 2 , 1 ) +
932     179          .                  ATEMP( 2 , 2 , 2 ) + ATEMP( 2 , 2 , 3 )
933     180           AA( 2 , 3 ) = AA0( 2 , 3 ) * 3.  + ATEMP( 2 , 3 , 1 ) +
934     181          .                  ATEMP( 2 , 3 , 2 ) + ATEMP( 2 , 3 , 3 )
935     182   C
936     183           AA( 3 , 1 ) = AA0( 3 , 1 ) * 3.  + ATEMP( 3 , 1 , 1 ) +
937     184          .                  ATEMP( 3 , 1 , 2 ) + ATEMP( 3 , 1 , 3 )
938     185           AA( 3 , 2 ) = AA0( 3 , 2 ) * 3.  + ATEMP( 3 , 2 , 1 ) +
939     186          .                  ATEMP( 3 , 2 , 2 ) + ATEMP( 3 , 2 , 3 )
940     187           AA( 3 , 3 ) = AA0( 3 , 3 ) * 3.  + ATEMP( 3 , 3 , 1 ) +
941     188          .                  ATEMP( 3 , 3 , 2 ) + ATEMP( 3 , 3 , 3 )
942     189   C
943     190           BB( 1 , 1 ) = BB0( 1 , 1 ) * 3.  + BTEMP( 1 , 1 , 1 ) +
944     191          .                  BTEMP( 1 , 1 , 2 ) + BTEMP( 1 , 1 , 3 )
945     192           BB( 1 , 2 ) = BB0( 1 , 2 ) * 3.  + BTEMP( 1 , 2 , 1 ) +
946     193          .                  BTEMP( 1 , 2 , 2 ) + BTEMP( 1 , 2 , 3 )
947     194           BB( 1 , 3 ) = BB0( 1 , 3 ) * 3.  + BTEMP( 1 , 3 , 1 ) +
948     195          .                  BTEMP( 1 , 3 , 2 ) + BTEMP( 1 , 3 , 3 )
949     196           BB( 1 , 4 ) = BB0( 1 , 4 ) * 3.  + BTEMP( 1 , 4 , 1 ) +
950     197          .                  BTEMP( 1 , 4 , 2 ) + BTEMP( 1 , 4 , 3 )
951     198   C
```

```
      BB( 2 , 1 ) = BBO( 2 , 1 )  * 3. + BTEMP( 2 , 1 , 1 ) +
     .              BTEMP( 2 , 1 , 2 ) + BTEMP( 2 , 1 , 3 )
      BB( 2 , 2 ) = BBO( 2 , 2 )  * 3. + BTEMP( 2 , 2 , 1 ) +
     .              BTEMP( 2 , 2 , 2 ) + BTEMP( 2 , 2 , 3 )
      BB( 2 , 3 ) = BBO( 2 , 3 )  * 3. + BTEMP( 2 , 3 , 1 ) +
     .              BTEMP( 2 , 3 , 2 ) + BTEMP( 2 , 3 , 3 )
      BB( 2 , 4 ) = BBO( 2 , 4 )  * 3. + BTEMP( 2 , 4 , 1 ) +
     .              BTEMP( 2 , 4 , 2 ) + BTEMP( 2 , 4 , 3 )
C
      BB( 3 , 1 ) = BBO( 3 , 1 )  * 3. + BTEMP( 3 , 1 , 1 ) +
     .              BTEMP( 3 , 1 , 2 ) + BTEMP( 3 , 1 , 3 )
      BB( 3 , 2 ) = BBO( 3 , 2 )  * 3. + BTEMP( 3 , 2 , 1 ) +
     .              BTEMP( 3 , 2 , 2 ) + BTEMP( 3 , 2 , 3 )
      BB( 3 , 3 ) = BBO( 3 , 3 )  * 3. + BTEMP( 3 , 3 , 1 ) +
     .              BTEMP( 3 , 3 , 2 ) + BTEMP( 3 , 3 , 3 )
      BB( 3 , 4 ) = BBO( 3 , 4 )  * 3. + BTEMP( 3 , 4 , 1 ) +
     .              BTEMP( 3 , 4 , 2 ) + BTEMP( 3 , 4 , 3 )
C
      DETERM = AA( 1 , 1 ) * ( AA( 2 , 2 ) * AA( 3 , 3 ) -
     .                         AA( 3 , 2 ) * AA( 2 , 3 ) ) +
     .         AA( 2 , 1 ) * ( AA( 1 , 3 ) * AA( 3 , 2 ) -
     .                         AA( 3 , 3 ) * AA( 1 , 2 ) ) +
     .         AA( 3 , 1 ) * ( AA( 1 , 2 ) * AA( 2 , 3 ) -
     .                         AA( 2 , 2 ) * AA( 1 , 3 ) )
C
      DTRMIN = 1. / DETERM
C
      AAA1 = AA( 2 , 3 ) * AA( 3 , 1 ) - AA( 2 , 1 ) * AA( 3 , 3 )
      AAA2 = AA( 3 , 3 ) * AA( 1 , 1 ) - AA( 3 , 1 ) * AA( 1 , 3 )
      AAA3 = AA( 1 , 3 ) * AA( 2 , 1 ) - AA( 1 , 1 ) * AA( 2 , 3 )
C
      AAA4 = AA( 2 , 1 ) * AA( 3 , 2 ) - AA( 3 , 1 ) * AA( 2 , 2 )
      AAA5 = AA( 3 , 1 ) * AA( 1 , 2 ) - AA( 1 , 1 ) * AA( 3 , 2 )
      AAA6 = AA( 1 , 1 ) * AA( 2 , 2 ) - AA( 2 , 1 ) * AA( 1 , 2 )
C
      RGRAD( IS , 1 ) = DTRMIN * ( BB( 1 , 1 ) * AAA1 +
     .                             BB( 2 , 1 ) * AAA2 +
     .                             BB( 3 , 1 ) * AAA3 )
C
      RGRAD( IS , 2 ) = DTRMIN * ( BB( 1 , 1 ) * AAA4 +
     .                             BB( 2 , 1 ) * AAA5 +
     .                             BB( 3 , 1 ) * AAA6 )
C
      UGRAD( IS , 1 ) = DTRMIN * ( BB( 1 , 2 ) * AAA1 +
     .                             BB( 2 , 2 ) * AAA2 +
     .                             BB( 3 , 2 ) * AAA3 )
C
      UGRAD( IS , 2 ) = DTRMIN * ( BB( 1 , 2 ) * AAA4 +
     .                             BB( 2 , 2 ) * AAA5 +
     .                             BB( 3 , 2 ) * AAA6 )
C
      VGRAD( IS , 1 ) = DTRMIN * ( BB( 1 , 3 ) * AAA1 +
     .                             BB( 2 , 3 ) * AAA2 +
     .                             BB( 3 , 3 ) * AAA3 )
C
      VGRAD( IS , 2 ) = DTRMIN * ( BB( 1 , 3 ) * AAA4 +
     .                             BB( 2 , 3 ) * AAA5 +
     .                             BB( 3 , 3 ) * AAA6 )
C
      PGRAD( IS , 1 ) = DTRMIN * ( BB( 1 , 4 ) * AAA1 +
     .                             BB( 2 , 4 ) * AAA2 +
     .                             BB( 3 , 4 ) * AAA3 )
C
      PGRAD( IS , 2 ) = DTRMIN * ( BB( 1 , 4 ) * AAA4 +
     .                             BB( 2 , 4 ) * AAA5 +
     .                             BB( 3 , 4 ) * AAA6 )
C
C
  105 CONTINUE
C
      NS1 = NS2 + 1
      NS2 = NS2 + NOFVES( INS + 1 )
   90 CONTINUE
C
C=======================================================================
```

```
1026    273   C                                                                1026
1027    274   C --- CALL THE MONOTONICITY LIMITER ----------------------------- 1027
1028    275   C                                                                1028
1029    276         CALL MONOTN                                                1029
1030    277   C                                                                1030
1031    278   C=================================================================1031
1032    279   C                                                                1032
1033    280   C                                                                1033
1034    281   C --- EXIT POINT FROM SUBROUTINE ------------------------------- 1034
1035    282   C                                                                1035
1036    283   C     ------                                                     1036
1037    284         RETURN                                                     1037
1038    285   C     ------                                                     1038
1039    286   C                                                                1039
1040    287   C     ---                                                        1040
1041    288         END                                                        1041
```



```
1042      1         SUBROUTINE MONOTN                                          1042
1043      2   C                                                                1043
1044      3   C-----------------------------------------------------------------I1044
1045      4   C                                                                I1045
1046      5   C        MONOTN LIMIT THE GRADIENTS SO THAT NO NEW EXTREMUM ARE  I1046
1047      6   C        CREATED ARTIFICIALY DURING THE PROJECTION PROCESS       I1047
1048      7   C                                                                I1048
1049      8   C-----------------------------------------------------------------I1049
1050      9   C                                                                1050
1051     10         include     'cmsh00.h'                                     1051
1052     11         include     'chyd00.h'                                     1052
1053     12         include     'cint00.h'                                     1053
1054     13         include     'cphs10.h'                                     1054
1055     14         include     'cphs20.h'                                     1055
1056     15   C                                                                1056
1057     16   C=================================================================1057
1058     17   C                                                                1058
1059     18         REAL RRMIDL(MBP),PPMIDL(MBP),UUMIDL(MBP),VVMIDL(MBP)       1059
1060     19         REAL RIGRAD(MBP),PIGRAD(MBP),UIGRAD(MBP),VIGRAD(MBP)       1060
1061     20         REAL RJGRAD(MBP),PJGRAD(MBP),UJGRAD(MBP),VJGRAD(MBP)       1061
1062     21         REAL RMAX(MBP),PMAX(MBP),UMAX(MBP),VMAX(MBP)               1062
1063     22         REAL RMIN(MBP),PMIN(MBP),UMIN(MBP),VMIN(MBP)               1063
1064     23         REAL RLEFTT(MBP),ULEFTT(MBP),VLEFTT(MBP),PLEFTT(MBP)       1064
1065     24         REAL RRIGHT(MBP),URIGHT(MBP),VRIGHT(MBP),PRIGHT(MBP)       1065
1066     25         REAL ROR(3),UOR(3),VOR(3),POR(3)                           1066
1067     26         REAL ROL(3),UOL(3),VOL(3),POL(3)                           1067
1068     27         REAL AA(3,3),BB(3,4),B(3),INDX(3),ATEMP(3,3,3),BTEMP(3,4,3)1068
1069     28         REAL AA0(3,3),BB0(3,4)                                     1069
1070     29   C                                                                1070
1071     30   C=================================================================1071
1072     31   C                                                                1072
1073     32   C --- LIMITER FOR GRADIENTS BEGINS ------------------------------ 1073
1074     33   C     USED TO PREVENT NEW MINIMA AND MAXIMA                      1074
1075     34   C     AT PROJECTED INTERFACE VALUES.                             1075
1076     35   C                                                                1076
1077     36         NS1 = 1                                                    1077
1078     37         NS2 = NOFVES( 1 )                                          1078
1079     38         DO 80 INS = 1 , NVEES                                      1079
1080     39   C                                                                1080
1081     40         DO 150 IS = NS1 , NS2                                      1081
1082     41          KS = IS - NS1 + 1                                         1082
1083     42   C                                                                1083
1084     43   C --- FIRST TRIANGLE EDGE --------------------------------------- 1084
1085     44   C                                                                1085
1086     45          IE = IABS( JS( 4 , IS ) )                                 1086
1087     46   C                                                                1087
1088     47          ISL = JE( 3 , IE )                                        1088
1089     48          ISR = JE( 4 , IE )                                        1089
1090     49   C                                                                1090
1091     50          RROL = HYDV( ISL , 1 )                                    1091
1092     51          UUOL = HYDV( ISL , 2 )                                    1092
1093     52          VVOL = HYDV( ISL , 3 )                                    1093
1094     53          PPOL = HYOV( ISL , 4 )                                    1094
1095     54   C                                                                1095
1096     55          IJE5 = JE( 5 , IE )                                       1096
```

```
1097      56          IF( IJE5 . EQ . 0 ) THEN                                    1097
1098      57    C                                                                 1098
1099      58          RROR = HYDV( ISR , 1 )                                      1099
1100      59          UUOR = HYDV( ISR , 2 )                                      1100
1101      60          VVOR = HYDV( ISR , 3 )                                      1101
1102      61          PPOR = HYDV( ISR , 4 )                                      1102
1103      62    C                                                                 1103
1104      63          ELSE                                                        1104
1105      64    C                                                                 1105
1106      65          RROR = RROL                                                 1106
1107      66          UUOR = UUOL                                                 1107
1108      67          VVOR = VVOL                                                 1108
1109      68          PPOR = PPOL                                                 1109
1110      69    C                                                                 1110
1111      70    C      IF( IJE5 . EQ . 6 . OR . IJE5 . EQ . 5 ) THEN              1111
1112      71    C      UUVV =   - ( UUOL * XN( IE ) + VVOL * YN( IE ) )           1112
1113      72    C      VVUU =     - UUOL * YN( IE ) + VVOL * XN( IE )             1113
1114      73    C      UUOR = UUVV * XN( IE ) - VVUU * YN( IE )                   1114
1115      74    C      VVOR = UUVV * YN( IE ) + VVUU * XN( IE )                   1115
1116      75    C                                                                 1116
1117      76    C      ELSE IF( IJE5 . EQ . 8 ) THEN                              1117
1118      77    C      RROR =   RIN                                               1118
1119      78    C      UUOR =   UIN                                               1119
1120      79    C      VVOR =   VIN                                               1120
1121      80    C      PPOR =   PIN                                               1121
1122      81    C      END IF                                                     1122
1123      82    C                                                                 1123
1124      83          END IF                                                      1124
1125      84    C                                                                 1125
1126      85          ROL( 1 ) = RROL                                             1126
1127      86          UOL( 1 ) = UUOL                                             1127
1128      87          VOL( 1 ) = VVOL                                             1128
1129      88          POL( 1 ) = PPOL                                             1129
1130      89    C                                                                 1130
1131      90          ROR( 1 ) = RROR                                             1131
1132      91          UOR( 1 ) = UUOR                                             1132
1133      92          VOR( 1 ) = VVOR                                             1133
1134      93          POR( 1 ) = PPOR                                             1134
1135      94    C                                                                 1135
1136      95    C --- SECOND TRIANGLE EDGE ----------------------------------------1136
1137      96    C                                                                 1137
1138      97          IE = IABS( JS( 5 , IS ) )                                   1138
1139      98    C                                                                 1139
1140      99          ISL = JE( 3 , IE )                                          1140
1141     100          ISR = JE( 4 , IE )                                          1141
1142     101    C                                                                 1142
1143     102          RROL = HYDV( ISL , 1 )                                      1143
1144     103          UUOL = HYDV( ISL , 2 )                                      1144
1145     104          VVOL = HYDV( ISL , 3 )                                      1145
1146     105          PPOL = HYDV( ISL , 4 )                                      1146
1147     106    C                                                                 1147
1148     107          IJE5 = JE( 5 , IE )                                         1148
1149     108          IF( IJE5 . EQ . 0 ) THEN                                    1149
1150     109    C                                                                 1150
1151     110          RROR = HYDV( ISR , 1 )                                      1151
1152     111          UUOR = HYDV( ISR , 2 )                                      1152
1153     112          VVOR = HYDV( ISR , 3 )                                      1153
1154     113          PPOR = HYDV( ISR , 4 )                                      1154
1155     114    C                                                                 1155
1156     115          ELSE                                                        1156
1157     116    C                                                                 1157
1158     117          RROR = RROL                                                 1158
1159     118          UUOR = UUOL                                                 1159
1160     119          VVOR = VVOL                                                 1160
1161     120          PPOR = PPOL                                                 1161
1162     121    C                                                                 1162
1163     122    C      IF( IJE5 . EQ . 6 . OR . IJE5 . EQ . 5 ) THEN              1163
1164     123    C      UUVV =   - ( UUOL * XN( IE ) + VVOL * YN( IE ) )           1164
1165     124    C      VVUU =     - UUOL * YN( IE ) + VVOL * XN( IE )             1165
1166     125    C      UUOR = UUVV * XN( IE ) - VVUU * YN( IE )                   1166
1167     126    C      VVOR = UUVV * YN( IE ) + VVUU * XN( IE )                   1167
1168     127    C                                                                 1168
1169     128    C      ELSE IF( IJE5 . EQ . 8 ) THEN                              1169
1170     129    C      RROR =   RIN                                               1170
```

```
1171     130   C       UUOR =   UIN
1172     131   C       VVOR =   VIN
1173     132   C       PPOR =   PIN
1174     133   C       END IF
1175     134   C
1176     135           END IF
1177     136   C
1178     137           ROL( 2 ) = RROL
1179     138           UOL( 2 ) = UUOL
1180     139           VOL( 2 ) = VVOL
1181     140           POL( 2 ) = PPOL
1182     141   C
1183     142           ROR( 2 ) = RROR
1184     143           UOR( 2 ) = UUOR
1185     144           VOR( 2 ) = VVOR
1186     145           POR( 2 ) = PPOR
1187     146   C
1188     147   C --- THIRD TRIANGLE EDGE ----------------------------------------------
1189     148   C
1190     149           IE = IABS( JS( 6 , IS ) )
1191     150   C
1192     151           ISL = JE( 3 , IE )
1193     152           ISR = JE( 4 , IE )
1194     153           RROL = HYDV( ISL , 1 )
1195     154           UUOL = HYDV( ISL , 2 )
1196     155           VVOL = HYDV( ISL , 3 )
1197     156           PPOL = HYDV( ISL , 4 )
1198     157   C
1199     158           IJE5 = JE( 5 , IE )
1200     159           IF( IJE5 . EQ . 0 ) THEN
1201     160   C
1202     161           RROR = HYDV( ISR , 1 )
1203     162           UUOR = HYDV( ISR , 2 )
1204     163           VVOR = HYDV( ISR , 3 )
1205     164           PPOR = HYDV( ISR , 4 )
1206     165   C
1207     166           ELSE
1208     167   C
1209     168           RROR = RROL
1210     169           UUOR = UUOL
1211     170           VVOR = VVOL
1212     171           PPOR = PPOL
1213     172   C
1214     173   C       IF( IJE5 . EQ . 6 . OR . IJE5 . EQ . 5 ) THEN
1215     174   C       UUVV =   - ( UUOL * XN( IE ) + VVOL * YN( IE ) )
1216     175   C       VVUU =     - UUOL * YN( IE ) + VVOL * XN( IE )
1217     176   C       UUOR = UUVV * XN( IE ) - VVUU * YN( IE )
1218     177   C       VVOR = UUVV * YN( IE ) + VVUU * XN( IE )
1219     178   C
1220     179   C       ELSE IF( IJE5 . EQ . 8 ) THEN
1221     180   C       RROR =   RIN
1222     181   C       UUOR =   UIN
1223     182   C       VVOR =   VIN
1224     183   C       PPOR =   PIN
1225     184   C       END IF
1226     185   C
1227     186           END IF
1228     187   C
1229     188           ROL( 3 ) = RROL
1230     189           UOL( 3 ) = UUOL
1231     190           VOL( 3 ) = VVOL
1232     191           POL( 3 ) = PPOL
1233     192   C
1234     193           ROR( 3 ) = RROR
1235     194           UOR( 3 ) = UUOR
1236     195           VOR( 3 ) = VVOR
1237     196           POR( 3 ) = PPOR
1238     197   C
1239     198   C --- FIND MAXIMA IN THE NEIGHBORHOOD OF A TRIANGLE --------------------
1240     199   C
1241     200           RMAX( KS ) = AMAX1( ROL( 1 ) , ROL( 2 ) , ROL( 3 ) ,
1242     201                               ROR( 1 ) , ROR( 2 ) , ROR( 3 ) )
1243     202           UMAX( KS ) = AMAX1( UOL( 1 ) , UOL( 2 ) , UOL( 3 ) ,
1244     203          .                    UOR( 1 ) , UOR( 2 ) , UOR( 3 ) )
```

```
      VMAX( KS ) = AMAX1( VOL( 1 ) , VOL( 2 ) , VOL( 3 ) ,
     .                    VOR( 1 ) , VOR( 2 ) , VOR( 3 ) )
      PMAX( KS ) = AMAX1( POL( 1 ) , POL( 2 ) , POL( 3 ) ,
     .                    POR( 1 ) , POR( 2 ) , POR( 3 ) )
C
C --- FIND MINIMA IN THE NEIGHBORHOOD OF A TRIANGLE --------------------
C
      RMIN( KS ) = AMIN1( ROL( 1 ) , ROL( 2 ) , ROL( 3 ) ,
     .                    ROR( 1 ) , ROR( 2 ) , ROR( 3 ) )
      UMIN( KS ) = AMIN1( UOL( 1 ) , UOL( 2 ) , UOL( 3 ) ,
     .                    UOR( 1 ) , UOR( 2 ) , UOR( 3 ) )
      VMIN( KS ) = AMIN1( VOL( 1 ) , VOL( 2 ) , VOL( 3 ) ,
     .                    VOR( 1 ) , VOR( 2 ) , VOR( 3 ) )
      PMIN( KS ) = AMIN1( POL( 1 ) , POL( 2 ) , POL( 3 ) ,
     .                    POR( 1 ) , POR( 2 ) , POR( 3 ) )
C
  150 CONTINUE
C
C --- FIND DIFFERENCES BETWEEN EXTREMA AND THE TRIANGLE CENTERED -------
C     QUANTITIES
C
      DO 180 IS = NS1 , NS2
         KS = IS - NS1 + 1
C
         RRR( KS ) = RMAX( KS ) - HYDV( IS , 1 )
         RRL( KS ) = RMIN( KS ) - HYDV( IS , 1 )
         UUR( KS ) = UMAX( KS ) - HYDV( IS , 2 )
         UUL( KS ) = UMIN( KS ) - HYDV( IS , 2 )
         VVR( KS ) = VMAX( KS ) - HYDV( IS , 3 )
         VVL( KS ) = VMIN( KS ) - HYDV( IS , 3 )
         PPR( KS ) = PMAX( KS ) - HYDV( IS , 4 )
         PPL( KS ) = PMIN( KS ) - HYDV( IS , 4 )
C
  180 CONTINUE
C
C --- FIND THE PROJECTED INCRAMENTS FOR INTERFACE BASED QUANTITIES -----
C
      DO 170 IS = NS1 , NS2
         KS = IS - NS1 + 1
C
C --- FIRST TRIANGLE EDGE ----------------------------------------------
C
         IE = IABS( JS( 4 , IS ) )
C
         ISL = JE( 3 , IE )
         ISR = JE( 4 , IE )
C
         XML = XMIDL( IE ) - XS( 1 , ISL )
         YML = YMIDL( IE ) - XS( 2 , ISL )
C
         RROL = 1.E-12 +
     .          RGRAD( ISL , 1 ) * XML + RGRAD( ISL , 2 ) * YML
         UUOL = 1.E-12 +
     .          UGRAD( ISL , 1 ) * XML + UGRAD( ISL , 2 ) * YML
         VVOL = 1.E-12 +
     .          VGRAD( ISL , 1 ) * XML + VGRAD( ISL , 2 ) * YML
         PPOL = 1.E-12 +
     .          PGRAD( ISL , 1 ) * XML + PGRAD( ISL , 2 ) * YML
C
         IJE5 = JE( 5 , IE )
         IF( IJE5 . EQ . 0 ) THEN
C
         XMR = XMIDL( IE ) - XS( 1 , ISR )
         YMR = YMIDL( IE ) - XS( 2 , ISR )
C
         RROR = 1.E-12 +
     .          RGRAD( ISR , 1 ) * XMR + RGRAD( ISR , 2 ) * YMR
         UUOR = 1.E-12 +
     .          UGRAD( ISR , 1 ) * XMR + UGRAD( ISR , 2 ) * YMR
         VVOR = 1.E-12 +
     .          VGRAD( ISR , 1 ) * XMR + VGRAD( ISR , 2 ) * YMR
         PPOR = 1.E-12 +
     .          PGRAD( ISR , 1 ) * XMR + PGRAD( ISR , 2 ) * YMR
C
```

```
1319     278          ELSE                                                                1319
1320     279    C                                                                         1320
1321     280          RROR = RROL                                                         1321
1322     281          UUOR = UUOL                                                         1322
1323     282          VVOR = VVOL                                                         1323
1324     283          PPOR = PPOL                                                         1324
1325     284    C                                                                         1325
1326     285          END IF                                                              1326
1327     286    C                                                                         1327
1328     287          ROL( 1 ) = 1. / RROL                                                1328
1329     288          UOL( 1 ) = 1. / UUOL                                                1329
1330     289          VOL( 1 ) = 1. / VVOL                                                1330
1331     290          POL( 1 ) = 1. / PPOL                                                1331
1332     291    C                                                                         1332
1333     292          ROR( 1 ) = 1. / RROR                                                1333
1334     293          UOR( 1 ) = 1. / UUOR                                                1334
1335     294          VOR( 1 ) = 1. / VVOR                                                1335
1336     295          POR( 1 ) = 1. / PPOR                                                1336
1337     296    C                                                                         1337
1338     297    C --- SECOND TRIANGLE EDGE ----------------------------------------------1338
1339     298    C                                                                         1339
1340     299          IE = IABS( JS( 5 , IS ) )                                           1340
1341     300    C                                                                         1341
1342     301          ISL = JE( 3 , IE )                                                  1342
1343     302          ISR = JE( 4 , IE )                                                  1343
1344     303    C                                                                         1344
1345     304          XML = XMIDL( IE ) - XS( 1 , ISL )                                   1345
1346     305          YML = YMIDL( IE ) - XS( 2 , ISL )                                   1346
1347     306    C                                                                         1347
1348     307          RROL = 1.E-12 +                                                     1348
1349     308         .          RGRAD( ISL , 1 ) * XML + RGRAD( ISL , 2 ) * YML          1349
1350     309          UUOL = 1.E-12 +                                                     1350
1351     310         .          UGRAD( ISL , 1 ) * XML + UGRAD( ISL , 2 ) * YML          1351
1352     311          VVOL = 1.E-12 +                                                     1352
1353     312         .          VGRAD( ISL , 1 ) * XML + VGRAD( ISL , 2 ) * YML          1353
1354     313          PPOL = 1.E-12 +                                                     1354
1355     314         .          PGRAD( ISL , 1 ) * XML + PGRAD( ISL , 2 ) * YML          1355
1356     315    C                                                                         1356
1357     316          IJE5 = JE( 5 , IE )                                                 1357
1358     317          IF( IJE5 . EQ . 0 ) THEN                                            1358
1359     318    C                                                                         1359
1360     319          XMR = XMIDL( IE ) - XS( 1 , ISR )                                   1360
1361     320          YMR = YMIDL( IE ) - XS( 2 , ISR )                                   1361
1362     321    C                                                                         1362
1363     322          RROR = 1.E-12 +                                                     1363
1364     323         .          RGRAD( ISR , 1 ) * XMR + RGRAD( ISR , 2 ) * YMR          1364
1365     324          UUOR = 1.E-12 +                                                     1365
1366     325         .          UGRAD( ISR , 1 ) * XMR + UGRAD( ISR , 2 ) * YMR          1366
1367     326          VVOR = 1.E-12 +                                                     1367
1368     327         .          VGRAD( ISR , 1 ) * XMR + VGRAD( ISR , 2 ) * YMR          1368
1369     328          PPOR = 1.E-12 +                                                     1369
1370     329         .          PGRAD( ISR , 1 ) * XMR + PGRAD( ISR , 2 ) * YMR          1370
1371     330    C                                                                         1371
1372     331          ELSE                                                                1372
1373     332    C                                                                         1373
1374     333          RROR = RROL                                                         1374
1375     334          UUOR = UUOL                                                         1375
1376     335          VVOR = VVOL                                                         1376
1377     336          PPOR = PPOL                                                         1377
1378     337    C                                                                         1378
1379     338          END IF                                                              1379
1380     339    C                                                                         1380
1381     340          ROL( 2 ) = 1. / RROL                                                1381
1382     341          UOL( 2 ) = 1. / UUOL                                                1382
1383     342          VOL( 2 ) = 1. / VVOL                                                1383
1384     343          POL( 2 ) = 1. / PPOL                                                1384
1385     344    C                                                                         1385
1386     345          ROR( 2 ) = 1. / RROR                                                1386
1387     346          UOR( 2 ) = 1. / UUOR                                                1387
1388     347          VOR( 2 ) = 1. / VVOR                                                1388
1389     348          POR( 2 ) = 1. / PPOR                                                1389
1390     349    C                                                                         1390
1391     350    C --- THIRD TRIANGLE EDGE -----------------------------------------------1391
1392     351    C                                                                         1392
```

```
1393  352          IE = IABS( JS( 6 , IS ) )                                  1393
1394  353    C                                                                1394
1395  354          ISL = JE( 3 , IE )                                         1395
1396  355          ISR = JE( 4 , IE )                                         1396
1397  356    C                                                                1397
1398  357          XML = XMIDL( IE ) - XS( 1 , ISL )                          1398
1399  358          YML = YMIDL( IE ) - XS( 2 , ISL )                          1399
1400  359    C                                                                1400
1401  360          RROL = 1.E-12 +                                            1401
1402  361         .          RGRAD( ISL , 1 ) * XML + RGRAD( ISL , 2 ) * YML  1402
1403  362          UUOL = 1.E-12 +                                            1403
1404  363         .          UGRAD( ISL , 1 ) * XML + UGRAD( ISL , 2 ) * YML  1404
1405  364          VVOL = 1.E-12 +                                            1405
1406  365         .          VGRAD( ISL , 1 ) * XML + VGRAD( ISL , 2 ) * YML  1406
1407  366          PPOL = 1.E-12 +                                            1407
1408  367         .          PGRAD( ISL , 1 ) * XML + PGRAD( ISL , 2 ) * YML  1408
1409  368    C                                                                1409
1410  369          IJE5 = JE( 5 , IE )                                        1410
1411  370          IF( IJE5 . EQ . 0 ) THEN                                   1411
1412  371    C                                                                1412
1413  372          XMR = XMIDL( IE ) - XS( 1 , ISR )                          1413
1414  373          YMR = YMIDL( IE ) - XS( 2 , ISR )                          1414
1415  374    C                                                                1415
1416  375          RROR = 1.E-12 +                                            1416
1417  376         .          RGRAD( ISR , 1 ) * XMR + RGRAD( ISR , 2 ) * YMR  1417
1418  377          UUOR = 1.E-12 +                                            1418
1419  378         .          UGRAD( ISR , 1 ) * XMR + UGRAD( ISR , 2 ) * YMR  1419
1420  379          VVOR = 1.E-12 +                                            1420
1421  380         .          VGRAD( ISR , 1 ) * XMR + VGRAD( ISR , 2 ) * YMR  1421
1422  381          PPOR = 1.E-12 +                                            1422
1423  382         .          PGRAD( ISR , 1 ) * XMR + PGRAD( ISR , 2 ) * YMR  1423
1424  383    C                                                                1424
1425  384          ELSE                                                       1425
1426  385    C                                                                1426
1427  386          RROR = RROL                                                1427
1428  387          UUOR = UUOL                                                1428
1429  388          VVOR = VVOL                                                1429
1430  389          PPOR = PPOL                                                1430
1431  390    C                                                                1431
1432  391          END IF                                                     1432
1433  392    C                                                                1433
1434  393          ROL( 3 ) = 1. / RROL                                       1434
1435  394          UOL( 3 ) = 1. / UUOL                                       1435
1436  395          VOL( 3 ) = 1. / VVOL                                       1436
1437  396          POL( 3 ) = 1. / PPOL                                       1437
1438  397    C                                                                1438
1439  398          ROR( 3 ) = 1. / RROR                                       1439
1440  399          UOR( 3 ) = 1. / UUOR                                       1440
1441  400          VOR( 3 ) = 1. / VVOR                                       1441
1442  401          POR( 3 ) = 1. / PPOR                                       1442
1443  402    C                                                                1443
1444  403          ISNR = SIGN( 1. , ROR( 1 ) )                               1444
1445  404          ISNL = SIGN( 1. , ROL( 1 ) )                               1445
1446  405    C                                                                1446
1447  406    C --- PERFORM THE LIMITING ON THE INCRAMENTS ------------------------ 1447
1448  407    C                                                                1448
1449  408          TEMPR = ( 1 + ISNR ) * RRR( KS ) +                         1449
1450  409         .        ( 1 - ISNR ) * RRL( KS )                           1450
1451  410          RUVPR1 = 0.5 * TEMPR * ROR( 1 )                            1451
1452  411    C                                                                1452
1453  412          TEMPL = ( 1 + ISNL ) * RRR( KS ) +                         1453
1454  413         .        ( 1 - ISNL ) * RRL( KS )                           1454
1455  414          RUVPL1 = 0.5 * TEMPL * ROL( 1 )                            1455
1456  415    C                                                                1456
1457  416          ISNR = SIGN( 1. , ROR( 2 ) )                               1457
1458  417          ISNL = SIGN( 1. , ROL( 2 ) )                               1458
1459  418    C                                                                1459
1460  419          TEMPR = ( 1 + ISNR ) * RRR( KS ) +                         1460
1461  420         .        ( 1 - ISNR ) * RRL( KS )                           1461
1462  421          RUVPR2 = 0.5 * TEMPR * ROR( 2 )                            1462
1463  422    C                                                                1463
1464  423          TEMPL = ( 1 + ISNL ) * RRR( KS ) +                         1464
1465  424         .        ( 1 - ISNL ) * RRL( KS )                           1465
1466  425          RUVPL2 = 0.5 * TEMPL * ROL( 2 )                            1466
```

```
1467     426  C                                                                  1467
1468     427        ISNR = SIGN( 1. , ROR( 3 ) )                                 1468
1469     428        ISNL = SIGN( 1. , ROL( 3 ) )                                 1469
1470     429  C                                                                  1470
1471     430        TEMPR = ( 1 + ISNR ) * RRR( KS ) +                           1471
1472     431       .        ( 1 - ISNR ) * RRL( KS )                             1472
1473     432        RUVPR3 = 0.5 * TEMPR * ROR( 3 )                              1473
1474     433  C                                                                  1474
1475     434        TEMPL = ( 1 + ISNL ) * RRR( KS ) +                           1475
1476     435       .        ( 1 - ISNL ) * RRL( KS )                             1476
1477     436        RUVPL3 = 0.5 * TEMPL * ROL( 3 )                              1477
1478     437  C                                                                  1478
1479     438        RMIN( KS ) = AMIN1( 1. , RUVPR1 , RUVPL1 , RUVPR2 , RUVPL2 , 1479
1480     439       .                                            RUVPR3 , RUVPL3 ) 1480
1481     440  C                                                                  1481
1482     441        ISNR = SIGN( 1. , UOR( 1 ) )                                 1482
1483     442        ISNL = SIGN( 1. , UOL( 1 ) )                                 1483
1484     443  C                                                                  1484
1485     444        TEMPR = ( 1 + ISNR ) * UUR( KS ) +                           1485
1486     445       .        ( 1 - ISNR ) * UUL( KS )                             1486
1487     446        RUVPR1 = 0.5 * TEMPR * UOR( 1 )                              1487
1488     447  C                                                                  1488
1489     448        TEMPL = ( 1 + ISNL ) * UUR( KS ) +                           1489
1490     449       .        ( 1 - ISNL ) * UUL( KS )                             1490
1491     450        RUVPL1 = 0.5 * TEMPL * UOL( 1 )                              1491
1492     451  C                                                                  1492
1493     452        ISNR = SIGN( 1. , UOR( 2 ) )                                 1493
1494     453        ISNL = SIGN( 1. , UOL( 2 ) )                                 1494
1495     454  C                                                                  1495
1496     455        TEMPR = ( 1 + ISNR ) * UUR( KS ) +                           1496
1497     456       .        ( 1 - ISNR ) * UUL( KS )                             1497
1498     457        RUVPR2 = 0.5 * TEMPR * UOR( 2 )                              1498
1499     458  C                                                                  1499
1500     459        TEMPL = ( 1 + ISNL ) * UUR( KS ) +                           1500
1501     460       .        ( 1 - ISNL ) * UUL( KS )                             1501
1502     461        RUVPL2 = 0.5 * TEMPL * UOL( 2 )                              1502
1503     462  C                                                                  1503
1504     463        ISNR = SIGN( 1. , UOR( 3 ) )                                 1504
1505     464        ISNL = SIGN( 1. , UOL( 3 ) )                                 1505
1506     465  C                                                                  1506
1507     466        TEMPR = ( 1 + ISNR ) * UUR( KS ) +                           1507
1508     467       .        ( 1 - ISNR ) * UUL( KS )                             1508
1509     468        RUVPR3 = 0.5 * TEMPR * UOR( 3 )                              15 )
1510     469  C                                                                  1510
1511     470        TEMPL = ( 1 + ISNL ) * UUR( KS ) +                           1511
1512     471       .        ( 1 - ISNL ) * UUL( KS )                             1512
1513     472        RUVPL3 = 0.5 * TEMPL * UOL( 3 )                              1513
1514     473  C                                                                  1514
1515     474        UMIN( KS ) = AMIN1( 1. , RUVPR1 , RUVPL1 , RUVPR2 , RUVPL2 , 1515
1516     475       .                                            RUVPR3 , RUVPL3 ) 1516
1517     476  C                                                                  1517
1518     477        ISNR = SIGN( 1. , VOR( 1 ) )                                 1518
1519     478        ISNL = SIGN( 1. , VOL( 1 ) )                                 1519
1520     479  C                                                                  1520
1521     480        TEMPR = ( 1 + ISNR ) * VVR( KS ) +                           1521
1522     481       .        ( 1 - ISNR ) * VVL( KS )                             1522
1523     482        RUVPR1 = 0.5 * TEMPR * VOR( 1 )                              1523
1524     483  C                                                                  1524
1525     484        TEMPL = ( 1 + ISNL ) * VVR( KS ) +                           1525
1526     485       .        ( 1 - ISNL ) * VVL( KS )                             1526
1527     486        RUVPL1 = 0.5 * TEMPL * VOL( 1 )                              1527
1528     487  C                                                                  1528
1529     488        ISNR = SIGN( 1. , VOR( 2 ) )                                 1529
1530     489        ISNL = SIGN( 1. , VOL( 2 ) )                                 1530
1531     490  C                                                                  1531
1532     491        TEMPR = ( 1 + ISNR ) * VVR( KS ) +                           1532
1533     492       .        ( 1 - ISNR ) * VVL( KS )                             1533
1534     493        RUVPR2 = 0.5 * TEMPR * VOR( 2 )                              1534
1535     494  C                                                                  1535
1536     495        TEMPL = ( 1 + ISNL ) * VVR( KS ) +                           1536
1537     496       .        ( 1 - ISNL ) * VVL( KS )                             1537
1538     497        RUVPL2 = 0.5 * TEMPL * VOL( 2 )                              1538
1539     498  C                                                                  1539
1540     499        ISNR = SIGN( 1. , VOR( 3 ) )                                 1540
```

```
1541    500          ISNL = SIGN( 1. , VOL( 3 ) )                                    1541
1542    501    C                                                                     1542
1543    502          TEMPR = ( 1 + ISNR ) * VVR( KS ) +                              1543
1544    503         .        ( 1 - ISNR ) * VVL( KS )                                1544
1545    504          RUVPR3 = 0.5 * TEMPR * VOR( 3 )                                 1545
1546    505    C                                                                     1546
1547    506          TEMPL = ( 1 + ISNL ) * VVR( KS ) +                              1547
1548    507         .        ( 1 - ISNL ) * VVL( KS )                                1548
1549    508          RUVPL3 = 0.5 * TEMPL * VOL( 3 )                                 1549
1550    509    C                                                                     1550
1551    510          VMIN( KS ) = AMIN1( 1. , RUVPR1 , RUVPL1 , RUVPR2 , RUVPL2 ,    1551
1552    511         .                                          RUVPR3 , RUVPL3 )    1552
1553    512    C                                                                     1553
1554    513          ISNR = SIGN( 1. , POR( 1 ) )                                    1554
1555    514          ISNL = SIGN( 1. , POL( 1 ) )                                    1555
1556    515    C                                                                     1556
1557    516          TEMPR = ( 1 + ISNR ) * PPR( KS ) +                              1557
1558    517         .        ( 1 - ISNR ) * PPL( KS )                                1558
1559    518          RUVPR1 = 0.5 * TEMPR * POR( 1 )                                 1559
1560    519    C                                                                     1560
1561    520          TEMPL = ( 1 + ISNL ) * PPR( KS ) +                              1561
1562    521         .        ( 1 - ISNL ) * PPL( KS )                                1562
1563    522          RUVPL1 = 0.5 * TEMPL * POL( 1 )                                 1563
1564    523    C                                                                     1564
1565    524          ISNR = SIGN( 1. , POR( 2 ) )                                    1565
1566    525          ISNL = SIGN( 1. , POL( 2 ) )                                    1566
1567    526    C                                                                     1567
1568    527          TEMPR = ( 1 + ISNR ) * PPR( KS ) +                              1568
1569    528         .        ( 1 - ISNR ) * PPL( KS )                                1569
1570    529          RUVPR2 = 0.5 * TEMPR * POR( 2 )                                 1570
1571    530    C                                                                     1571
1572    531          TEMPL = ( 1 + ISNL ) * PPR( KS ) +                              1572
1573    532         .        ( 1 - ISNL ) * PPL( KS )                                1573
1574    533          RUVPL2 = 0.5 * TEMPL * POL( 2 )                                 1574
1575    534    C                                                                     1575
1576    535          ISNR = SIGN( 1. , POR( 3 ) )                                    1576
1577    536          ISNL = SIGN( 1. , POL( 3 ) )                                    1577
1578    537    C                                                                     1578
1579    538          TEMPR = ( 1 + ISNR ) * PPR( KS ) +                              1579
1580    539         .        ( 1 - ISNR ) * PPL( KS )                                1580
1581    540          RUVPR3 = 0.5 * TEMPR * POR( 3 )                                 1581
1582    541    C                                                                     1582
1583    542          TEMPL = ( 1 + ISNL ) * PPR( KS ) +                              1583
1584    543         .        ( 1 - ISNL ) * PPL( KS )                                1584
1585    544          RUVPL3 = 0.5 * TEMPL * POL( 3 )                                 1585
1586    545    C                                                                     1586
1587    546          PMIN( KS ) = AMIN1( 1. , RUVPR1 , RUVPL1 , RUVPR2 , RUVPL2 ,    1587
1588    547         .                                          RUVPR3 , RUVPL3 )    1588
1589    548    C                                                                     1589
1590    549     170  CONTINUE                                                        1590
1591    550    C                                                                     1591
1592    551    C --- LIMIT THE ACTUAL GRADIENTS ------------------------------------ 1592
1593    552    C                                                                     1593
1594    553          DO 330 IH = 1 , 2                                               1594
1595    554    C                                                                     1595
1596    555          DO 330 IS = NS1 , NS2                                           1596
1597    556             KS = IS - NS1 + 1                                            1597
1598    557    C                                                                     1598
1599    558          RGRAD( IS , IH ) = RGRAD( IS , IH ) * RMIN( KS ) * FLATDR       1599
1600    559          UGRAD( IS , IH ) = UGRAD( IS , IH ) * UMIN( KS ) * FLATDR       1600
1601    560          VGRAD( IS , IH ) = VGRAD( IS , IH ) * VMIN( KS ) * FLATDR       1601
1602    561          PGRAD( IS , IH ) = PGRAD( IS , IH ) * PMIN( KS ) * FLATDR       1602
1603    562    C                                                                     1603
1604    563     330  CONTINUE                                                        1604
1605    564    C                                                                     1605
1606    565          NS1 = NS2 + 1                                                   1606
1607    566          NS2 = NS2 + NOFVES( INS + 1 )                                   1607
1608    567     80   CONTINUE                                                        1608
1609    568    C                                                                     1609
1610    569    C=====================================================================1610
1611    570    C                                                                     1611
1612    571    C --- CALL THE CHARECTERISTIC LIMITER ------------------------------- 1612
1613    572    C                                                                     1613
1614    573          CALL FCHART                                                     1614
```

```
1615   574  C                                                                 1615
1616   575  C=================================================================1616
1617   576  C                                                                 1617
1618   577  C                                                                 1618
1619   578  C --- EXIT POINT FROM SUBROUTINE ---------------------------------1619
1620   579  C                                                                 1620
1621   580  C     ------                                                      1621
1622   581        RETURN                                                      1622
1623   582  C     ------                                                      1623
1624   583  C                                                                 1624
1625   584  C     ---                                                         1625
1626   585        END                                                         1626
```



```
1627     1        SUBROUTINE GRADNG                                          1627
1628     2  C                                                                1628
1629     3  C-----------------------------------------------------------------I1629
1630     4  C                                                                 I1630
1631     5  C      GRADNG COMPUTE THE GRADIENT FOR SECOND ORDER CALCULATION   I1631
1632     6  C             USING THE INFORMATION STORED ASSOCIATED WITH THE    I1632
1633     7  C             VERTICIES OF THE TRIANGLE TO COMPUTE THE GRADIENT   I1633
1634     8  C                                                                 I1634
1635     9  C-----------------------------------------------------------------I1635
1636    10  C                                                                1636
1637    11        include     'cmsh00.h'                                     1637
1638    12        include     'chyd00.h'                                     1638
1639    13        include     'cint00.h'                                     1639
1640    14        include     'cphs10.h'                                     1640
1641    15        include     'cphs20.h'                                     1641
1642    16  C                                                                1642
1643    17  C=================================================================1643
1644    18  C                                                                1644
1645    19  C --- BEGIN LOOP OVER ALL CELLS IN THE DOMAIN --------------------1645
1646    20  C                                                                1646
1647    21        NS1 = 1                                                    1647
1648    22        NS2 = NOFVES( 1 )                                          1648
1649    23        DO 90 INS = 1 , NVEES                                      1649
1650    24  C                                                                1650
1651    25  C --- FETCH HYDRO QUANTITIES ------------------------------------1651
1652    26  C                                                                1652
1653    27        DO 105 IS = NS1 , NS2                                      1653
1654    28           KS = IS - NS1 + 1                                       1654
1655    29  C                                                                1655
1656    30         IV1 = JS( 1 , IS )                                        1656
1657    31         IV2 = JS( 2 , IS )                                        1657
1658    32         IV3 = JS( 3 , IS )                                        1658
1659    33         XV1 = XV( 1 , IV1 )                                       1659
1660    34         XV2 = XV( 1 , IV2 )                                       1660
1661    35         XV3 = XV( 1 , IV3 )                                       1661
1662    36         YV1 = XV( 2 , IV1 )                                       1662
1663    37         YV2 = XV( 2 , IV2 )                                       1663
1664    38         YV3 = XV( 2 , IV3 )                                       1664
1665    39         C = ( XV2 - XV1 ) * ( YV3 - YV2 ) - ( XV3 - XV2 ) * ( YV2 - YV1 )1665
1666    40         CINV = 1. / C                                             1666
1667    41  C                                                                1667
1668    42         RRMDL1 = HYDVVV( IV1 , 1 )                                1668
1669    43         UUMDL1 = HYDVVV( IV1 , 2 ) / RRMDL1                       1669
1670    44         VVMDL1 = HYDVVV( IV1 , 3 ) / RRMDL1                       1670
1671    45         PPMDL1 = ( HYDVVV( IV1 , 4 ) - .5 * RRMDL1 * ( UUMDL1 * UUMDL1 +1671
1672    46       .            VVMDL1 * VVMDL1 ) ) * ( HYDVVV( IV1 , 5 ) - 1. )1672
1673    47  C                                                                1673
1674    48         RRMDL2 = HYDVVV( IV2 , 1 )                                1674
1675    49         UUMDL2 = HYDVVV( IV2 , 2 ) / RRMDL2                       1675
1676    50         VVMDL2 = HYDVVV( IV2 , 3 ) / RRMDL2                       1676
1677    51         PPMDL2 = ( HYDVVV( IV2 , 4 ) - .5 * RRMDL2 * ( UUMDL2 * UUMDL2 +1677
1678    52       .            VVMDL2 * VVMDL2 ) ) * ( HYDVVV( IV2 , 5 ) - 1. )1678
1679    53  C                                                                1679
1680    54         RRMDL3 = HYDVVV( IV3 , 1 )                                1680
1681    55         UUMDL3 = HYDVVV( IV3 , 2 ) / RRMDL3                       1681
1682    56         VVMDL3 = HYDVVV( IV3 , 3 ) / RRMDL3                       1682
1683    57         PPMDL3 = ( HYDVVV( IV3 , 4 ) - .5 * RRMDL3 * ( UUMDL3 * UUMDL3 +1683
1684    58       .            VVMDL3 * VVMDL3 ) ) * ( HYDVVV( IV3 , 5 ) - 1. )1684
1685    59  C                                                                1685
```

```
1686      60          ZV1 = RRMDL1                                                  1686
1687      61          ZV2 = RRMDL2                                                  1687
1688      62          ZV3 = RRMDL3                                                  1688
1689      63          A = ( YV2 - YV1 ) * ( ZV3 - ZV2 ) - ( YV3 - YV2 ) * ( ZV2 - ZV1 )  1689
1690      64          B = ( ZV2 - ZV1 ) * ( XV3 - XV2 ) - ( ZV3 - ZV2 ) * ( XV2 - XV1 )  1690
1691      65    C                                                                   1691
1692      66          RGRAD( IS , 1 ) = - A * CINV                                  1692
1693      67          RGRAD( IS , 2 ) = - B * CINV                                  1693
1694      68    C                                                                   1694
1695      69          ZV1 = UUMDL1                                                  1695
1696      70          ZV2 = UUMDL2                                                  1696
1697      71          ZV3 = UUMDL3                                                  1697
1698      72          A = ( YV2 - YV1 ) * ( ZV3 - ZV2 ) - ( YV3 - YV2 ) * ( ZV2 - ZV1 )  1698
1699      73          B = ( ZV2 - ZV1 ) * ( XV3 - XV2 ) - ( ZV3 - ZV2 ) * ( XV2 - XV1 )  1699
1700      74    C                                                                   1700
1701      75          UGRAD( IS , 1 ) = - A * CINV                                  1701
1702      76          UGRAD( IS , 2 ) = - B * CINV                                  1702
1703      77    C                                                                   1703
1704      78          ZV1 = VVMDL1                                                  1704
1705      79          ZV2 = VVMDL2                                                  1705
1706      80          ZV3 = VVMDL3                                                  1706
1707      81          A = ( YV2 - YV1 ) * ( ZV3 - ZV2 ) - ( YV3 - YV2 ) * ( ZV2 - ZV1 )  1707
1708      82          B = ( ZV2 - ZV1 ) * ( XV3 - XV2 ) - ( ZV3 - ZV2 ) * ( XV2 - XV1 )  1708
1709      83    C                                                                   1709
1710      84          VGRAD( IS , 1 ) = - A * CINV                                  1710
1711      85          VGRAD( IS , 2 ) = - B * CINV                                  1711
1712      86    C                                                                   1712
1713      87          ZV1 = PPMDL1                                                  1713
1714      88          ZV2 = PPMDL2                                                  1714
1715      89          ZV3 = PPMDL3                                                  1715
1716      90          A = ( YV2 - YV1 ) * ( ZV3 - ZV2 ) - ( YV3 - YV2 ) * ( ZV2 - ZV1 )  1716
1717      91          B = ( ZV2 - ZV1 ) * ( XV3 - XV2 ) - ( ZV3 - ZV2 ) * ( XV2 - XV1 )  1717
1718      92    C                                                                   1718
1719      93          PGRAD( IS , 1 ) = - A * CINV                                  1719
1720      94          PGRAD( IS , 2 ) = - B * CINV                                  1720
1721      95    C                                                                   1721
1722      96    105   CONTINUE                                                      1722
1723      97    C                                                                   1723
1724      98          NS1 = NS2 + 1                                                 1724
1725      99          NS2 = NS2 + NOFVES( INS + 1 )                                 1725
1726     100     90   CONTINUE                                                      1726
1727     101    C                                                                   1727
1728     102    C=================================================================  1728
1729     103    C                                                                   1729
1730     104    C --- CALL THE MONOTONICITY LIMITER ------------------------------  1730
1731     105    C                                                                   1731
1732     106          CALL MONOTN                                                   1732
1733     107    C                                                                   1733
1734     108    C=================================================================  1734
1735     109    C                                                                   1735
1736     110    C                                                                   1736
1737     111    C --- EXIT POINT FROM SUBROUTINE ---------------------------------  1737
1738     112    C                                                                   1738
1739     113    C     ------                                                        1739
1740     114          RETURN                                                        1740
1741     115    C     ------                                                        1741
1742     116    C                                                                   1742
1743     117    C     ---                                                           1743
1744     118          END                                                           1744
```

```
      SUBROUTINE GRADNO
C
C-----------------------------------------------------------------I
C                                                                 I
C     GRADNO COMPUTE THE GRADIENT FOR SECOND ORDER CALCULATION    I
C           USING THE INFORMATION STORED ASSOCIATED WITH THE      I
C           VERTICIES OF THE TRIANGLE TO COMPUTE THE GRADIENT     I
C           APPLYING THE GRADIENT THEOREM                         I
C                                                                 I
C-----------------------------------------------------------------I
C
      include     'cmsh00.h'
      include     'chyd00.h'
      include     'cint00.h'
      include     'cphs10.h'
      include     'cphs20.h'
C
C=================================================================
C
      REAL RRMIDL(MBP),PPMIDL(MBP),UUMIDL(MBP),VVMIDL(MBP)
      REAL RIGRAD(MBP),PIGRAD(MBP),UIGRAD(MBP),VIGRAD(MBP)
      REAL RJGRAD(MBP),PJGRAD(MBP),UJGRAD(MBP),VJGRAD(MBP)
      REAL RMAX(MBP),PMAX(MBP),UMAX(MBP),VMAX(MBP)
      REAL RMIN(MBP),PMIN(MBP),UMIN(MBP),VMIN(MBP)
      REAL RLEFTT(MBP),ULEFTT(MBP),VLEFTT(MBP),PLEFTT(MBP)
      REAL RRIGHT(MBP),URIGHT(MBP),VRIGHT(MBP),PRIGHT(MBP)
      REAL ROR(3),UOR(3),VOR(3),POR(3)
      REAL ROL(3),UOL(3),VOL(3),POL(3)
      REAL AA(3,3),BB(3,4),B(3),INDX(3),ATEMP(3,3,3),BTEMP(3,4,3)
      REAL AA0(3,3),BB0(3,4)
C
C=================================================================
C
C --- BEGIN LOOP OVER ALL CELLS IN THE DOMAIN -------------------
C
      DO 120 IH = 1 , 2
      DO 120 IS = 1 , NS
      RGRAD( IS , IH ) = 0.
      UGRAD( IS , IH ) = 0.
      VGRAD( IS , IH ) = 0.
      PGRAD( IS , IH ) = 0.
120   CONTINUE
C
      NE1 = 1
      NE2 = NOFVEE( 1 )
      DO 90 INE = 1 , NVEEE
C
C --- FETCH HYDRO QUANTITIES ------------------------------------
C
      DO 105 IE = NE1 , NE2
         KE = IE - NE1 + 1
C
       IV1 = JE( 1 , IE )
       IV2 = JE( 2 , IE )
       RRMDL = ( HYDVVV( IV1 , 1 ) + HYDVVV( IV2 , 1 ) ) * .5
       UUMDL = ( HYDVVV( IV1 , 2 ) + HYDVVV( IV2 , 2 ) ) * .5 / RRMDL
       VVMDL = ( HYDVVV( IV1 , 3 ) + HYDVVV( IV2 , 3 ) ) * .5 / RRMDL
       PPMDL = ( HYDVVV( IV1 , 4 ) + HYDVVV( IV2 , 4 ) ) * .5
       GGMDL = ( HYDVVV( IV1 , 5 ) + HYDVVV( IV2 , 5 ) ) * .5
       PPMDL = ( PPMDL - .5 * RRMDL *
     .         ( UUMDL * UUMDL + VVMDL * VVMDL ) ) * ( GGMDL - 1. )
C
       RRMIDL( KE ) = RRMDL
       UUMIDL( KE ) = UUMDL
       VVMIDL( KE ) = VVMDL
       PPMIDL( KE ) = PPMDL
C
105   CONTINUE
C
      DO 110 IE = NE1 , NE2
         KE = IE - NE1 + 1
C
      XEXN = XE( 1 , IE ) * XN( IE )
      XEYN = XE( 1 , IE ) * YN( IE )
```

```
      C
            RIGRAD( KE ) = RRMIDL( KE ) * XEXN
            UIGRAD( KE ) = UUMIDL( KE ) * XEXN
            VIGRAD( KE ) = VVMIDL( KE ) * XEXN
            PIGRAD( KE ) = PPMIDL( KE ) * XEXN
      C
            RJGRAD( KE ) = RRMIDL( KE ) * XEYN
            UJGRAD( KE ) = UUMIDL( KE ) * XEYN
            VJGRAD( KE ) = VVMIDL( KE ) * XEYN
            PJGRAD( KE ) = PPMIDL( KE ) * XEYN
      C
  110   CONTINUE
      C
            DO 130 IE = NE1 , NE2
               KE = IE - NE1 + 1
      C
             ISL = JE( 3 , IE )
             ISR = JE( 4 , IE )
             IJE5 = JE( 5 , IE )
      C
             IF( IJE5 . EQ . 0 ) THEN
      C
            RGRAD( ISL , 1 ) = RGRAD( ISL , 1 ) + RIGRAD( KE )
            RGRAD( ISR , 1 ) = RGRAD( ISR , 1 ) - RIGRAD( KE )
            RGRAD( ISL , 2 ) = RGRAD( ISL , 2 ) + RJGRAD( KE )
            RGRAD( ISR , 2 ) = RGRAD( ISR , 2 ) - RJGRAD( KE )
            UGRAD( ISL , 1 ) = UGRAD( ISL , 1 ) + UIGRAD( KE )
            UGRAD( ISR , 1 ) = UGRAD( ISR , 1 ) - UIGRAD( KE )
            UGRAD( ISL , 2 ) = UGRAD( ISL , 2 ) + UJGRAD( KE )
            UGRAD( ISR , 2 ) = UGRAD( ISR , 2 ) - UJGRAD( KE )
            VGRAD( ISL , 1 ) = VGRAD( ISL , 1 ) + VIGRAD( KE )
            VGRAD( ISR , 1 ) = VGRAD( ISR , 1 ) - VIGRAD( KE )
            VGRAD( ISL , 2 ) = VGRAD( ISL , 2 ) + VJGRAD( KE )
            VGRAD( ISR , 2 ) = VGRAD( ISR , 2 ) - VJGRAD( KE )
            PGRAD( ISL , 1 ) = PGRAD( ISL , 1 ) + PIGRAD( KE )
            PGRAD( ISR , 1 ) = PGRAD( ISR , 1 ) - PIGRAD( KE )
            PGRAD( ISL , 2 ) = PGRAD( ISL , 2 ) + PJGRAD( KE )
            PGRAD( ISR , 2 ) = PGRAD( ISR , 2 ) - PJGRAD( KE )
      C
            ELSE
      C
            RGRAD( ISL , 1 ) = RGRAD( ISL , 1 ) + RIGRAD( KE )
            RGRAD( ISL , 2 ) = RGRAD( ISL , 2 ) + RJGRAD( KE )
            UGRAD( ISL , 1 ) = UGRAD( ISL , 1 ) + UIGRAD( KE )
            UGRAD( ISL , 2 ) = UGRAD( ISL , 2 ) + UJGRAD( KE )
            VGRAD( ISL , 1 ) = VGRAD( ISL , 1 ) + VIGRAD( KE )
            VGRAD( ISL , 2 ) = VGRAD( ISL , 2 ) + VJGRAD( KE )
            PGRAD( ISL , 1 ) = PGRAD( ISL , 1 ) + PIGRAD( KE )
            PGRAD( ISL , 2 ) = PGRAD( ISL , 2 ) + PJGRAD( KE )
      C
            END IF
      C
  130   CONTINUE
            NE1 = NE2 + 1
            NE2 = NE2 + NOFVEE( INE + 1 )
   90   CONTINUE
      C
            DO 140 IH = 1 , 2
            DO 140 IS = 1 , NS
            RGRAD( IS , IH ) = RGRAD( IS , IH ) * SAREA( IS )
            UGRAD( IS , IH ) = UGRAD( IS , IH ) * SAREA( IS )
            VGRAD( IS , IH ) = VGRAD( IS , IH ) * SAREA( IS )
            PGRAD( IS , IH ) = PGRAD( IS , IH ) * SAREA( IS )
  140   CONTINUE
      C
      C=======================================================================
      C
      C --- CALL THE MONOTONICITY LIMITER ------------------------------
      C
            CALL MONOTN
      C
      C=======================================================================
      C
      C
```

```
1893    149   C --- EXIT POINT FROM SUBROUTINE ----------------------------------------
1894    150   C
1895    151   C     ------
1896    152         RETURN
1897    153   C     ------
1898    154   C
1899    155   C     ---
1900    156         END
```



```
1901      1         SUBROUTINE GRADNS
1902      2   C
1903      3   C-------------------------------------------------------------------I
1904      4   C                                                                   I
1905      5   C      GRADNS COMPUTE THE GRADIENT FOR SECOND ORDER CALCULATION     I
1906      6   C             USING THE INFORMATION ASSOCIATE WITH THE BARICENTER I
1907      7   C             OF THE TWO TRIANGLES FROM THE TWO SIDE OF EACH       |
1908      8   C             EDGE COMPUTING THE VALUE FOR THE EDGE AND APPLYING   I
1909      9   C             THE GRADIENT THEOREM TO COMPUTE THE GRADIENT         I
1910     10   C                                                                   I
1911     11   C-------------------------------------------------------------------I
1912     12   C
1913     13         include     'cmsh00.h'
1914     14         include     'chyd00.h'
1915     15         include     'cint00.h'
1916     16         include     'cphs10.h'
1917     17         include     'cphs20.h'
1918     18   C
1919     19   C=====================================================================
1920     20   C
1921     21         REAL RRMIDL(MBP),PPMIDL(MBP),UUMIDL(MBP),VVMIDL(MBP)
1922     22         REAL RIGRAD(MBP),PIGRAD(MBP),UIGRAD(MBP),VIGRAD(MBP)
1923     23         REAL RJGRAD(MBP),PJGRAD(MBP),UJGRAD(MBP),VJGRAD(MBP)
1924     24         REAL RMAX(MBP),PMAX(MBP),UMAX(MBP),VMAX(MBP)
1925     25         REAL RMIN(MBP),PMIN(MBP),UMIN(MBP),VMIN(MBP)
1926     26         REAL RLEFTT(MBP),ULEFTT(MBP),VLEFTT(MBP),PLEFTT(MBP)
1927     27         REAL RRIGHT(MBP),URIGHT(MBP),VRIGHT(MBP),PRIGHT(MBP)
1928     28         REAL ROR(3),UOR(3),VOR(3),POR(3)
1929     29         REAL ROL(3),UOL(3),VOL(3),POL(3)
1930     30         REAL AA(3,3),BB(3,4),B(3),INDX(3),ATEMP(3,3,3),BTEMP(3,4,3)
1931     31         REAL AA0(3,3),BB0(3,4)
1932     32   C
1933     33   C=====================================================================
1934     34   C
1935     35   C --- BEGIN LOOP OVER ALL CELLS IN THE DOMAIN -------------------------
1936     36   C
1937     37         DO 120 IH = 1 , 2
1938     38         DO 120 IS = 1 , NS
1939     39         RGRAD( IS , IH ) = 0.
1940     40         UGRAD( IS , IH ) = 0.
1941     41         VGRAD( IS , IH ) = 0.
1942     42         PGRAD( IS , IH ) = 0.
1943     43   120   CONTINUE
1944     44   C
1945     45         NE1 = 1
1946     46         NE2 = NOFVEE( 1 )
1947     47         DO 90 INE = 1 , NVEEE
1948     48   C
1949     49   C --- FETCH HYDRO QUANTITIES ------------------------------------------
1950     50   C
1951     51         DO 105 IE = NE1 , NE2
1952     52            KE = IE - NE1 + 1
1953     53   C
1954     54          ISL = JE( 3 , IE )
1955     55          ISR = JE( 4 , IE )
1956     56          IJE5 = JE( 5 , IE )
1957     57   C
1958     58          IF( IJE5 . EQ . 0 ) THEN
1959     59
1960     60          RRMDL = XYMIDL( IE ) * ( HYDV( ISR , 1 ) -
1961     61        .                          HYDV( ISL , 1 ) ) + HYDV( ISL , 1 )
1962     62          UUMDL = XYMIDL( IE ) * ( HYDV( ISR , 2 ) -
1963     63        .                          HYDV( ISL , 2 ) ) + HYDV( ISL , 2 )
```

```
1964      64          VVMDL = XYMIDL( IE ) * ( HYDV( ISR , 3 ) -
1965      65         .                         HYDV( ISL , 3 ) ) + HYDV( ISL , 3 )
1966      66          PPMDL = XYMIDL( IE ) * ( HYDV( ISR , 4 ) -
1967      67         .                         HYDV( ISL , 4 ) ) + HYDV( ISL , 4 )
1968      68    C
1969      69          ELSE
1970      70    C
1971      71          RRMDL = HYDV( ISL , 1 )
1972      72          UUMDL = HYDV( ISL , 2 )
1973      73          VVMDL = HYDV( ISL , 3 )
1974      74          PPMDL = HYDV( ISL , 4 )
1975      75    C
1976      76          END IF
1977      77    C
1978      78          RRMIDL( KE ) = RRMDL
1979      79          UUMIDL( KE ) = UUMDL
1980      80          VVMIDL( KE ) = VVMDL
1981      81          PPMIDL( KE ) = PPMDL
1982      82    C
1983      83    105   CONTINUE
1984      84    C
1985      85          DO 110 IE = NE1 , NE2
1986      86             KE = IE - NE1 + 1
1987      87    C
1988      88          XEXN = XE( 1 , IE ) * XN( IE )
1989      89          XEYN = XE( 1 , IE ) * YN( IE )
1990      90    C
1991      91          RIGRAD( KE ) = RRMIDL( KE ) * XEXN
1992      92          UIGRAD( KE ) = UUMIDL( KE ) * XEXN
1993      93          VIGRAD( KE ) = VVMIDL( KE ) * XEXN
1994      94          PIGRAD( KE ) = PPMIDL( KE ) * XEXN
1995      95    C
1996      96          RJGRAD( KE ) = RRMIDL( KE ) * XEYN
1997      97          UJGRAD( KE ) = UUMIDL( KE ) * XEYN
1998      98          VJGRAD( KE ) = VVMIDL( KE ) * XEYN
1999      99          PJGRAD( KE ) = PPMIDL( KE ) * XEYN
2000     100    C
2001     101    110   CONTINUE
2002     102    C
2003     103          DO 130 IE = NE1 , NE2
2004     104             KE = IE - NE1 + 1
2005     105    C
2006     106           ISL = JE( 3 , IE )
2007     107           ISR = JE( 4 , IE )
2008     108           IJE5 = JE( 5 , IE )
2009     109    C
2010     110           IF( IJE5 . EQ . 0 ) THEN
2011     111    C
2012     112          RGRAD( ISL , 1 ) = RGRAD( ISL , 1 ) + RIGRAD( KE )
2013     113          RGRAD( ISR , 1 ) = RGRAD( ISR , 1 ) - RIGRAD( KE )
2014     114          RGRAD( ISL , 2 ) = RGRAD( ISL , 2 ) + RJGRAD( KE )
2015     115          RGRAD( ISR , 2 ) = RGRAD( ISR , 2 ) - RJGRAD( KE )
2016     116          UGRAD( ISL , 1 ) = UGRAD( ISL , 1 ) + UIGRAD( KE )
2017     117          UGRAD( ISR , 1 ) = UGRAD( ISR , 1 ) - UIGRAD( KE )
2018     118          UGRAD( ISL , 2 ) = UGRAD( ISL , 2 ) + UJGRAD( KE )
2019     119          UGRAD( ISR , 2 ) = UGRAD( ISR , 2 ) - UJGRAD( KE )
2020     120          VGRAD( ISL , 1 ) = VGRAD( ISL , 1 ) + VIGRAD( KE )
2021     121          VGRAD( ISR , 1 ) = VGRAD( ISR , 1 ) - VIGRAD( KE )
2022     122          VGRAD( ISL , 2 ) = VGRAD( ISL , 2 ) + VJGRAD( KE )
2023     123          VGRAD( ISR , 2 ) = VGRAD( ISR , 2 ) - VJGRAD( KE )
2024     124          PGRAD( ISL , 1 ) = PGRAD( ISL , 1 ) + PIGRAD( KE )
2025     125          PGRAD( ISR , 1 ) = PGRAD( ISR , 1 ) - PIGRAD( KE )
2026     126          PGRAD( ISL , 2 ) = PGRAD( ISL , 2 ) + PJGRAD( KE )
2027     127          PGRAD( ISR , 2 ) = PGRAD( ISR , 2 ) - PJGRAD( KE )
2028     128    C
2029     129          ELSE
2030     130    C
2031     131          RGRAD( ISL , 1 ) = RGRAD( ISL , 1 ) + RIGRAD( KE )
2032     132          RGRAD( ISL , 2 ) = RGRAD( ISL , 2 ) + RJGRAD( KE )
2033     133          UGRAD( ISL , 1 ) = UGRAD( ISL , 1 ) + UIGRAD( KE )
2034     134          UGRAD( ISL , 2 ) = UGRAD( ISL , 2 ) + UJGRAD( KE )
2035     135          VGRAD( ISL , 1 ) = VGRAD( ISL , 1 ) + VIGRAD( KE )
2036     136          VGRAD( ISL , 2 ) = VGRAD( ISL , 2 ) + VJGRAD( KE )
2037     137          PGRAD( ISL , 1 ) = PGRAD( ISL , 1 ) + PIGRAD( KE )
```

```
2038  138        PGRAD( ISL , 2 ) = PGRAD( ISL , 2 ) + PJGRAD( KE )
2039  139  C
2040  140        END IF
2041  141  C
2042  142  130   CONTINUE
2043  143        NE1 = NE2 + 1
2044  144        NE2 = NE2 + NOFVEE( INE + 1 )
2045  145   90   CONTINUE
2046  146  C
2047  147        DO 140 IH = 1 , 2
2048  148        DO 140 IS = 1 , NS
2049  149        RGRAD( IS , IH ) = RGRAD( IS , IH ) * SAREA( IS )
2050  150        UGRAD( IS , IH ) = UGRAD( IS , IH ) * SAREA( IS )
2051  151        VGRAD( IS , IH ) = VGRAD( IS , IH ) * SAREA( IS )
2052  152        PGRAD( IS , IH ) = PGRAD( IS , IH ) * SAREA( IS )
2053  153  140   CONTINUE
2054  154  C
2055  155  C=================================================================
2056  156  C
2057  157  C --- CALL THE MONOTONICITY LIMITER ------------------------------
2058  158  C
2059  159        CALL MONOTN
2060  160  C
2061  161  C=================================================================
2062  162  C
2063  163  C
2064  164  C --- EXIT POINT FROM SUBROUTINE ---------------------------------
2065  165  C
2066  166  C     ------
2067  167        RETURN
2068  168  C     ------
2069  169  C
2070  170  C     ---
2071  171        END
```



```
2072    1        SUBROUTINE LUDCMP(A,N,NP,INDX,D)
2073    2  C
2074    3  C-------------------------------------------------------------I
2075    4  C                                                             I
2076    5  C      PERFORM AN L U DECOMPOSITION OF THE A MATRIX           I
2077    6  C                                                             I
2078    7  C-------------------------------------------------------------I
2079    8  C
2080    9        PARAMETER (NMAX=100,TINY=1.0E-20)
2081   10        DIMENSION A(NP,NP),INDX(N),VV(NMAX)
2082   11        D=1.
2083   12        DO 12 I=1,N
2084   13          AAMAX=0.
2085   14          DO 11 J=1,N
2086   15            IF (ABS(A(I,J)).GT.AAMAX) AAMAX=ABS(A(I,J))
2087   16  11      CONTINUE
2088   17          IF (AAMAX.EQ.0.) PAUSE 'Singular matrix.'
2089   18          VV(I)=1./AAMAX
2090   19  12    CONTINUE
2091   20        DO 19 J=1,N
2092   21          IF (J.GT.1) THEN
2093   22            DO 14 I=1,J-1
2094   23              SUM=A(I,J)
2095   24              IF (I.GT.1)THEN
2096   25                DO 13 K=1,I-1
2097   26                  SUM=SUM-A(I,K)*A(K,J)
2098   27  13              CONTINUE
2099   28                A(I,J)=SUM
2100   29              ENDIF
2101   30  14        CONTINUE
2102   31          ENDIF
2103   32          AAMAX=0.
2104   33          DO 16 I=J,N
2105   34            SUM=A(I,J)
2106   35            IF (J.GT.1)THEN
2107   36              DO 15 K=1,J-1
2108   37                SUM=SUM-A(I,K)*A(K,J)
```

```
2109      38   15          CONTINUE                                          2109
2110      39               A(I,J)=SUM                                        2110
2111      40             ENDIF                                               2111
2112      41             DUM=VV(I)*ABS(SUM)                                  2112
2113      42             IF (DUM.GE.AAMAX) THEN                              2113
2114      43               IMAX=I                                            2114
2115      44               AAMAX=DUM                                         2115
2116      45             ENDIF                                               2116
2117      46   16      CONTINUE                                              2117
2118      47           IF (J.NE.IMAX)THEN                                    2118
2119      48             DO 17 K=1,N                                         2119
2120      49               DUM=A(IMAX,K)                                     2120
2121      50               A(IMAX,K)=A(J,K)                                  2121
2122      51               A(J,K)=DUM                                        2122
2123      52   17        CONTINUE                                            2123
2124      53             D=-D                                                2124
2125      54             VV(IMAX)=VV(J)                                      2125
2126      55           ENDIF                                                 2126
2127      56           INDX(J)=IMAX                                          2127
2128      57           IF(J.NE.N)THEN                                        2128
2129      58             IF(A(J,J).EQ.0.)A(J,J)=TINY                         2129
2130      59             DUM=1./A(J,J)                                       2130
2131      60             DO 18 I=J+1,N                                       2131
2132      61               A(I,J)=A(I,J)*DUM                                 2132
2133      62   18        CONTINUE                                            2133
2134      63           ENDIF                                                 2134
2135      64   19    CONTINUE                                                2135
2136      65         IF(A(N,N).EQ.0.)A(N,N)=TINY                             2136
2137      66         RETURN                                                  2137
2138      67         END                                                     2138
2139      68   c                                                            2139
```



```
2140       1         SUBROUTINE LUBKSB(A,N,NP,INDX,B)                       2140
2141       2         DIMENSION A(NP,NP),INDX(N),B(N)                        2141
2142       3         II=0                                                   2142
2143       4         DO 12 I=1,N                                            2143
2144       5           LL=INDX(I)                                           2144
2145       6           SUM=B(LL)                                            2145
2146       7           B(LL)=B(I)                                           2146
2147       8           IF (II.NE.0)THEN                                     2147
2148       9             DO 11 J=II,I-1                                     2148
2149      10               SUM=SUM-A(I,J)*B(J)                              2149
2150      11   11        CONTINUE                                            2150
2151      12           ELSE IF (SUM.NE.0.) THEN                             2151
2152      13             II=I                                               2152
2153      14           ENDIF                                                2153
2154      15           B(I)=SUM                                             2154
2155      16   12    CONTINUE                                                2155
2156      17         DO 14 I=N,1,-1                                          2156
2157      18           SUM=B(I)                                             2157
2158      19           IF(I.LT.N)THEN                                       2158
2159      20             DO 13 J=I+1,N                                      2159
2160      21               SUM=SUM-A(I,J)*B(J)                              2160
2161      22   13        CONTINUE                                            2161
2162      23           ENDIF                                                2162
2163      24           B(I)=SUM/A(I,I)                                      2163
2164      25   14    CONTINUE                                                2164
2165      26         RETURN                                                  2165
2166      27         END                                                     2166
```

```
      1         SUBROUTINE FIRST
      2   C
      3   C-----------------------------------------------------------------I
      4   C                                                                 I
      5   C      FIRST IS USED TO FIND THE LEFT AND RIGHT INTERFACE         I
      6   C            QUANTITIES TO FIRST ORDER WITHOUT USING EITHER THE   I
      7   C            GRADIENT OR THE CHARACTERISTICS.                     I
      8   C                                                                 I
      9   C-----------------------------------------------------------------I
     10   C
     11         include     'cmsh00.h'
     12         include     'chyd00.h'
     13         include     'cint00.h'
     14         include     'cphs10.h'
     15         include     'cphs20.h'
     16   C
     17   C=================================================================
     18   C
     19         DO 110 IE = 1 , NE
     20          ISL = JE( 3 , IE )
     21          ISR = JE( 4 , IE )
     22            IJE5 = JE( 5 , IE )
     23              RL( IE ) =   HYDV( ISL , 1 )
     24              UL( IE ) =   HYDV( ISL , 2 ) * XN( IE )
     25         .                 + HYDV( ISL , 3 ) * YN( IE )
     26              VL( IE ) = - HYDV( ISL , 2 ) * YN( IE )
     27         .                 + HYDV( ISL , 3 ) * XN( IE )
     28              PL( IE ) =   HYDV( ISL , 4 )
     29   C
     30   C --- EDGES IN THE COMPUTATIONAL DOMAIN ---------------------------------
     31   C
     32         IF( IJE5 . EQ . 0 ) THEN
     33              RR( IE ) =   HYDV( ISR , 1 )
     34              UR( IE ) =   HYDV( ISR , 2 ) * XN( IE )
     35         .                 + HYDV( ISR , 3 ) * YN( IE )
     36              VR( IE ) = - HYDV( ISR , 2 ) * YN( IE )
     37         .                 + HYDV( ISR , 3 ) * XN( IE )
     38              PR( IE ) =   HYDV( ISR , 4 )
     39   C
     40   C --- EDGES ON THE BOUNDARY WITH ENFORCED CONDITIONS --------------------
     41   C
     42   C           IJE5 = 6 A WALL WITH REFLECTING NORMAL COMPONENTS
     43   C                = 7 SUPERSONIC OUTFLOW ZERO NORMAL DERIVATIVE
     44   C                = 8 INFLOW WITH PRESPECIFIED VALUES (RIN,UIN,VIN,PIN)
     45   C
     46         ELSEIF( IJE5 . EQ . 8 ) THEN
     47              RR( IE ) =   RIN
     48              UR( IE ) =   UIN * XN( IE ) + VIN * YN( IE )
     49              VR( IE ) = - UIN * YN( IE ) + VIN * XN( IE )
     50              PR( IE ) =   PIN
     51   C
     52         ELSEIF( IJE5 . EQ . 7 ) THEN
     53              RR( IE ) =   RL( IE )
     54              UR( IE ) =   UL( IE )
     55              VR( IE ) =   VL( IE )
     56              PR( IE ) =   PL( IE )
     57   C
     58         ELSEIF( IJE5 . EQ . 6 . OR . IJE5 . EQ . 5 ) THEN
     59              RR( IE ) =   RL( IE )
     60              UR( IE ) = - UL( IE )
     61              VR( IE ) =   VL( IE )
     62              PR( IE ) =   PL( IE )
     63   C
     64         END IF
     65    110  CONTINUE
     66   C
     67   C=================================================================
     68   C
     69   C --- EXIT POINT FROM SUBROUTINE ----------------------------------------
     70   C
     71   C     ------
     72         RETURN
     73   C     ------
     74   C
```

```
2241      75  C     ---                                                          2241
2242      76        END                                                          2242
```



```
2243       1        SUBROUTINE FCHART                                            2243
2244       2  C                                                                  2244
2245       3  C-------------------------------------------------------------I    2245
2246       4  C                                                             I    2246
2247       5  C      FCHART LIMITS THE PROJECTED INTERFACE VALUES ACCORDING TO I    2247
2248       6  C      CHARACTERISTICS.                                       I    2248
2249       7  C                                                             I    2249
2250       8  C-------------------------------------------------------------I    2250
2251       9  C                                                                  2251
2252      10        include     'cmsh00.h'                                       2252
2253      11        include     'chyd00.h'                                       2253
2254      12        include     'cint00.h'                                       2254
2255      13        include     'cphs10.h'                                       2255
2256      14        include     'cphs20.h'                                       2256
2257      15  C                                                                  2257
2258      16  C=================================================================2258
2259      17  C                                                                  2259
2260      18        REAL ZZLEFT(MBP),ZOLEFT(MBP),ZMLEFT(MBP)                     2260
2261      19        REAL ZZRIGT(MBP),ZORIGT(MBP),ZPRIGT(MBP)                     2261
2262      20        REAL UPLEFT(MBP),UMLEFT(MBP),URLEFT(MBP),SQGMTL(MBP)         2262
2263      21        REAL UPRIGT(MBP),UMRIGT(MBP),URRIGT(MBP),SQGMTR(MBP)         2263
2264      22        REAL UVLEFT(MBP),UVRIGT(MBP),CNLEFT(MBP),CNRIGT(MBP)         2264
2265      23        REAL RLEFTT(MBP),ULEFTT(MBP),VLEFTT(MBP),PLEFTT(MBP)         2265
2266      24        REAL RRIGHT(MBP),URIGHT(MBP),VRIGHT(MBP),PRIGHT(MBP)         2266
2267      25  C                                                                  2267
2268      26  C=================================================================2268
2269      27  C                                                                  2269
2270      28        NE1 = 1                                                      2270
2271      29        NE2 = NOFVEE( 1 )                                            2271
2272      30        DO 90 INE = 1 , NVEEE                                        2272
2273      31  C                                                                  2273
2274      32        DO 110 IE = NE1 , NE2                                        2274
2275      33           KE = IE - NE1 + 1                                         2275
2276      34  C                                                                  2276
2277      35         ISL = JE( 3 , IE )                                         2277
2278      36         ISR = JE( 4 , IE )                                         2278
2279      37         GAMAL( KE ) = HYDV( ISL , 5 )                              2279
2280      38  C                                                                  2280
2281      39         CNLFTS = GAMAL( KE ) * HYDV( ISL , 4 ) / HYDV( ISL , 1 )   2281
2282      40         CNLFT = SQRT( CNLFTS )                                     2282
2283      41         UVLFT = HYDV( ISL , 2 ) * XXN( IE ) +                      2283
2284      42     .           HYDV( ISL , 3 ) * YYN( IE )                        2284
2285      43  C                                                                  2285
2286      44         IJE5 = JE( 5 , IE )                                        2286
2287      45         IF( IJE5 . EQ . 0 ) THEN                                   2287
2288      46  C                                                                  2288
2289      47         GAMAR( KE ) = HYDV( ISR , 5 )                              2289
2290      48         CNRGTS = GAMAR( KE ) * HYDV( ISR , 4 ) / HYDV( ISR , 1 )   2290
2291      49         CNRGT = SQRT( CNRGTS )                                     2291
2292      50  C                                                                  2292
2293      51         UVRGT = HYDV( ISR , 2 ) * XXN( IE ) +                      2293
2294      52     .           HYDV( ISR , 3 ) * YYN( IE )                        2294
2295      53  C                                                                  2295
2296      54         ELSE                                                       2296
2297      55  C                                                                  2297
2298      56          GAMAR( KE ) = GAMAL( KE )                                 2298
2299      57          CNRGT = CNLFT                                             2299
2300      58          UVRGT = UVLFT                                             2300
2301      59  C                                                                  2301
2302      60         END IF                                                     2302
2303      61  C                                                                  2303
2304      62           CNLEFT( KE ) = CNLFT                                     2304
2305      63           CNRIGT( KE ) = CNRGT                                     2305
2306      64  C                                                                  2306
2307      65           UVLEFT( KE ) = UVLFT                                     2307
2308      66           UVRIGT( KE ) = UVRGT                                     2308
2309      67  C                                                                  2309
2310      68    110  CONTINUE                                                   2310
2311      69  C                                                                  2311
```

```
      DO 130 KE = 1 , NOFVEE( INE )
C
      ZZLEFT( KE ) =   .5 * ( UVLEFT( KE ) + CNLEFT( KE ) ) * DTT
      ZZRIGT( KE ) = - .5 * ( UVRIGT( KE ) - CNRIGT( KE ) ) * DTT
C
 130  CONTINUE
C
C  CHARACTERISTICS LOCATIONS
C
      DO 140 KE = 1 , NOFVEE( INE )
C
      IF( ZZLEFT( KE ) . LT . 0. ) ZZLEFT( KE ) = 0.
      IF( ZZRIGT( KE ) . LT . 0. ) ZZRIGT( KE ) = 0.
C
 140  CONTINUE
C
C      DO 150 KE = 1 , NOFVEE( INE )
C
C      ZOLEFT( KE ) =   .5 * UVLEFT( KE ) * DTT
C      ZORIGT( KE ) = - .5 * UVRIGT( KE ) * DTT
C      ZPRIGT( KE ) = - .5 * ( UVRIGT( KE ) + CNRIGT( KE ) ) * DTT
C      ZMLEFT( KE ) =   .5 * ( UVLEFT( KE ) - CNLEFT( KE ) ) * DTT
C
C 150  CONTINUE
C
C  FIRST GUESS LEFT AND RIGHT VARIABLES, LINEAR INTERPOLATON
C
      DO 160 IE = NE1 , NE2
         KE = IE - NE1 + 1
C
      ISL = JE( 3 , IE )
      ISR = JE( 4 , IE )
C
      XX = XMIDL( IE ) - ZZLEFT( KE ) * XXN( IE ) - XS( 1 , ISL )
      YY = YMIDL( IE ) - ZZLEFT( KE ) * YYN( IE ) - XS( 2 , ISL )
C
      HRRL =  HYDV( ISL , 1 ) +
     .        RGRAD( ISL , 1 ) * XX + RGRAD( ISL , 2 ) * YY
      HUUL =  HYDV( ISL , 2 ) +
     .        UGRAD( ISL , 1 ) * XX + UGRAD( ISL , 2 ) * YY
      HVVL =  HYDV( ISL , 3 ) +
     .        VGRAD( ISL , 1 ) * XX + VGRAD( ISL , 2 ) * YY
      HPPL =  HYDV( ISL , 4 ) +
     .        PGRAD( ISL , 1 ) * XX + PGRAD( ISL , 2 ) * YY
C
      GMTLFT = GAMAL( KE ) * HRRL * HPPL
      SQGMTL( KE ) = SQRT( GMTLFT )
C
C      UMLFT = 0.
C      IF( UVLEFT( KE ) - CNLEFT( KE ) . GT . 0. ) THEN
C      XX = ( ZMLEFT( KE ) - ZZLEFT( KE ) ) * XXN( IE )
C      YY = ( ZMLEFT( KE ) - ZZLEFT( KE ) ) * YYN( IE )
C      UUU = UGRAD( ISL , 1 ) * XX + UGRAD( ISL , 2 ) * YY
C      VVV = VGRAD( ISL , 1 ) * XX + VGRAD( ISL , 2 ) * YY
C      UVU = UUU * XXN( IE ) + VVV * YYN( IE )
C      PPP = PGRAD( ISL , 1 ) * XX + PGRAD( ISL , 2 ) * YY
C      UMLFT =   .5 * ( UVU - PPP / SQGMTL( KE ) ) / SQGMTL( KE )
C      END IF
C
C      URLFT = 0.
C      IF( UVLEFT( KE ) . GT . 0. ) THEN
C      XX = ( ZOLEFT( KE ) - ZZLEFT( KE ) ) * XXN( IE )
C      YY = ( ZOLEFT( KE ) - ZZLEFT( KE ) ) * YYN( IE )
C      PPP = PGRAD( ISL , 1 ) * XX + PGRAD( ISL , 2 ) * YY
C      XX = XMIDL( IE ) - ZOLEFT( KE ) * XXN( IE ) - XS( 1 , ISL )
C      YY = YMIDL( IE ) - ZOLEFT( KE ) * YYN( IE ) - XS( 2 , ISL )
C      RRRR = HYDV( ISL , 1 ) +
C     .        RGRAD( ISL , 1 ) * XX + RGRAD( ISL , 2 ) * YY
C      URLFT = PPP / GMTLFT + 1. / HRRL - 1. / RRRR
C      END IF
C
      IJE5 = JE( 5 , IE )
      IF( IJE5 . EQ . 0 ) THEN
C
```

```
2386    144          XX = XMIDL( IE ) + ZZRIGT( KE ) * XXN( IE ) - XS( 1 , ISR )                2386
2387    145          YY = YMIDL( IE ) + ZZRIGT( KE ) * YYN( IE ) - XS( 2 , ISR )                2387
2388    146    C                                                                                2388
2389    147          HRRR =  HYDV( ISR , 1 ) +                                                  2389
2390    148         .        RGRAD( ISR , 1 ) * XX + RGRAD( ISR , 2 ) * YY                      2390
2391    149          HUUR =  HYDV( ISR , 2 ) +                                                  2391
2392    150         .        UGRAD( ISR , 1 ) * XX + UGRAD( ISR , 2 ) * YY                      2392
2393    151          HVVR =  HYDV( ISR , 3 ) +                                                  2393
2394    152         .        VGRAD( ISR , 1 ) * XX + VGRAD( ISR , 2 ) * YY                      2394
2395    153          HPPR =  HYDV( ISR , 4 ) +                                                  2395
2396    154         .        PGRAD( ISR , 1 ) * XX + PGRAD( ISR , 2 ) * YY                      2396
2397    155    C                                                                                2397
2398    156          GMTRGT = GAMAR( KE ) * HRRR * HPPR                                         2398
2399    157          SQGMTR( KE ) = SQRT( GMTRGT )                                              2399
2400    158    C                                                                                2400
2401    159    C      UPRGT = 0.                                                                2401
2402    160    C      IF( UVRIGT( KE ) + CNRIGT( KE ) . LT . 0. ) THEN                          2402
2403    161    C      XX = ( ZZRIGT( KE ) - ZPRIGT( KE ) ) * XXN( IE )                          2403
2404    162    C      YY = ( ZZRIGT( KE ) - ZPRIGT( KE ) ) * YYN( IE )                          2404
2405    163    C      UUU = UGRAD( ISR , 1 ) * XX + UGRAD( ISR , 2 ) * YY                       2405
2406    164    C      VVV = VGRAD( ISR , 1 ) * XX + VGRAD( ISR , 2 ) * YY                       2406
2407    165    C      UVU = UUU * XXN( IE ) + VVV * YYN( IE )                                   2407
2408    166    C      PPP = PGRAD( ISR , 1 ) * XX + PGRAD( ISR , 2 ) * YY                       2408
2409    167    C      UPRGT = - .5 * ( UVU + PPP / SQGMTR( KE ) ) / SQGMTR( KE )                2409
2410    168    C      END IF                                                                    2410
2411    169    C                                                                                2411
2412    170    C      URRGT = 0.                                                                2412
2413    171    C      IF( UVRIGT( KE ) . LT . 0. ) THEN                                         2413
2414    172    C      XX = ( ZZRIGT( KE ) - ZORIGT( KE ) ) * XXN( IE )                          2414
2415    173    C      YY = ( ZZRIGT( KE ) - ZORIGT( KE ) ) * YYN( IE )                          2415
2416    174    C      PPP = PGRAD( ISR , 1 ) * XX + PGRAD( ISR , 2 ) * YY                       2416
2417    175    C      XX = XMIDL( IE ) + ZORIGT( KE ) * XXN( IE ) - XS( 1 , ISR )               2417
2418    176    C      YY = YMIDL( IE ) + ZORIGT( KE ) * YYN( IE ) - XS( 2 , ISR )               2418
2419    177    C      RRRR = HYDV( ISR , 1 ) +                                                  2419
2420    178    C     .       RGRAD( ISR , 1 ) * XX + RGRAD( ISR , 2 ) * YY                      2420
2421    179    C      URRGT = PPP / GMTRGT + 1. / HRRR - 1. / RRRR                              2421
2422    180    C      END IF                                                                    2422
2423    181    C                                                                                2423
2424    182          ELSE                                                                       2424
2425    183    C                                                                                2425
2426    184           HRRR =  HRRL                                                              2426
2427    185           HUUR =  HUUL                                                              2427
2428    186           HVVR =  HVVL                                                              2428
2429    187           HPPR =  HPPL                                                              2429
2430    188    C                                                                                2430
2431    189    C      UPRGT = UMLFT                                                             2431
2432    190    C      URRGT = URLFT                                                             2432
2433    191    C                                                                                2433
2434    192          END IF                                                                     2434
2435    193    C                                                                                2435
2436    194          RRL( KE ) = HRRL                                                           2436
2437    195          UUL( KE ) =   HUUL * XN( IE ) + HVVL * YN( IE )                            2437
2438    196          VVL( KE ) = - HUUL * YN( IE ) + HVVL * XN( IE )                            2438
2439    197          PPL( KE ) = HPPL                                                           2439
2440    198    C                                                                                2440
2441    199          RRR( KE ) = HRRR                                                           2441
2442    200          UUR( KE ) =   HUUR * XN( IE ) + HVVR * YN( IE )                            2442
2443    201          VVR( KE ) = - HUUR * YN( IE ) + HVVR * XN( IE )                            2443
2444    202          PPR( KE ) = HPPR                                                           2444
2445    203    C                                                                                2445
2446    204    C      UMLEFT( KE ) = UMLFT                                                      2446
2447    205    C      URLEFT( KE ) = URLFT                                                      2447
2448    206    C                                                                                2448
2449    207    C      UPRIGT( KE ) = UPRGT                                                      2449
2450    208    C      URRIGT( KE ) = URRGT                                                      2450
2451    209    C                                                                                2451
2452    210     160  CONTINUE                                                                  2452
2453    211    C                                                                                2453
2454    212    C  FINAL VALUES FOR RIGHT AND LEFT STATES                                        2454
2455    213    C                                                                                2455
2456    214    C      DO 180 KE = 1 , NOFVEE( INE )                                             2456
2457    215    C                                                                                2457
2458    216    C       GMTLFT = SQGMTL( KE ) * SQGMTL( KE )                                     2458
2459    217    C       GMTRGT = SQGMTR( KE ) * SQGMTR( KE )                                     2459
```

```
2460    218   C                                                                2460
2461    219   C       RRL( KE ) = 1. / ( 1. / RRL( KE ) - ( UMLEFT( KE ) +    2461
2462    220   C     .                                        URLEFT( KE ) ) )  2462
2463    221   C       UUL( KE ) = UUL( KE ) - SQGMTL( KE ) * UMLEFT( KE )      2463
2464    222   C       PPL( KE ) = PPL( KE ) + GMTLFT * UMLEFT( KE )            2464
2465    223   C                                                                2465
2466    224   C       RRR( KE ) = 1. / ( 1. / RRR( KE ) - ( UPRIGT( KE ) +    2466
2467    225   C     .                                        URRIGT( KE ) ) )  2467
2468    226   C       UUR( KE ) = UUR( KE ) + SQGMTR( KE ) * UPRIGT( KE )      2468
2469    227   C       PPR( KE ) = PPR( KE ) + GMTRGT * UPRIGT( KE )            2469
2470    228   C                                                                2470
2471    229   C 180  CONTINUE                                                  2471
2472    230   C                                                                2472
2473    231         DO 200 IE = NE1 , NE2                                      2473
2474    232            KE = IE - NE1 + 1                                       2474
2475    233   C                                                                2475
2476    234          ISL = JE( 3 , IE )                                        2476
2477    235          ISR = JE( 4 , IE )                                        2477
2478    236   C                                                                2478
2479    237          IJE5 = JE( 5 , IE )                                       2479
2480    238   C                                                                2480
2481    239   C --- PROJECTED VALUES ON THE LEFT SIDE OF THE INTERFACE ---------2481
2482    240   C                                                                2482
2483    241          RL( IE ) = RRL( KE )                                      2483
2484    242          UL( IE ) = UUL( KE )                                      2484
2485    243          VL( IE ) = VVL( KE )                                      2485
2486    244          PL( IE ) = PPL( KE )                                      2486
2487    245   C                                                                2487
2488    246   C --- PROJECTED VALUES ON THE RIGHT SIDE OF THE INTERFACE --------2488
2489    247   C                                                                2489
2490    248   C --- EDGES IN THE COMPUTATIONAL DOMAIN -------------------------2490
2491    249   C                                                                2491
2492    250         IF( IJE5 . EQ . 0 ) THEN                                   2492
2493    251            RR( IE ) = RRR( KE )                                    2493
2494    252            UR( IE ) = UUR( KE )                                    2494
2495    253            VR( IE ) = VVR( KE )                                    2495
2496    254            PR( IE ) = PPR( KE )                                    2496
2497    255   C                                                                2497
2498    256   C --- EDGES ON THE BOUNDARY -------------------------------------2498
2499    257   C                                                                2499
2500    258         ELSEIF( IJE5 . EQ . 8 ) THEN                               2500
2501    259            RR( IE ) =   RIN                                        2501
2502    260            UR( IE ) =   UIN * XN( IE ) + VIN * YN( IE )            2502
2503    261            VR( IE ) = - UIN * YN( IE ) + VIN * XN( IE )            2503
2504    262            PR( IE ) =   PIN                                        2504
2505    263   C                                                                2505
2506    264         ELSEIF( IJE5 . EQ . 7 ) THEN                               2506
2507    265            RR( IE ) = RL( IE )                                     2507
2508    266            UR( IE ) = UL( IE )                                     2508
2509    267            VR( IE ) = VL( IE )                                     2509
2510    268            PR( IE ) = PL( IE )                                     2510
2511    269   C                                                                2511
2512    270         ELSEIF( IJE5 . EQ . 6 . OR . IJE5 . EQ . 5 ) THEN          2512
2513    271            RR( IE ) = RL( IE )                                     2513
2514    272            UR( IE ) = - UL( IE )                                   2514
2515    273            VR( IE ) = VL( IE )                                     2515
2516    274            PR( IE ) = PL( IE )                                     2516
2517    275   C                                                                2517
2518    276         END IF                                                     2518
2519    277    200  CONTINUE                                                  2519
2520    278   C                                                                2520
2521    279         NE1 = NE2 + 1                                              2521
2522    280         NE2 = NE2 + NOFVEE( INE + 1 )                              2522
2523    281    90   CONTINUE                                                  2523
2524    282   C                                                                2524
2525    283   C*****************************************************************2525
2526    284   C                                                                2526
2527    285   C --- EXIT POINT FROM SUBROUTINE --------------------------------2527
2528    286   C                                                                2528
2529    287   C     ------                                                     2529
2530    288         RETURN                                                     2530
2531    289   C     ------                                                     2531
2532    290   C                                                                2532
2533    291   C     ---                                                        2533
```

```
2534    292       END                                                          2534
```



```
2535      1       SUBROUTINE PRLCTN                                            2535
2536      2 C                                                                  2536
2537      3 C-----------------------------------------------------------------I 2537
2538      4 C                                                                 I 2538
2539      5 C     PRLCTN INITIALIZE PARTICLES LOCATION IN THE COMPUTATION     I 2539
2540      6 C           DOMAIN FOR THE FIRST TIME                             I 2540
2541      7 C                                                                 I 2541
2542      8 C-----------------------------------------------------------------I 2542
2543      9 C                                                                  2543
2544     10       include     'cmsh00.h'                                       2544
2545     11       include     'chyd00.h'                                       2545
2546     12       include     'cint00.h'                                       2546
2547     13       include     'cphs10.h'                                       2547
2548     14       include     'cphs20.h'                                       2548
2549     15 C                                                                  2549
2550     16 C=================================================================2550
2551     17 C                                                                  2551
2552     18       IPT = 0                                                      2552
2553     19       DO 110 IPRTCL = 1 , NPT                                      2553
2554     20 C                                                                  2554
2555     21       IDUM = 0                                                     2555
2556     22       DO 130 IS = 1 , NS                                           2556
2557     23       IF( IDUM . EQ . 0 ) THEN                                     2557
2558     24 C                                                                  2558
2559     25       IV1 = JS( 1 , IS )                                           2559
2560     26       IV2 = JS( 2 , IS )                                           2560
2561     27       IV3 = JS( 3 , IS )                                           2561
2562     28 C                                                                  2562
2563     29       X1 = XV( 1 , IV1 )                                           2563
2564     30       Y1 = XV( 2 , IV1 )                                           2564
2565     31       X2 = XV( 1 , IV2 )                                           2565
2566     32       Y2 = XV( 2 , IV2 )                                           2566
2567     33 C                                                                  2567
2568     34       XX = ( X2 - X1 )                                             2568
2569     35       XXP = ( XPRTCL( 1 , IPRTCL ) - X1 )                          2569
2570     36 C                                                                  2570
2571     37       YY = ( Y2 - Y1 )                                             2571
2572     38       YYP = ( XPRTCL( 2 , IPRTCL ) - Y1 )                          2572
2573     39 C                                                                  2573
2574     40       A1 = XX * YYP - YY * XXP                                     2574
2575     41 C                                                                  2575
2576     42       X1 = XV( 1 , IV2 )                                           2576
2577     43       Y1 = XV( 2 , IV2 )                                           2577
2578     44       X2 = XV( 1 , IV3 )                                           2578
2579     45       Y2 = XV( 2 , IV3 )                                           2579
2580     46 C                                                                  2580
2581     47       XX = ( X2 - X1 )                                             2581
2582     48       XXP = ( XPRTCL( 1 , IPRTCL ) - X1 )                          2582
2583     49 C                                                                  2583
2584     50       YY = ( Y2 - Y1 )                                             2584
2585     51       YYP = ( XPRTCL( 2 , IPRTCL ) - Y1 )                          2585
2586     52 C                                                                  2586
2587     53       A2 = XX * YYP - YY * XXP                                     2587
2588     54 C                                                                  2588
2589     55       X1 = XV( 1 , IV3 )                                           2589
2590     56       Y1 = XV( 2 , IV3 )                                           2590
2591     57       X2 = XV( 1 , IV1 )                                           2591
2592     58       Y2 = XV( 2 , IV1 )                                           2592
2593     59 C                                                                  2593
2594     60       XX = ( X2 - X1 )                                             2594
2595     61       XXP = ( XPRTCL( 1 , IPRTCL ) - X1 )                          2595
2596     62 C                                                                  2596
2597     63       YY = ( Y2 - Y1 )                                             2597
2598     64       YYP = ( XPRTCL( 2 , IPRTCL ) - Y1 )                          2598
2599     65 C                                                                  2599
2600     66       A3 = XX * YYP - YY * XXP                                     2600
2601     67 C                                                                  2601
2602     68       IA1 = INT( SIGN( 1.1 , A1 ) )                                2602
2603     69       IA2 = INT( SIGN( 1.1 , A2 ) )                                2603
2604     70       IA3 = INT( SIGN( 1.1 , A3 ) )                                2604
```

```
2605      71          IAJ = IA1 + IA2 + IA3                                    2605
2606      72    C                                                              2606
2607      73          IF( IAJ . EQ . 3 )  THEN                                 2607
2608      74          IPT = IPT + 1                                            2608
2609      75          IJKPRT( IPT ) = IS                                       2609
2610      76          XPRTCL( 1 , IPT ) = XPRTCL( 1 , IPRTCL )                 2610
2611      77          XPRTCL( 2 , IPT ) = XPRTCL( 2 , IPRTCL )                 2611
2612      78    C      PRINT *, XPRTCL(1,IPT),XPRTCL(2,IPT),IJKPRT(IPT)        2612
2613      79          IDUM = 1                                                 2613
2614      80          END IF                                                   2614
2615      81          END IF                                                   2615
2616      82    C                                                              2616
2617      83     130  CONTINUE                                                 2617
2618      84     110  CONTINUE                                                 2618
2619      85          NPT = IPT                                                2619
2620      86    C       PRINT *,   NPT,(XPRTCL(1,IPT),XPRTCL(2,IPT),IPT=1,NPT) 2620
2621      87    C       WRITE (10.*)  NPT,(XPRTCL(1,IPT),XPRTCL(2,IPT),IPT=1,NPT) 2621
2622      88    C                                                              2622
2623      89    C                                                              2623
2624      90    C --- EXIT POINT FROM SUBROUTINE -----------------------------------  2624
2625      91    C                                                              2625
2626      92    C     ------                                                   2626
2627      93          RETURN                                                   2627
2628      94    C     ------                                                   2628
2629      95    C                                                              2629
2630      96    C     ---                                                      2630
2631      97          END                                                      2631
```



```
2632       1          SUBROUTINE PRPTHC                                        2632
2633       2    C                                                              2633
2634       3    C---------------------------------------------------------------I  2634
2635       4    C                                                              I  2635
2636       5    C      PRPTHC TRACE PARTICLES PATH IN THE COMPUTATION DOMAIN    I  2636
2637       6    C                                                              I  2637
2638       7    C---------------------------------------------------------------I  2638
2639       8    C                                                              2639
2640       9          include     'cmsh00.h'                                   2640
2641      10          include     'chyd00.h'                                   2641
2642      11          include     'cint00.h'                                   2642
2643      12          include     'cphs10.h'                                   2643
2644      13          include     'cphs20.h'                                   2644
2645      14    C                                                              2645
2646      15          DO 110 IPRTCL = 1 , NPT                                  2646
2647      16          KFIND = 0                                                2647
2648      17    C                                                              2648
2649      18          DO 110 IK = 1 , 3                                        2649
2650      19          KFIND = 0                                                2650
2651      20          IJE5 = 0                                                 2651
2652      21          IS = IJKPRT( IPRTCL )                                    2652
2653      22          XP = XPRTCL( 1 , IPRTCL )                                2653
2654      23          YP = XPRTCL( 2 , IPRTCL )                                2654
2655      24    C                                                              2655
2656      25          DO 120 IJ = 1 , 3                                        2656
2657      26          IE = JS( IJ + 3 , IS )                                   2657
2658      27    C                                                              2658
2659      28          IF( IE . GT . 0 ) THEN                                   2659
2660      29    C                                                              2660
2661      30          IV1 = JE( 1 , IE )                                       2661
2662      31          IV2 = JE( 2 , IE )                                       2662
2663      32    C                                                              2663
2664      33          X1 = XV( 1 , IV1 )                                       2664
2665      34          Y1 = XV( 2 , IV1 )                                       2665
2666      35          X2 = XV( 1 , IV2 )                                       2666
2667      36          Y2 = XV( 2 , IV2 )                                       2667
2668      37    C                                                              2668
2669      38          XX = ( X2 - X1 )                                         2669
2670      39          XXP = ( XP - X1 )                                        2670
2671      40    C                                                              2671
2672      41          YY = ( Y2 - Y1 )                                         2672
2673      42          YYP = ( YP - Y1 )                                        2673
2674      43    C                                                              2674
2675      44          A = XX * YYP - YY * XXP                                  2675
```

```
2676      45          IF( A . LT . 0. )  THEN                                    2676
2677      46          IJKPRT( IPRTCL ) = JE( 4 , IE )                            2677
2678      47          IJE5 = JE( 5 , IE )                                        2678
2679      48          XREV = 1. / XE( 1 , IE )                                   2679
2680      49          KFIND = KFIND + 1                                          2680
2681      50          END IF                                                     2681
2682      51    C                                                                2682
2683      52          ELSE                                                       2683
2684      53    C                                                                2684
2685      54          IV1 = JE( 2 , - IE )                                       2685
2686      55          IV2 = JE( 1 , - IE )                                       2686
2687      56    C                                                                2687
2688      57          X1 = XV( 1 , IV1 )                                         2688
2689      58          Y1 = XV( 2 , IV1 )                                         2689
2690      59          X2 = XV( 1 , IV2 )                                         2690
2691      60          Y2 = XV( 2 , IV2 )                                         2691
2692      61    C                                                                2692
2693      62          XX = ( X2 - X1 )                                           2693
2694      63          XXP = ( XP - X1 )                                          2694
2695      64    C                                                                2695
2696      65          YY = ( Y2 - Y1 )                                           2696
2697      66          YYP = ( YP - Y1 )                                          2697
2698      67    C                                                                2698
2699      68          A = XX * YYP - YY * XXP                                    2699
2700      69          IF( A . LT . 0. )  THEN                                    2700
2701      70          IJKPRT( IPRTCL ) = JE( 3 , - IE )                          2701
2702      71          IJE5 = JE( 5 , - IE )                                      2702
2703      72          XREV = 1. / XE( 1 , - IE )                                 2703
2704      73          KFIND = KFIND + 1                                          2704
2705      74          END IF                                                     2705
2706      75          END IF                                                     2706
2707      76    C                                                                2707
2708      77     120  CONTINUE                                                   2708
2709      78    C                                                                2709
2710      79          IF( KFIND . GT . 0 . AND . IJE5 . NE . 0 ) THEN            2710
2711      80          IJKPRT( IPRTCL ) = IS                                      2711
2712      81    C                                                                2712
2713      82          AA = X2 - X1                                               2713
2714      83          BB = Y2 - Y1                                               2714
2715      84          CC = XP - X1                                               2715
2716      85          DD = YP - Y1                                               2716
2717      86          TREV = ( CC * AA + DD * BB ) * XREV * XREV                 2717
2718      87          IF( BB . NE . 0. ) THEN                                    2718
2719      88          XPRTCP = X1 + TREV * AA                                    2719
2720      89          XPRTCL( 1 , IPRTCL ) = XP + 1.1 * ( XPRTCP - XP )          2720
2721      90          END IF                                                     2721
2722      91          IF( AA . NE . 0. ) THEN                                    2722
2723      92          YPRTCP = Y1 + TREV * BB                                    2723
2724      93          XPRTCL( 2 , IPRTCL ) = YP + 1.1 * ( YPRTCP - YP )          2724
2725      94          END IF                                                     2725
2726      95    C                                                                2726
2727      96          END IF                                                     2727
2728      97     110  CONTINUE                                                   2728
2729      98    C                                                                2729
2730      99          DO 180 IPRTCL = 1 , NPT                                    2730
2731     100    C                                                                2731
2732     101          IS = IJKPRT( IPRTCL )                                      2732
2733     102          UPRTCL = HYDV( IS , 2 )                                    2733
2734     103          VPRTCL = HYDV( IS , 3 )                                    2734
2735     104    C                                                                2735
2736     105          XPRTCL( 1 , IPRTCL ) = XPRTCL( 1 , IPRTCL ) + UPRTCL * DTT 2736
2737     106          XPRTCL( 2 , IPRTCL ) = XPRTCL( 2 , IPRTCL ) + VPRTCL * DTT 2737
2738     107          WPRTCL( 1 , IPRTCL ) = UPRTCL                              2738
2739     108          WPRTCL( 2 , IPRTCL ) = VPRTCL                              2739
2740     109    C                                                                2740
2741     110          DO 180 IK = 1 , 3                                          2741
2742     111          IS = IJKPRT( IPRTCL )                                      2742
2743     112          XP = XPRTCL( 1 , IPRTCL )                                  2743
2744     113          YP = XPRTCL( 2 , IPRTCL )                                  2744
2745     114          KFIND = 0                                                  2745
2746     115          IJE5 = 0                                                   2746
2747     116    C                                                                2747
2748     117          DO 170 IJ = 1 , 3                                          2748
2749     118          IE = JS( IJ + 3 , IS )                                     2749
```

```
2750     119   C                                                                2750
2751     120         IF( IE . GT . 0 ) THEN                                     2751
2752     121   C                                                                2752
2753     122         IV1 = JE( 1 , IE )                                         2753
2754     123         IV2 = JE( 2 , IE )                                         2754
2755     124   C                                                                2755
2756     125         X1 = XV( 1 , IV1 )                                         2756
2757     126         Y1 = XV( 2 , IV1 )                                         2757
2758     127         X2 = XV( 1 , IV2 )                                         2758
2759     128         Y2 = XV( 2 , IV2 )                                         2759
2760     129   C                                                                2760
2761     130         XX = ( X2 - X1 )                                           2761
2762     131         XXP = ( XP - X1 )                                          2762
2763     132   C                                                                2763
2764     133         YY = ( Y2 - Y1 )                                           2764
2765     134         YYP = ( YP - Y1 )                                          2765
2766     135   C                                                                2766
2767     136         A = XX * YYP - YY * XXP                                    2767
2768     137         IF( A . LT . 0. )  THEN                                    2768
2769     138         IJKPRT( IPRTCL ) = JE( 4 , IE )                            2769
2770     139         IJE5 = JE( 5 , IE )                                        2770
2771     140         XREV = 1. / XE( 1 , IE )                                   2771
2772     141         KFIND = KFIND + 1                                          2772
2773     142         END IF                                                     2773
2774     143   C                                                                2774
2775     144         ELSE                                                       2775
2776     145   C                                                                2776
2777     146         IV1 = JE( 2 , - IE )                                       2777
2778     147         IV2 = JE( 1 , - IE )                                       2778
2779     148   C                                                                2779
2780     149         X1 = XV( 1 , IV1 )                                         2780
2781     150         Y1 = XV( 2 , IV1 )                                         2781
2782     151         X2 = XV( 1 , IV2 )                                         2782
2783     152         Y2 = XV( 2 , IV2 )                                         2783
2784     153   C                                                                2784
2785     154         XX = ( X2 - X1 )                                           2785
2786     155         XXP = ( XP - X1 )                                          2786
2787     156   C                                                                2787
2788     157         YY = ( Y2 - Y1 )                                           2788
2789     158         YYP = ( YP - Y1 )                                          2789
2790     159   C                                                                2790
2791     160         A = XX * YYP - YY * XXP                                    2791
2792     161         IF( A . LT . 0. )  THEN                                    2792
2793     162         IJKPRT( IPRTCL ) = JE( 3 , - IE )                          2793
2794     163         IJE5 = JE( 5 , - IE )                                      2794
2795     164         XREV = 1. / XE( 1 , - IE )                                 2795
2796     165         KFIND = KFIND + 1                                          2796
2797     166         END IF                                                     2797
2798     167   C                                                                2798
2799     168         END IF                                                     2799
2800     169    170  CONTINUE                                                   2800
2801     170   C                                                                2801
2802     171         IF( KFIND . GT . 0 . AND . IJE5 . NE . 0 ) THEN            2802
2803     172         IJKPRT( IPRTCL ) = IS                                      2803
2804     173   C                                                                2804
2805     174         AA = X2 - X1                                               2805
2806     175         BB = Y2 - Y1                                               2806
2807     176         CC = XP - X1                                               2807
2808     177         DD = YP - Y1                                               2808
2809     178         TREV = ( CC * AA + DD * BB ) * XREV * XREV                 2809
2810     179         IF( BB . NE . 0. ) THEN                                    2810
2811     180         XPRTCP = X1 + TREV * AA                                    2811
2812     181         XPRTCL( 1 , IPRTCL ) = XP + 1.1 * ( XPRTCP - XP )          2812
2813     182         END IF                                                     2813
2814     183         IF( AA . NE . 0. ) THEN                                    2814
2815     184         YPRTCP = Y1 + TREV * BB                                    2815
2816     185         XPRTCL( 2 , IPRTCL ) = YP + 1.1 * ( YPRTCP - YP )          2816
2817     186         END IF                                                     2817
2818     187   C                                                                2818
2819     188         END IF                                                     2819
2820     189    180  CONTINUE                                                   2820
2821     190   C                                                                2821
2822     191   C                                                                2822
2823     192   C --- EXIT POINT FROM SUBROUTINE ----------------------------------- 2823
```

```
 2824     193   C
 2825     194   C     ------
 2826     195         RETURN
 2827     196   C     ------
 2828     197   C
 2829     198   C     ---
 2830     199         END
```

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#	routine	page
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```
      SUBROUTINE VERCEN( IT )
C
C-----------------------------------------------------------------I
C                                                                 I
C       VERCEN ADD A VERTEX IN THE IT TRIANGLE. THE VERTEX        I
C       IS ADDED IN THE CENTROID OF THE TRIANGLE.                 I
C                                                                 I
C-----------------------------------------------------------------I
C
          IMPLICIT REAL (A-H,O-Z)
C
      include     'cmsh00.h'
      include     'chyd00.h'
      include     'cint00.h'
      include     'cphs10.h'
      include     'cphs20.h'
C
C       SET UP THE NEW TRIANGLE BOOKKEEPING.
C
          IV1 = JS( 1 , IT )
          IV2 = JS( 2 , IT )
          IV3 = JS( 3 , IT )
C
          IE1 = JS( 4 , IT )
          IE2 = JS( 5 , IT )
          IE3 = JS( 6 , IT )
          IE1A = IABS( IE1 )
          IE2A = IABS( IE2 )
          IE3A = IABS( IE3 )
C
C       PUT IN NEW TRIANGLES
C
          NV = NV + 1
          XV( 1 , NV ) = ( XV( 1 , IV1 ) + XV( 1 , IV2 ) +
     .                                     XV( 1 , IV3 ) ) * THIRD
          XV( 2 , NV ) = ( XV( 2 , IV1 ) + XV( 2 , IV2 ) +
     .                                     XV( 2 , IV3 ) ) * THIRD
          JV( 1 , NV ) = 0
C
          DO 110 IR = 1 , MHQ
          HYDVVV( NV , IR ) = ( HYDVVV( IV1 , IR ) +
     .                          HYDVVV( IV2 , IR ) +
     .                          HYDVVV( IV3 , IR ) ) * THIRD
110       CONTINUE
C
          NE = NE + 1
          JE( 1 , NE ) = NV
          JE( 2 , NE ) = IV1
          JE( 5 , NE ) = 0
          NE = NE + 1
          JE( 1 , NE ) = NV
          JE( 2 , NE ) = IV2
          JE( 5 , NE ) = 0
          NE = NE + 1
          JE( 1 , NE ) = NV
          JE( 2 , NE ) = IV3
          JE( 5 , NE ) = 0
          NEM1 = NE - 1
          NEM2 = NE - 2
C
C         TRIANGLE ONE, THE ORIGINAL IT.
C
          JS( 3 , IT ) = NV
          JS( 5 , IT ) = - NEM1
          JS( 6 , IT ) = NEM2
C
C         TRIANGLE TWO.
C
          NS = NS + 1
          JS( 1 , NS ) = IV2
          JS( 2 , NS ) = IV3
          JS( 3 , NS ) = NV
          JS( 4 , NS ) = IE2
```

```
                JS( 5 , NS ) = - NE
                JS( 6 , NS ) = NEM1
C
C       TRIANGLE THREE.
C
                NS = NS + 1
                JS( 1 , NS ) = IV3
                JS( 2 , NS ) = IV1
                JS( 3 , NS ) = NV
                JS( 4 , NS ) = IE3
                JS( 5 , NS ) = - NEM2
                JS( 6 , NS ) = NE
C
C       NOW FIX THE LEFT AND RIGHT FOR EDGES.
C
                NSM1 = NS - 1
                IF( JE( 4 , IE2A ) . EQ . IT ) JE( 4 , IE2A ) = NSM1
                IF( JE( 3 , IE2A ) . EQ . IT ) JE( 3 , IE2A ) = NSM1
                IF( JE( 4 , IE3A ) . EQ . IT ) JE( 4 , IE3A ) = NS
                IF( JE( 3 , IE3A ) . EQ . IT ) JE( 3 , IE3A ) = NS
                JE( 4 , NEM2 ) = NS
                JE( 3 , NEM2 ) = IT
                JE( 4 , NEM1 ) = IT
                JE( 3 , NEM1 ) = NSM1
                JE( 4 , NE ) = NSM1
                JE( 3 , NE ) = NS
C
                JV( 2 , NV ) = NE
C
                XSAREA = XS( 3 , IT ) * THIRD
                XS( 3 , IT ) = XSAREA
                XS( 3 , NSM1 ) = XSAREA
                XS( 3 , NS ) = XSAREA
C
                XS( 1 , IT ) = ( XV( 1 , IV1 ) + XV( 1 , IV2 ) +
     .                           XV( 1 , NV ) ) * THIRD
                XS( 1 , NSM1 ) = ( XV( 1 , IV2 ) + XV( 1 , IV3 ) +
     .                             XV( 1 , NV ) ) * THIRD
                XS( 1 , NS ) = ( XV( 1 , IV3 ) + XV( 1 , IV1 ) +
     .                           XV( 1 , NV ) ) * THIRD
                XS( 2 , IT ) = ( XV( 2 , IV1 ) + XV( 2 , IV2 ) +
     .                           XV( 2 , NV ) ) * THIRD
                XS( 2 , NSM1 ) = ( XV( 2 , IV2 ) + XV( 2 , IV3 ) +
     .                             XV( 2 , NV ) ) * THIRD
                XS( 2 , NS ) = ( XV( 2 , IV3 ) + XV( 2 , IV1 ) +
     .                           XV( 2 , NV ) ) * THIRD
C
                XSAREA = 1. / XS( 3 , IT )
                SAREA( IT ) = XSAREA
                SAREA( NS ) = XSAREA
                SAREA( NSM1 ) = XSAREA
C
                DO 630 IR = 1 , MHQ
                HYDV( IT , IR ) = ( HYDVVV( IV1 , IR ) +
     .                              HYDVVV( IV2 , IR ) +
     .                              HYDVVV( NV , IR ) ) * THIRD
                HYDV( NS , IR ) = ( HYDVVV( IV3 , IR ) +
     .                              HYDVVV( IV1 , IR ) +
     .                              HYDVVV( NV , IR ) ) * THIRD
                HYDV( NSM1 , IR ) = ( HYDVVV( IV2 , IR ) +
     .                                HYDVVV( IV3 , IR ) +
     .                                HYDVVV( NV , IR ) ) * THIRD
630             CONTINUE
C
                HDUM          = 1. / ( HYDV( IT , 1 ) + 1.E-12 )
                HYDV( IT , 2 ) = HYDV( IT , 2 ) * HDUM
                HYDV( IT , 3 ) = HYDV( IT , 3 ) * HDUM
                HYDV( IT , 4 ) = ( HYDV( IT , 4 )  -
     .                          .5 * HYDV( IT , 1 ) *
     .          ( HYDV( IT , 2 ) * HYDV( IT , 2 ) +
     .            HYDV( IT , 3 ) * HYDV( IT , 3 ) ) ) *
     .                           ( HYDV( IT , 5 ) - 1. )
C
                HDUM          = 1. / ( HYDV( NS , 1 ) + 1.E-12 )
```

```
148  148           HYDV( NS , 2 ) = HYDV( NS , 2 ) * HDUM                          148
149  149           HYDV( NS , 3 ) = HYDV( NS , 3 ) * HDUM                          149
150  150           HYDV( NS , 4 ) = ( HYDV( NS , 4 )  -                            150
151  151     .                       .5 * HYDV( NS , 1 ) *                         151
152  152     .     ( HYDV( NS , 2 ) * HYDV( NS , 2 ) +                             152
153  153     .       HYDV( NS , 3 ) * HYDV( NS , 3 ) ) ) *                         153
154  154     .                        ( HYDV( NS , 5 ) - 1. )                      154
155  155     C                                                                     155
156  156           HDUM              = 1. / ( HYDV( NSM1 , 1 ) + 1.E-12 )          156
157  157           HYDV( NSM1 , 2 ) = HYDV( NSM1 , 2 ) * HDUM                      157
158  158           HYDV( NSM1 , 3 ) = HYDV( NSM1 , 3 ) * HDUM                      158
159  159           HYDV( NSM1 , 4 ) = ( HYDV( NSM1 , 4 )  -                        159
160  160     .                       .5 * HYDV( NSM1 , 1 ) *                       160
161  161     .     ( HYDV( NSM1 , 2 ) * HYDV( NSM1 , 2 ) +                         161
162  162     .       HYDV( NSM1 , 3 ) * HYDV( NSM1 , 3 ) ) ) *                     162
163  163     .                        ( HYDV( NSM1 , 5 ) - 1. )                    163
164  164     C                                                                     164
165  165           DO 114 IR = 1 , 2                                               165
166  166           RGRAD( NS , IR ) = RGRAD( IT , IR )                             166
167  167           RGRAD( NSM1 , IR ) = RGRAD( IT , IR )                           167
168  168     C                                                                     168
169  169           UGRAD( NS , IR ) = UGRAD( IT , IR )                             169
170  170           UGRAD( NSM1 , IR ) = UGRAD( IT , IR )                           170
171  171     C                                                                     171
172  172           VGRAD( NS , IR ) = VGRAD( IT , IR )                             172
173  173           VGRAD( NSM1 , IR ) = VGRAD( IT , IR )                           173
174  174     C                                                                     174
175  175           PGRAD( NS , IR ) = PGRAD( IT , IR )                             175
176  176           PGRAD( NSM1 , IR ) = PGRAD( IT , IR )                           176
177  177     114   CONTINUE                                                        177
178  178     C                                                                     178
179  179           JEN( 1 ) = IE1A                                                 179
180  180           JEN( 2 ) = IE2A                                                 180
181  181           JEN( 3 ) = IE3A                                                 181
182  182           JEN( 4 ) = NEM2                                                 182
183  183           JEN( 5 ) = NEM1                                                 183
184  184           JEN( 6 ) = NE                                                   184
185  185     C                                                                     185
186  186           DO 30 IENN = 1 , 6                                              186
187  187           IEN = JEN( IENN )                                               187
188  188           JV1 = JE( 1 , IEN )                                             188
189  189           JV2 = JE( 2 , IEN )                                             189
190  190           AX = XV( 1 , JV2 ) - XV( 1 , JV1 )                              190
191  191           AY = XV( 2 , JV2 ) - XV( 2 , JV1 )                              191
192  192           XE( 1 , IEN ) = SQRT( AX * AX + AY * AY )                       192
193  193           XEREV = 1. / XE( 1 , IEN )                                      193
194  194           XN( IEN ) = AY * XEREV                                          194
195  195           YN( IEN ) = - AX * XEREV                                        195
196  196           ISSR = JE( 4 , IEN )                                            196
197  197           ISSL = JE( 3 , IEN )                                            197
198  198     C                                                                     198
199  199         IJE5 = JE( 5 , IEN )                                              199
200  200         IF( IJE5 . NE . 0 ) THEN                                          200
201  201     C                                                                     201
202  202           AA = XV( 1 , JV2 ) - XV( 1 , JV1 )                              202
203  203           BB = XV( 2 , JV2 ) - XV( 2 , JV1 )                              203
204  204           XEL = XS( 1 , ISSL )                                            204
205  205           YEL = XS( 2 , ISSL )                                            205
206  206           CC = XEL - XV( 1 , JV1 )                                        206
207  207           DD = YEL - XV( 2 , JV1 )                                        207
208  208           EE = ( AA * CC + BB * DD ) * XEREV * XEREV                      208
209  209           XER = XV( 1 , JV1 ) + AA * EE                                   209
210  210           YER = XV( 2 , JV1 ) + BB * EE                                   210
211  211           AX = XER - XEL                                                  211
212  212           AY = YER - YEL                                                  212
213  213           XE( 2 , IEN ) = SQRT( AX * AX + AY * AY )                       213
214  214           XEREV = 1. / XE( 2 , IEN )                                      214
215  215           XXN( IEN ) = AX * XEREV                                         215
216  216           YYN( IEN ) = AY * XEREV                                         216
217  217           XE( 2 , IEN ) = 2. * XE( 2 , IEN )                              217
218  218           XYMIDL( IEN ) = .5                                              218
219  219           XMIDL( IEN ) = XER                                              219
220  220           YMIDL( IEN ) = YER                                              220
221  221     C                                                                     221
```

```
222  222            ELSE                                                    222
223  223  C                                                                 223
224  224            XER = XS( 1 , ISSR )                                    224
225  225            YER = XS( 2 , ISSR )                                    225
226  226            XEL = XS( 1 , ISSL )                                    226
227  227            YEL = XS( 2 , ISSL )                                    227
228  228  C                                                                 228
229  229            AA = XV( 1 , JV2 ) - XV( 1 , JV1 )                      229
230  230            BB = XV( 2 , JV2 ) - XV( 2 , JV1 )                      230
231  231            CC = XEL - XER                                          231
232  232            DD = YEL - YER                                          232
233  233            ACA = XER - XV( 1 , JV1 )                               233
234  234            DBD = YER - XV( 2 , JV1 )                               234
235  235            EE = ( ACA * DD - DBD * CC ) / ( AA * DD - BB * CC )    235
236  236            XMIDL( IEN ) = XV( 1 , JV1 ) + AA * EE                  236
237  237            YMIDL( IEN ) = XV( 2 , JV1 ) + BB * EE                  237
238  238  C                                                                 238
239  239            XEMID = XMIDL( IEN ) - XEL                              239
240  240            YEMID = YMIDL( IEN ) - YEL                              240
241  241  C                                                                 241
242  242            AX = XER - XEL                                          242
243  243            AY = YER - YEL                                          243
244  244            XE( 2 , IEN ) = SQRT( AX * AX + AY * AY )               244
245  245            XEREV = 1. / XE( 2 , IEN )                              245
246  246            XXN( IEN ) = AX * XEREV                                 246
247  247            YYN( IEN ) = AY * XEREV                                 247
248  248  C                                                                 248
249  249            XYMIDL( IEN ) = SQRT( XEMID * XEMID + YEMID * YEMID ) * XEREV  249
250  250  C                                                                 250
251  251            END IF                                                  251
252  252  C                                                                 252
253  253   30     CONTINUE                                                  253
254  254  C                                                                 254
255  255  C --- EXIT POINT FROM SUBROUTINE ----------------------   ---------- 255
256  256  C                                                                 256
257  257  C      -----                                                      257
258  258         RETURN                                                     258
259  259  C      ------                                                     259
260  260  C                                                                 260
261  261  C      ---                                                        261
262  262         END                                                        262
```



```
263    1         SUBROUTINE DISECT ( N , IDONE , IDUMP )                   263
264    2  C                                                                264
265    3  C-----------------------------------------------------------------I 265
266    4  C                                                                 I 266
267    5  C         DISECT DISECTS THE LINE N TO CREATE TWO NEW TRIANGLES AND I 267
268    6  C         A NEW VERTEX.  IF THE LINE N IS ON A SOLID BOUNDARY, ONLY I 268
269    7  C         ONE NEW TRIANGLE IS CREATED.                            I 269
270    8  C                                                                 I 270
271    9  C         DISECT CANNOT BE USED FOR PERIODIC SIDES.  HOWEVER, A   I 271
272   10  C         CALL TO TSHIFT CAN BE USED TO MAKE THOSE SIDES INTERNAL I 272
273   11  C         BEFORE CALLING DISECT.                                  I 273
274   12  C                                                                 I 274
275   13  C         INPUT:  N  - THE SIDE TO BE DISECTED.                   I 275
276   14  C                                                                 I 276
277   15  C         OUTPUT: N3 - THE SECOND HALF OF WHAT WAS N.  WHEN N IS  I 277
278   16  C                      DISECTED, THE INDEX N IS RETAINED FOR ONE OF I 278
279   17  C                      THE NEW SIDES, THE OTHER IS N3.            I 279
280   18  C                                                                 I 280
281   19  C                 I1 - THE STARTING VERTEX OF THE INPUT LINE N;   I 281
282   20  C                 I2 - THE ENDING VERTEX OF THE INPUT LINE N;     I 282
283   21  C                 I3 - THE THIRD VERTEX IN THE TRIANGLE TO THE RIGHT; I 283
284   22  C                 I4 - THE THIRD VERTEX IN THE TRIANGLE TO THE LEFT; I 284
285   23  C                 I5 - THE NEW VERTEX.                            I 285
286   24  C                                                                 I 286
287   25  C-----------------------------------------------------------------I 287
288   26  C                                                                 288
289   27            IMPLICIT REAL (A-H,O-Z)                                 289
290   28  C                                                                 290
291   29        include     'cmsh00.h'                                      291
292   30        include     'chyd00.h'                                      292
```

```
      include     'cint00.h'
      include     'cphs10.h'
      include     'cphs20.h'
C
          INTEGER IS(2), IVS(2)
C
          ITRING = 0
          IDONE = 0
          IJE5 = JE( 5 , N )
          IF( IJE5 . NE . 0 ) ITRING = 1
          I5     = 0
          IEROR = 0
          EROR = 1.0E-3
C
C         FIND THE VERTICES OF THE LINE N.
C
          I1 = JE( 1 , N )
          I2 = JE( 2 , N )
          IT1   = JE( 4 , N )
          IT2   = JE( 3 , N )
C
C         FIND THE TWO VERTICES TO WHICH THE NEW LINES WILL BE DRAWN.
C         THESE ARE THE VERTICES OTHER THAN I1 AND I2 IN THE
C         TRIANGLES TO EITHER SIDE OF N.  IVS STORES THE INDEX OF
C         THESE VERTICES AND  IS STORES WHETHER THEY ARE VERTEX 1, 2
C         OR 3 IN THE TRIANGLE IT.
C
          DO 10 I = 1 , 2
             IVS(I) = 0
             IT     = JE( 5-I , N )
             IF( IT . NE . 0 ) THEN
                DO 20 J = 1 , 3
                   IV = JS( J , IT )
                   IF( IV . NE . I1 .AND. IV . NE . I2 ) THEN
                      IVS( I ) = IV
                      IS( I )  = J
                   END IF
20                 CONTINUE
             END IF
10        CONTINUE
          I3  = IVS(1)
          I4  = IVS(2)
          IS1 = IS(1)
          IS2 = IS(2)
C
C     COMPARE OPPOSING ANGLE PAIRS IN THE QUADRILATERAL
C
          IF( ITRING . EQ . 0 ) THEN
          AX = XV( 1 , I3 ) - XV( 1 , I1 )
          AY = XV( 2 , I3 ) - XV( 2 , I1 )
          BX = XV( 1 , I4 ) - XV( 1 , I1 )
          BY = XV( 2 , I4 ) - XV( 2 , I1 )
          CX = XV( 1 , I4 ) - XV( 1 , I2 )
          CY = XV( 2 , I4 ) - XV( 2 , I2 )
          DX = XV( 1 , I3 ) - XV( 1 , I2 )
          DY = XV( 2 , I3 ) - XV( 2 , I2 )
          AI2 = AX * BY - AY * BX
          AI1 = CX * DY - CY * DX
          XLN = XE( 1 , N )
          ROUNDF = EROR * XLN * XLN
          IF( AI2 . LT . ROUNDF . OR . AI1 . LT . ROUNDF ) RETURN
          END IF
C
C         CREATE A NEW VERTEX MIDWAY ON LINE N.
C
          IDONE = 1
          NV      = NV + 1
          I5      = NV
C
C         CHANGE THE LINE N SO THAT IT STARTS AT THE SAME VERTEX,
C         BUT NOW ENDS AT I5.
C
          JE( 2 , N ) = I5
C
```

```
      C        DRAW THE THREE NEW LINES, ALL ENDING AT I5.
      C
               DO 30 I = 1 , 2
                  IF( JE( 5 - I , N ) . NE . 0 ) THEN
               NE           = NE + 1
               JE( 1 , NE ) = IVS( I )
               JE( 2 , NE ) = I5
      C
                    JE( 5 , NE ) = 0
                    IF( I . EQ . 1 ) N1 = NE
                    IF( I . EQ . 2 ) N2 = NE
                  END IF
           30 CONTINUE
      C
      C        WE NEED TO HANDLE THE LINE FROM I2 TO I5 SEPARATELY,
      C        SINCE WE ARE NOT ADDING A LINE TO I2, BUT REPLACING
      C        THE OLD ONE.
      C
               NE           = NE + 1
      C
               JE( 5 , NE )   = JE( 5 , N )
               N3             = NE
               JE( 3 , N3 )   = 0
               JE( 4 , N3 )   = 0
      C
      C        RESET THE OLD TRIANGLES AND SET UP THE NEW TRIANGLES.
      C
      C        N WAS ORIGINALLY DRAWN FROM I1 TO I2 -- NOW FROM I1 TO I5.
      C        N1 IS THE NEW LINE FROM I3 TO I5.
      C        N2 IS THE NEW LINE FROM I4 TO I5.
      C        N3 IS THE NEW LINE FROM I2 TO I5.
      C        NAA IS THE OLD LINE FROM I4 TO I1.
      C        NBB IS THE OLD LINE FROM I1 TO I3.
      C        NCC IS THE OLD LINE FROM I3 TO I2.
      C        NDD IS THE OLD LINE FROM I2 TO I4.
      C        THE DIRECTIONS OF LINES NAA THROUGH NDD ARE NOT
      C            EXPLICITLY USED.
      C
               IF(  IT1 . NE . 0 ) THEN
                  NCC                 = JS( IS1 + 3 , IT1 )
                  JS( IS1 + 3 , IT1 ) = N1
                  J                   = MOD( IS1 , 3 ) + 1
                  IF( JS( J , IT1 ) . NE . I2 ) THEN
                     IEROR = 2
                     J1    = J
                  END IF
                  JS( J , IT1 ) = I5
      C
                 JJ  = MOD( IS1 + 1 , 3 ) + 1
                 NBB = IABS( JS( JJ + 3 , IT1 ) )
      C
                  NS           = NS + 1
                  JS( 1 , NS ) = I2
                  JS( 2 , NS ) = I5
                  JS( 3 , NS ) = I3
                  JS( 4 , NS ) = N3
                  JS( 5 , NS ) = - N1
                  JS( 6 , NS ) = NCC
                  JE( 3 , N3 ) = NS
                  JE( 4 , N1 ) = NS
                  JE( 3 , N1 ) = IT1
                  NCC          = IABS( NCC )
                  IF( JE( 4 , NCC ) . EQ . IT1 ) JE( 4 , NCC ) = NS
                  IF( JE( 3 , NCC ) . EQ . IT1 ) JE( 3 , NCC ) = NS
      C
               END IF
      C
               IF( IT2 . NE . 0 ) THEN
                  J            = MOD( IS2 + 1 , 3 ) + 1
                  NDD          = JS( J + 3 , IT2 )
                  JS( J + 3 , IT2 ) = - N2
                  IF( JS( J , IT2 ) . NE . I2 ) THEN
                     IEROR = 3
                     J2    = J
```

```
441     179               END IF                                                  441
442     180               JS( J , IT2 ) = I5                                      442
443     181   C                                                                   443
444     182              NAA = IABS( JS( IS2 + 3 , IT2 ) )                        444
445     183   C                                                                   445
446     184               NS           = NS + 1                                   446
447     185               JS( 1 , NS ) = I2                                       447
448     186               JS( 2 , NS ) = I4                                       448
449     187               JS( 3 , NS ) = I5                                       449
450     188               JS( 4 , NS ) = NDD                                      450
451     189               JS( 5 , NS ) = N2                                       451
452     190   C                                                                   452
453     191            IF( ITRING . EQ . 0 ) THEN                                 453
454     192   C                                                                   454
455     193            JE( 1 , N3 )   = I2                                        455
456     194            JE( 2 , N3 )   = I5                                        456
457     195               JS( 6 , NS ) = - N3                                     457
458     196               JE( 4 , N3 ) = NS                                       458
459     197   C                                                                   459
460     198            ELSE                                                       460
461     199   C                                                                   461
462     200            JE( 1 , N3 )   = I5                                        462
463     201            JE( 2 , N3 )   = I2                                        463
464     202               JS( 6 , NS ) = N3                                       464
465     203               JE( 3 , N3 ) = NS                                       465
466     204   C                                                                   466
467     205            END IF                                                     467
468     206   C                                                                   468
469     207               JE( 3 , N2 ) = NS                                       469
470     208               JE( 4 , N2 ) = IT2                                      470
471     209               NDD          = IABS( NDD )                              471
472     210               IF( JE( 4 , NDD ) . EQ . IT2 ) JE( 4 , NDD ) = NS       472
473     211               IF( JE( 3 , NDD ) . EQ . IT2 ) JE( 3 , NDD ) = NS       473
474     212   C                                                                   474
475     213            END IF                                                     475
476     214   C                                                                   476
477     215            NSM1 = NS - 1                                              477
478     216            NEM1 = NE - 1                                              478
479     217            NEM2 = NE - 2                                              479
480     218   C                                                                   480
481     219            IF(  ITRING . EQ . 0 ) THEN                                481
482     220            XV( 1 , I5 ) = 0.25 * ( XV( 1 , I1 ) + XV( 1 , I2 ) +      482
483     221           .                        XV( 1 , I3 ) + XV( 1 , I4 ) )      483
484     222            XV( 2 , I5 ) = 0.25 * ( XV( 2 , I1 ) + XV( 2 , I2 ) +      484
485     223           .                        XV( 2 , I3 ) + XV( 2 , I4 ) )      485
486     224            JV( 1 , I5 ) = 0                                           486
487     225   C                                                                   487
488     226            DO 85 IR = 1 , MHQ                                         488
489     227            HYDVVV( I5 , IR ) = 0.25 * ( HYDVVV( I1 , IR ) +           489
490     228           .                             HYDVVV( I2 , IR ) +           490
491     229           .                             HYDVVV( I3 , IR ) +           491
492     230           .                             HYDVVV( I4 , IR ) )           492
493     231    85     CONTINUE                                                   493
494     232   C                                                                   494
495     233            JV( 2 , NV ) = N                                           495
496     234            IF( JV( 2 , I2 ) . GT . 0 ) JV( 2 , I2 ) = N3              496
497     235   C                                                                   497
498     236            DX = XV( 1 , I3 ) - XV( 1 , I1 )                           498
499     237            DXX = XV( 1 , I5 ) - XV( 1 , I1 )                          499
500     238            DY = XV( 2 , I3 ) - XV( 2 , I1 )                           500
501     239            DYY = XV( 2 , I5 ) - XV( 2 , I1 )                          501
502     240            XS( 3 , IT1 ) = .5 * ( DX * DYY - DXX * DY )               502
503     241            DX = XV( 1 , I2 ) - XV( 1 , I3 )                           503
504     242            DXX = XV( 1 , I5 ) - XV( 1 , I3 )                          504
505     243            DY = XV( 2 , I2 ) - XV( 2 , I3 )                           505
506     244            DYY = XV( 2 , I5 ) - XV( 2 , I3 )                          506
507     245            XS( 3 , NSM1 ) = .5 * ( DX * DYY - DXX * DY )              507
508     246            DX = XV( 1 , I4 ) - XV( 1 , I2 )                           508
509     247            DXX = XV( 1 , I5 ) - XV( 1 , I2 )                          509
510     248            DY = XV( 2 , I4 ) - XV( 2 , I2 )                           510
511     249            DYY = XV( 2 , I5 ) - XV( 2 , I2 )                          511
512     250            XS( 3 , NS ) = .5 * ( DX * DYY - DXX * DY )                512
513     251            DX = XV( 1 , I1 ) - XV( 1 , I4 )                           513
514     252            DXX = XV( 1 , I5 ) - XV( 1 , I4 )                          514
```

```
      DY = XV( 2 , I1 ) - XV( 2 , I4 )
      DYY = XV( 2 , I5 ) - XV( 2 , I4 )
      XS( 3 , IT2 ) = .5 * ( DX * DYY - DXX * DY )
C
      XS( 1 , IT1 ) = ( XV( 1 , I1 ) + XV( 1 , I3 ) +
     .                  XV( 1 , NV ) ) * THIRD
      XS( 1 , NSM1 ) = ( XV( 1 , I3 ) + XV( 1 , I2 ) +
     .                   XV( 1 , NV ) ) * THIRD
      XS( 2 , IT1 ) = ( XV( 2 , I1 ) + XV( 2 , I3 ) +
     .                  XV( 2 , NV ) ) * THIRD
      XS( 2 , NSM1 ) = ( XV( 2 , I3 ) + XV( 2 , I2 ) +
     .                   XV( 2 , NV ) ) * THIRD
C
      XS( 1 , NS ) = ( XV( 1 , I2 ) + XV( 1 , I4 ) +
     .                 XV( 1 , NV ) ) * THIRD
      XS( 1 , IT2 ) = ( XV( 1 , I4 ) + XV( 1 , I1 ) +
     .                  XV( 1 , NV ) ) * THIRD
      XS( 2 , NS ) = ( XV( 2 , I2 ) + XV( 2 , I4 ) +
     .                 XV( 2 , NV ) ) * THIRD
      XS( 2 , IT2 ) = ( XV( 2 , I4 ) + XV( 2 , I1 ) +
     .                  XV( 2 , NV ) ) * THIRD
C
      DO 94 IR = 1 , MHQ
      HYDV( IT1 , IR ) = ( HYDVVV( I1 , IR ) +
     .                     HYDVVV( I3 , IR ) +
     .                     HYDVVV( NV , IR ) ) * THIRD
      HYDV( NSM1 , IR ) = ( HYDVVV( I3 , IR ) +
     .                      HYDVVV( I2 , IR ) +
     .                      HYDVVV( NV , IR ) ) * THIRD
      HYDV( IT2 , IR ) = ( HYDVVV( I4 , IR ) +
     .                     HYDVVV( I1 , IR ) +
     .                     HYDVVV( NV , IR ) ) * THIRD
      HYDV( NS , IR ) = ( HYDVVV( I2 , IR ) +
     .                    HYDVVV( I4 , IR ) +
     .                    HYDVVV( NV , IR ) ) * THIRD
 94   CONTINUE
C
      HDUM          = 1. / ( HYDV( IT1 , 1 ) + 1.E-12 )
      HYDV( IT1 , 2 ) = HYDV( IT1 , 2 ) * HDUM
      HYDV( IT1 , 3 ) = HYDV( IT1 , 3 ) * HDUM
      HYDV( IT1 , 4 ) = ( HYDV( IT1 , 4 )  -
     .                  .5 * HYDV( IT1 , 1 ) *
     .  ( HYDV( IT1 , 2 ) * HYDV( IT1 , 2 ) +
     .    HYDV( IT1 , 3 ) * HYDV( IT1 , 3 ) ) ) *
     .                    ( HYDV( IT1 , 5 ) - 1. )
C
      HDUM          = 1. / ( HYDV( NSM1 , 1 ) + 1.E-12 )
      HYDV( NSM1 , 2 ) = HYDV( NSM1 , 2 ) * HDUM
      HYDV( NSM1 , 3 ) = HYDV( NSM1 , 3 ) * HDUM
      HYDV( NSM1 , 4 ) = ( HYDV( NSM1 , 4 )  -
     .                   .5 * HYDV( NSM1 , 1 ) *
     .  ( HYDV( NSM1 , 2 ) * HYDV( NSM1 , 2 ) +
     .    HYDV( NSM1 , 3 ) * HYDV( NSM1 , 3 ) ) ) *
     .                     ( HYDV( NSM1 , 5 ) - 1. )
C
      HDUM          = 1. / ( HYDV( IT2 , 1 ) + 1.E-12 )
      HYDV( IT2 , 2 ) = HYDV( IT2 , 2 ) * HDUM
      HYDV( IT2 , 3 ) = HYDV( IT2 , 3 ) * HDUM
      HYDV( IT2 , 4 ) = ( HYDV( IT2 , 4 )  -
     .                  .5 * HYDV( IT2 , 1 ) *
     .  ( HYDV( IT2 , 2 ) * HYDV( IT2 , 2 ) +
     .    HYDV( IT2 , 3 ) * HYDV( IT2 , 3 ) ) ) *
     .                    ( HYDV( IT2 , 5 ) - 1. )
C
      HDUM          = 1. / ( HYDV( NS , 1 ) + 1.E-12 )
      HYDV( NS , 2 ) = HYDV( NS , 2 ) * HDUM
      HYDV( NS , 3 ) = HYDV( NS , 3 ) * HDUM
      HYDV( NS , 4 ) = ( HYDV( NS , 4 )  -
     .                 .5 * HYDV( NS , 1 ) *
     .  ( HYDV( NS , 2 ) * HYDV( NS , 2 ) +
     .    HYDV( NS , 3 ) * HYDV( NS , 3 ) ) ) *
     .                   ( HYDV( NS , 5 ) - 1. )
C
      SAREA( IT1 ) = 1. / XS( 3 , IT1 )
```

```
589     327            SAREA( NSM1 ) = 1. / XS( 3 , NSM1 )                    589
590     328            SAREA( IT2 ) = 1. / XS( 3 , IT2 )                      590
591     329            SAREA( NS ) = 1. / XS( 3 , NS )                        591
592     330    C                                                              592
593     331            DO 112 IR = 1 , 2                                      593
594     332            RGRAD( NS , IR ) = RGRAD( IT2 , IR )                   594
595     333            RGRAD( NSM1 , IR ) = RGRAD( IT1 , IR )                 595
596     334            UGRAD( NS , IR ) = UGRAD( IT2 , IR )                   596
597     335            UGRAD( NSM1 , IR ) = UGRAD( IT1 , IR )                 597
598     336            VGRAD( NS , IR ) = VGRAD( IT2 , IR )                   598
599     337            VGRAD( NSM1 , IR ) = VGRAD( IT1 , IR )                 599
600     338            PGRAD( NS , IR ) = PGRAD( IT2 , IR )                   600
601     339            PGRAD( NSM1 , IR ) = PGRAD( IT1 , IR )                 601
602     340    112     CONTINUE                                               602
603     341    C                                                              603
604     342            KSDELT( NS ) = IDUMP                                   604
605     343            KSDELT( NSM1 ) = IDUMP                                 605
606     344            KSDELT( IT1 ) = IDUMP                                  606
607     345            KSDELT( IT2 ) = IDUMP                                  607
608     346    C                                                              608
609     347            JEN( 1 ) = NAA                                         609
610     348            JEN( 2 ) = NBB                                         610
611     349            JEN( 3 ) = NCC                                         611
612     350            JEN( 4 ) = NDD                                         612
613     351            JEN( 5 ) = N                                           613
614     352            JEN( 6 ) = N1                                          614
615     353            JEN( 7 ) = N2                                          615
616     354            JEN( 8 ) = N3                                          616
617     355            JENN = 8                                               617
618     356    C                                                              618
619     357          ELSE                                                     619
620     358    C                                                              620
621     359            XV( 1 , I5 ) = 0.5 * ( XV( 1 , I1 ) + XV( 1 , I2 ) )   621
622     360            XV( 2 , I5 ) = 0.5 * ( XV( 2 , I1 ) + XV( 2 , I2 ) )   622
623     361            JV( 1 , I5 ) = 0                                       623
624     362    C                                                              624
625     363            IF( IOSPCL . EQ . 1 . AND . IJE5 . EQ . 6 ) THEN       625
626     364            ANGL = 1.570796327                                     626
627     365            DXX = XV( 1 , I5 ) - 1.5                               627
628     366            IF( DXX . NE . 0. )  ANGL = ATAN2( XV( 2 , I5 ) , DXX ) 628
629     367            XV( 1 , I5 ) = COS( ANGL ) + 1.5                       629
630     368            XV( 2 , I5 ) = SIN( ANGL )                             630
631     369            END IF                                                 631
632     370    C                                                              632
633     371            DO 80 IR = 1 , MHQ                                     633
634     372            HYDVVV( I5 , IR ) = 0.5 * ( HYDVVV( I1 , IR ) +        634
635     373           .                            HYDVVV( I2 , IR ) )        635
636     374     80     CONTINUE                                               636
637     375    C                                                              637
638     376            JV( 2 , I1 ) = - N                                     638
639     377            JV( 2 , NV ) = - N3                                    639
640     378    C                                                              640
641     379            XSAREA = .5 * XS( 3 , IT2 )                            641
642     380            XS( 3 , IT2 ) = XSAREA                                 642
643     381            XS( 3 , NS ) = XSAREA                                  643
644     382    C                                                              644
645     383            XS( 1 , NS ) = ( XV( 1 , I2 ) + XV( 1 , I4 ) +         645
646     384           .                 XV( 1 , NV ) ) * THIRD                646
647     385            XS( 1 , IT2 ) = ( XV( 1 , I4 ) + XV( 1 , I1 ) +        647
648     386           .                 XV( 1 , NV ) ) * THIRD                648
649     387            XS( 2 , NS ) = ( XV( 2 , I2 ) + XV( 2 , I4 ) +         649
650     388           .                 XV( 2 , NV ) ) * THIRD                650
651     389            XS( 2 , IT2 ) = ( XV( 2 , I4 ) + XV( 2 , I1 ) +        651
652     390           .                 XV( 2 , NV ) ) * THIRD                652
653     391    C                                                              653
654     392            DO 92 IR = 1 , MHQ                                     654
655     393            HYDV( IT2 , IR ) = ( HYDVVV( I4 , IR ) +               655
656     394           .                     HYDVVV( I1 , IR ) +               656
657     395           .                     HYDVVV( NV , IR ) ) * THIRD       657
658     396            HYDV( NS , IR ) = ( HYDVVV( I2 , IR ) +                658
659     397           .                    HYDVVV( I4 , IR ) +                659
660     398           .                    HYDVVV( NV , IR ) ) * THIRD        660
661     399     92     CONTINUE                                               661
662     400    C                                                              662
```

```
663     401             HDUM          = 1. / ( HYDV( IT2 , 1 ) + 1.E-12 )
664     402             HYDV( IT2 , 2 ) = HYDV( IT2 , 2 ) * HDUM
665     403             HYDV( IT2 , 3 ) = HYDV( IT2 , 3 ) * HDUM
666     404             HYDV( IT2 , 4 ) = ( HYDV( IT2 , 4 )  -
667     405      .                       .5 * HYDV( IT2 , 1 ) *
668     406      .      ( HYDV( IT2 , 2 ) * HYDV( IT2 , 2 ) +
669     407      .        HYDV( IT2 , 3 ) * HYDV( IT2 , 3 ) ) ) *
670     408      .                         ( HYDV( IT2 , 5 ) - 1. )
671     409     C
672     410             HDUM          = 1. / ( HYDV( NS , 1 ) + 1.E-12 )
673     411             HYDV( NS , 2 ) = HYDV( NS , 2 ) * HDUM
674     412             HYDV( NS , 3 ) = HYDV( NS , 3 ) * HDUM
675     413             HYDV( NS , 4 ) = ( HYDV( NS , 4 )  -
676     414      .                       .5 * HYDV( NS , 1 ) *
677     415      .      ( HYDV( NS , 2 ) * HYDV( NS , 2 ) +
678     416      .        HYDV( NS , 3 ) * HYDV( NS , 3 ) ) ) *
679     417      .                         ( HYDV( NS , 5 ) - 1. )
680     418     C
681     419             XSYREA = 1. / XSAREA
682     420             SAREA( IT2 ) = XSYREA
683     421             SAREA( NS ) = XSYREA
684     422     C
685     423             DO 122 IR = 1 , 2
686     424             RGRAD( NS , IR ) = RGRAD( IT2 , IR )
687     425             UGRAD( NS , IR ) = UGRAD( IT2 , IR )
688     426             VGRAD( NS , IR ) = VGRAD( IT2 , IR )
689     427             PGRAD( NS , IR ) = PGRAD( IT2 , IR )
690     428     122     CONTINUE
691     429     C
692     430             KSDELT( NS ) = IDUMP
693     431             KSDELT( IT2 ) = IDUMP
694     432     C
695     433             JEN( 1 ) = NAA
696     434             JEN( 2 ) = NDO
697     435             JEN( 3 ) = N2
698     436             JEN( 4 ) = N3
699     437             JEN( 5 ) = N
700     438             JENN = 5
701     439     C
702     440             END IF
703     441     C
704     442             DO 90 IENN = 1 , JENN
705     443             IEN = JEN( IENN )
706     444             JV1 = JE( 1 , IEN )
707     445             JV2 = JE( 2 , IEN )
708     446             AX = XV( 1 , JV2 ) - XV( 1 , JV1 )
709     447             AY = XV( 2 , JV2 ) - XV( 2 , JV1 )
710     448             XE( 1 , IEN ) = SQRT( AX * AX + AY * AY )
711     449             XEREV = 1. / XE( 1 , IEN )
712     450             XN( IEN ) = AY * XEREV
713     451             YN( IEN ) = - AX * XEREV
714     452             ISSR = JE( 4 , IEN )
715     453             ISSL = JE( 3 , IEN )
716     454     C
717     455             IJE5 = JE( 5 , IEN )
718     456             IF( IJE5 . NE . 0 ) THEN
719     457     C
720     458             AA = XV( 1 , JV2 ) - XV( 1 , JV1 )
721     459             BB = XV( 2 , JV2 ) - XV( 2 , JV1 )
722     460             XEL = XS( 1 , ISSL )
723     461             YEL = XS( 2 , ISSL )
724     462             CC = XEL - XV( 1 , JV1 )
725     463             DD = YEL - XV( 2 , JV1 )
726     464             EE = ( AA * CC + BB * DD ) * XEREV * XEREV
727     465             XER = XV( 1 , JV1 ) + AA * EE
728     466             YER = XV( 2 , JV1 ) + BB * EE
729     467             AX = XER - XEL
730     468             AY = YER - YEL
731     469             XE( 2 , IEN ) = SQRT( AX * AX + AY * AY )
732     470             XEREV = 1. / XE( 2 , IEN )
733     471             XXN( IEN ) = AX * XEREV
734     472             YYN( IEN ) = AY * XEREV
735     473             XE( 2 , IEN ) = 2. * XE( 2 , IEN )
736     474             XYMIDL( IEN ) = .5
```

```
737   475              XMIDL( IEN ) = XER                                                    737
738   476              YMIDL( IEN ) = YER                                                    738
739   477   C                                                                               739
740   478              ELSE                                                                  740
741   479   C                                                                               741
742   480              XER = XS( 1 , ISSR )                                                  742
743   481              YER = XS( 2 , ISSR )                                                  743
744   482              XEL = XS( 1 , ISSL )                                                  744
745   483              YEL = XS( 2 , ISSL )                                                  745
746   484   C                                                                               746
747   485              AA = XV( 1 , JV2 ) - XV( 1 , JV1 )                                    747
748   486              BB = XV( 2 , JV2 ) - XV( 2 , JV1 )                                    748
749   487              CC = XEL - XER                                                        749
750   488              DD = YEL - YER                                                        750
751   489              ACA = XER - XV( 1 , JV1 )                                             751
752   490              DBD = YER - XV( 2 , JV1 )                                             752
753   491              EE = ( ACA * DD - DBD * CC ) / ( AA * DD - BB * CC )                  753
754   492              XMIDL( IEN ) = XV( 1 , JV1 ) + AA * EE                                754
755   493              YMIDL( IEN ) = XV( 2 , JV1 ) + BB * EE                                755
756   494   C                                                                               756
757   495              XEMID = XMIDL( IEN ) - XEL                                            757
758   496              YEMID = YMIDL( IEN ) - YEL                                            758
759   497   C                                                                               759
760   498              AX = XER - XEL                                                        760
761   499              AY = YER - YEL                                                        761
762   500              XE( 2 , IEN ) = SQRT( AX * AX + AY * AY )                             762
763   501              XEREV = 1. / XE( 2 , IEN )                                            763
764   502              XXN( IEN ) = AX * XEREV                                               764
765   503              YYN( IEN ) = AY * XEREV                                               765
766   504   C                                                                               766
767   505              XYMIDL( IEN ) = SQRT( XEMID * XEMID + YEMID * YEMID ) * XEREV         767
768   506   C                                                                               768
769   507              END IF                                                                769
770   508   C                                                                               770
771   509    90      CONTINUE                                                              771
772   510   C                                                                               772
773   511              IF( IEROR.NE.0 ) THEN                                                 773
774   512                 WRITE (6,1000) N                                                   774
775   513                 IF( IEROR.EQ.2 ) WRITE (6,1002) I2, J1, IT1, I5                    775
776   514                 IF( IEROR.EQ.3 ) WRITE (6,1003) I2, J2, IT2, I5                    776
777   515                 STOP                                                               777
778   516              END IF                                                                778
779   517   C                                                                               779
780   518   C --- EXIT POINT FROM SUBROUTINE ----------------------------------------       780
781   519   C                                                                               781
782   520   C      ------                                                                   782
783   521          RETURN                                                                   783
784   522   C      ------                                                                   784
785   523   C                                                                               785
786   524   C --- FORMATS ------------------------------------------------------------      786
787   525   C                                                                               787
788   526    1000      FORMAT(/'0 TROUBLE WITH BOOKKEEPING DATA FOUND IN DISECT ',          788
789   527     .                'FOR LINE ', I5///)                                          789
790   528    1002      FORMAT(' DISECT  I2= ',I5,' J= ',I5,' IT1= ',I5,' I5= ',I5)          790
791   529    1003      FORMAT(' DISECT  I2= ',I5,' J= ',I5,' IT2= ',I5,' I5= ',I5)          791
792   530   C                                                                               792
793   531   C      ---                                                                      793
794   532          END                                                                      794
```

```
      SUBROUTINE DYNPTN( DAREA , NOFDIV , IDUMP , LTRIG )
C
C-----------------------------------------------------------------------I
C                                                                       I
C     DYNPTN ADAPT THE GRID DYNAMICALLY, ADD VERTECES                   I
C                                                                       I
C-----------------------------------------------------------------------I
C
         IMPLICIT REAL (A-H,O-Z)
C
      include     'cmsh00.h'
      include     'chyd00.h'
      include     'cint00.h'
      include     'cphs10.h'
      include     'cphs20.h'
C
      INTEGER JTRIG(MEM),KTRIG(MEM),IRECNC(MEM)
      INTEGER JSE(MEM),JEE(MEM),IOFDVS(10),NOFDVS(10)
C
      EQUIVALENCE (UL,JTRIG)
      EQUIVALENCE (VR,KTRIG)
      EQUIVALENCE (VL,IRECNC)
      EQUIVALENCE (PR,JSE)
      EQUIVALENCE (PL,JEE)
C
       SMINVG = SAREVG * DAREA
       RMINVG = .7 * SMINVG
       DO 115 IS = 1 , NS
       JEE( IS ) = 0
 115   CONTINUE
C
       NSS = 0
       FLUXPP = .00001 * HYDMOM( 4 )
       FLUXUU = .00001 * HYDMOM( 2 )
       FLUXRR = .00001 * HYDMOM( 1 )
       DO 120 IS = 1 , NS
       PCRTRY = HYDFLX( IS , 4 ) - FLUXPP
       IPCRTR = SIGN( 1. , PCRTRY )
       UCRTRY = HYDFLX( IS , 2 ) - FLUXUU
       IUCRTR = SIGN( 1. , UCRTRY )
       RCRTRY = HYDFLX( IS , 1 ) - FLUXRR
       IRCRTR = SIGN( 1. , RCRTRY )
       IF( (
     .       IPCRTR . EQ . 1 . OR .
     .       IUCRTR . EQ . 1 . OR .
     .       IRCRTR . EQ . 1 ) . AND .
     .       KSDELT( IS ) . LT . IDUMP ) THEN
       KSDELT( IS ) = IDUMP
       JEE( IS ) = 1
       NSS = NSS + 1
       JTRIG( NSS ) = IS
       END IF
 120   CONTINUE
C
       DO 130 IS = 1 , NSS
       JSE( IS ) = JTRIG( IS )
 130   CONTINUE
C
       MSS = NSS
       DO 140 KDIV = 1 , NOFDIV
       ITRIG = 0
       DO 150 KS = 1 , NSS
C
       ISS = JSE( KS )
C
       DO 160 KR = 1 , 3
       IVV = JS( KR , ISS )
C
          IE = JV( 2 , IVV )
          IF( IE . GT . 0 ) THEN
C
          IV1 = JE( 1 , IE )
          IF( IV1 . EQ . IVV ) THEN
          ISI = JE( 3 , IE )
```

```
      ELSE
      ISI = JE( 4 , IE )
      END IF
      IS = ISI
C
750   CONTINUE
C
      JES = JEE( IS )
      XAS = XS( 3 , IS )
      IF( JES . EQ . 0 . AND . XAS . LT . SAREVG ) THEN
      ITRIG = ITRIG + 1
      KTRIG( ITRIG ) = IS
      KSDELT( IS ) = IDUMP
      JEE( IS ) = 1
      END IF
C
      DO 760 IR = 1 , 3
      JR = MOD( IR , 3 ) + 1
      IEA = IABS( JS( JR + 3 , IS ) )
      IF( IEA . EQ . IE ) THEN
      JJR = MOD( JR + 1 , 3 ) + 4
      IER = IABS( JS( JJR , IS ) )
C
      IV1 = JE( 1 , IER )
      IF( IV1 . EQ . IVV ) THEN
      ISR = JE( 3 , IER )
      ELSE
      ISR = JE( 4 , IER )
      END IF
      END IF
C
760   CONTINUE
C
      IF( ISR . NE . ISI ) THEN
      IS = ISR
      IE = IER
      GO TO 750
      END IF
C
      ELSE
C
      IE = - IE
      IV1 = JE( 1 , IE )
      IF( IV1 . EQ . IVV ) THEN
      ISI = JE( 3 , IE )
      ELSE
      ISI = JE( 4 , IE )
      END IF
      IS = ISI
      ISI = 0
      IIE = IE
C
650   CONTINUE
C
      JES = JEE( IS )
      XAS = XS( 3 , IS )
      IF( JES . EQ . 0 . AND . XAS . LT . SAREVG ) THEN
      ITRIG = ITRIG + 1
      KTRIG( ITRIG ) = IS
      KSDELT( IS ) = IDUMP
      JEE( IS ) = 1
      END IF
C
      DO 660 IR = 1 , 3
      JR = MOD( IR , 3 ) + 1
      IEA = IABS( JS( JR + 3 , IS ) )
      IF( IEA . EQ . IE ) THEN
      JJR = MOD( JR + 1 , 3 ) + 4
      IER = IABS( JS( JJR , IS ) )
C
      IV1 = JE( 1 , IER )
      IF( IV1 . EQ . IVV ) THEN
      ISR = JE( 3 , IER )
      ELSE
```

```
 943     149            ISR = IE( 4 , IER )                                                    943
 944     150            END IF                                                                 944
 945     151            END IF                                                                 945
 946     152  C                                                                                946
 947     153  660       CONTINUE                                                               947
 948     154  C                                                                                948
 949     155            IF( ISR . NE . ISI ) THEN                                              949
 950     156            IS = ISR                                                               950
 951     157            IE = IER                                                               951
 952     158            GO TO 650                                                              952
 953     159            END IF                                                                 953
 954     160  C                                                                                954
 955     161            END IF                                                                 955
 956     162   160   CONTINUE                                                                 956
 957     163  C                                                                                957
 958     164   150   CONTINUE                                                                 958
 959     165  C                                                                                959
 960     166         DO 170 IS = 1 , ITRIG                                                    960
 961     167         JTRIG( IS + MSS ) = KTRIG( IS )                                          961
 962     168         JSE( IS ) = KTRIG( IS )                                                  962
 963     169   170   CONTINUE                                                                 963
 964     170         NSS = ITRIG                                                              964
 965     171         MSS = MSS + ITRIG                                                        965
 966     172  C                                                                                966
 967     173   140   CONTINUE                                                                 967
 968     174         NSS = MSS                                                                968
 969     175  C                                                                                969
 970     176         DO 300 KDIV = 1 , 1                                                      970
 971     177         LTRIG = NSS                                                              971
 972     178  C                                                                                972
 973     179         DO 310 IS = 1 , NSS                                                      973
 974     180         ISS = JTRIG( IS )                                                        974
 975     181         XSAREA = XS( 3 , ISS )                                                   975
 976     182         IF( XSAREA . GE . RMINVG ) THEN                                          976
 977     183  C                                                                                977
 978     184         DO 335 IR = 4 , 6                                                        978
 979     185         IE = IABS( JS( IR , ISS ) )                                              979
 980     186         IJE5 = JE( 5 , IE )                                                      980
 981     187         IF( IJE5 . NE . 0 ) THEN                                                 981
 982     188         JR2 = MOD( IR - 3 , 3 ) + 4                                              982
 983     189         IE2 = IABS( JS( JR2 , ISS ) )                                            983
 984     190         JR3 = MOD( IR - 2 , 3 ) + 4                                              984
 985     191         IE3 = IABS( JS( JR3 , ISS ) )                                            985
 986     192         XE1 = XE( 1 , IE )                                                       986
 987     193         XE2 = XE( 1 , IE2 )                                                      987
 988     194         XE3 = XE( 1 , IE3 )                                                      988
 989     195         XEDIST = 1. / XE1                                                        989
 990     196         YE2 = XE2 * XEDIST                                                       990
 991     197         YE3 = XE3 * XEDIST                                                       991
 992     198         ZE2 = ( YE2 - 1.5 ) * ( YE2 - .1 )                                       992
 993     199         ZE3 = ( YE3 - 1.5 ) * ( YE3 - .  )                                       993
 994     200         YY2 = XE1 * XE1 + XE2 * XE2 + .35 * XE1 * XE2 - XE3 * XE3                994
 995     201         YY3 = XE1 * XE1 + XE3 * XE3 + .35 * XE1 * XE3 - XE2 * XE2                995
 996     202         IF( ZE2 . LT . .0 . AND . ZE3 . LT . 0. . AND .                          996
 997     203        .     YY2 . GT . 0. . AND . YY3 . GT . 0. ) THEN                          997
 998     204         CALL DISECT ( IE , IDONE , IDUMP )                                       998
 999     205  C                                                                                999
1000     206         LTRIG = LTRIG + 1                                                       1000
1001     207         JTRIG( LTRIG ) = NS                                                     1001
1002     208         KSDELT( NS ) = IDUMP                                                    1002
1003     209  C                                                                               1003
1004     210         END IF                                                                  1004
1005     211         END IF                                                                  1005
1006     212  335    CONTINUE                                                                1006
1007     213         END IF                                                                  1007
1008     214  310    CONTINUE                                                                1008
1009     215  C                                                                               1009
1010     216         NSS = LTRIG                                                             1010
1011     217         IEDGE = 0                                                               1011
1012     218         NCOLOR = 0                                                              1012
1013     219  C                                                                               1013
1014     220         DO 295 IE = 1 , NE                                                      1014
1015     221         JSE( IE ) = 0                                                           1015
1016     222   295   CONTINUE                                                                1016
```

```
1017    223  C                                                              1017
1018    224        DO 320 IS = 1 , NSS                                      1018
1019    225        ISS = JTRIG( IS )                                        1019
1020    226        XSAREA = XS( 3 , ISS )                                   1020
1021    227  C                                                              1021
1022    228        XXS = XS( 1 , ISS )                                      1022
1023    229        YYS = XS( 2 , ISS )                                      1023
1024    230        IZZ = 1                                                  1024
1025    231        IF( IWINDW . EQ . 1 ) THEN                               1025
1026    232        XXSS = - XXS * XXS + XXS + .75                           1026
1027    233        YYSS = - YYS * YYS + 1.                                  1027
1028    234        IZZ = INT( SIGN( 1. , XXSS * YYSS ) )                    1028
1029    235        END IF                                                   1029
1030    236  C                                                              1030
1031    237        IF( XSAREA . GT . RMINVG . AND . IZZ . EQ . 1 ) THEN     1031
1032    238  C                                                              1032
1033    239        DO 735 IR = 4 , 6                                        1033
1034    240        IE = IABS( JS( IR , ISS ) )                              1034
1035    241        IF( JSE( IE ) . EQ . 0 ) THEN                            1035
1036    242        IEDGE = IEDGE + 1                                        1036
1037    243        IRECNC( IEDGE ) = IE                                     1037
1038    244        NCOLOR = NCOLOR + 1                                      1038
1039    245        JEE( NCOLOR ) = IE                                       1039
1040    246        JSE( IE ) = 1                                            1040
1041    247        END IF                                                   1041
1042    248  735   CONTINUE                                                 1042
1043    249  C                                                              1043
1044    250        AREAXS = SAREA( ISS )                                    1044
1045    251        IE1 = IABS( JS( 4 , ISS ) )                              1045
1046    252        XE1 = XE( 1 , IE1 )                                      1046
1047    253        HD1 = AREAXS * XE1 * XE1                                 1047
1048    254        IJE5 = JE( 5 , IE1 )                                     1048
1049    255        IE2 = IABS( JS( 5 , ISS ) )                              1049
1050    256        XE2 = XE( 1 , IE2 )                                      1050
1051    257        HD2 = AREAXS * XE2 * XE2                                 1051
1052    258        IJE5 = IJE5 + JE( 5 , IE2 )                              1052
1053    259        IE3 = IABS( JS( 6 , ISS ) )                              1053
1054    260        XE3 = XE( 1 , IE3 )                                      1054
1055    261        HD3 = AREAXS * XE3 * XE3                                 1055
1056    262        IJE5 = IJE5 + JE( 5 , IE3 )                              1056
1057    263        RATIO = AMAX1( HD1 , HD2 , HD3 )                         1057
1058    264        IRATIO = 0                                               1058
1059    265        IF( RATIO . LE . 7. . AND . IJE5 . EQ . 0 . AND .        1059
1060    266       .                                XSAREA . GT . SMINVG ) IRATIO = 1  1060
1061    267        IF( IJE5 . GT . 0 ) IRATIO = 2                           1061
1062    268  C                                                              1062
1063    269        IF( IRATIO . EQ . 2 ) THEN                               1063
1064    270        IJE51 = JE( 5 , IE1 )                                    1064
1065    271        IJE52 = JE( 5 , IE2 )                                    1065
1066    272        IJE53 = JE( 5 , IE3 )                                    1066
1067    273        IF( IJE51 . NE . 0 ) THEN                                1067
1068    274        IEDIST = IE1                                             1068
1069    275        XE1 = XE( 1 , IE1 )                                      1069
1070    276        XE2 = XE( 1 , IE2 )                                      1070
1071    277        XE3 = XE( 1 , IE3 )                                      1071
1072    278        END IF                                                   1072
1073    279        IF( IJE52 . NE . 0 ) THEN                                1073
1074    280        IEDIST = IE2                                             1074
1075    281        XE1 = XE( 1 , IE2 )                                      1075
1076    282        XE2 = XE( 1 , IE1 )                                      1076
1077    283        XE3 = XE( 1 , IE3 )                                      1077
1078    284        END IF                                                   1078
1079    285        IF( IJE53 . NE . 0 ) THEN                                1079
1080    286        IEDIST = IE3                                             1080
1081    287        XE1 = XE( 1 , IE3 )                                      1081
1082    288        XE2 = XE( 1 , IE2 )                                      1082
1083    289        XE3 = XE( 1 , IE1 )                                      1083
1084    290        END IF                                                   1084
1085    291        XEDIST = 1. / XE( 1 , IEDIST )                           1085
1086    292        YE2 = XE2 * XEDIST                                       1086
1087    293        YE3 = XE3 * XEDIST                                       1087
1088    294        ZE2 = ( YE2 - 1.5 ) * ( YE2 - .1 )                       1088
1089    295        ZE3 = ( YE3 - 1.5 ) * ( YE3 - .1 )                       1089
1090    296        YY2 = XE1 * XE1 + XE2 * XE2 + .35 * XE1 * XE2 - XE3 * XE3  1090
```

```
      YY3 = XE1 * XE1 + XE3 * XE3 + .35 * XE1 * XE2 - XE2 * XE2
      IF( ZE2 . LT . .0 . AND . ZE3 . LT . 0. . AND .
     .    YY2 . GT . 0. . AND . YY3 . GT . 0. ) THEN
      CALL DISECT ( IEDIST , IDONE , IDUMP )
C
      LTRIG = LTRIG + 1
      JTRIG( LTRIG ) = NS
      KSDELT( NS ) = IDUMP
C
      IEDGE = IEDGE + 1
      IRECNC( IEDGE ) = NE
      NCOLOR = NCOLOR + 1
      JEE( NCOLOR ) = NE
      JSE( NE ) = 1
      IEDGE = IEDGE + 1
      IRECNC( IEDGE ) = NE - 1
      NCOLOR = NCOLOR + 1
      JEE( NCOLOR ) = NE - 1
      JSE( NE - 1 ) = 1
C
      END IF
      END IF
C
      IF( IRATIO . EQ . 1 ) THEN
C
      CALL VERCEN( ISS )
      KSDELT( ISS ) = IDUMP
      LTRIG = LTRIG + 1
      JTRIG( LTRIG ) = NS - 1
      KSDELT( NS - 1 ) = IDUMP
C
      LTRIG = LTRIG + 1
      JTRIG( LTRIG ) = NS
      KSDELT( NS ) = IDUMP
C
      IEDGE = IEDGE + 1
      IRECNC( IEDGE ) = NE
      NCOLOR = NCOLOR + 1
      JEE( NCOLOR ) = NE
      JSE( NE ) = 1
      IEDGE = IEDGE + 1
      IRECNC( IEDGE ) = NE - 1
      NCOLOR = NCOLOR + 1
      JEE( NCOLOR ) = NE - 1
      JSE( NE - 1 ) = 1
      IEDGE = IEDGE + 1
      IRECNC( IEDGE ) = NE - 2
      NCOLOR = NCOLOR + 1
      JEE( NCOLOR ) = NE - 2
      JSE( NE - 2 ) = 1
C
      ELSE
C
      IDISCT = 0
      DO 545 KK = 4 , 6
      IEE = JS( KK , ISS )
      IEF = IABS( IEE )
      IJE55 = JE( 5 , IEF )
      IF( IJE55 . EQ . 0 ) THEN
      IF( IEE . GT . 0 ) THEN
      ISI = JE( 4 , IEE )
      ELSE
      ISI = JE( 3 , IEF )
      END IF
      AREAXS = SAREA( ISI )
      IE1 = IABS( JS( 4 , ISI ) )
      XE1 = XE( 1 , IE1 )
      IJE55 = JE( 5 , IE1 )
      HD1 = AREAXS * XE1 * XE1
       E2 = IABS( JS( 5 , ISI ) )
      XE2 = XE( 1 , IE2 )
      IJE55 = IJE55 + JE( 5 , IE2 )
      HD2 = AREAXS * XE2 * XE2
      IE3 = IABS( JS( 6 , ISI ) )
```

```
1165     371          XE3 = XE( 1 , IE3 )                                                  1165
1166     372          IJE55 = IJE55 + JE( 5 , IE3 )                                        1166
1167     373          HD3 = AREAXS * XE3 * XE3                                             1167
1168     374          RATIO = AMAX1( HD1 , HD2 , HD3 )                                     1168
1169     375          YSAREA = XS( 3 , ISI )                                               1169
1170     376          IF( RATIO . LT . 7. . AND . YSAREA . GT . SMINVG . AND .             1170
1171     377         .                                    IJE55 . EQ . 0 ) THEN           1171
1172     378          IDISCT = 1                                                           1172
1173     379          DO 435 IR = 4 , 6                                                    1173
1174     380          IE = IABS( JS( IR , ISI ) )                                          1174
1175     381          IF( JSE( IE ) . EQ . 0 ) THEN                                        1175
1176     382          IEDGE = IEDGE + 1                                                    1176
1177     383          IRECNC( IEDGE ) = IE                                                 1177
1178     384          NCOLOR = NCOLOR + 1                                                  1178
1179     385          JEE( NCOLOR ) = IE                                                   1179
1180     386          JSE( IE ) = 1                                                        1180
1181     387          END IF                                                               1181
1182     388  435     CONTINUE                                                             1182
1183     389          CALL VERCEN( ISI )                                                   1183
1184     390          KSDELT( ISI ) = IDUMP                                                1184
1185     391          LTRIG = LTRIG + 1                                                    1185
1186     392          JTRIG( LTRIG ) = NS - 1                                              1186
1187     393          KSDELT( NS - 1 ) = IDUMP                                             1187
1188     394  C                                                                            1188
1189     395          LTRIG = LTRIG + 1                                                    1189
1190     396          JTRIG( LTRIG ) = NS                                                  1190
1191     397          KSDELT( NS ) = IDUMP                                                 1191
1192     398  C                                                                            1192
1193     399          IEDGE = IEDGE + 1                                                    1193
1194     400          IRECNC( IEDGE ) = NE                                                 1194
1195     401          NCOLOR = NCOLOR + 1                                                  1195
1196     402          JEE( NCOLOR ) = NE                                                   1196
1197     403          JSE( NE ) = 1                                                        1197
1198     404          IEDGE = IEDGE + 1                                                    1198
1199     405          IRECNC( IEDGE ) = NE - 1                                             1199
1200     406          NCOLOR = NCOLOR + 1                                                  1200
1201     407          JEE( NCOLOR ) = NE - 1                                               1201
1202     408          JSE( NE - 1 ) = 1                                                    1202
1203     409          IEDGE = IEDGE + 1                                                    1203
1204     410          IRECNC( IEDGE ) = NE - 2                                             1204
1205     411          NCOLOR = NCOLOR + 1                                                  1205
1206     412          JEE( NCOLOR ) = NE - 2                                               1206
1207     413          JSE( NE - 2 ) = 1                                                    1207
1208     414          END IF                                                               1208
1209     415          END IF                                                               1209
1210     416  545     CONTINUE                                                             1210
1211     417  C                                                                            1211
1212     418          IF( IDISCT . EQ . 0 ) THEN                                           1212
1213     419          IE1 = IABS( JS( 4 , ISS ) )                                          1213
1214     420          XE1 = XE( 1 , IE1 )                                                  1214
1215     421          IE2 = IABS( JS( 5 , ISS ) )                                          1215
1216     422          XE2 = XE( 1 , IE2 )                                                  1216
1217     423          IE3 = IABS( JS( 6 , ISS ) )                                          1217
1218     424          XE3 = XE( 1 , IE3 )                                                  1218
1219     425          IEDIST = IE1                                                         1219
1220     426          XEDIST = XE1                                                         1220
1221     427          IF( XE2 . GT . XEDIST ) THEN                                         1221
1222     428          XEDIST = XE2                                                         1222
1223     429          IEDIST = IE2                                                         1223
1224     430          END IF                                                               1224
1225     431          IF( XE3 . GT . XEDIST ) THEN                                         1225
1226     432          XEDIST = XE3                                                         1226
1227     433          IEDIST = IE3                                                         1227
1228     434          END IF                                                               1228
1229     435          ISL = JE( 3 , IEDIST )                                               1229
1230     436          ISR = JE( 4 , IEDIST )                                               1230
1231     437          XSISL = XS( 3 , ISL )                                                1231
1232     438          XSISR = XS( 3 , ISR )                                                1232
1233     439          IJE5 = JE( 5 , IEDIST )                                              1233
1234     440          IF( XSISL . GT . RMINVG . AND . XSISR . GT . RMINVG . AND .          1234
1235     441         .     IJE5 . EQ . 0 . AND . IRATIO . NE . 2 )  THEN                   1235
1236     442          IF( ISS . NE . ISL ) THEN                                            1236
1237     443          DO 345 IR = 4 , 6                                                    1237
1238     444          IE = IABS( JS( IR , ISL ) )                                          1238
```

```
1239     445          IF( JSE( IE ) . EQ . 0 ) THEN                                  1239
1240     446          IEDGE = IEDGE + 1                                              1240
1241     447          IRECNC( IEDGE ) = IE                                           1241
1242     448          NCOLOR = NCOLOR + 1                                            1242
1243     449          JEE( NCOLOR ) = IE                                             1243
1244     450          JSE( IE ) = 1                                                  1244
1245     451          END IF                                                         1245
1246     452   345    CONTINUE                                                       1246
1247     453          END IF                                                         1247
1248     454   C                                                                     1248
1249     455          IF( ISS . NE . ISR ) THEN                                      1249
1250     456          DO 355 IR = 4 , 6                                              1250
1251     457          IE = IABS( JS( IR , ISR ) )                                    1251
1252     458          IF( JSE( IE ) . EQ . 0 ) THEN                                  1252
1253     459          IEDGE = IEDGE + 1                                              1253
1254     460          IRECNC( IEDGE ) = IE                                           1254
1255     461          NCOLOR = NCOLOR + 1                                            1255
1256     462          JEE( NCOLOR ) = IE                                             1256
1257     463          JSE( IE ) = 1                                                  1257
1258     464          END IF                                                         1258
1259     465   355    CONTINUE                                                       1259
1260     466          END IF                                                         1260
1261     467   C                                                                     1261
1262     468          IDONE = 0                                                      1262
1263     469          CALL DISECT ( IEDIST , IDONE , IDUMP )                         1263
1264     470          IF( IDONE . EQ . 1 ) THEN                                      1264
1265     471   C                                                                     1265
1266     472          LTRIG = LTRIG + 1                                              1266
1267     473          JTRIG( LTRIG ) = NS                                            1267
1268     474          KSDELT( NS ) = IDUMP                                           1268
1269     475          LTRIG = LTRIG + 1                                              1269
1270     476          JTRIG( LTRIG ) = NS - 1                                        1270
1271     477          KSDELT( NS - 1 ) = IDUMP                                       1271
1272     478   C                                                                     1272
1273     479          IEDGE = IEDGE + 1                                              1273
1274     480          IRECNC( IEDGE ) = NE                                           1274
1275     481          NCOLOR = NCOLOR + 1                                            1275
1276     482          JEE( NCOLOR ) = NE                                             1276
1277     483          JSE( NE ) = 1                                                  1277
1278     484          IEDGE = IEDGE + 1                                              1278
1279     485          IRECNC( IEDGE ) = NE - 1                                       1279
1280     486          NCOLOR = NCOLOR + 1                                            1280
1281     487          JEE( NCOLOR ) = NE - 1                                         1281
1282     488          JSE( NE - 1 ) = 1                                              1282
1283     489          IEDGE = IEDGE + 1                                              1283
1284     490          IRECNC( IEDGE ) = NE - 2                                       1284
1285     491          NCOLOR = NCOLOR + 1                                            1285
1286     492          JEE( NCOLOR ) = NE - 2                                         1286
1287     493          JSE( NE - 2 ) = 1                                              1287
1288     494          END IF                                                         1288
1289     495   C                                                                     1289
1290     496          END IF                                                         1290
1291     497          END IF                                                         1291
1292     498          END IF                                                         1292
1293     499          END IF                                                         1293
1294     500   C                                                                     1294
1295     501    320   CONTINUE                                                       1295
1296     502   C                                                                     1296
1297     503          DO 340 IEM = 1 , NCOLOR                                        1297
1298     504          IE = JEE( IEM )                                                1298
1299     505   C                                                                     1299
1300     506          ISL = JE( 3 , IE )                                             1300
1301     507          YSAREA = XS( 3 , ISL )                                         1301
1302     508          IJE5 = JE( 5 , IE )                                            1302
1303     509          IF( YSAREA . GE . RMINVG . AND . IJE5 . NE . 0 ) THEN          1303
1304     510          IE1 = IABS( JS( 4 , ISL ) )                                    1304
1305     511          IE2 = IABS( JS( 5 , ISL ) )                                    1305
1306     512          IE3 = IABS( JS( 6 , ISL ) )                                    1306
1307     513          IJE51 = JE( 5 , IE1 )                                          1307
1308     514          IJE52 = JE( 5 , IE2 )                                          1308
1309     515          IJE53 = JE( 5 , IE3 )                                          1309
1310     516          IF( IJE51 . NE . 0 ) THEN                                      1310
1311     517          IEDIST = IE1                                                   1311
1312     518          XE1 = XE( 1 , IE1 )                                            1312
```

```
1313  519        XE2 = XE( 1 , IE2 )                                                    1313
1314  520        XE3 = XE( 1 , IE3 )                                                    1314
1315  521        END IF                                                                 1315
1316  522        IF( IJE52 . NE . 0 ) THEN                                              1316
1317  523        IEDIST = IE2                                                           1317
1318  524        XE1 = XE( 1 , IE2 )                                                    1318
1319  525        XE2 = XE( 1 , IE1 )                                                    1319
1320  526        XE3 = XE( 1 , IE3 )                                                    1320
1321  527        END IF                                                                 1321
1322  528        IF( IJE53 . NE . 0 ) THEN                                              1322
1323  529        IEDIST = IE3                                                           1323
1324  530        XE1 = XE( 1 , IE3 )                                                    1324
1325  531        XE2 = XE( 1 , IE2 )                                                    1325
1326  532        XE3 = XE( 1 , IE1 )                                                    1326
1327  533        END IF                                                                 1327
1328  534        XEDIST = 1. / XE( 1 , IEDIST )                                         1328
1329  535        YE2 = XE2 * XEDIST                                                     1329
1330  536        YE3 = XE3 * XEDIST                                                     1330
1331  537        ZE2 = ( YE2 - 1.5 ) * ( YE2 - .1 )                                     1331
1332  538        ZE3 = ( YE3 - 1.5 ) * ( YE3 - .1 )                                     1332
1333  539        YY2 = XE1 * XE1 + XE2 * XE2 + .35 * XE1 * XE2 - XE3 * XE3              1333
1334  540        YY3 = XE1 * XE1 + XE3 * XE3 + .35 * XE1 * XE3 - XE2 * XE2              1334
1335  541        IF( ZE2 . LT . .0 . AND . ZE3 . LT . 0. . AND .                        1335
1336  542       .     YY2 . GT . 0. . AND . YY3 . GT . 0. ) THEN                        1336
1337  543        CALL DISECT ( IEDIST , IDONE , IDUMP )                                 1337
1338  544   C                                                                           1338
1339  545        LTRIG = LTRIG + 1                                                      1339
1340  546        JTRIG( LTRIG ) = NS                                                    1340
1341  547        KSDELT( NS ) = IDUMP                                                   1341
1342  548   C                                                                           1342
1343  549        IEDGE = IEDGE + 1                                                      1343
1344  550        IRECNC( IEDGE ) = NE                                                   1344
1345  551        NCOLOR = NCOLOR + 1                                                    1345
1346  552        JEE( NCOLOR ) = NE                                                     1346
1347  553        JSE( NE ) = 1                                                          1347
1348  554        IEDGE = IEDGE + 1                                                      1348
1349  555        IRECNC( IEDGE ) = NE - 1                                               1349
1350  556        NCOLOR = NCOLOR + 1                                                    1350
1351  557        JEE( NCOLOR ) = NE - 1                                                 1351
1352  558        JSE( NE - 1 ) = 1                                                      1352
1353  559   C                                                                           1353
1354  560         ELSE                                                                  1354
1355  661   C                                                                           1355
1356  562        IEDIST = IE1                                                           1356
1357  563        XEDIST = XE1                                                           1357
1358  564        IF( XE2 . GT . XEDIST ) THEN                                           1358
1359  565        XEDIST = XE2                                                           1359
1360  566        IEDIST = IE2                                                           1360
1361  567        END IF                                                                 1361
1362  568        IF( XE3 . GT . XEDIST ) THEN                                           1362
1363  569        XEDIST = XE3                                                           1363
1364  570        IEDIST = IE3                                                           1364
1365  571        END IF                                                                 1365
1366  572        ISL = JE( 3 , IEDIST )                                                 1366
1367  573        ISR = JE( 4 , IEDIST )                                                 1367
1368  574        XSISL = XS( 3 , ISL )                                                  1368
1369  575        XSISR = XS( 3 , ISR )                                                  1369
1370  576        IJE5 = JE( 5 , IEDIST )                                                1370
1371  577        IF( XSISL . GT . RMINVG . AND . XSISR . GT . RMINVG . AND .            1371
1372  578       .                                      IJE5 . EQ . 0 )  THEN           1372
1373  579        DO 645 IR = 4 , 6                                                      1373
1374  580        IE = IABS( JS( IR , ISL ) )                                            1374
1375  581        IF( JSE( IE ) . EQ . 0 ) THEN                                          1375
1376  582        IEDGE = IEDGE + 1                                                      1376
1377  583        IRECNC( IEDGE ) = IE                                                   1377
1378  584        NCOLOR = NCOLOR + 1                                                    1378
1379  585        JEE( NCOLOR ) = IE                                                     1379
1380  586        JSE( IE ) = 1                                                          1380
1381  587        END IF                                                                 1381
1382  588   645  CONTINUE                                                              1382
1383  589        DO 655 IR = 4 , 6                                                      1383
1384  590        IE = IABS( JS( IR , ISR ) )                                            1384
1385  591        IF( JSE( IE ) . EQ . 0 ) THEN                                          1385
1386  592        IEDGE = IEDGE + 1                                                      1386
```

```
1387  593          IRECNC( IEDGE ) = IE                                                    1387
1388  594          NCOLOR = NCOLOR + 1                                                     1388
1389  595          JEE( NCOLOR ) = IE                                                      1389
1390  596          JSE( IE ) = 1                                                           1390
1391  597          END IF                                                                  1391
1392  598   655    CONTINUE                                                                1392
1393  599   C                                                                              1393
1394  600          IDONE = 0                                                               1394
1395  601          CALL DISECT ( IEDIST , IDONE , IDUMP )                                  1395
1396  602          IF( IDONE . EQ . 1 ) THEN                                               1396
1397  603   C                                                                              1397
1398  604          LTRIG = LTRIG + 1                                                       1398
1399  605          JTRIG( LTRIG ) = NS                                                     1399
1400  606          KSDELT( NS ) = IDUMP                                                    1400
1401  607          LTRIG = LTRIG + 1                                                       1401
1402  608          JTRIG( LTRIG ) = NS - 1                                                 1402
1403  609          KSDELT( NS - 1 ) = IDUMP                                                1403
1404  610   C                                                                              1404
1405  611          IEDGE = IEDGE + 1                                                       1405
1406  612          IRECNC( IEDGE ) = NE                                                    1406
1407  613          NCOLOR = NCOLOR + 1                                                     1407
1408  614          JEE( NCOLOR ) = NE                                                      1408
1409  615          JSE( NE ) = 1                                                           1409
1410  616          IEDGE = IEDGE + 1                                                       1410
1411  617          IRECNC( IEDGE ) = NE - 1                                                1411
1412  618          NCOLOR = NCOLOR + 1                                                     1412
1413  619          JEE( NCOLOR ) = NE - 1                                                  1413
1414  620          JSE( NE - 1 ) = 1                                                       1414
1415  621          IEDGE = IEDGE + 1                                                       1415
1416  622          IRECNC( IEDGE ) = NE - 2                                                1416
1417  623          NCOLOR = NCOLOR + 1                                                     1417
1418  624          JEE( NCOLOR ) = NE - 2                                                  1418
1419  625          JSE( NE - 2 ) = 1                                                       1419
1420  626          END IF                                                                  1420
1421  627   C                                                                              1421
1422  628          END IF                                                                  1422
1423  629          END IF                                                                  1423
1424  630          END IF                                                                  1424
1425  631    340   CONTINUE                                                                1425
1426  632   C                                                                              1426
1427  633          NSS = LTRIG                                                             1427
1428  634   C                                                                              1428
1429  635          DO 370 IEM = 1 , NCOLOR                                                 1429
1430  636          IE = JEE( IEM )                                                         1430
1431  637          CALL RECNC( IE , IDONE , ITL , ITR , JA , JB , JC , JD )                1431
1432  638          CALL RECNC( JA , JADONE , ITL , ITR , JAA , JAB , JAC , JAD )           1432
1433  639          CALL RECNC( JB , JBDONE , ITL , ITR , JBA , JBB , JBC , JBD )           1433
1434  640          CALL RECNC( JC , JCDONE , ITL , ITR , JCA , JCB , JCC , JCD )           1434
1435  641          CALL RECNC( JD , JDDONE , ITL , ITR , JDA , JDB , JDC , JDD )           1435
1436  642   370    CONTINUE                                                                1436
1437  643   C                                                                              1437
1438  644   300    CONTINUE                                                                1438
1439  645   C                                                                              1439
1440  646        NVECE = NE / MBL                                                        1440
1441  647        NREME = NE - NVECE * MBL                                                1441
1442  648        NVECS = NS / MBL                                                        1442
1443  649        NREMS = NS - NVECS * MBL                                                1443
1444  650        NVECV = NV / MBL                                                        1444
1445  651        NREMV = NV - NVECV * MBL                                                1445
1446  652   C                                                                              1446
1447  653        DO 400 INE = 1 , NVECE                                                  1447
1448  654        NOFVEE( INE ) = MBL                                                     1448
1449  655   400  CONTINUE                                                                1449
1450  656        NVEEE = NVECE                                                           1450
1451  657        IF( NREME . GT . 0 ) THEN                                               1451
1452  658        NVEEE = NVECE + 1                                                       1452
1453  659        NOFVEE( NVEEE ) = NREME                                                 1453
1454  660        END IF                                                                  1454
1455  661   C                                                                              1455
1456  662        DO 410 INS = 1 , NVECS                                                  1456
1457  663        NOFVES( INS ) = MBL                                                     1457
1458  664   410  CONTINUE                                                                1458
1459  665        NVEES = NVECS                                                           1459
1460  666        IF( NREMS . GT . 0 ) THEN                                               1460
```

```
                NVEES = NVECS + 1
                NOFVES( NVEES ) = NREMS
                END IF
C
                DO 420 INV = 1 , NVECV
                NOFVEV( INV ) = MBL
420             CONTINUE
                NVEEV = NVECV
                IF( NREMV . GT . 0 ) THEN
                NVEEV = NVECV + 1
                NOFVEV( NVEEV ) = NREMV
                END IF
C
                 PRINT*,NV,NE,NS
C
C --- EXIT POINT FROM SUBROUTINE ------------------------------------
C
C       ------
                RETURN
C       ------
C
C       ---
                END
```



```
                SUBROUTINE DYYPTN( DAREA , NOFDIV , IDUMP , LTRIG )
C
C-------------------------------------------------------------------I
C                                                                   I
C       DYYPTN ADAPT THE GRID DYNAMICALLY, ADD VERTECES             I
C       SUB DIVIDE THE TRIANGLE THAT WERE FLAGED IN DYNPTN          I
C                                                                   I
C-------------------------------------------------------------------I
C
                IMPLICIT REAL (A-H,O-Z)
C
              include     'cmsh00.h'
              include     'chyd00.h'
              include     'cint00.h'
              include     'cphs10.h'
              include     'cphs20.h'
C
              INTEGER JTRIG(MEM),KTRIG(MEM),IRECNC(MEM)
              INTEGER JSE(MEM),JEE(MEM),IOFDVS(10),NOFDVS(10)
C
              EQUIVALENCE (UL,JTRIG)
              EQUIVALENCE (VR,KTRIG)
              EQUIVALENCE (VL,IRECNC)
              EQUIVALENCE (PR,JSE)
              EQUIVALENCE (PL,JEE)
C
               SMINVG = SAREVG * DAREA
               AMINVG = SAREVG * THIRD
               RMINVG = .7 * SMINVG
               DO 115 IS = 1 , NS
               JEE( IS ) = 0
115            CONTINUE
               MSS = 0
               NSS = LTRIG
C
               DO 140 KDIV = 1 , NOFDIV
               ITRIG = 0
               DO 150 KS = 1 , NSS
C
               ISS = JTRIG( KS )
               IF( ISS . NE . 0 ) THEN
C
               DO 160 KR = 1 , 3
               IVV = JS( KR , ISS )
C
                  IE = JV( 2 , IVV )
                  IF( IE . GT . 0 ) THEN
C
```

```
1532    49              IV1 = JE( 1 , IE )                                      1532
1533    50              IF( IV1 . EQ . IVV ) THEN                               1533
1534    51              ISI = JE( 3 , IE )                                      1534
1535    52              ELSE                                                    1535
1536    53              ISI = JE( 4 , IE )                                      1536
1537    54              END IF                                                  1537
1538    55              IS = ISI                                                1538
1539    56  C                                                                   1539
1540    57  750         CONTINUE                                                1540
1541    58  C                                                                   1541
1542    59              JES = JEE( IS )                                         1542
1543    60              XAS = XS( 3 , IS )                                      1543
1544    61              IF( JES . EQ . 0 . AND . XAS . GT . RMINVG ) THEN       1544
1545    62              ITRIG = ITRIG + 1                                       1545
1546    63              KTRIG( ITRIG ) = IS                                     1546
1547    64              KSDELT( IS ) = IDUMP                                    1547
1548    65              JEE( IS ) = 1                                           1548
1549    66              END IF                                                  1549
1550    67  C                                                                   1550
1551    68              DO 760 IR = 1 , 3                                       1551
1552    69              JR = MOD( IR , 3 ) + 1                                  1552
1553    70              IEA = IABS( JS( JR + 3 , IS ) )                         1553
1554    71              IF( IEA . EQ . IE ) THEN                                1554
1555    72              JJR = MOD( JR + 1 , 3 ) + 4                             1555
1556    73              IER = IABS( JS( JJR , IS ) )                            1556
1557    74  C                                                                   1557
1558    75              IV1 = JE( 1 , IER )                                     1558
1559    76              IF( IV1 . EQ . IVV ) THEN                               1559
1560    77              ISR = JE( 3 , IER )                                     1560
1561    78              ELSE                                                    1561
1562    79              ISR = JE( 4 , IER )                                     1562
1563    80              END IF                                                  1563
1564    81              END IF                                                  1564
1565    82  C                                                                   1565
1566    83  760         CONTINUE                                                1566
1567    84  C                                                                   1567
1568    85              IF( ISR . NE . ISI ) THEN                               1568
1569    86              IS = ISR                                                1569
1570    87              IE = IER                                                1570
1571    88              GO TO 750                                               1571
1572    89              END IF                                                  1572
1573    90  C                                                                   1573
1574    91              ELSE                                                    1574
1575    92  C                                                                   1575
1576    93              IE = - IE                                               1576
1577    94              IV1 = JE( 1 , IE )                                      1577
1578    95              IF( IV1 . EQ . IVV ) THEN                               1578
1579    96              ISI = JE( 3 , IE )                                      1579
1580    97              ELSE                                                    1580
1581    98              ISI = JE( 4 , IE )                                      1581
1582    99              END IF                                                  1582
1583   100              IS = ISI                                                1583
1584   101              ISI = 0                                                 1584
1585   102              IIE = IE                                                1585
1586   103  C                                                                   1586
1587   104  650         CONTINUE                                                1587
1588   105  C                                                                   1588
1589   106              JES = JEE( IS )                                         1589
1590   107              XAS = XS( 3 , IS )                                      1590
1591   108              IF( JES . EQ . 0 . AND . XAS . GT . RMINVG ) THEN       1591
1592   109              ITRIG = ITRIG + 1                                       1592
1593   110              KTRIG( ITRIG ) = IS                                     1593
1594   111              KSDELT( IS ) = IDUMP                                    1594
1595   112              JEE( IS ) = 1                                           1595
1596   113              END IF                                                  1596
1597   114  C                                                                   1597
1598   115              DO 660 IR = 1 , 3                                       1598
1599   116              JR = MOD( IR , 3 ) + 1                                  1599
1600   117              IEA = IABS( JS( JR + 3 , IS ) )                         1600
1601   118              IF( IEA . EQ . IE ) THEN                                1601
1602   119              JJR = MOD( JR + 1 , 3 ) + 4                             1602
1603   120              IER = IABS( JS( JJR , IS ) )                            1603
1604   121  C                                                                   1604
1605   122              IV1 = JE( 1 , IER )                                     1605
```

```
1606    123             IF( IV1 . EQ . IVV ) THEN                                1606
1607    124             ISR = JE( 3 , IER )                                      1607
1608    125             ELSE                                                     1608
1609    126             ISR = JE( 4 , IER )                                      1609
1610    127             END IF                                                   1610
1611    128             END IF                                                   1611
1612    129     C                                                                1612
1613    130     660     CONTINUE                                                 1613
1614    131     C                                                                1614
1615    132             IF( ISR . NE . ISI ) THEN                                1615
1616    133             IS = ISR                                                 1616
1617    134             IE = IER                                                 1617
1618    135             GO TO 650                                                1618
1619    136             END IF                                                   1619
1620    137     C                                                                1620
1621    138             END IF                                                   1621
1622    139      160    CONTINUE                                                 1622
1623    140     C                                                                1623
1624    141             END IF                                                   1624
1625    142      150    CONTINUE                                                 1625
1626    143     C                                                                1626
1627    144             DO 170 IS = 1 , ITRIG                                    1627
1628    145             JTRIG( IS + MSS ) = KTRIG( IS )                          1628
1629    146      170    CONTINUE                                                 1629
1630    147             NSS = ITRIG                                              1630
1631    148             MSS = MSS + ITRIG                                        1631
1632    149     C                                                                1632
1633    150      140    CONTINUE                                                 1633
1634    151             NSS = MSS                                                1634
1635    152     C                                                                1635
1636    153             DO 300 KDIV = 1 , 1                                      1636
1637    154             LTRIG = NSS                                              1637
1638    155     C                                                                1638
1639    156             DO 310 IS = 1 , NSS                                      1639
1640    157             ISS = JTRIG( IS )                                        1640
1641    158             XSAREA = XS( 3 , ISS )                                   1641
1642    159             IF( XSAREA . GE . RMINVG ) THEN                          1642
1643    160     C                                                                1643
1644    161             DO 335 IR = 4 , 6                                        1644
1645    162             IE = IABS( JS( IR , ISS ) )                              1645
1646    163             IJE5 = JE( 5 , IE )                                      1646
1647    164             IF( IJE5 . NE . 0 ) THEN                                 1647
1648    165             JR2 = MOD( IR - 3 , 3 ) + 4                              1648
1649    166             IE2 = IABS( JS( JR2 , ISS ) )                            1649
1650    167             JR3 = MOD( IR - 2 , 3 ) + 4                              1650
1651    168             IE3 = IABS( JS( JR3 , ISS ) )                            1651
1652    169             XE1 = XE( 1 , IE )                                       1652
1653    170             XE2 = XE( 1 , IE2 )                                      1653
1654    171             XE3 = XE( 1 , IE3 )                                      1654
1655    172             XEDIST = 1. / XE1                                        1655
1656    173             YE2 = XE2 * XEDIST                                       1656
1657    174             YE3 = XE3 * XEDIST                                       1657
1658    175             ZE2 = ( YE2 - 1.5 ) * ( YE2 - .1 )                       1658
1659    176             ZE3 = ( YE3 - 1.5 ) * ( YE3 - .1 )                       1659
1660    177             YY2 = XE1 * XE1 + XE2 * XE2 + .35 * XE1 * XE2 - XE3 * XE3 1660
1661    178             YY3 = XE1 * XE1 + XE3 * XE3 + .35 * XE1 * XE3 - XE2 * XE2 1661
1662    179             IF( ZE2 . LT . .0 . AND . ZE3 . LT . 0. . AND .          1662
1663    180            .    YY2 . GT . 0. . AND . YY3 . GT . 0. ) THEN           1663
1664    181             CALL DISECT ( IE , IDONE , IDUMP )                       1664
1665    182     C                                                                1665
1666    183             LTRIG = LTRIG + 1                                        1666
1667    184             JTRIG( LTRIG ) = NS                                      1667
1668    185             KSDELT( NS ) = IDUMP                                     1668
1669    186     C                                                                1669
1670    187             END IF                                                   1670
1671    188             END IF                                                   1671
1672    189     335     CONTINUE                                                 1672
1673    190             END IF                                                   1673
1674    191     310     CONTINUE                                                 1674
1675    192     C                                                                1675
1676    193             NSS = LTRIG                                              1676
1677    194             IEDGE = 0                                                1677
1678    195             NCOLOR = 0                                               1678
1679    196     C                                                                1679
```

```
      DO 295 IE = 1 , NE
      JSE( IE ) = 0
  295 CONTINUE
C
      DO 320 IS = 1 , NSS
      ISS = JTRIG( IS )
      XSAREA = XS( 3 , ISS )
C
      IF( XSAREA . GT . RMINVG ) THEN
C
      DO 735 IR = 4 , 6
      IE = IABS( JS( IR , ISS ) )
      IF( JSE( IE ) . EQ . 0 ) THEN
      IEDGE = IEDGE + 1
      IRECNC( IEDGE ) = IE
      NCOLOR = NCOLOR + 1
      JEE( NCOLOR ) = IE
      JSE( IE ) = 1
      END IF
  735 CONTINUE
C
      AREAXS = SAREA( ISS )
      IE1 = IABS( JS( 4 , ISS ) )
      XE1 = XE( 1 , IE1 )
      HD1 = AREAXS * XE1 * XE1
      IJE5 = JE( 5 , IE1 )
      IE2 = IABS( JS( 5 , ISS ) )
      XE2 = XE( 1 , IE2 )
      HD2 = AREAXS * XE2 * XE2
      IJE5 = IJE5 + JE( 5 , IE2 )
      IE3 = IABS( JS( 6 , ISS ) )
      XE3 = XE( 1 , IE3 )
      HD3 = AREAXS * XE3 * XE3
      IJE5 = IJE5 + JE( 5 , IE3 )
      RATIO = AMAX1( HD1 , HD2 , HD3 )
      IRATIO = 0
      IF( RATIO . LE . 7. . AND . IJE5 . EQ . 0 . AND .
     .                              XSAREA . GT . SMINVG ) IRATIO = 1
      IF( IJE5 . GT . 0 ) IRATIO = 2
C
      IF( IRATIO . EQ . 2 ) THEN
      IJE51 = JE( 5 , IE1 )
      IJE52 = JE( 5 , IE2 )
      IJE53 = JE( 5 , IE3 )
      IF( IJE51 . NE . 0 ) THEN
      IEDIST = IE1
      XE1 = XE( 1 , IE1 )
      XE2 = XE( 1 , IE2 )
      XE3 = XE( 1 , IE3 )
      END IF
      IF( IJE52 . NE . 0 ) THEN
      IEDIST = IE2
      XE1 = XE( 1 , IE2 )
      XE2 = XE( 1 , IE1 )
      XE3 = XE( 1 , IE3 )
      END IF
      IF( IJE53 . NE . 0 ) THEN
      IEDIST = IE3
      XE1 = XE( 1 , IE3 )
      XE2 = XE( 1 , IE2 )
      XE3 = XE( 1 , IE1 )
      END IF
      XEDIST = 1. / XE( 1 , IEDIST )
      YE2 = XE2 * XEDIST
      YE3 = XE3 * XEDIST
      ZE2 = ( YE2 - 1.5 ) * ( YE2 - .1 )
      ZE3 = ( YE3 - 1.5 ) * ( YE3 - .1 )
      YY2 = XE1 * XE1 + XE2 * XE2 + .35 * XE1 * XE2 - XE3 * XE3
      YY3 = XE1 * XE1 + XE3 * XE3 + .35 * XE1 * XE3 - XE2 * XE2
      IF( ZE2 . LT . .0 . AND . ZE3 . LT . 0. . AND .
     .    YY2 . GT . 0. . AND . YY3 . GT . 0. ) THEN
      CALL DISECT ( IEDIST , IDONE , IDUMP )
C
      LTRIG = LTRIG + 1
```

```
1754  271          JTRIG( LTRIG ) = NS                                    1754
1755  272          KSDELT( NS ) = IDUMP                                   1755
1756  273    C                                                            1756
1757  274          IEDGE = IEDGE + 1                                      1757
1758  275          IRECNC( IEDGE ) = NE                                   1758
1759  276          NCOLOR = NCOLOR + 1                                    1759
1760  277          JEE( NCOLOR ) = NE                                     1760
1761  278          JSE( NE ) = 1                                          1761
1762  279          IEDGE = IEDGE + 1                                      1762
1763  280          IRECNC( IEDGE ) = NE - 1                               1763
1764  281          NCOLOR = NCOLOR + 1                                    1764
1765  282          JEE( NCOLOR ) = NE - 1                                 1765
1766  283          JSE( NE - 1 ) = 1                                      1766
1767  284    C                                                            1767
1768  285          END IF                                                 1768
1769  286          END IF                                                 1769
1770  287    C                                                            1770
1771  288          IF( IRATIO . EQ . 1 ) THEN                             1771
1772  289    C                                                            1772
1773  290          CALL VERCEN( ISS )                                     1773
1774  291          KSDELT( ISS ) = IDUMP                                  1774
1775  292          LTRIG = LTRIG + 1                                      1775
1776  293          JTRIG( LTRIG ) = NS - 1                                1776
1777  294          KSDELT( NS - 1 ) = IDUMP                               1777
1778  295    C                                                            1778
1779  296          LTRIG = LTRIG + 1                                      1779
1780  297          JTRIG( LTRIG ) = NS                                    1780
1781  298          KSDELT( NS ) = IDUMP                                   1781
1782  299    C                                                            1782
1783  300          IEDGE = IEDGE + 1                                      1783
1784  301          IRECNC( IEDGE ) = NE                                   1784
1785  302          NCOLOR = NCOLOR + 1                                    1785
1786  303          JEE( NCOLOR ) = NE                                     1786
1787  304          JSE( NE ) = 1                                          1787
1788  305          IEDGE = IEDGE + 1                                      1788
1789  306          IRECNC( IEDGE ) = NE - 1                               1789
1790  307          NCOLOR = NCOLOR + 1                                    1790
1791  308          JEE( NCOLOR ) = NE - 1                                 1791
1792  309          JSE( NE - 1 ) = 1                                      1792
1793  310          IEDGE = IEDGE + 1                                      1793
1794  311          IRECNC( IEDGE ) = NE - 2                               1794
1795  312          NCOLOR = NCOLOR + 1                                    1795
1796  313          JEE( NCOLOR ) = NE - 2                                 1796
1797  314          JSE( NE - 2 ) = 1                                      1797
1798  315    C                                                            1798
1799  316          ELSE                                                   1799
1800  317    C                                                            1800
1801  318          IDISCT = 0                                             1801
1802  319          DO 545 KK = 4 , 6                                      1802
1803  320          IEE = JS( KK , ISS )                                   1803
1804  321          IEF = IABS( IEE )                                      1804
1805  322          IJE55 = JE( 5 , IEF )                                  1805
1806  323          IF( IJE55 . EQ . 0 ) THEN                              1806
1807  324          IF( IEE . GT . 0 ) THEN                                1807
1808  325          ISI = JE( 4 , IEE )                                    1808
1809  326          ELSE                                                   1809
1810  327          ISI = JE( 3 , IEF )                                    1810
1811  328          END IF                                                 1811
1812  329          AREAXS = SAREA( ISI )                                  1812
1813  330          IE1 = IABS( JS( 4 , ISI ) )                            1813
1814  331          XE1 = XE( 1 , IE1 )                                    1814
1815  332          IJE55 = JE( 5 , IE1 )                                  1815
1816  333          HD1 = AREAXS * XE1 * XE1                               1816
1817  334          IE2 = IABS( JS( 5 , ISI ) )                            1817
1818  335          XE2 = XE( 1 , IE2 )                                    1818
1819  336          IJE55 = IJE55 + JE( 5 , IE2 )                          1819
1820  337          HD2 = AREAXS * XE2 * XE2                               1820
1821  338          IE3 = IABS( JS( 6 , ISI ) )                            1821
1822  339          XE3 = XE( 1 , IE3 )                                    1822
1823  340          IJE55 = IJE55 + JE( 5 , IE3 )                          1823
1824  341          HD3 = AREAXS * XE3 * XE3                               1824
1825  342          RATIO = AMAX1( HD1 , HD2 , HD3 )                       1825
1826  343          YSAREA = XS( 3 , ISI )                                 1826
1827  344          IF( RATIO . LT . 7. . AND . YSAREA . GT . SMINVG . AND .  1827
```

```
1828  345         .                                  IJE55 . EQ . 0 ) THEN
1829  346           IDISCT = 1
1830  347           DO 435 IR = 4 , 6
1831  348           IE = IABS( JS( IR , ISI ) )
1832  349           IF( JSE( IE ) . EQ . 0 ) THEN
1833  350           IEDGE = IEDGE + 1
1834  351           IRECNC( IEDGE ) = IE
1835  352           NCOLOR = NCOLOR + 1
1836  353           JEE( NCOLOR ) = IE
1837  354           JSE( IE ) = 1
1838  355           END IF
1839  356   435     CONTINUE
1840  357           CALL VERCEN( ISI )
1841  358           KSDELT( ISI ) = IDUMP
1842  359           LTRIG = LTRIG + 1
1843  360           JTRIG( LTRIG ) = NS - 1
1844  361           KSDELT( NS - 1 ) = IDUMP
1845  362   C
1846  363           LTRIG = LTRIG + 1
1847  364           JTRIG( LTRIG ) = NS
1848  365           KSDELT( NS ) = IDUMP
1849  366   C
1850  367           IEDGE = IEDGE + 1
1851  368           IRECNC( IEDGE ) = NE
1852  369           NCOLOR = NCOLOR + 1
1853  370           JEE( NCOLOR ) = NE
1854  371           JSE( NE ) = 1
1855  372           IEDGE = IEDGE + 1
1856  373           IRECNC( IEDGE ) = NE - 1
1857  374           NCOLOR = NCOLOR + 1
1858  375           JEE( NCOLOR ) = NE - 1
1859  376           JSE( NE - 1 ) = 1
1860  377           IEDGE = IEDGE + 1
1861  378           IRECNC( IEDGE ) = NE - 2
1862  379           NCOLOR = NCOLOR + 1
1863  380           JEE( NCOLOR ) = NE - 2
1864  381           JSE( NE - 2 ) = 1
1865  382           END IF
1866  383           END IF
1867  384   545     CONTINUE
1868  385   C
1869  386           IF( IDISCT . EQ . 0 ) THEN
1870  387           IE1 = IABS( JS( 4 , ISS ) )
1871  388           XE1 = XE( 1 , IE1 )
1872  389           IE2 = IABS( JS( 5 , ISS ) )
1873  390           XE2 = XE( 1 , IE2 )
1874  391           IE3 = IABS( JS( 6 , ISS ) )
1875  392           XE3 = XE( 1 , IE3 )
1876  393           IEDIST = IE1
1877  394           XEDIST = XE1
1878  395           IF( XE2 . GT . XEDIST ) THEN
1879  396           XEDIST = XE2
1880  397           IEDIST = IE2
1881  398           END IF
1882  399           IF( XE3 . GT . XEDIST ) THEN
1883  400           XEDIST = XE3
1884  401           IEDIST = IE3
1885  402           END IF
1886  403           ISL = JE( 3 , IEDIST )
1887  404           ISR = JE( 4 , IEDIST )
1888  405           XSISL = XS( 3 , ISL )
1889  406           XSISR = XS( 3 , ISR )
1890  407           IJE5 = JE( 5 , IEDIST )
1891  408           IF( XSISL . GT . RMINVG . AND . XSISR . GT . RMINVG . AND .
1892  409         .     IJE5 . EQ . 0 . AND . IRATIO . NE . 2 )  THEN
1893  410           IF( ISS . NE . ISL ) THEN
1894  411           DO 345 IR = 4 , 6
1895  412           IE = IABS( JS( IR , ISL ) )
1896  413           IF( JSE( IE ) . EQ . 0 ) THEN
1897  414           IEDGE = IEDGE + 1
1898  415           IRECNC( IEDGE ) = IE
1899  416           NCOLOR = NCOLOR + 1
1900  417           JEE( NCOLOR ) = IE
1901  418           JSE( IE ) = 1
```

```
1902     419          END IF                                                    1902
1903     420   345    CONTINUE                                                  1903
1904     421          END IF                                                    1904
1905     422   C                                                                1905
1906     423          IF( ISS . NE . ISR ) THEN                                 1906
1907     424          DO 355 IR = 4 , 6                                         1907
1908     425          IE = IABS( JS( IR , ISR ) )                               1908
1909     426          IF( JSE( IE ) . EQ . 0 ) THEN                             1909
1910     427          IEDGE = IEDGE + 1                                         1910
1911     428          IRECNC( IEDGE ) = IE                                      1911
1912     429          NCOLOR = NCOLOR + 1                                       1912
1913     430          JEE( NCOLOR ) = IE                                        1913
1914     431          JSE( IE ) = 1                                             1914
1915     432          END IF                                                    1915
1916     433   355    CONTINUE                                                  1916
1917     434          END IF                                                    1917
1918     435   C                                                                1918
1919     436          IDONE = 0                                                 1919
1920     437          CALL DISECT ( IEDIST , IDONE , IDUMP )                    1920
1921     438          IF( IDONE . EQ . 1 ) THEN                                 1921
1922     439   C                                                                1922
1923     440          LTRIG = LTRIG + 1                                         1923
1924     441          JTRIG( LTRIG ) = NS                                       1924
1925     442          KSDELT( NS ) = IDUMP                                      1925
1926     443          LTRIG = LTRIG + 1                                         1926
1927     444          JTRIG( LTRIG ) = NS - 1                                   1927
1928     445          KSDELT( NS - 1 ) = IDUMP                                  1928
1929     446   C                                                                1929
1930     447          IEDGE = IEDGE + 1                                         1930
1931     448          IRECNC( IEDGE ) = NE                                      1931
1932     449          NCOLOR = NCOLOR + 1                                       1932
1933     450          JEE( NCOLOR ) = NE                                        1933
1934     451          JSE( NE ) = 1                                             1934
1935     452          IEDGE = IEDGE + 1                                         1935
1936     453          IRECNC( IEDGE ) = NE - 1                                  1936
1937     454          NCOLOR = NCOLOR + 1                                       1937
1938     455          JEE( NCOLOR ) = NE - 1                                    1938
1939     456          JSE( NE - 1 ) = 1                                         1939
1940     457          IEDGE = IEDGE + 1                                         1940
1941     458          IRECNC( IEDGE ) = NE - 2                                  1941
1942     459          NCOLOR = NCOLOR + 1                                       1942
1943     460          JEE( NCOLOR ) = NE - 2                                    1943
1944     461          JSE( NE - 2 ) = 1                                         1944
1945     462          END IF                                                    1945
1946     463   C                                                                1946
1947     464          END IF                                                    1947
1948     465          END IF                                                    1948
1949     466          END IF                                                    1949
1950     467          END IF                                                    1950
1951     468   C                                                                1951
1952     469    320   CONTINUE                                                  1952
1953     470   C                                                                1953
1954     471          DO 340 IEM = 1 , NCOLOR                                   1954
1955     472          IE = JEE( IEM )                                           1955
1956     473   C                                                                1956
1957     474          ISL = JE( 3 , IE )                                        1957
1958     475          YSAREA = XS( 3 , ISL )                                    1958
1959     476          IJE5 = JE( 5 , IE )                                       1959
1960     477          IF( YSAREA . GE . RMINVG . AND . IJE5 . NE . 0 ) THEN     1960
1961     478          IE1 = IABS( JS( 4 , ISL ) )                               1961
1962     479          IE2 = IABS( JS( 5 , ISL ) )                               1962
1963     480          IE3 = IABS( JS( 6 , ISL ) )                               1963
1964     481          IJE51 = JE( 5 , IE1 )                                     1964
1965     482          IJE52 = JE( 5 , IE2 )                                     1965
1966     483          IJE53 = JE( 5 , IE3 )                                     1966
1967     484          IF( IJE51 . NE . 0 ) THEN                                 1967
1968     485          IEDIST = IE1                                              1968
1969     486          XE1 = XE( 1 , IE1 )                                       1969
1970     487          XE2 = XE( 1 , IE2 )                                       1970
1971     488          XE3 = XE( 1 , IE3 )                                       1971
1972     489          END IF                                                    1972
1973     490          IF( IJE52 . NE . 0 ) THEN                                 1973
1974     491          IEDIST = IE2                                              1974
1975     492          XE1 = XE( 1 , IE2 )                                       1975
```

```
1976    493          XE2 = XE( 1 , IE1 )                                                    1976
1977    494          XE3 = XF( 1 , IE3 )                                                    1977
1978    495          END IF                                                                 1978
1979    496          IF( IJE53 . NE . 0 ) THEN                                              1979
1980    497          IEDIST = IE3                                                           1980
1981    498          XE1 = XE( 1 , IE3 )                                                    1981
1982    499          XE2 = XE( 1 , IE2 )                                                    1982
1983    500          XE3 = XE( 1 , IE1 )                                                    1983
1984    501          END IF                                                                 1984
1985    502          XEDIST = 1. / XE( 1 , IEDIST )                                         1985
1986    503          YE2 = XE2 * XEDIST                                                     1986
1987    504          YE3 = XE3 * XEDIST                                                     1987
1988    505          ZE2 = ( YE2 - 1.5 ) * ( YE2 - .1 )                                     1988
1989    506          ZE3 = ( YE3 - 1.5 ) * ( YE3 - .1 )                                     1989
1990    507          YY2 = XE1 * XE1 + XE2 * XE2 + .35 * XE1 * XE2 - XE3 * XE3              1990
1991    508          YY3 = XE1 * XE1 + XE3 * XE3 + .35 * XE1 * XE3 - XE2 * XE2              1991
1992    509          IF( ZE2 . LT . .0 . AND . ZE3 . LT . 0. . AND .                        1992
1993    510         .     YY2 . GT . 0. . AND . YY3 . GT . 0. ) THEN                       1993
1994    511          CALL DISECT ( IEDIST , IDONE , IDUMP )                                 1994
1995    512  C                                                                              1995
1996    513          LTRIG = LTRIG + 1                                                      1996
1997    514          JTRIG( LTRIG ) = NS                                                    1997
1998    515          KSDELT( NS ) = IDUMP                                                   1998
1999    516  C                                                                              1999
2000    517          IEDGE = IEDGE + 1                                                      2000
2001    518          IRECNC( IEDGE ) = NE                                                   2001
2002    519          NCOLOR = NCOLOR + 1                                                    2002
2003    520          JEE( NCOLOR ) = NE                                                     2003
2004    521          JSE( NE ) = 1                                                          2004
2005    522          IEDGE = IEDGE + 1                                                      2005
2006    523          IRECNC( IEDGE ) = NE - 1                                               2006
2007    524          NCOLOR = NCOLOR + 1                                                    2007
2008    525          JEE( NCOLOR ) = NE - 1                                                 2008
2009    526          JSE( NE - 1 ) = 1                                                      2009
2010    527  C                                                                              2010
2011    528           ELSE                                                                  2011
2012    529  C                                                                              2012
2013    530          IEDIST = IE1                                                           2013
2014    531          XEDIST = XE1                                                           2014
2015    532          IF( XE2 . GT . XEDIST ) THEN                                           2015
2016    533          XEDIST = XE2                                                           2016
2017    534          IEDIST = IE2                                                           2017
2018    535          END IF                                                                 2018
2019    536          IF( XE3 . GT . XEDIST ) THEN                                           2019
2020    537          XEDIST = XE3                                                           2020
2021    538          IEDIST = IE3                                                           2021
2022    539          END IF                                                                 2022
2023    540          ISL = JE( 3 , IEDIST )                                                 2023
2024    541          ISR = JE( 4 , IEDIST )                                                 2024
2025    542          XSISL = XS( 3 , ISL )                                                  2025
2026    543          XSISR = XS( 3 , ISR )                                                  2026
2027    544          IJE5 = JE( 5 , IEDIST )                                                2027
2028    545          IF( XSISL . GT . RMINVG . AND . XSISR . GT . RMINVG . AND .            2028
2029    546         .                                          IJE5 . EQ . 0 )  THEN       2029
2030    547          DO 645 IR = 4 , 6                                                      2030
2031    548          IE = IABS( JS( IR , ISL ) )                                            2031
2032    549          IF( JSE( IE ) . EQ . 0 ) THEN                                          2032
2033    550          IEDGE = IEDGE + 1                                                      2033
2034    551          IRECNC( IEDGE ) = IE                                                   2034
2035    552          NCOLOR = NCOLOR + 1                                                    2035
2036    553          JEE( NCOLOR ) = IE                                                     2036
2037    554          JSE( IE ) = 1                                                          2037
2038    555          END IF                                                                 2038
2039    556  645     CONTINUE                                                               2039
2040    557          DO 655 IR = 4 , 6                                                      2040
2041    558          IE = IABS( JS( IR , ISR ) )                                            2041
2042    559          IF( JSE( IE ) . EQ . 0 ) THEN                                          2042
2043    560          IEDGE = IEDGE + 1                                                      2043
2044    561          IRECNC( IEDGE ) = IE                                                   2044
2045    562          NCOLOR = NCOLOR + 1                                                    2045
2046    563          JEE( NCOLOR ) = IE                                                     2046
2047    564          JSE( IE ) = 1                                                          2047
2048    565          END IF                                                                 2048
2049    566  655     CONTINUE                                                               2049
```

```
2050     567   C                                                                2050
2051     568         IDONE = 0                                                  2051
2052     569         CALL DISECT ( IEDIST , IDONE , IDUMP )                     2052
2053     570         IF( IDONE . EQ . 1 ) THEN                                  2053
2054     571   C                                                                2054
2055     572         LTRIG = LTRIG + 1                                          2055
2056     573         JTRIG( LTRIG ) = NS                                        2056
2057     574         KSDELT( NS ) = IDUMP                                       2057
2058     575         LTRIG = LTRIG + 1                                          2058
2059     576         JTRIG( LTRIG ) = NS - 1                                    2059
2060     577         KSDELT( NS - 1 ) = IDUMP                                   2060
2061     578   C                                                                2061
2062     579         IEDGE = IEDGE + 1                                          2062
2063     580         IRECNC( IEDGE ) = NE                                       2063
2064     581         NCOLOR = NCOLOR + 1                                        2064
2065     582         JEE( NCOLOR ) = NE                                         2065
2066     583         JSE( NE ) = 1                                              2066
2067     584         IEDGE = IEDGE + 1                                          2067
2068     585         IRECNC( IEDGE ) = NE - 1                                   2068
2069     586         NCOLOR = NCOLOR + 1                                        2069
2070     587         JEE( NCOLOR ) = NE - 1                                     2070
2071     588         JSE( NE - 1 ) = 1                                          2071
2072     589         IEDGE = IEDGE + 1                                          2072
2073     590         IRECNC( IEDGE ) = NE - 2                                   2073
2074     591         NCOLOR = NCOLOR + 1                                        2074
2075     592         JEE( NCOLOR ) = NE - 2                                     2075
2076     593         JSE( NE - 2 ) = 1                                          2076
2077     594         END IF                                                     2077
2078     595   C                                                                2078
2079     596         END IF                                                     2079
2080     597         END IF                                                     2080
2081     598         END IF                                                     2081
2082     599    340  CONTINUE                                                   2082
2083     600   C                                                                2083
2084     601         NSS = LTRIG                                                2084
2085     602   C                                                                2085
2086     603         DO 370 IEM = 1 , NCOLOR                                    2086
2087     604         IE = JEE( IEM )                                            2087
2088     605         CALL RECNC( IE , IDONE , ITL , ITR , JA , JB , JC , JD )   2088
2089     606         CALL RECNC( JA , JADONE , ITL , ITR , JAA , JAB , JAC , JAD ) 2089
2090     607         CALL RECNC( JB , JBDONE , ITL , ITR , JBA , JBB , JBC , JBD ) 2090
2091     608         CALL RECNC( JC , JCDONE , ITL , ITR , JCA , JCB , JCC , JCD ) 2091
2092     609         CALL RECNC( JD , JDDONE , ITL , ITR , JDA , JDB , JDC , JDD ) 2092
2093     610   370   CONTINUE                                                   2093
2094     611   C                                                                2094
2095     612   300   CONTINUE                                                   2095
2096     613   C                                                                2096
2097     614         NVECE = NE / MBL                                           2097
2098     615         NREME = NE - NVECE * MBL                                   2098
2099     616         NVECS = NS / MBL                                           2099
2100     617         NREMS = NS - NVECS * MBL                                   2100
2101     618         NVECV = NV / MBL                                           2101
2102     619         NREMV = NV - NVECV * MBL                                   2102
2103     620   C                                                                2103
2104     621         DO 400 INE = 1 , NVECE                                     2104
2105     622         NOFVEE( INE ) = MBL                                        2105
2106     623   400   CONTINUE                                                   2106
2107     624         NVEEE = NVECE                                              2107
2108     625         IF( NREME . GT . 0 ) THEN                                  2108
2109     626         NVEEE = NVECE + 1                                          2109
2110     627         NOFVEE( NVEEE ) = NREME                                    2110
2111     628         END IF                                                     2111
2112     629   C                                                                2112
2113     630         DO 410 INS = 1 , NVECS                                     2113
2114     631         NOFVES( INS ) = MBL                                        2114
2115     632   410   CONTINUE                                                   2115
2116     633         NVEES = NVECS                                              2116
2117     634         IF( NREMS . GT . 0 ) THEN                                  2117
2118     635         NVEES = NVECS + 1                                          2118
2119     636         NOFVES( NVEES ) = NREMS                                    2119
2120     637         END IF                                                     2120
2121     638   C                                                                2121
2122     639         DO 420 INV = 1 , NVECV                                     2122
2123     640         NOFVEV( INV ) = MBL                                        2123
```

```
2124     641   420   CONTINUE                                                  2124
2125     642         NVEEV = NVECV                                             2125
2126     643         IF( NREMV . GT . 0 ) THEN                                 2126
2127     644         NVEEV = NVECV + 1                                         2127
2128     645         NOFVEV( NVEEV ) = NREMV                                   2128
2129     646         END IF                                                    2129
2130     647   C                                                               2130
2131     648          PRINT*,NV,NE,NS                                          2131
2132     649   C                                                               2132
2133     650   C --- EXIT POINT FROM SUBROUTINE ----------------------------------- 2133
2134     651   C                                                               2134
2135     652   C     ------                                                    2135
2136     653         RETURN                                                    2136
2137     654   C     ------                                                    2137
2138     655   C                                                               2138
2139     656   C     ---                                                       2139
2140     657         END                                                       2140
```



```
2141       1         SUBROUTINE INTPTN( DAREA , NOFDIV , IDUMP , LTRIG )       2141
2142       2   C                                                               2142
2143       3   C-----------------------------------------------------------------| 2143
2144       4   C                                                               I 2144
2145       5   C      INTPTN ADAPT THE GRID DYNAMICALLY, ADD VERTECES          I 2145
2146       6   C      SUB DIVIDE TO REFINE AT THE INITIAL STAGE OF THE SIMULATION I 2146
2147       7   C                                                               I 2147
2148       8   C-----------------------------------------------------------------I 2148
2149       9   C                                                               2149
2150      10             IMPLICIT REAL (A-H,O-Z)                              2150
2151      11   C                                                               2151
2152      12         include     'cmsh00.h'                                    2152
2153      13         include     'chyd00.h'                                    2153
2154      14         include     'cint00.h'                                    2154
2155      15         include     'cphs10.h'                                    2155
2156      16         include     'cphs20.h'                                    2156
2157      17   C                                                               2157
2158      18         INTEGER JTRIG(MEM),KTRIG(MEM),IRECNC(MEM)                 2158
2159      19         INTEGER JSE(MEM),JEE(MEM),IOFDVS(10),NOFDVS(10)           2159
2160      20   C                                                               2160
2161      21         EQUIVALENCE (UL,JTRIG)                                    2161
2162      22         EQUIVALENCE (VR,KTRIG)                                    2162
2163      23         EQUIVALENCE (VL,IRECNC)                                   2163
2164      24         EQUIVALENCE (PR,JSE)                                      2164
2165      25         EQUIVALENCE (PL,JEE)                                      2165
2166      26   C                                                               2166
2167      27          SMINVG = SAREVG * DAREA                                  2167
2168      28          RMINVG = .7 * SMINVG                                     2168
2169      29   C                                                               2169
2170      30          DO 115 IS = 1 , NS                                       2170
2171      31          JEE( IS ) = 0                                            2171
2172      32    115   CONTINUE                                                 2172
2173      33   C                                                               2173
2174      34          NSS = 0                                                  2174
2175      35          DO 120 IS = 1 , NS                                       2175
2176      36   C       DO 120 IR = 4 , 6                                       2176
2177      37   C       IE = IABS( JS( IR , IS ) )                              2177
2178      38   C       IJE5 = JE( 5 , IE )                                     2178
2179      39          XSS = XS( 1 , IS )                                       2179
2180      40          IF( XSS . GT . -.05 . AND . XSS . LT . .05 . AND .       2180
2181      41         .     KSDELT( IS ) . LT . IDUMP ) THEN                    2181
2182      42   C       IF( IJE5 . EQ . 8 ) THEN                                2182
2183      43          KSDELT( IS ) = IDUMP                                     2183
2184      44          JEE( IS ) = 1                                            2184
2185      45          NSS = NSS + 1                                            2185
2186      46          JTRIG( NSS ) = IS                                        2186
2187      47          END IF                                                   2187
2188      48    120   CONTINUE                                                 2188
2189      49   C                                                               2189
2190      50          DO 130 IS = 1 , NSS                                      2190
2191      51          JSE( IS ) = JTRIG( IS )                                  2191
2192      52    130   CONTINUE                                                 2192
2193      53   C                                                               2193
2194      54          MSS = NSS                                                2194
```

```
2195      55          DO 140 KDIV = 1 , NOFDIV                                  2195
2196      56          ITRIG = 0                                                 2196
2197      57          DO 150 KS = 1 , NSS                                       2197
2198      58  C                                                                 2198
2199      59          ISS = JSE( KS )                                           2199
2200      60  C                                                                 2200
2201      61          DO 160 KR = 1 , 3                                         2201
2202      62          IVV = JS( KR , ISS )                                      2202
2203      63  C                                                                 2203
2204      64             IE = JV( 2 , IVV )                                     2204
2205      65             IF( IE . GT . 0 ) THEN                                 2205
2206      66  C                                                                 2206
2207      67             IV1 = JE( 1 , IE )                                     2207
2208      68             IF( IV1 . EQ . IVV ) THEN                              2208
2209      69             ISI = JE( 3 , IE )                                     2209
2210      70             ELSE                                                   2210
2211      71             ISI = JE( 4 , IE )                                     2211
2212      72             END IF                                                 2212
2213      73             IS = ISI                                               2213
2214      74  C                                                                 2214
2215      75  750        CONTINUE                                               2215
2216      76  C                                                                 2216
2217      77             JES = JEE( IS )                                        2217
2218      78             XAS = XS( 3 ,  S )                                     2218
2219      79             IF( JES . EQ . 0 . AND . XAS . LT . SAREVG ) THEN      2219
2220      80             ITRIG = ITRIG + 1                                      2220
2221      81             KTRIG( ITRIG ) = IS                                    2221
2222      82             KSDELT( IS ) = IDUMP                                   2222
2223      83             JEE( IS ) = 1                                          2223
2224      84             END IF                                                 2224
2225      85  C                                                                 2225
2226      86             DO 760 IR = 1 , 3                                      2226
2227      87             JR = MOD( IR , 3 ) + 1                                 2227
2228      88             IEA = IABS( JS( JR + 3 , IS ) )                        2228
2229      89             IF( IEA . EQ . IE ) THEN                               2229
2230      90             JJR = MOD( JR + 1 , 3 ) + 4                            2230
2231      91             IER = IABS( JS( JJR , IS ) )                           2231
2232      92  C                                                                 2232
2233      93             IV1 = JE( 1 , IER )                                    2233
2234      94             IF( IV1 . EQ . IVV ) THEN                              2234
2235      95             ISR = JE( 3 , IER )                                    2235
2236      96             ELSE                                                   2236
2237      97             ISR = JE( 4 , IER )                                    2237
2238      98             END IF                                                 2238
2239      99             END IF                                                 2239
2240     100  760        CONTINUE                                               2240
2241     101  C                                                                 2241
2242     102             IF( ISR . NE . ISI ) THEN                              2242
2243     103             IS = ISR                                               2243
2244     104             IE = IER                                               2244
2245     105  C                                                                 2245
2246     106             GO TO 750                                              2246
2247     107             END IF                                                 2247
2248     108  C                                                                 2248
2249     109             ELSE                                                   2249
2250     110  C                                                                 2250
2251     111             IE = - IE                                              2251
2252     112             IV1 = JE( 1 , IE )                                     2252
2253     113             IF( IV1 . EQ . IVV ) THEN                              2253
2254     114             ISI = JE( 3 , IE )                                     2254
2255     115             ELSE                                                   2255
2256     116             ISI = JE( 4 , IE )                                     2256
2257     117             END IF                                                 2257
2258     118             IS = ISI                                               2258
2259     119             ISI = 0                                                2259
2260     120  C                                                                 2260
2261     121  650        CONTINUE                                               2261
2262     122  C                                                                 2262
2263     123             JES = JEE( IS )                                        2263
2264     124             XAS = XS( 3 , IS )                                     2264
2265     125             IF( JES . EQ . 0 . AND . XAS . LT . SAREVG ) THEN      2265
2266     126             ITRIG = ITRIG + 1                                      2266
2267     127             KTRIG( ITRIG ) = IS                                    2267
2268     128             KSDELT( IS ) = IDUMP                                   2268
```

```
2269     129              JEE( IS ) = 1                                                                  2269
2270     130              END IF                                                                         2270
2271     131    C                                                                                       2271
2272     132              DO 660 IR = 1 , 3                                                              2272
2273     133              JR = MOD( IR , 3 ) + 1                                                         2273
2274     134              IEA = IABS( JS( JR + 3 , IS ) )                                                2274
2275     135              IF( IEA . EQ . IE ) THEN                                                       2275
2276     136              JJR = MOD( JR + 1 , 3 ) + 4                                                    2276
2277     137              IER = IABS( JS( JJR , IS ) )                                                   2277
2278     138    C                                                                                       2278
2279     139              IV1 = JE( 1 , IER )                                                            2279
2280     140              IF( IV1 . EQ . IVV ) THEN                                                      2280
2281     141              ISR = JE( 3 , IER )                                                            2281
2282     142              ELSE                                                                           2282
2283     143              ISR = JE( 4 , IER )                                                            2283
2284     144              END IF                                                                         2284
2285     145              END IF                                                                         2285
2286     146    C                                                                                       2286
2287     147    660       CONTINUE                                                                      2287
2288     148    C                                                                                       2288
2289     149              IF( ISR . NE . ISI ) THEN                                                      2289
2290     150              IS = ISR                                                                       2290
2291     151              IE = IER                                                                       2291
2292     152              GO TO 650                                                                      2292
2293     153              END IF                                                                         2293
2294     154              END IF                                                                         2294
2295     155     160   CONTINUE                                                                         2295
2296     156    C                                                                                       2296
2297     157     150   CONTINUE                                                                         2297
2298     158    C                                                                                       2298
2299     159           DO 170 IS = 1 , ITRIG                                                           2299
2300     160           JTRIG( IS + MSS ) = KTRIG( IS )                                                 2300
2301     161           JSE( IS ) = KTRIG( IS )                                                         2301
2302     162     170   CONTINUE                                                                        2302
2303     163           NSS = ITRIG                                                                     2303
2304     164           MSS = MSS + ITRIG                                                               2304
2305     165    C                                                                                      2305
2306     166     140   CONTINUE                                                                       2306
2307     167           NSS = MSS                                                                      2307
2308     168    C                                                                                      2308
2309     169           DO 300 KDIV = 1 , 1                                                            2309
2310     170           LTRIG = NSS                                                                    2310
2311     171           IEDGE = 0                                                                      2311
2312     172           NCOLOR = 0                                                                     2312
2313     173    C                                                                                      2313
2314     174           DO 290 IE = 1 , NE                                                             2314
2315     175           JSE( IE ) = 0                                                                  2315
2316     176     290   CONTINUE                                                                       2316
2317     177    C                                                                                      2317
2318     178           DO 310 IS = 1 , NSS                                                            2318
2319     179           ISS = JTRIG( IS )                                                              2319
2320     180           XSAREA = XS( 3 , ISS )                                                         2320
2321     181           IF( XSAREA . GE . RMINVG ) THEN                                                2321
2322     182    C                                                                                      2322
2323     183           DO 335 IR = 4 , 6                                                              2323
2324     184           IE = IABS( JS( IR , ISS ) )                                                    2324
2325     185           IJE5 = JE( 5 , IE )                                                            2325
2326     186           IF( IJE5 . NE . 0 ) THEN                                                       2326
2327     187           JR2 = MOD( IR - 3 , 3 ) + 4                                                    2327
2328     188           IE2 = IABS( JS( JR2 , ISS ) )                                                  2328
2329     189           JR3 = MOD( IR - 2 , 3 ) + 4                                                    2329
2330     190           IE3 = IABS( JS( JR3 , ISS ) )                                                  2330
2331     191           XE1 = XE( 1 , IE )                                                             2331
2332     192           XE2 = XE( 1 , IE2 )                                                            2332
2333     193           XE3 = XE( 1 , IE3 )                                                            2333
2334     194           XEDIST = 1. / XE1                                                              2334
2335     195           YE2 = XE2 * XEDIST                                                             2335
2336     196           YE3 = XE3 * XEDIST                                                             2336
2337     197           ZE2 = ( YE2 - 1.5 ) * ( YE2 - .1 )                                             2337
2338     198           ZE3 = ( YE3 - 1.5 ) * ( YE3 - .1 )                                             2338
2339     199           YY2 = XE1 * XE1 + XE2 * XE2 + .35 * XE1 * XE2 - XE3 * XE3                      2339
2340     200           YY3 = XE1 * XE1 + XE3 * XE3 + .35 * XE1 * XE3 - XE2 * XE2                      2340
2341     201           IF( ZE2 . LT . .0 . AND . ZE3 . LT . 0. . AND .                                2341
2342     202          .     YY2 . GT . 0. . AND . YY3 . GT . 0. ) THEN                                2342
```

```
2343    203          CALL DISECT ( IE , IDONE , IDUMP )                    2343
2344    204   C                                                            2344
2345    205          LTRIG = LTRIG + 1                                     2345
2346    206          JTRIG( LTRIG ) = NS                                   2346
2347    207          KSOELT( NS ) = IDUMP                                  2347
2348    208   C                                                            2348
2349    209          IEDGE = IEDGE + 1                                     2349
2350    210          IRECNC( IEDGE ) = NE                                  2350
2351    211          NCOLOR = NCOLOR + 1                                   2351
2352    212          JEE( NCOLOR ) = NE                                    2352
2353    213          JSE( NE ) = 1                                         2353
2354    214          IEDGE = IEDGE + 1                                     2354
2355    215          IRECNC( IEDGE ) = NE - 1                              2355
2356    216          NCOLOR = NCOLOR + 1                                   2356
2357    217          JEE( NCOLOR ) = NE - 1                                2357
2358    218          JSE( NE - 1 ) = 1                                     2358
2359    219   C                                                            2359
2360    220          END IF                                                2360
2361    221          END IF                                                2361
2362    222   335    CONTINUE                                              2362
2363    223          END IF                                                2363
2364    224   310    CONTINUE                                              2364
2365    225   C                                                            2365
2366    226          NSS = LTRIG                                           2366
2367    227          IEDGE = 0                                             2367
2368    228          NCOLOR = 0                                            2368
2369    229   C                                                            2369
2370    230          DO 295 IE = 1 , NE                                    2370
2371    231          JSE( IE ) = 0                                         2371
2372    232    295   CONTINUE                                              2372
2373    233   C                                                            2373
2374    234          DO 320 IS = 1 , NSS                                   2374
2375    235          ISS = JTRIG( IS )                                     2375
2376    236          XSAREA = XS( 3 , ISS )                                2376
2377    237   C                                                            2377
2378    238          DO 735 IR = 4 , 6                                     2378
2379    239          IE = IABS( JS( IR , ISS ) )                           2379
2380    240          IF( JSE( IE ) . EQ . 0 ) THEN                         2380
2381    241          IEDGE = IEDGE + 1                                     2381
2382    242          IRECNC( IEDGE ) = IE                                  2382
2383    243          NCOLOR = NCOLOR + 1                                   2383
2384    244          JEE( NCOLOR ) = IE                                    2384
2385    245          JSE( IE ) = 1                                         2385
2386    246          END IF                                                2386
2387    247   735    CONTINUE                                              2387
2388    248   C                                                            2388
2389    249          IF( XSAREA . GT . RMINVG ) THEN                       2389
2390    250   C                                                            2390
2391    251          AREAXS = SAREA( ISS )                                 2391
2392    252          IE1 = IABS( JS( 4 , ISS ) )                           2392
2393    253          XE1 = XE( 1 , IE1 )                                   2393
2394    254          HD1 = AREAXS * XE1 * XE1                              2394
2395    255          IJE5 = JE( 5 , IE1 )                                  2395
2396    256          IE2 = IABS( JS( 5 , ISS ) )                           2396
2397    257          XE2 = XE( 1 , IE2 )                                   2397
2398    258          HD2 = AREAXS * XE2 * XE2                              2398
2399    259          IJE5 = IJE5 + JE( 5 , IE2 )                           2399
2400    260          IE3 = IABS( JS( 6 , ISS ) )                           2400
2401    261          XE3 = XE( 1 , IE3 )                                   2401
2402    262          HD3 = AREAXS * XE3 * XE3                              2402
2403    263          IJE5 = IJE5 + JE( 5 , IE3 )                           2403
2404    264          RATIO = AMAX1( HD1 , HD2 , HD3 )                      2404
2405    265          IRATIO = 0                                            2405
2406    266          IF( RATIO . LE . 7. . AND . IJE5 . EQ . 0 . AND .     2406
2407    267       .                              XSAREA . GT . SMINVG ) IRATIO = 1  2407
2408    268          IF( IJE5 . GT . 0 ) IRATIO = 2                        2408
2409    269   C                                                            2409
2410    270          IF( IRATIO . EQ . 2 ) THEN                            2410
2411    271          IJE51 = JE( 5 , IE1 )                                 2411
2412    272          IJE52 = JE( 5 , IE2 )                                 2412
2413    273          IJE53 = JE( 5 , IE3 )                                 2413
2414    274          IF( IJE51 . NE . 0 ) THEN                             2414
2415    275          IEDIST = IE1                                          2415
2416    276          XE1 = XE( 1 , IE1 )                                   2416
```

```
2417     277          XE2 = XE( 1 , IE2 )
2418     278          XE3 = XE( 1 , IE3 )
2419     279          END IF
2420     280          IF( IJE52 . NE . 0 ) THEN
2421     281          IEDIST = IE2
2422     282          XE1 = XE( 1 , IE2 )
2423     283          XE2 = XE( 1 , IE1 )
2424     284          XE3 = XE( 1 , IE3 )
2425     285          END IF
2426     286          IF( IJE53 . NE . 0 ) THEN
2427     287          IEDIST = IE3
2428     288          XE1 = XE( 1 , IE3 )
2429     289          XE2 = XE( 1 , IE2 )
2430     290          XE3 = XE( 1 , IE1 )
2431     291          END IF
2432     292          XEDIST = 1. / XE( 1 , IEDIST )
2433     293          YE2 = XE2 * XEDIST
2434     294          YE3 = XE3 * XEDIST
2435     295          ZE2 = ( YE2 - 1.5 ) * ( YE2 - .1 )
2436     296          ZE3 = ( YE3 - 1.5 ) * ( YE3 - .1 )
2437     297          YY2 = XE1 * XE1 + XE2 * XE2 + .35 * XE1 * XE2 - XE3 * XE3
2438     298          YY3 = XE1 * XE1 + XE3 * XE3 + .35 * XE1 * XE3 - XE2 * XE2
2439     299          YY3 = XE1 * XE1 + XE3 * XE3 - XE2 * XE2
2440     300          IF( ZE2 . LT . .0 . AND . ZE3 . LT . 0. . AND .
2441     301         .     YY2 . GT . 0. . AND . YY3 . GT . 0. ) THEN
2442     302          CALL DISECT ( IEDIST , IDONE , IDUMP )
2443     303   C
2444     304          LTRIG = LTRIG + 1
2445     305          JTRIG( LTRIG ) = NS
2446     306          KSDELT( NS ) = IDUMP
2447     307   C
2448     308          IEDGE = IEDGE + 1
2449     309          IRECNC( IEDGE ) = NE
2450     310          NCOLOR = NCOLOR + 1
2451     311          JEE( NCOLOR ) = NE
2452     312          JSE( NE ) = 1
2453     313          IEDGE = IEDGE + 1
2454     314          IRECNC( IEDGE ) = NE - 1
2455     315          NCOLOR = NCOLOR + 1
2456     316          JEE( NCOLOR ) = NE - 1
2457     317          JSE( NE - 1 ) = 1
2458     318   C
2459     319          END IF
2460     320          END IF
2461     321   C
2462     322          IF( IRATIO . EQ . 1 ) THEN
2463     323   C
2464     324          CALL VERCEN( ISS )
2465     325          KSDELT( ISS ) = IDUMP
2466     326          LTRIG = LTRIG + 1
2467     327          JTRIG( LTRIG ) = NS - 1
2468     328          KSDELT( NS - 1 ) = IDUMP
2469     329   C
2470     330          LTRIG = LTRIG + 1
2471     331          JTRIG( LTRIG ) = NS
2472     332          KSDELT( NS ) = IDUMP
2473     333   C
2474     334          IEDGE = IEDGE + 1
2475     335          IRECNC( IEDGE ) = NE
2476     336          NCOLOR = NCOLOR + 1
2477     337          JEE( NCOLOR ) = NE
2478     338          JSE( NE ) = 1
2479     339          IEDGE = IEDGE + 1
2480     340          IRECNC( IEDGE ) = NE - 1
2481     341          NCOLOR = NCOLOR + 1
2482     342          JEE( NCOLOR ) = NE - 1
2483     343          JSE( NE - 1 ) = 1
2484     344          IEDGE = IEDGE + 1
2485     345          IRECNC( IEDGE ) = NE - 2
2486     346          NCOLOR = NCOLOR + 1
2487     347          JEE( NCOLOR ) = NE - 2
2488     348          JSE( NE - 2 ) = 1
2489     349   C
2490     350          ELSE
```

```
2491     351   C                                                              2491
2492     352         IDISCT = 0                                               2492
2493     353         DO 545 KK = 4 , 6                                        2493
2494     354         IEE = JS( KK , ISS )                                     2494
2495     355         IEF = IABS( IEE )                                        2495
2496     356         IJE55 = JE( 5 , IEF )                                    2496
2497     357         IF( IJE55 . EQ . 0 ) THEN                                2497
2498     358         IF( IEE . GT . 0 ) THEN                                  2498
2499     359         ISI = JE( 4 , IEE )                                      2499
2500     360         ELSE                                                     2500
2501     361         ISI = JE( 3 , IEF )                                      2501
2502     362         END IF                                                   2502
2503     363         AREAXS = SAREA( ISI )                                    2503
2504     364         IE1 = IABS( JS( 4 , ISI ) )                              2504
2505     365         XE1 = XE( 1 , IE1 )                                      2505
2506     366         IJE55 = JE( 5 , IE1 )                                    2506
2507     367         HD1 = AREAXS * XE1 * XE1                                 2507
2508     368         IE2 = IABS( JS( 5 , ISI ) )                              2508
2509     369         XE2 = XE( 1 , IE2 )                                      2509
2510     370         IJE55 = IJE55 + JE( 5 , IE2 )                            2510
2511     371         HD2 = AREAXS * XE2 * XE2                                 2511
2512     372         IE3 = IABS( JS( 6 , ISI ) )                              2512
2513     373         XE3 = XE( 1 , IE3 )                                      2513
2514     374         IJE55 = IJE55 + JE( 5 , IE3 )                            2514
2515     375         HD3 = AREAXS * XE3 * XE3                                 2515
2516     376         RATIO = AMAX1( HD1 , HD2 , HD3 )                         2516
2517     377         YSAREA = XS( 3 , ISI )                                   2517
2518     378         IF( RATIO . LT . 7. . AND . YSAREA . GT . SMINVG . AND .  2518
2519     379        .                                IJE55 . EQ . 0 ) THEN    2519
2520     380         IDISCT = 1                                               2520
2521     381         DO 435 IR = 4 , 6                                        2521
2522     382         IE = IABS( JS( IR , ISI ) )                              2522
2523     383         IF( JSE( IE ) . EQ . 0 ) THEN                            2523
2524     384         IEDGE = IEDGE + 1                                        2524
2525     385         IRECNC( IEDGE ) = IE                                     2525
2526     386         NCOLOR = NCOLOR + 1                                      2526
2527     387         JEE( NCOLOR ) = IE                                       2527
2528     388         JSE( IE ) = 1                                            2528
2529     389         END IF                                                   2529
2530     390   435   CONTINUE                                                 2530
2531     391         CALL VERCEN( ISI )                                       2531
2532     392         KSDELT( ISI ) = IDUMP                                    2532
2533     393         LTRIG = LTRIG + 1                                        2533
2534     394         JTRIG( LTRIG ) = NS - 1                                  2534
2535     395         KSDELT( NS - 1 ) = IDUMP                                 2535
2536     396   C                                                              2536
2537     397         LTRIG = LTRIG + 1                                        2537
2538     398         JTRIG( LTRIG ) = NS                                      2538
2539     399         KSDELT( NS ) = IDUMP                                     2539
2540     400   C                                                              2540
2541     401         IEDGE = IEDGE + 1                                        2541
2542     402         IRECNC( IEDGE ) = NE                                     2542
2543     403         NCOLOR = NCOLOR + 1                                      2543
2544     404         JEE( NCOLOR ) = NE                                       2544
2545     405         JSE( NE ) = 1                                            2545
2546     406         IEDGE = IEDGE + 1                                        2546
2547     407         IRECNC( IEDGE ) = NE - 1                                 2547
2548     408         NCOLOR = NCOLOR + 1                                      2548
2549     409         JEE( NCOLOR ) = NE - 1                                   2549
2550     410         JSE( NE - 1 ) = 1                                        2550
2551     411         IEDGE = IEDGE + 1                                        2551
2552     412         IRECNC( IEDGE ) = NE - 2                                 2552
2553     413         NCOLOR = NCOLOR + 1                                      2553
2554     414         JEE( NCOLOR ) = NE - 2                                   2554
2555     415         JSE( NE - 2 ) = 1                                        2555
2556     416         END IF                                                   2556
2557     417         END IF                                                   2557
2558     418   545   CONTINUE                                                 2558
2559     419   C                                                              2559
2560     420         IF( IDISCT . EQ . 0 ) THEN                               2560
2561     421         IE1 = IABS( JS( 4 , ISS ) )                              2561
2562     422         XE1 = XE( 1 , IE1 )                                      2562
2563     423         IE2 = IABS( JS( 5 , ISS ) )                              2563
2564     424         XE2 = XE( 1 , IE2 )                                      2564
```

```
2565     425          IE3 = IABS( JS( 6 , ISS ) )                                    2565
2566     426          XE3 = XE( 1 , IE3 )                                            2566
2567     427          IEDIST = IE1                                                   2567
2568     428          XEDIST = XE1                                                   2568
2569     429          IF( XE2 . GT . XEDIST ) THEN                                   2569
2570     430          XEDIST = XE2                                                   2570
2571     431          IEDIST = IE2                                                   2571
2572     432          END IF                                                         2572
2573     433          IF( XE3 . GT . XEDIST ) THEN                                   2573
2574     434          XEDIST = XE3                                                   2574
2575     435          IEDIST = IE3                                                   2575
2576     436          END IF                                                         2576
2577     437          ISL = JE( 3 , IEDIST )                                         2577
2578     438          ISR = JE( 4 , IEDIST )                                         2578
2579     439          XSISL = XS( 3 , ISL )                                          2579
2580     440          XSISR = XS( 3 , ISR )                                          2580
2581     441          IJE5 = JE( 5 , IEDIST )                                        2581
2582     442          IF( XSISL . GT . RMINVG . AND . XSISR . GT . RMINVG . AND .    2582
2583     443         .     IJE5 . EQ . 0 . AND . IRATIO . NE . 2 )  THEN             2583
2584     444          IF( ISS . NE . ISL ) THEN                                      2584
2585     445          DO 345 IR = 4 , 6                                              2585
2586     446          IE = IABS( JS( IR , ISL ) )                                    2586
2587     447          IF( JSE( IE ) . EQ . 0 ) THEN                                  2587
2588     448          IEDGE = IEDGE + 1                                              2588
2589     449          IRECNC( IEDGE ) = IE                                           2589
2590     450          NCOLOR = NCOLOR + 1                                            2590
2591     451          JEE( NCOLOR ) = IE                                             2591
2592     452          JSE( IE ) = 1                                                  2592
2593     453          END IF                                                         2593
2594     454  345     CONTINUE                                                       2594
2595     455          END IF                                                         2595
2596     456  C                                                                      2596
2597     457          IF( ISS . NE . ISR ) THEN                                      2597
2598     458          DO 355 IR = 4 , 6                                              2598
2599     459          IE = IABS( JS( IR , ISR ) )                                    2599
2600     460          IF( JSE( IE ) . EQ . 0 ) THEN                                  2600
2601     461          IEDGE = IEDGE + 1                                              2601
2602     462          IRECNC( IEDGE ) = IE                                           2602
2603     463          NCOLOR = NCOLOR + 1                                            2603
2604     464          JEE( NCOLOR ) = IE                                             2604
2605     465          JSE( IE ) = 1                                                  2605
2606     466          END IF                                                         2606
2607     467  355     CONTINUE                                                       2607
2608     468          END IF                                                         2608
2609     469  C                                                                      2609
2610     470          IDONE = 0                                                      2610
2611     471          CALL DISECT ( IEDIST , IDONE , IDUMP )                         2611
2612     472          IF( IDONE . EQ . 1 ) THEN                                      2612
2613     473  C                                                                      2613
2614     474          LTRIG = LTRIG + 1                                              2614
2615     475          JTRIG( LTRIG ) = NS                                            2615
2616     476          KSDELT( NS ) = IDUMP                                           2616
2617     477          LTRIG = LTRIG + 1                                              2617
2618     478          JTRIG( LTRIG ) = NS - 1                                        2618
2619     479          KSDELT( NS - 1 ) = IDUMP                                       2619
2620     480  C                                                                      2620
2621     481          IEDGE = IEDGE + 1                                              2621
2622     482          IRECNC( IEDGE ) = NE                                           2622
2623     483          NCOLOR = NCOLOR + 1                                            2623
2624     484          JEE( NCOLOR ) = NE                                             2624
2625     485          JSE( NE ) = 1                                                  2625
2626     486          IEDGE = IEDGE + 1                                              2626
2627     487          IRECNC( IEDGE ) = NE - 1                                       2627
2628     488          NCOLOR = NCOLOR + 1                                            2628
2629     489          JEE( NCOLOR ) = NE - 1                                         2629
2630     490          JSE( NE - 1 ) = 1                                              2630
2631     491          IEDGE = IEDGE + 1                                              2631
2632     492          IRECNC( IEDGE ) = NE - 2                                       2632
2633     493          NCOLOR = NCOLOR + 1                                            2633
2634     494          JEE( NCOLOR ) = NE - 2                                         2634
2635     495          JSE( NE - 2 ) = 1                                              2635
2636     496          END IF                                                         2636
2637     497  C                                                                      2637
2638     498          END IF                                                         2638
```

```
2639     499          END IF                                                    2639
2640     500          END IF                                                    2640
2641     501          END IF                                                    2641
2642     502    C                                                               2642
2643     503     320  CONTINUE                                                  2643
2644     504    C                                                               2644
2645     505          DO 340 IEM = 1 , NCOLOR                                   2645
2646     506          IE = JEE( IEM )                                           2646
2647     507    C                                                               2647
2648     508          ISL = JE( 3 , IE )                                        2648
2649     509          YSAREA = XS( 3 , ISL )                                    2649
2650     510          IJE5 = JE( 5 , IE )                                       2650
2651     511          IF( YSAREA . GE . RMINVG . AND . IJE5 . NE . 0 ) THEN      2651
2652     512          IE1 = IABS( JS( 4 , ISL ) )                               2652
2653     513          IE2 = IABS( JS( 5 , ISL ) )                               2653
2654     514          IE3 = IABS( JS( 6 , ISL ) )                               2654
2655     515          IJE51 = JE( 5 , IE1 )                                     2655
2656     516          IJE52 = JE( 5 , IE2 )                                     2656
2657     517          IJE53 = JE( 5 , IE3 )                                     2657
2658     518          IF( IJE51 . NE . 0 ) THEN                                 2658
2659     519          IEDIST = IE1                                              2659
2660     520          XE1 = XE( 1 , IE1 )                                       2660
2661     521          XE2 = XE( 1 , IE2 )                                       2661
2662     522          XE3 = XE( 1 , IE3 )                                       2662
2663     523          END IF                                                    2663
2664     524          IF( IJE52 . NE . 0 ) THEN                                 2664
2665     525          IEDIST = IE2                                              2665
2666     526          XE1 = XE( 1 , IE2 )                                       2666
2667     527          XE2 = XE( 1 , IE1 )                                       2667
2668     528          XE3 = XE( 1 , IE3 )                                       2668
2669     529          END IF                                                    2669
2670     530          IF( IJE53 . NE . 0 ) THEN                                 2670
2671     531          IEDIST = IE3                                              2671
2672     532          XE1 = XE( 1 , IE3 )                                       2672
2673     533          XE2 = XE( 1 , IE2 )                                       2673
2674     534          XE3 = XE( 1 , IE1 )                                       2674
2675     535          END IF                                                    2675
2676     536          XEDIST = 1. / XE( 1 , IEDIST )                            2676
2677     537          YE2 = XE2 * XEDIST                                        2677
2678     538          YE3 = XE3 * XEDIST                                        2678
2679     539          ZE2 = ( YE2 - 1.5 ) * ( YE2 - .1 )                        2679
2680     540          ZE3 = ( YE3 - 1.5 ) * ( YE3 - .1 )                        2680
2681     541          YY2 = XE1 * XE1 + XE2 * XE2 + .35 * XE1 * XE2 - XE3 * XE3 2681
2682     542          YY3 = XE1 * XE1 + XE3 * XE3 + .35 * XE1 * XE3 - XE2 * XE2 2682
2683     543          IF( ZE2 . LT . .0 . AND . ZE3 . LT . 0. . AND .           2683
2684     544         .     YY2 . GT . 0. . AND . YY3 . GT . 0. ) THEN           2684
2685     545          CALL DISECT ( IEDIST , IDONE , IDUMP )                    2685
2686     546    C                                                               2686
2687     547          LTRIG = LTRIG + 1                                         2687
2688     548          JTRIG( LTRIG ) = NS                                       2688
2689     549          KSDELT( NS ) = IDUMP                                      2689
2690     550    C                                                               2690
2691     551          IEDGE = IEDGE + 1                                         2691
2692     552          IRECNC( IEDGE ) = NE                                      2692
2693     553          NCOLOR = NCOLOR + 1                                       2693
2694     554          JEE( NCOLOR ) = NE                                        2694
2695     555          JSE( NE ) = 1                                             2695
2696     556          IEDGE = IEDGE + 1                                         2696
2697     557          IRECNC( IEDGE ) = NE - 1                                  2697
2698     558          NCOLOR = NCOLOR + 1                                       2698
2699     559          JEE( NCOLOR ) = NE - 1                                    2699
2700     560          JSE( NE - 1 ) = 1                                         2700
2701     561    C                                                               2701
2702     562           ELSE                                                     2702
2703     563    C                                                               2703
2704     564          IEDIST = IE1                                              2704
2705     565          XEDIST = XE1                                              2705
2706     566          IF( XE2 . GT . XEDIST ) THEN                              2706
2707     567          XEDIST = XE2                                              2707
2708     568          IEDIST = IE2                                              2708
2709     569          END IF                                                    2709
2710     570          IF( XE3 . GT . XEDIST ) THEN                              2710
2711     571          XEDIST = XE3                                              2711
2712     572          IEDIST = IE3                                              2712
```

```
2713     573          END IF                                                    2713
2714     574          ISL = JE( 3 , IEDIST )                                    2714
2715     575          ISR = JE( 4 , IEDIST )                                    2715
2716     576          XSISL = XS( 3 , ISL )                                     2716
2717     577          XSISR = XS( 3 , ISR )                                     2717
2718     578          IJE5 = JE( 5 , IEDIST )                                   2718
2719     579          IF( XSISL . GT . RMINVG . AND . XSISR . GT . RMINVG . AND .2719
2720     580         .     IJE5 . EQ . 0 )  THEN                                2720
2721     581          DO 645 IR = 4 , 6                                         2721
2722     582          IE = IABS( JS( IR , ISL ) )                               2722
2723     583          IF( JSE( IE ) . EQ . 0 ) THEN                             2723
2724     584          IEDGE = IEDGE + 1                                         2724
2725     585          IRECNC( IEDGE ) = IE                                      2725
2726     586          NCOLOR = NCOLOR + 1                                       2726
2727     587          JEE( NCOLOR ) = IE                                        2727
2728     588          JSE( IE ) = 1                                             2728
2729     589          END IF                                                    2729
2730     590   645    CONTINUE                                                  2730
2731     591          DO 655 IR = 4 , 6                                         2731
2732     592          IE = IABS( JS( IR , ISR ) )                               2732
2733     593          IF( JSE( IE ) . EQ . 0 ) THEN                             2733
2734     594          IEDGE = IEDGE + 1                                         2734
2735     595          IRECNC( IEDGE ) = IE                                      2735
2736     596          NCOLOR = NCOLOR + 1                                       2736
2737     597          JEE( NCOLOR ) = IE                                        2737
2738     598          JSE( IE ) = 1                                             2738
2739     599          END IF                                                    2739
2740     600   655    CONTINUE                                                  2740
2741     601   C                                                               2741
2742     602          IDONE = 0                                                 2742
2743     603          CALL DISECT ( IEDIST , IDONE , IDUMP )                    2743
2744     604          IF( IDONE . EQ . 1 ) THEN                                 2744
2745     605   C                                                               2745
2746     606          LTRIG = LTRIG + 1                                         2746
2747     607          JTRIG( LTRIG ) = NS                                       2747
2748     608          KSDELT( NS ) = IDUMP                                      2748
2749     609          LTRIG = LTRIG + 1                                         2749
2750     610          JTRIG( LTRIG ) = NS - 1                                   2750
2751     611          KSDELT( NS - 1 ) = IDUMP                                  2751
2752     612   C                                                               2752
2753     613          IEDGE = IEDGE + 1                                         2753
2754     614          IRECNC( IEDGE ) = NE                                      2754
2755     615          NCOLOR = NCOLOR + 1                                       2755
2756     616          JEE( NCOLOR ) = NE                                        2756
2757     617          JSE( NE ) = 1                                             2757
2758     618          IEDGE = IEDGE + 1                                         2758
2759     619          IRECNC( IEDGE ) = NE - 1                                  2759
2760     620          NCOLOR = NCOLOR + 1                                       2760
2761     621          JEE( NCOLOR ) = NE - 1                                    2761
2762     622          JSE( NE - 1 ) = 1                                         2762
2763     623          IEDGE = IEDGE + 1                                         2763
2764     624          IRECNC( IEDGE ) = NE - 2                                  2764
2765     625          NCOLOR = NCOLOR + 1                                       2765
2766     626          JEE( NCOLOR ) = NE - 2                                    2766
2767     627          JSE( NE - 2 ) = 1                                         2767
2768     628   C                                                               2768
2769     629          END IF                                                    2769
2770     630          END IF                                                    2770
2771     631          END IF                                                    2771
2772     632          END IF                                                    2772
2773     633    340   CONTINUE                                                  2773
2774     634   C                                                               2774
2775     635          NSS = LTRIG                                               2775
2776     636   C                                                               2776
2777     637          DO 370 IEM = 1 , NCOLOR                                   2777
2778     638          IE = JEE( IEM )                                           2778
2779     639          CALL RECNC( IE , IDONE , ITL , ITR , JA , JB , JC , JD )  2779
2780     640          CALL RECNC( JA , JADONE , ITL , ITR , JAA , JAB , JAC , JAD )2780
2781     641          CALL RECNC( JB , JBDONE , ITL , ITR , JBA , JBB , JBC , JBD )2781
2782     642          CALL RECNC( JC , JCDONE , ITL , ITR , JCA , JCB , JCC , JCD )2782
2783     643          CALL RECNC( JD , JDDONE , ITL , ITR , JDA , JDB , JDC , JDD )2783
2784     644   370    CONTINUE                                                  2784
2785     645   C                                                               2785
2786     646   300    CONTINUE                                                  2786
```

```
2787     647   C                                                              2787
2788     648         NVECE = NE / MBL                                         2788
2789     649         NREME = NE - NVECE * MBL                                 2789
2790     650         NVECS = NS / MBL                                         2790
2791     651         NREMS = NS - NVECS * MBL                                 2791
2792     652         NVECV = NV / MBL                                         2792
2793     653         NREMV = NV - NVECV * MBL                                 2793
2794     654   C                                                              2794
2795     655         DO 400 INE = 1 , NVECE                                   2795
2796     656         NOFVEE( INE ) = MBL                                      2796
2797     657   400   CONTINUE                                                 2797
2798     658         NVEEE = NVECE                                            2798
2799     659         IF( NREME . GT . 0 ) THEN                                2799
2800     660         NVEEE = NVECE + 1                                        2800
2801     661         NOFVEE( NVEEE ) = NREME                                  2801
2802     662         END IF                                                   2802
2803     663   C                                                              2803
2804     664         DO 410 INS = 1 , NVECS                                   2804
2805     665         NOFVES( INS ) = MBL                                      2805
2806     666   410   CONTINUE                                                 2806
2807     667         NVEES = NVECS                                            2807
2808     668         IF( NREMS . GT . 0 ) THEN                                2808
2809     669         NVEES = NVECS + 1                                        2809
2810     670         NOFVES( NVEES ) = NREMS                                  2810
2811     671         END IF                                                   2811
2812     672   C                                                              2812
2813     673         DO 420 INV = 1 , NVECV                                   2813
2814     674         NOFVEV( INV ) = MBL                                      2814
2815     675   420   CONTINUE                                                 2815
2816     676         NVEEV = NVECV                                            2816
2817     677         IF( NREMV . GT . 0 ) THEN                                2817
2818     678         NVEEV = NVECV + 1                                        2818
2819     679         NOFVEV( NVEEV ) = NREMV                                  2819
2820     680         END IF                                                   2820
2821     681   C                                                              2821
2822     682          PRINT*,NV,NE,NS                                         2822
2823     683   C                                                              2823
2824     684   C --- EXIT POINT FROM SUBROUTINE ------------------------------2824
2825     685   C                                                              2825
2826     686   C     ------                                                   2826
2827     687         RETURN                                                   2827
2828     688   C     ------                                                   2828
2829     689   C                                                              2829
2830     690   C     ---                                                      2830
2831     691         END                                                      2831
```

```
      SUBROUTINE DELPTNT( DAREA , IDUMP )
C
C-----------------------------------------------------------------I
C                                                                 I
C     DELPTN ADAPT THE GRID DYNAMICALLY, DELETE VERTECES          I
C     WILL FLAGED TRIANGLES FOR DELETION                          I
C                                                                 I
C-----------------------------------------------------------------I
C
         IMPLICIT REAL (A-H,O-Z)
C
      include     'cmsh00.h'
      include     'chyd00.h'
      include     'cint00.h'
      include     'cphs10.h'
      include     'cphs20.h'
C
      INTEGER JTRIG(MEM),KTRIG(MEM),IRECNC(MEM)
      INTEGER JSE(MEM),JEE(MEM),IOFDVS(10),NOFDVS(10)
      INTEGER IITRIG(200)
      REAL ADFCTR(8),DLFCTR(8)
C
      EQUIVALENCE (UL,JTRIG)
      EQUIVALENCE (VR,KTRIG)
      EQUIVALENCE (VL,IRECNC)
      EQUIVALENCE (PR,JSE)
      EQUIVALENCE (PL,JEE)
C
       DLFCTR( 1 ) = DAREA
       DLFCTR( 2 ) = .4
       DLFCTR( 3 ) = .5
       DLFCTR( 4 ) = .65
       DLFCTR( 5 ) = .8
C
       SMINVG = SAREVG * DAREA
       DO 112 IS = 1 , NS
       JSDELT( IS  ) = 0
 112   CONTINUE
       ISDELT = 0
C
       NSS = 0
       FLUXPP = .00001 * HYDMOM( 4 )
       FLUXUU = .00001 * HYDMOM( 2 )
       FLUXRR = .00001 * HYDMOM( 1 )
       DO 120 IS = 1 , NS
       PCRTRY = HYDFLX( IS , 4 ) - FLUXPP
       IPCRTR = SIGN( 1. , PCRTRY )
       UCRTRY = HYDFLX( IS , 2 ) - FLUXUU
       IUCRTR = SIGN( 1. , UCRTRY )
       RCRTRY = HYDFLX( IS , 1 ) - FLUXRR
       IRCRTR = SIGN( 1. , RCRTRY )
       NIDUMP = IDUMP - NAREAD
       IF(
     .     IPCRTR . EQ . - 1 . AND .
     .     IUCRTR . EQ . - 1 . AND .
     .     IRCRTR . EQ . - 1 . AND .
     .     KSDELT( IS ) . LE . NIDUMP . AND .
     .     KSDELT( IS ) . NE . 0 ) THEN
       NSS = NSS + 1
       JTRIG( NSS ) = IS
       END IF
 120   CONTINUE
C
       PRINT*,NV,NE,NS,NSS
C
       ISDELT = NSS
       DO 210 IS = 1 , NSS
       JSDELT( IS ) = JTRIG( IS )
 210   CONTINUE
C
       DO 300 KDIV = 1 , 1
       ILOOP = 1
310    CONTINUE
       ISS = JSDELT( ILOOP )
```

```
2906      75          XSAREA = XS( 3 , ISS )                                    2906
2907      76          INDCTR = 0                                                2907
2908      77          IF( XSAREA . LT . SMINVG ) THEN                           2908
2909      78    C                                                               2909
2910      79          CALL VERDELT( ISS , INDCTR , NIDUMP , JJTRIG , IITRIG )   2910
2911      80          IF( INDCTR . EQ . 1 ) THEN                                2911
2912      81          ILOOP = 1                                                 2912
2913      82          ELSE                                                      2913
2914      83          JSDELT( ILOOP ) = 0                                       2914
2915      84          ILOOP = ILOOP + 1                                         2915
2916      85          END IF                                                    2916
2917      86          ELSE                                                      2917
2918      87          JSDELT( ILOOP ) = 0                                       2918
2919      88          ILOOP = ILOOP + 1                                         2919
2920      89          END IF                                                    2920
2921      90    C                                                               2921
2922      91          IF( ISDELT . GT . ILOOP ) GO TO 310                       2922
2923      92          PRINT *,KDIV,NV,NE,NS,DLFCTR(KDIV)                        2923
2924      93    300   CONTINUE                                                  2924
2925      94    C                                                               2925
2926      95          NVECE = NE / MBL                                          2926
2927      96          NREME = NE - NVECE * MBL                                  2927
2928      97          NVECS = NS / MBL                                          2928
2929      98          NREMS = NS - NVECS * MBL                                  2929
2930      99          NVECV = NV / MBL                                          2930
2931     100          NREMV = NV - NVECV * MBL                                  2931
2932     101    C                                                               2932
2933     102          DO 400 INE = 1 , NVECE                                    2933
2934     103          NOFVEE( INE ) = MBL                                       2934
2935     104    400   CONTINUE                                                  2935
2936     105          NVEEE = NVECE                                             2936
2937     106          IF( NREME . GT . 0 ) THEN                                 2937
2938     107          NVEEE = NVECE + 1                                         2938
2939     108          NOFVEE( NVEEE ) = NREME                                   2939
2940     109          END IF                                                    2940
2941     110    C                                                               2941
2942     111          DO 410 INS = 1 , NVECS                                    2942
2943     112          NOFVES( INS ) = MBL                                       2943
2944     113    410   CONTINUE                                                  2944
2945     114          NVEES = NVECS                                             2945
2946     115          IF( NREMS . GT . 0 ) THEN                                 2946
2947     116          NVEES = NVECS + 1                                         2947
2948     117          NOFVES( NVEES ) = NREMS                                   2948
2949     118          END IF                                                    2949
2950     119    C                                                               2950
2951     120          DO 420 INV = 1 , NVECV                                    2951
2952     121          NOFVEV( INV ) = MBL                                       2952
2953     122    420   CONTINUE                                                  2953
2954     123          NVEEV = NVECV                                             2954
2955     124          IF( NREMV . GT . 0 ) THEN                                 2955
2956     125          NVEEV = NVECV + 1                                         2956
2957     126          NOFVEV( NVEEV ) = NREMV                                   2957
2958     127          END IF                                                    2958
2959     128    C                                                               2959
2960     129           PRINT*,NV,NE,NS                                          2960
2961     130    C                                                               2961
2962     131    C --- EXIT POINT FROM SUBROUTINE ------------------------------- 2962
2963     132    C                                                               2963
2964     133    C     ------                                                    2964
2965     134          RETURN                                                    2965
2966     135    C     ------                                                    2966
2967     136    C                                                               2967
2968     137    C     ---                                                       2968
2969     138          END                                                       2969
```

```
      SUBROUTINE RELAXY( IV )
      IMPLICIT REAL (A-H,O-Z)
C
C-----------------------------------------------------------------I
C                                                                 I
C     THIS ROUTINE RELAX THE GRID AFTER DELETION                  |
C                                                                 I
C-----------------------------------------------------------------I
C
      include     'cmsh00.h'
      include     'chyd00.h'
      include     'cint00.h'
      include     'cphs10.h'
      include     'cphs20.h'
          ITRIG = 0
          IETRIG = 0
          IE = JV( 2 , IV )
          IF( IE . GT . 0 ) THEN
C
          IV1 = JE( 1 , IE )
          IV2 = JE( 2 , IE )
          IF( IV1 . EQ . IV ) THEN
          ISI = JE( 3 , IE )
          ELSE
          ISI = JE( 4 , IE )
          END IF
          IS = ISI
C
 75       CONTINUE
C
          DO 65 IR = 1 , 3
          JR = MOD( IR , 3 ) + 1
          IEA = IABS( JS( JR + 3 , IS ) )
          IF( IEA . EQ . IE ) THEN
          IIR = MOD( JR , 3 ) + 4
          IEI = JS( IIR , IS )
          IEII = IABS( IEI )
          IETRIG = IETRIG + 1
          JECRSS( IETRIG ) = IEII
          JJR = MOD( JR + 1 , 3 ) + 4
          IEM = JS( JJR , IS )
          IER = IABS( IEM )
          IETRIG = IETRIG + 1
          JECRSS( IETRIG ) = IER
C
          IV1 = JE( 1 , IER )
          IV2 = JE( 2 , IER )
          IF( IV1 . EQ . IV ) THEN
          ISR = JE( 3 , IER )
          ITRIG = ITRIG + 1
          IICOLR( ITRIG ) = IV2
          JSCRSS( ITRIG ) = ISR
          ELSE
          ISR = JE( 4 , IER )
          ITRIG = ITRIG + 1
          IICOLR( ITRIG ) = IV1
          JSCRSS( ITRIG ) = ISR
          END IF
          END IF
 65       CONTINUE
C
          IF( ISR . NE . ISI ) THEN
          IS = ISR
          IE = IER
          GO TO 75
          END IF
C
          DO 510 IE = 1 , ITRIG
C
          IEM = MOD( IE - 1 , ITRIG ) + 1
          IEP = MOD( IE , ITRIG ) + 1
          IEI = MOD( IE + 1 , ITRIG ) + 1
C
          IV1 = IICOLR( IEM )
```

```
3044      75              IV2 = IICOLR( IEP )                                     3044
3045      76              IV3 = IICOLR( IEI )                                     3045
3046      77    C                                                                 3046
3047      78              X1 = XV( 1 , IV1 ) - XV( 1 , IV2 )                      3047
3048      79              Y1 = XV( 2 , IV1 ) - XV( 2 , IV2 )                      3048
3049      80              X2 = XV( 1 , IV3 ) - XV( 1 , IV2 )                      3049
3050      81              Y2 = XV( 2 , IV3 ) - XV( 2 , IV2 )                      3050
3051      82              XSIN = ( X2 * Y1 - X1 * Y2 )                            3051
3052      83              XCOS = ( X1 * X2 + Y1 * Y2 )                            3052
3053      84              ANGLE( IE ) = XSIN / ( ABS( XCOS ) + 1.E-7 )            3053
3054      85              IF( ANGLE( IE ) . LT . 0. ) RETURN                      3054
3055      86    C                                                                 3055
3056      87    510       CONTINUE                                                3056
3057      88    C                                                                 3057
3058      89              XSUM = 0.                                               3058
3059      90              YSUM = 0.                                               3059
3060      91              HSUMR = 0.                                              3060
3061      92              HSUMU = 0.                                              3061
3062      93              HSUMV = 0.                                              3062
3063      94              HSUMP = 0.                                              3063
3064      95              HSUMG = 0.                                              3064
3065      96    C                                                                 3065
3066      97              DO 110 IT = 1 , ITRIG                                   3066
3067      98              IVV = IICOLR( IT )                                      3067
3068      99    C                                                                 3068
3069     100              XSUM = XSUM + XV( 1 , IVV )                             3069
3070     101              YSUM = YSUM + XV( 2 , IVV )                             3070
3071     102    C                                                                 3071
3072     103              HSUMR  = HSUMR + HYDVVV( IVV , 1 )                      3072
3073     104              HSUMU  = HSUMU + HYDVVV( IVV , 2 )                      3073
3074     105              HSUMV  = HSUMV + HYDVVV( IVV , 3 )                      3074
3075     106              HSUMP  = HSUMP + HYDVVV( IVV , 4 )                      3075
3076     107              HSUMG  = HSUMG + HYDVVV( IVV , 5 )                      3076
3077     108     110      CONTINUE                                                3077
3078     109    C                                                                 3078
3079     110              XINVRG = 1. / ITRIG                                     3079
3080     111              XV( 1 , IV ) = XSUM * XINVRG                            3080
3081     112              XV( 2 , IV ) = YSUM * XINVRG                            3081
3082     113              HYDVVV( IV , 1 ) = HSUMR * XINVRG                       3082
3083     114              HYDVVV( IV , 2 ) = HSUMU * XINVRG                       3083
3084     115              HYDVVV( IV , 3 ) = HSUMV * XINVRG                       3084
3085     116              HYDVVV( IV , 4 ) = HSUMP * XINVRG                       3085
3086     117              HYDVVV( IV , 5 ) = HSUMG * XINVRG                       3086
3087     118    C                                                                 3087
3088     119              ELSE                                                    3088
3089     120    C                                                                 3089
3090     121              IE = - IE                                               3090
3091     122              IV1 = JE( 1 , IE )                                      3091
3092     123              IV2 = JE( 2 , IE )                                      3092
3093     124              IF( IV1 . EQ . IV ) THEN                                3093
3094     125              ISI = JE( 3 , IE )                                      3094
3095     126              ITRIG = ITRIG + 1                                       3095
3096     127              JSCRSS( ITRIG ) = ISI                                   3096
3097     128              IICOLR( ITRIG ) = IV2                                   3097
3098     129              ELSE                                                    3098
3099     130              ISI = JE( 4 , IE )                                      3099
3100     131              ITRIG = ITRIG + 1                                       3100
3101     132              JSCRSS( ITRIG ) = ISI                                   3101
3102     133              IICOLR( ITRIG ) = IV1                                   3102
3103     134              END IF                                                  3103
3104     135    C                                                                 3104
3105     136              IS = ISI                                                3105
3106     137              ISI = 0                                                 3106
3107     138              IIE = IE                                                3107
3108     139              IETRIG = IETRIG + 1                                     3108
3109     140              JECRSS( IETRIG ) = IE                                   3109
3110     141    C                                                                 3110
3111     142    670       CONTINUE                                                3111
3112     143    C                                                                 3112
3113     144              DO 680 IR = 1 , 3                                       3113
3114     145              JR = MOD( IR , 3 ) + 1                                  3114
3115     146              IEA = IABS( JS( JR + 3 , IS ) )                         3115
3116     147              IF( IEA . EQ . IE ) THEN                                3116
3117     148              IIR = MOD( JR , 3 ) + 4                                 3117
```

```
3118    149             IEI = JS( IIR , IS )                                    3118
3119    150             IEII = IABS( IEI )                                      3119
3120    151             IETRIG = IETRIG + 1                                     3120
3121    152             JECRSS( IETRIG ) = IEII                                 3121
3122    153             JJR = MOD( JR + 1 , 3 ) + 4                             3122
3123    154             IEM = JS( JJR , IS )                                    3123
3124    155             IER = IABS( IEM )                                       3124
3125    156             IETRIG = IETRIG + 1                                     3125
3126    157             JECRSS( IETRIG ) = IER                                  3126
3127    158     C                                                               3127
3128    159             IV1 = JE( 1 , IER )                                     3128
3129    160             IV2 = JE( 2 , IER )                                     3129
3130    161             IF( IV1 . EQ . IV ) THEN                                3130
3131    162             ISR = JE( 3 , IER )                                     3131
3132    163             ITRIG = ITRIG + 1                                       3132
3133    164             IICOLR( ITRIG ) = IV2                                   3133
3134    165             JSCRSS( ITRIG ) = ISR                                   3134
3135    166             ELSE                                                    3135
3136    167             ISR = JE( 4 , IER )                                     3136
3137    168             ITRIG = ITRIG + 1                                       3137
3138    169             IICOLR( ITRIG ) = IV1                                   3138
3139    170             JSCRSS( ITRIG ) = ISR                                   3139
3140    171             END IF                                                  3140
3141    172             END IF                                                  3141
3142    173     C                                                               3142
3143    174     680     CONTINUE                                                3143
3144    175     C                                                               3144
3145    176             IF( ISR . NE . ISI ) THEN                               3145
3146    177             IS = ISR                                                3146
3147    178             IE = IER                                                3147
3148    179             GO TO 670                                               3148
3149    180             END IF                                                  3149
3150    181             ITRIG = ITRIG - 1                                       3150
3151    182     C                                                               3151
3152    183             IV1 = JE( 1 , IIE )                                     3152
3153    184             IV2 = JE( 2 , IIE )                                     3153
3154    185     C                                                               3154
3155    186             IV3 = JE( 1 , IER )                                     3155
3156    187             IV4 = JE( 2 , IER )                                     3156
3157    188     C                                                               3157
3158    189             X1 = XV( 1 , IV1 ) - XV( 1 , IV2 )                      3158
3159    190             Y1 = XV( 2 , IV1 ) - XV( 2 , IV2 )                      3159
3160    191             X2 = XV( 1 , IV4 ) - XV( 1 , IV3 )                      3160
3161    192             Y2 = XV( 2 , IV4 ) - XV( 2 , IV3 )                      3161
3162    193             XSIN = ( X2 * Y1 - X1 * Y2 )                            3162
3163    194             XCOS = ( X1 * X2 + Y1 * Y2 )                            3163
3164    195             XANGLE = XSIN / ( ABS( XCOS ) + 1.E-7 )                 3164
3165    196     C                                                               3165
3166    197             IF( ABS( XANGLE ) . GT . 1.E-3 ) RETURN                 3166
3167    198     C                                                               3167
3168    199             IVI = IV1                                               3168
3169    200             IF( IV . EQ . IV1 ) IVI = IV2                           3169
3170    201             IVL = IV3                                               3170
3171    202             IF( IV . EQ . IV3 ) IVL = IV4                           3171
3172    203             IVTRIG = ITRIG + 1                                      3172
3173    204             IICOLR( IVTRIG ) = IVL                                  3173
3174    205     C                                                               3174
3175    206             DO 512 IE = 1 , IVTRIG                                  3175
3176    207     C                                                               3176
3177    208             IEM = MOD( IE - 1 , IVTRIG ) + 1                        3177
3178    209             IEP = MOD( IE , IVTRIG ) + 1                            3178
3179    210             IEI = MOD( IE + 1 , IVTRIG ) + 1                        3179
3180    211     C                                                               3180
3181    212             IV1 = IICOLR( IEM )                                     3181
3182    213             IV2 = IICOLR( IEP )                                     3182
3183    214             IV3 = IICOLP( IEI )                                     3183
3184    215     C                                                               3184
3185    216             X1 = XV( 1 , IV1 ) - XV( 1 , IV2 )                      3185
3186    217             Y1 = XV( 2 , IV1 ) - XV( 2 , IV2 )                      3186
3187    218             X2 = XV( 1 , IV3 ) - XV( 1 , IV2 )                      3187
3188    219             Y2 = XV( 2 , IV3 ) - XV( 2 , IV2 )                      3188
3189    220             XSIN = ( X2 * Y1 - X1 * Y2 )                            3189
3190    221             XCOS = ( X1 * X2 + Y1 * Y2 )                            3190
3191    222             ANGLE( IE ) = XSIN / ( ABS( XCOS ) + 1.E-7 )            3191
```

```
3192    223             IF( ANGLE( IE ) . LT . 0. ) RETURN                                3192
3193    224     C                                                                         3193
3194    225     512     CONTINUE                                                          3194
3195    226     C                                                                         3195
3196    227             XV( 1 , IV ) = .5 * ( XV( 1 , IVI ) + XV( 1 , IVL ) )             3196
3197    228             XV( 2 , IV ) = .5 * ( XV( 2 , IVI ) + XV( 2 , IVL ) )             3197
3198    229             HYDVVV( IV , 1 ) = .5 * ( HYDVVV( IVI , 1 ) +                     3198
3199    230            .                          HYDVVV( IVL , 1 ) )                     3199
3200    231             HYDVVV( IV , 2 ) = .5 * ( HYDVVV( IVI , 2 ) +                     3200
3201    232            .                          HYDVVV( IVL , 2 ) )                     3201
3202    233             HYDVVV( IV , 3 ) = .5 * ( HYDVVV( IVI , 3 ) +                     3202
3203    234            .                          HYDVVV( IVL , 3 ) )                     3203
3204    235             HYDVVV( IV , 4 ) = .5 * ( HYDVVV( IVI , 4 ) +                     3204
3205    236            .                          HYDVVV( IVL , 4 ) )                     3205
3206    237             HYDVVV( IV , 5 ) = .5 * ( HYDVVV( IVI , 5 ) +                     3206
3207    238            .                          HYDVVV( IVL , 5 ) )                     3207
3208    239     C                                                                         3208
3209    240             END IF                                                            3209
3210    241     C                                                                         3210
3211    242             DO 120 ISNN = 1 , ITRIG                                           3211
3212    243             INS = JSCRSS( ISNN )                                              3212
3213    244     C                                                                         3213
3214    245             IV1 = JS( 1 , INS )                                               3214
3215    246             IV2 = JS( 2 , INS )                                               3215
3216    247             IV3 = JS( 3 , INS )                                               3216
3217    248             AX = XV( 1 , IV2 ) - XV( 1 , IV1 )                                3217
3218    249             AY = XV( 2 , IV2 ) - XV( 2 , IV1 )                                3218
3219    250             BX = XV( 1 , IV3 ) - XV( 1 , IV1 )                                3219
3220    251             BY = XV( 2 , IV3 ) - XV( 2 , IV1 )                                3220
3221    252             XS( 3 , INS ) = 0.5 * ( AX * BY - AY * BX )                       3221
3222    253     C                                                                         3222
3223    254             SAREA( INS ) = 1. / XS( 3 , INS )                                 3223
3224    255             HYDFLX( INS , 4 ) = 0.                                            3224
3225    256             HYDFLX( INS , 1 ) = 0.                                            3225
3226    257             HYDFLX( INS , 2 ) = 0.                                            3226
3227    258             KSDELT( INS ) = 1                                                 3227
3228    259     C                                                                         3228
3229    260             XXC = ( XV( 1 , IV1 ) + XV( 1 , IV2 ) + XV( 1 , IV3 ) ) *         3229
3230    261            .       THIRD                                                      3230
3231    262             YYC = ( XV( 2 , IV1 ) + XV( 2 , IV2 ) + XV( 2 , IV3 ) ) *         3231
3232    263            .       THIRD                                                      3232
3233    264             XS( 1 , INS ) = XXC                                               3233
3234    265             XS( 2 , INS ) = YYC                                               3234
3235    266     C                                                                         3235
3236    267             DO 130 IR = 1 , MHQ                                               3236
3237    268             HYDV( INS , IR ) = ( HYDVVV( IV1 , IR ) +                         3237
3238    269            .                     HYDVVV( IV2 , IR ) +                         3238
3239    270            .                     HYDVVV( IV3 , IR ) ) * THIRD                 3239
3240    271     130     CONTINUE                                                          3240
3241    272     C                                                                         3241
3242    273             HDUM          = 1. / ( HYDV( INS , 1 ) + 1.E-12 )                 3242
3243    274             HYDV( INS , 2 ) = HYDV( INS , 2 ) * HDUM                          3243
3244    275             HYDV( INS , 3 ) = HYDV( INS , 3 ) * HDUM                          3244
3245    276             HYDV( INS , 4 ) = ( HYDV( INS , 4 )  -                            3245
3246    277            .                  .5 * HYDV( INS , 1 ) *                          3246
3247    278            . ( HYDV( INS , 2 ) * HYDV( INS , 2 ) +                           3247
3248    279            .   HYDV( INS , 3 ) * HYDV( INS , 3 ) ) ) *                       3248
3249    280            .                     ( HYDV( INS , 5 ) - 1. )                    3249
3250    281     C                                                                         3250
3251    282     120     CONTINUE                                                          3251
3252    283     C                                                                         3252
3253    284             DO 140 IENN = 1 , IETRIG                                          3253
3254    285             IEN = JECRSS( IENN )                                              3254
3255    286     C                                                                         3255
3256    287             JV1 = JE( 1 , IEN )                                               3256
3257    288             JV2 = JE( 2 , IEN )                                               3257
3258    289             AX = XV( 1 , JV2 ) - XV( 1 , JV1 )                                3258
3259    290             AY = XV( 2 , JV2 ) - XV( 2 , JV1 )                                3259
3260    291             XE( 1 , IEN ) = SQRT( AX * AX + AY * AY )                         3260
3261    292             XEREV = 1. / XE( 1 , IEN )                                        3261
3262    293             XN( IEN ) = AY * XEREV                                            3262
3263    294             YN( IEN ) = - AX * XEREV                                          3263
3264    295             ISSR = JE( 4 , IEN )                                              3264
3265    296             ISSL = JE( 3 , IEN )                                              3265
```

```
3266     297   C                                                                3266
3267     298               IF( JE( 5 , IEN ) . NE . 0 ) THEN                    3267
3268     299   C                                                                3268
3269     300               AA = XV( 1 , JV2 ) - XV( 1 , JV1 )                   3269
3270     301               BB = XV( 2 , JV2 ) - XV( 2 , JV1 )                   3270
3271     302               XEL = XS( 1 , ISSL )                                 3271
3272     303               YEL = XS( 2 , ISSL )                                 3272
3273     304               CC = XEL - XV( 1 , JV1 )                             3273
3274     305               DD = YEL - XV( 2 , JV1 )                             3274
3275     306               EE = ( AA * CC + BB * DD ) * XEREV * XEREV           3275
3276     307               XER = XV( 1 , JV1 ) + AA * EE                        3276
3277     308               YER = XV( 2 , JV1 ) + BB * EE                        3277
3278     309               AX = XER - XEL                                       3278
3279     310               AY = YER - YEL                                       3279
3280     311               XE( 2 , IEN ) = SQRT( AX * AX + AY * AY )            3280
3281     312               XEREV = 1. / XE( 2 , IEN )                           3281
3282     313               XXN( IEN ) = AX * XEREV                              3282
3283     314               YYN( IEN ) = AY * XEREV                              3283
3284     315               XE( 2 , IEN ) = 2. * XE( 2 , IEN )                   3284
3285     316               XYMIDL( IEN ) = .5                                   3285
3286     317               XMIDL( IEN ) = XER                                   3286
3287     318               YMIDL( IEN ) = YER                                   3287
3288     319   C                                                                3288
3289     320               ELSE                                                 3289
3290     321   C                                                                3290
3291     322               XER = XS( 1 , ISSR )                                 3291
3292     323               YER = XS( 2 , ISSR )                                 3292
3293     324               XEL = XS( 1 , ISSL )                                 3293
3294     325               YEL = XS( 2 , ISSL )                                 3294
3295     326   C                                                                3295
3296     327               AA = XV( 1 , JV2 ) - XV( 1 , JV1 )                   3296
3297     328               BB = XV( 2 , JV2 ) - XV( 2 , JV1 )                   3297
3298     329               CC = XEL - XER                                       3298
3299     330               DD = YEL - YER                                       3299
3300     331               ACA = XER - XV( 1 , JV1 )                            3300
3301     332               DBD = YER - XV( 2 , JV1 )                            3301
3302     333               EE = ( ACA * DD - DBD * CC ) / ( AA * DD - BB * CC ) 3302
3303     334               XMIDL( IEN ) = XV( 1 , JV1 ) + AA * EE               3303
3304     335               YMIDL( IEN ) = XV( 2 , JV1 ) + BB * EE               3304
3305     336   C                                                                3305
3306     337               XEMID = XMIDL( IEN ) - XEL                           3306
3307     338               YEMID = YMIDL( IEN ) - YEL                           3307
3308     339   C                                                                3308
3309     340               AX = XER - XEL                                       3309
3310     341               AY = YER - YEL                                       3310
3311     342               XE( 2 , IEN ) = SQRT( AX * AX + AY * AY )            3311
3312     343               XEREV = 1. / XE( 2 , IEN )                           3312
3313     344               XXN( IEN ) = AX * XEREV                              3313
3314     345               YYN( IEN ) = AY * XEREV                              3314
3315     346   C                                                                3315
3316     347               XYMIDL( IEN ) = SQRT( XEMID * XEMID + YEMID * YEMID ) * XEREV 3316
3317     348   C                                                                3317
3318     349               END IF                                               3318
3319     350   C                                                                3319
3320     351   140         CONTINUE                                             3320
3321     352   C                                                                3321
3322     353               DO 142 IENN = 1 , IETRIG                             3322
3323     354               IE = JECRSS( IENN )                                  3323
3324     355               CALL RECNC( IE , IDONE , ITL , ITR , JA , JB , JC , JD ) 3324
3325     356               CALL RECNC( JA , JADONE , ITL , ITR , JAA , JAB , JAC , JAD ) 3325
3326     357               CALL RECNC( JB , JBDONE , ITL , ITR , JBA , JBB , JBC , JBD ) 3326
3327     358               CALL RECNC( JC , JCDONE , ITL , ITR , JCA , JCB , JCC , JCD ) 3327
3328     359               CALL RECNC( JD , JDDONE , ITL , ITR , JDA , JDB , JDC , JDD ) 3328
3329     360   142         CONTINUE                                             3329
3330     361   C                                                                3330
3331     362   C --- EXIT POINT FROM SUBROUTINE ----------------------------------- 3331
3332     363   C                                                                3332
3333     364   C     ------                                                     3333
3334     365         RETURN                                                     3334
3335     366   C     ------                                                     3335
3336     367   C                                                                3336
3337     368   C     ---                                                        3337
3338     369         END                                                        3338
```

```
      1         SUBROUTINE LAPLAC
      2   C
      3   C-------------------------------------------------------------------I
      4   C                                                                   I
      5   C            LAPLAC COMPUTE THE LAPLACIAN FOR GRID ADAPTATION       I
      6   C                                                                   I
      7   C-------------------------------------------------------------------I
      8   C
      9         include     'cmsh00.h'
     10         include     'chyd00.h'
     11         include     'cint00.h'
     12         include     'cphs10.h'
     13         include     'cphs20.h'
     14   C
     15         REAL RRMIDL(MBP),PPMIDL(MBP)
     16         REAL ROR(3),UOR(3),VOR(3),POR(3)
     17         REAL ROL(3),UOL(3),VOL(3),POL(3)
     18   C
     19         EPSLON = .025
     20   C
     21         DO 120 IS = 1 , NS
     22         RR( IS ) = 0.
     23         RL( IS ) = 0.
     24    120  CONTINUE
     25   C
     26   C --- BEGIN LOOP OVER ALL EDGES IN THE DOMAIN ----------------------
     27   C
     28         NE1 = 1
     29         NE2 = NOFVEE( 1 )
     30         DO 90 INE = 1 , NVEEE
     31   C
     32   C --- FETCH HYDRO QUANTITIES --------------------------------------
     33   C
     34         DO 105 IE = NE1 , NE2
     35             KE = IE - NE1 + 1
     36   C
     37          ISL = JE( 3 , IE )
     38          ISR = JE( 4 , IE )
     39   C
     40         IF( JE ( 5 , IE ) . EQ . 0 ) THEN
     41   C
     42            RRMDL = XYMIDL( IE ) * ( RGRAD( ISR , 1 ) -
     43        .           RGRAD( ISL , 1 ) ) + RGRAD( ISL , 1 )
     44            RLMDL = XYMIDL( IE ) * ( RGRAD( ISR , 2 ) -
     45        .           RGRAD( ISL , 2 ) ) + RGRAD( ISL , 2 )
     46            PRMDL = XYMIDL( IE ) * ( PGRAD( ISR , 1 ) -
     47        .           PGRAD( ISL , 1 ) ) + PGRAD( ISL , 1 )
     48            PLMDL = XYMIDL( IE ) * ( PGRAD( ISR , 2 ) -
     49        .           PGRAD( ISL , 2 ) ) + PGRAD( ISL , 2 )
     50   C
     51         ELSE
     52   C
     53            RRMDL = RGRAD( ISL , 1 )
     54            RLMDL = RGRAD( ISL , 2 )
     55            PRMDL = PGRAD( ISL , 1 )
     56            PLMDL = PGRAD( ISL , 2 )
     57   C
     58         END IF
     59   C
     60            RRMIDL( KE ) = ( RRMDL * XN( IE ) + RLMDL * YN( IE ) ) *
     61        .                                              XE( 1 , IE )
     62            PPMIDL( KE ) = ( PRMDL * XN( IE ) + PLMDL * YN( IE ) ) *
     63        .                                              XE( 1 , IE )
     64   C
     65    105  CONTINUE
     66   C
     67         DO 130 IE = NE1 , NE2
     68             KE = IE - NE1 + 1
     69   C
     70          ISL = JE( 3 , IE )
     71          ISR = JE( 4 , IE )
     72   C
     73         IF( JE( 5 , IE ) . EQ . 0 ) THEN
     74   C
```

```
3413      75          RR( ISL ) = RR( ISL ) + RRMIDL( KE )                                3413
3414      76          RR( ISR ) = RR( ISR ) - RRMIDL( KE )                                3414
3415      77          RL( ISL ) = RL( ISL ) + PPMIDL( KE )                                3415
3416      78          RL( ISR ) = RL( ISR ) - PPMIDL( KE )                                3416
3417      79    C                                                                         3417
3418      80          ELSE                                                                3418
3419      81    C                                                                         3419
3420      82          RR( ISL ) = RR( ISL ) + RRMIDL( KE )                                3420
3421      83          RL( ISL ) = RL( ISL ) + PPMIDL( KE )                                3421
3422      84    C                                                                         3422
3423      85          END IF                                                              3423
3424      86    C                                                                         3424
3425      87     130  CONTINUE                                                            3425
3426      88    C                                                                         3426
3427      89          NE1 = NE2 + 1                                                       3427
3428      90          NE2 = NE2 + NOFVEE( INE + 1 )                                       3428
3429      91     90   CONTINUE                                                            3429
3430      92    C                                                                         3430
3431      93          DO 135 IS = 1 , NS                                                  3431
3432      94          ZRR = ABS( RR( IS ) ) * SAREA( IS )                                 3432
3433      95          ZPR = ABS( RL( IS ) ) * SAREA( IS )                                 3433
3434      96          RR( IS ) = ZRR * SAREVG                                             3434
3435      97          RL( IS ) = ZPR * SAREVG                                             3435
3436      98     135  CONTINUE                                                            3436
3437      99    C                                                                         3437
3438     100          DO 140 IS = 1 , NS                                                  3438
3439     101          ZRL = ( RGRAD( IS , 1 ) * RGRAD( IS , 1 ) +                         3439
3440     102         .        RGRAD( IS , 2 ) * RGRAD( IS , 2 ) ) * SAREVG                3440
3441     103          ZPL = ( PGRAD( IS , 1 ) * PGRAD( IS , 1 ) +                         3441
3442     104         .        PGRAD( IS , 2 ) * PGRAD( IS , 2 ) ) * SAREVG                3442
3443     105          ZRR = ABS( HYDV( IS , 1 ) ) * EPSLON                                3443
3444     106          ZPP = ABS( HYDV( IS , 4 ) ) * EPSLON                                3444
3445     107          RR( IS ) = RR( IS ) / ( ZRL + ZRR )                                 3445
3446     108          RL( IS ) = RL( IS ) / ( ZPL + ZPP )                                 3446
3447     109     140  CONTINUE                                                            3447
3448     110    C                                                                         3448
3449     111    C --- EXIT POINT FROM SUBROUTINE ------------------------------------     3449
3450     112    C                                                                         3450
3451     113    C     ------                                                              3451
3452     114          RETURN                                                              3452
3453     115    C     ------                                                              3453
3454     116    C                                                                         3454
3455     117    C     ---                                                                 3455
3456     118          END                                                                 3456
```

```
3457      1          SUBROUTINE RECNC( IE , IDONE , ITL , ITR , JA , JB , JC , JD )                3457
3458      2          IMPLICIT REAL (A-H,O-Z)                                                       3458
3459      3    C                                                                                   3459
3460      4    C-------------------------------------------------------------------I              3460
3461      5    C                                                                   I              3461
3462      6    C     THIS ROUTINE CHECKS FOR RECONNECTION OF EDGE NUMBER IE        I              3462
3463      7    C     TO GET A BETTER CONNECTIVITY BETWEEN ADJACENT TRIANGLES       I              3463
3464      8    C     USED AFTER ADDITION AND DELETION                              I              3464
3465      9    C                                                                   I              3465
3466     10    C-------------------------------------------------------------------I              3466
3467     11    C                                                                                   3467
3468     12          include     'cmsh00.h'                                                        3468
3469     13          include     'chyd00.h'                                                        3469
3470     14          include     'cint00.h'                                                        3470
3471     15          include     'cphs10.h'                                                        3471
3472     16          include     'cphs20.h'                                                        3472
3473     17    C                                                                                   3473
3474     18              EROR = 1.0E-3                                                           3474
3475     19    C                                                                                   3475
3476     20              IDONE = 0                                                               3476
3477     21              IF( IE . EQ . 0 ) RETURN                                                3477
3478     22              IF( JE( 5 , IE ) . NE . 0 ) RETURN                                      3478
3479     23              ITR = JE( 4 , IE )                                                      3479
3480     24              ITL = JE( 3 , IE )                                                      3480
3481     25    C                                                                                   3481
3482     26    C     IDENTIFY VERTICES                                                           3482
3483     27    C                                                                                   3483
3484     28              I1 = JE( 1 , IE )                                                       3484
3485     29              I2 = JE( 2 , IE )                                                       3485
3486     30              DO 1 IV = 1 , 3                                                         3486
3487     31              ID = JS( IV , ITL )                                                     3487
3488     32              IF( ID . NE . I1 . AND . ID . NE . I2 ) THEN                            3488
3489     33              I4 = ID                                                                 3489
3490     34              IV4 = IV                                                                3490
3491     35              END IF                                                                  3491
3492     36    1         CONTINUE                                                                3492
3493     37    C                                                                                   3493
3494     38              DO 3 IV = 1 , 3                                                         3494
3495     39              ID = JS( IV , ITR )                                                     3495
3496     40              IF( ID . NE . I1 . AND . ID . NE . I2 ) THEN                            3496
3497     41              I3 = ID                                                                 3497
3498     42              IV3 = IV                                                                3498
3499     43              END IF                                                                  3499
3500     44    3         CONTINUE                                                                3500
3501     45    C     IT MAY HAPPEN THAT I3 IS I4.                                                3501
3502     46              IF( I3 . EQ . I4 ) GO TO 999                                            3502
3503     47    C                                                                                   3503
3504     48    C     COMPARE OPPOSING ANGLE PAIRS IN THE QUADRILATERAL AND RECONNECT TO          3504
3505     49    C     PRESERVE DIAGONAL DOMINANCE OF THE POISSON SOLVER.                          3505
3506     50    C                                                                                   3506
3507     51              AX = XV( 1 , I3 ) - XV( 1 , I1 )                                        3507
3508     52              AY = XV( 2 , I3 ) - XV( 2 , I1 )                                        3508
3509     53              BX = XV( 1 , I4 ) - XV( 1 , I1 )                                        3509
3510     54              BY = XV( 2 , I4 ) - XV( 2 , I1 )                                        3510
3511     55              CX = XV( 1 , I4 ) - XV( 1 , I2 )                                        3511
3512     56              CY = XV( 2 , I4 ) - XV( 2 , I2 )                                        3512
3513     57              DX = XV( 1 , I3 ) - XV( 1 , I2 )                                        3513
3514     58              DY = XV( 2 , I3 ) - XV( 2 , I2 )                                        3514
3515     59              AI2 = AX * BY - AY * BX                                                 3515
3516     60              AI1 = CX * DY - CY * DX                                                 3516
3517     61              XLN = XE( 1 , IE )                                                      3517
3518     62              ROUNDF = EROR * XLN * XLN                                               3518
3519     63    C                                                                                   3519
3520     64    C     IA IS BETWEEN I1 AND I3                                                     3520
3521     65    C     IB IS BETWEEN I1 AND I4                                                     3521
3522     66    C     IC IS BETWEEN I2 AND I4                                                     3522
3523     67    C     ID IS BETWEEN I2 AND I3                                                     3523
3524     68    C                                                                                   3524
3525     69              IB = JS( IV4 + 3 , ITL )                                                3525
3526     70              ID = JS( IV3 + 3 , ITR )                                                3526
3527     71              IV4 = MOD( IV4 + 1 , 3 ) + 1                                            3527
3528     72              IV3 = MOD( IV3 + 1 , 3 ) + 1                                            3528
3529     73              IC = JS( IV4 + 3 , ITL )                                                3529
3530     74              IA = JS( IV3 + 3 , ITR )                                                3530
```

```
3531     75   C                                                                  3531
3532     76            JB = IABS( IB )                                           3532
3533     77            JD = IABS( ID )                                           3533
3534     78            JA = IABS( IA )                                           3534
3535     79            JC = IABS( IC )                                           3535
3536     80            IF( AI2 . LT . ROUNDF . OR . AI1 . LT . ROUNDF ) RETURN   3536
3537     81   C                                                                  3537
3538     82            XL1 = XE( 1 , JA )                                        3538
3539     83            XL2 = XE( 1 , JB )                                        3539
3540     84            XL3 = XE( 1 , JC )                                        3540
3541     85            XL4 = XE( 1 , JD )                                        3541
3542     86   C                                                                  3542
3543     87            XX = XV( 1 , I3 ) - XV( 1 , I4 )                          3543
3544     88            YY = XV( 2 , I3 ) - XV( 2 , I4 )                          3544
3545     89            XLL = SQRT( XX * XX + YY * YY )                           3545
3546     90   C                                                                  3546
3547     91            AREATL = SAREA( ITL )                                     3547
3548     92            AREATR = SAREA( ITR )                                     3548
3549     93            ASP2 = AREATL * XL2 * XL2                                 3549
3550     94            ASP3 = AREATL * XL3 * XL3                                 3550
3551     95            ASPTL = AREATL * XLN * XLN                                3551
3552     96            ASP1 = AREATR * XL1 * XL1                                 3552
3553     97            ASP4 = AREATR * XL4 * XL4                                 3553
3554     98            ASPTR = AREATR * XLN * XLN                                3554
3555     99            ASPN = AMAX1( ASPTL , ASPTR , ASP1 , ASP2 , ASP3 , ASP4 ) 3555
3556    100   C                                                                  3556
3557    101            XSISR = 0.5 * AI2                                         3557
3558    102            XSINSR = 1. / XSISR                                       3558
3559    103   C                                                                  3559
3560    104            XSISL = 0.5 * AI1                                         3560
3561    105            XSINSL = 1. / XSISL                                       3561
3562    106   C                                                                  3562
3563    107            ASP2 = XSINSR * XL2 * XL2                                 3563
3564    108            ASP1 = XSINSR * XL1 * XL1                                 3564
3565    109            ASPSR = XSINSR * XLL * XLL                                3565
3566    110            ASP3 = XSINSL * XL3 * XL3                                 3566
3567    111            ASP4 = XSINSL * XL4 * XL4                                 3567
3568    112            ASPSL = XSINSL * XLL * XLL                                3568
3569    113            ASPL = AMAX1( ASPSL , ASPSR , ASP1 , ASP2 , ASP3 , ASP4 ) 3569
3570    114   C                                                                  3570
3571    115               IF( ASPN . LT . ASPL ) RETURN                          3571
3572    116   C     YES, REDRAW LINE- THE OLD CONNECTION VIOLATES DIAGONAL DOMINANCE. 3572
3573    117   C     DRAW LINE DIRECTED FROM I4 TO I3                             3573
3574    118   C     WE HAVE LEFT JE( 3 , IE ) THE SAME SINCE IE IS STILL INTERNAL. 3574
3575    119               IDONE = 1                                              3575
3576    120               JE( 1 , IE ) = I4                                      3576
3577    121               JE( 2 , IE ) = I3                                      3577
3578    122               XE( 1 , IE ) = XLL                                     3578
3579    123   C                                                                  3579
3580    124   C     ITR IS STILL TO THE RIGHT, ITL TO THE LEFT OF THE NEW LINE IE . 3580
3581    125   C     FIND THE OTHER DIRECTED LINE SEGMENTS                        3581
3582    126   C                                                                  3582
3583    127               DO 30 I = 1 , 2                                        3583
3584    128               IM5 = 5 - I                                            3584
3585    129               IF( JE( IM5 , JB ) . NE . ITL ) GO TO 26               3585
3586    130               JE( IM5 , JB ) = ITR                                   3586
3587    131    26         CONTINUE                                               3587
3588    132               IF( JE( IM5 , JD ) . NE . ITR ) GO TO 28               3588
3589    133               JE( IM5 , JD ) = ITL                                   3589
3590    134    28         CONTINUE                                               3590
3591    135    30         CONTINUE                                               3591
3592    136   C                                                                  3592
3593    137   C     RESET JS( 1 - 6 , ITL AND ITR )                              3593
3594    138   C     START BOTH TRIANGLES AT I4 WITH ( AND PUT IN COUNTERCLOCKWISE 3594
3595    139   C     MANNER)                                                      3595
3596    140               JS( 4 , ITR ) = IB                                     3596
3597    141               JS( 5 , ITR ) = IA                                     3597
3598    142               JS( 6 , ITR ) = - IE                                   3598
3599    143               JS( 1 , ITR ) = I4                                     3599
3600    144               JS( 2 , ITR ) = I1                                     3600
3601    145               JS( 3 , ITR ) = I3                                     3601
3602    146               JS( 4 , ITL ) = IE                                     3602
3603    147               JS( 5 , ITL ) = ID                                     3603
3604    148               JS( 6 , ITL ) = IC                                     3604
```

```
3605     149           JS( 1 , ITL ) = I4                                                3605
3606     150           JS( 2 , ITL ) = I3                                                3606
3607     151           JS( 3 , ITL ) = I2                                                3607
3608     152   C                                                                         3608
3609     153           IF( JV( 2 , I1 ) . GT . 0 ) JV( 2 , I1 ) = JA                     3609
3610     154           IF( JV( 2 , I2 ) . GT . 0 ) JV( 2 , I2 ) = JC                     3610
3611     155   C                                                                         3611
3612     156           XEL = ( XV( 1 , I3 ) + XV( 1 , I2 ) + XV( 1 , I4 ) ) * THIRD      3612
3613     157           YEL = ( XV( 2 , I3 ) + XV( 2 , I2 ) + XV( 2 , I4 ) ) * THIRD      3613
3614     158           XER = ( XV( 1 , I3 ) + XV( 1 , I1 ) + XV( 1 , I4 ) ) * THIRD      3614
3615     159           YER = ( XV( 2 , I3 ) + XV( 2 , I1 ) + XV( 2 , I4 ) ) * THIRD      3615
3616     160   C                                                                         3616
3617     161           DO 92 IR = 1 , MHQ                                                3617
3618     162           HYDV( ITL , IR ) = ( HYDVVV( I3 , IR ) +                          3618
3619     163          .                     HYDVVV( I2 , IR ) +                          3619
3620     164          .                     HYDVVV( I4 , IR ) ) * THIRD                  3620
3621     165   C                                                                         3621
3622     166           HYDV( ITR , IR ) = ( HYDVVV( I3 , IR ) +                          3622
3623     167          .                     HYDVVV( I1 , IR ) +                          3623
3624     168          .                     HYDVVV( I4 , IR ) ) * THIRD                  3624
3625     169    92     CONTINUE                                                          3625
3626     170   C                                                                         3626
3627     171           HDUM          = 1. / ( HYDV( ITL , 1 ) + 1.E-12 )                 3627
3628     172           HYDV( ITL , 2 ) = HYDV( ITL , 2 ) * HDUM                          3628
3629     173           HYDV( ITL , 3 ) = HYDV( ITL , 3 ) * HDUM                          3629
3630     174           HYDV( ITL , 4 ) = ( HYDV( ITL , 4 )  -                            3630
3631     175          .                  .5 * HYDV( ITL , 1 ) *                        3631
3632     176          . ( HYDV( ITL , 2 ) * HYDV( ITL , 2 ) +                          3632
3633     177          .   HYDV( ITL , 3 ) * HYDV( ITL , 3 ) ) ) *                      3633
3634     178          .                     ( HYDV( ITL , 5 ) - 1. )                    3634
3635     179   C                                                                         3635
3636     180           HDUM          = 1. / ( HYDV( ITR , 1 ) + 1.E-12 )                 3636
3637     181           HYDV( ITR , 2 ) = HYDV( ITR , 2 ) * HDUM                          3637
3638     182           HYDV( ITR , 3 ) = HYDV( ITR , 3 ) * HDUM                          3638
3639     183           HYDV( ITR , 4 ) = ( HYDV( ITR , 4 )  -                            3639
3640     184          .                  .5 * HYDV( ITR , 1 ) *                        3640
3641     185          . ( HYDV( ITR , 2 ) * HYDV( ITR , 2 ) +                          3641
3642     186          .   HYDV( ITR , 3 ) * HYDV( ITR , 3 ) ) ) *                      3642
3643     187          .                     ( HYDV( ITR , 5 ) - 1. )                    3643
3644     188   C                                                                         3644
3645     189           RGRAD1 = RGRAD( ITL , 1 ) + RGRAD( ITR , 1 )                      3645
3646     190           RGRAD2 = RGRAD( ITL , 2 ) + RGRAD( ITR , 2 )                      3646
3647     191           RGRAD( ITL , 1 ) = .5 * RGRAD1                                    3647
3648     192           RGRAD( ITR , 1 ) = .5 * RGRAD1                                    3648
3649     193           RGRAD( ITL , 2 ) = .5 * RGRAD2                                    3649
3650     194           RGRAD( ITR , 2 ) = .5 * RGRAD2                                    3650
3651     195   C                                                                         3651
3652     196           UGRAD1 = UGRAD( ITL , 1 ) + UGRAD( ITR , 1 )                      3652
3653     197           UGRAD2 = UGRAD( ITL , 2 ) + UGRAD( ITR , 2 )                      3653
3654     198           UGRAD( ITL , 1 ) = .5 * UGRAD1                                    3654
3655     199           UGRAD( ITR , 1 ) = .5 * UGRAD1                                    3655
3656     200           UGRAD( ITL , 2 ) = .5 * UGRAD2                                    3656
3657     201           UGRAD( ITR , 2 ) = .5 * UGRAD2                                    3657
3658     202   C                                                                         3658
3659     203           VGRAD1 = VGRAD( ITL , 1 ) + VGRAD( ITR , 1 )                      3659
3660     204           VGRAD2 = VGRAD( ITL , 2 ) + VGRAD( ITR , 2 )                      3660
3661     205           VGRAD( ITL , 1 ) = .5 * VGRAD1                                    3661
3662     206           VGRAD( ITR , 1 ) = .5 * VGRAD1                                    3662
3663     207           VGRAD( ITL , 2 ) = .5 * VGRAD2                                    3663
3664     208           VGRAD( ITR , 2 ) = .5 * VGRAD2                                    3664
3665     209   C                                                                         3665
3666     210           PGRAD1 = PGRAD( ITL , 1 ) + PGRAD( ITR , 1 )                      3666
3667     211           PGRAD2 = PGRAD( ITL , 2 ) + PGRAD( ITR , 2 )                      3667
3668     212           PGRAD( ITL , 1 ) = .5 * PGRAD1                                    3668
3669     213           PGRAD( ITR , 1 ) = .5 * PGRAD1                                    3669
3670     214           PGRAD( ITL , 2 ) = .5 * PGRAD2                                    3670
3671     215           PGRAD( ITR , 2 ) = .5 * PGRAD2                                    3671
3672     216   C                                                                         3672
3673     217           XS( 1 , ITL ) = XEL                                               3673
3674     218           XS( 2 , ITL ) = YEL                                               3674
3675     219           XS( 1 , ITR ) = XER                                               3675
3676     220           XS( 2 , ITR ) = YER                                               3676
3677     221   C                                                                         3677
3678     222           XS( 3 , ITR ) = XSISR                                             3678
```

```
3679    223             XS( 3 , ITL ) = XSISL                                   3679
3680    224   C                                                                 3680
3681    225             SAREA( ITL ) = XSINSL                                   3681
3682    226             SAREA( ITR ) = XSINSR                                   3682
3683    227   C                                                                 3683
3684    228             JEN( 1 ) = JA                                           3684
3685    229             JEN( 2 ) = JB                                           3685
3686    230             JEN( 3 ) = JC                                           3686
3687    231             JEN( 4 ) = JD                                           3687
3688    232             JEN( 5 ) = IE                                           3688
3689    233   C                                                                 3689
3690    234             DO 80 IENN = 1 , 5                                      3690
3691    235             IEN = JEN( IENN )                                       3691
3692    236             JV1 = JE( 1 , IEN )                                     3692
3693    237             JV2 = JE( 2 , IEN )                                     3693
3694    238             AX = XV( 1 , JV2 ) - XV( 1 , JV1 )                      3694
3695    239             AY = XV( 2 , JV2 ) - XV( 2 , JV1 )                      3695
3696    240             XEREV = 1. / XE( 1 , IEN )                              3696
3697    241             XN( IEN ) = AY * XEREV                                  3697
3698    242             YN( IEN ) = - AX * XEREV                                3698
3699    243             ISSR = JE( 4 , IEN )                                    3699
3700    244             ISSL = JE( 3 , IEN )                                    3700
3701    245             IJE5 = JE( 5 , IEN )                                    3701
3702    246             IF( IJE5 . NE . 0 ) THEN                                3702
3703    247   C                                                                 3703
3704    248             AA = XV( 1 , JV2 ) - XV( 1 , JV1 )                      3704
3705    249             BB = XV( 2 , JV2 ) - XV( 2 , JV1 )                      3705
3706    250             XEL = XS( 1 , ISSL )                                    3706
3707    251             YEL = XS( 2 , ISSL )                                    3707
3708    252             CC = XEL - XV( 1 , JV1 )                                3708
3709    253             DD = YEL - XV( 2 , JV1 )                                3709
3710    254             EE = ( AA * CC + BB * DD ) * XEREV * XEREV              3710
3711    255             XER = XV( 1 , JV1 ) + AA * EE                           3711
3712    256             YER = XV( 2 , JV1 ) + BB * EE                           3712
3713    257             AX = XER - XEL                                          3713
3714    258             AY = YER - YEL                                          3714
3715    259             XE( 2 , IEN ) = SQRT( AX * AX + AY * AY )               3715
3716    260             XEREV = 1. / XE( 2 , IEN )                              3716
3717    261             XXN( IEN ) = AX * XEREV                                 3717
3718    262             YYN( IEN ) = AY * XEREV                                 3718
3719    263             XE( 2 , IEN ) = 2. * XE( 2 , IEN )                      3719
3720    264             XYMIDL( IEN ) = .5                                      3720
3721    265             XMIDL( IEN ) = XER                                      3721
3722    266             YMIDL( IEN ) = YER                                      3722
3723    267   C                                                                 3723
3724    268             ELSE                                                    3724
3725    269   C                                                                 3725
3726    270             XER = XS( 1 , ISSR )                                    3726
3727    271             YER = XS( 2 , ISSR )                                    3727
3728    272             XEL = XS( 1 , ISSL )                                    3728
3729    273             YEL = XS( 2 , ISSL )                                    3729
3730    274   C                                                                 3730
3731    275             AA = XV( 1 , JV2 ) - XV( 1 , JV1 )                      3731
3732    276             BB = XV( 2 , JV2 ) - XV( 2 , JV1 )                      3732
3733    277             CC = XEL - XER                                          3733
3734    278             DD = YEL - YER                                          3734
3735    279             ACA = XER - XV( 1 , JV1 )                               3735
3736    280             DBD = YER - XV( 2 , JV1 )                               3736
3737    281             EE = ( ACA * DD - DBD * CC ) / ( AA * DD - BB * CC )    3737
3738    282             XMIDL( IEN ) = XV( 1 , JV1 ) + AA * EE                  3738
3739    283             YMIDL( IEN ) = XV( 2 , JV1 ) + BB * EE                  3739
3740    284   C                                                                 3740
3741    285             XEMID = XMIDL( IEN ) - XEL                              3741
3742    286             YEMID = YMIDL( IEN ) - YEL                              3742
3743    287   C                                                                 3743
3744    288             AX = XER - XEL                                          3744
3745    289             AY = YER - YEL                                          3745
3746    290             XE( 2 , IEN ) = SQRT( AX * AX + AY * AY )               3746
3747    291             XEREV = 1. / XE( 2 , IEN )                              3747
3748    292             XXN( IEN ) = AX * XEREV                                 3748
3749    293             YYN( IEN ) = AY * XEREV                                 3749
3750    294   C                                                                 3750
3751    295             XYMIDL( IEN ) = SQRT( XEMID * XEMID + YEMID * YEMID ) * XEREV   3751
3752    296   C                                                                 3752
```

```
      END IF
C
 80   CONTINUE
C
        RETURN
C
 999    WRITE (6,1000) IE
C
C --- EXIT POINT FROM SUBROUTINE ----------------------------------------
C
C     ------
      RETURN
C     ------
C
C --- FORMATS -----------------------------------------------------------
C
 1000 FORMAT('OITS ABOUT TO BOMB--RECNC ON EDGE ',I5)
C
C     ---
      END
```



```
      SUBROUTINE EOS (RRR,EEE,N,GAMMA)
C
C-----------------------------------------------------------------I
C                                                                 I
C     AIR IS ASSUMED TO BE CALORICALLY IMPERFECT, THERMALLY       |
C     PERFECT. THEREFORE, INCLUDE IMPERFECTIONS VIA A VARIABLE    |
C     GAMMA DEPENDENTON DENSITY AND INTERNAL ENERGY.              |
C     THIS ROUTINE PERFORMS A TABLE LOOK UP FOR GAMMA.            |
C                                                                 I
C-----------------------------------------------------------------I
C
C     INPUT VARIBLE DEFINITIONS.
C     RRR = MASS DENSITY
C     EEE = INTERNAL ENERGY PER UNIT VOLUME
C           (CONVERTED FOR INTERNAL *CALL TO ENERGY PER UNIT MASS)
C     N   = NUMBER OF ENTRIES IN ARRAYS RRR & EEE
C
      PARAMETER (M = 64 )
C
      DIMENSION RRR(N), EEE(N), GAMMA(N)
      DIMENSION T11(M), T12(M), T21(M), T22(M), RHO(M), E(M)
      DIMENSION OMP(M), Q(M), I(M), J(M)
      DIMENSION G1(168),G2(112),G3(112),G4(112),G5(112),
     |          G6(112),G7(112),GF(840)
C
C     NOTE:  THE TABLE LOOK UP TREATS ARRAY GF AS THOUGH IT
C     WERE DIMENSIONED (8,105).
C
      EQUIVALENCE (G1(1),GF(  1)), (G2(1),GF(169)), (G3(1),GF(281)),
     |            (G4(1),GF(393)), (G5(1),GF(505)), (G6(1),GF(617)),
     |            (G7(1),GF(729))
C
      DATA XL16E  /2.772588722239774483568908181041479110717773437 5/
C-----------------------------------------------------------------
C     G = GAMMA - 1.0 IS STORED FOR 32 BIT WORD MACHINES IN POWERS OF
C     16 ACROSS FOR MASS DENSITY VARIATION AND INTERMEDIATE VALUES
C     1 - 16 FOR POWERS OF 16 VERTICALLY WHICH REPRESENT THE INTERNAL
C     ENERGY VARIATION.
C
C     16**(2)  .GE. RHO .GE. 16**(-6)
C     16**(15) .GE.  E  .GE. 16**(8)
C-----------------------------------------------------------------
      DATA G1 /8*.4222,8*.4152,8*.4110,8*.4081,8*.4058,8*.4040,
     |         8*.4024,8*.4011,8*.3998,8*.3988,8*.3978,8*.3969,
     |         8*.3961,8*.3953,8*.3935,8*.3918,
     |        .3723,..3715,..3707,..3699,..3690,..3680,..3663,..3637,
     |        .3555,..3538,..3522,..3502,..3476,..3430,..3344,..3238,
     |        .3370,..3370,..3370,..3364,..3347,..3277,..3099,..2885,
     |        .3257,..3227,..3201,..3134,..3062,..3014,..2884,..2591,
     |        .3166,..3110,..3063,..2946,..2831,..2783,..2677,..2358/
      DATA G2/.3111,..3006,..2940,..2787,..2635,..2588,..2502,..2236,
```

```
3824  52        !        .3075,.2906,.2810,.2665,.2466,.2418,.2350,.2131,                3824
3825  53        !        .3043,.2819,.2695,.2554,.2317,.2269,.2216,.2038,                3825
3826  54        !        .2929,.2740,.2593,.2455,.2206,.2136,.2097,.1955,                3826
3827  55        !        .2840,.2672,.2500,.2366,.2166,.2015,.1988,.1879,                3827
3828  56        !        .2764,.2611,.2429,.2285,.2125,.1890,.1890,.1811,                3828
3829  57        !        .2714,.2555,.2384,.2210,.2079,.1818,.1799,.1747,                3829
3830  58        !        .2669,.2504,.2343,.2141,.2037,.1822,.1709,.1689,                3830
3831  59        !        .2624,.2473,.2304,.2096,.1998,.1828,.1684,.1639,                3831
3832  60        !        .2599,.2446,.2268,.2087,.1961,.1834,.1673,.1601,                3832
3833  61        !        .2401,.2191,.1972,.1775,.1592,.1444,.1358,.1203,                3833
3834  62        !        .2002,.1960,.1749,.1536,.1376,.1252,.1107,.1044,                3834
3835  63        !        .1911,.1829,.1633,.1420,.1266,.1101,.1012,.0933,                3835
3836  64        !        .1950,.1781,.1566,.1415,.1241,.1118,.1009,.0948/                3836
3837  65         DATA G3/.2001,.1789,.1594,.1443,.1306,.1189,.1095,.1013,               3837
3838  66        !        .2040,.1826,.1657,.1494,.1338,.1177,.1081,.0980,                3838
3839  67        !        .2034,.1854,.1683,.1497,.1322,.1169,.1051,.0946,                3839
3840  68        !        .1969,.1855,.1685,.1487,.1304,.1149,.1024,.0916,                3840
3841  69        !        .1899,.1837,.1677,.1475,.1287,.1126,.1002,.0900,                3841
3842  70        !        .1841,.1817,.1667,.1464,.1272,.1109,.0983,.0888,                3842
3843  71        !        .1800,.1800,.1659,.1455,.1262,.1097,.0965,.0878,                3843
3844  72        !        .1779,.1787,.1657,.1450,.1254,.1087,.0949,.0868,                3844
3845  73        !        .1773,.1778,.1656,.1447,.1250,.1080,.0939,.0859,                3845
3846  74        !        .1783,.1778,.1658,.1448,.1248,.1076,.0933,.0851,                3846
3847  75        !        .1808,.1781,.1667,.1451,.1248,.1074,.0930,.0843,                3847
3848  76        !        .2134,.2040,.1978,.1782,.1565,.1368,.1206,.1074,                3848
3849  77        !        .2210,.2072,.1957,.1739,.1516,.1312,.1137,.1000,                3849
3850  78        !        .2245,.2109,.1989,.1772,.1563,.1390,.1247,.1133/                3850
3851  79         DATA G4/.2299,.2132,.2017,.1795,.1579,.1384,.1221,.1090,               3851
3852  80        !        .2350,.2157,.2023,.1798,.1575,.1370,.1197,.1057,                3852
3853  81        !        .2397,.2194,.2034,.1796,.1572,.1372,.1205,.1070,                3853
3854  82        !        .2452,.2227,.2050,.1805,.1576,.1379,.1236,.1118,                3854
3855  83        !        .2510,.2256,.2069,.1814,.1581,.1383,.1231,.1103,                3855
3856  84        !        .2560,.2282,.2091,.1822,.1585,.1385,.1226,.1083,                3856
3857  85        !        .2605,.2312,.2111,.1829,.1588,.1386,.1222,.1070,                3857
3858  86        !        .2677,.2358,.2129,.1836,.1592,.1386,.1218,.1071,                3858
3859  87        !        .2759,.2403,.2145,.1857,.1598,.1389,.1219,.1078,                3859
3860  88        !        .2834,.2445,.2160,.1878,.1603,.1394,.1223,.1084,                3860
3861  89        !        .2905,.2484,.2175,.1898,.1613,.1399,.1226,.1090,                3861
3862  90        !        .2963,.2531,.2199,.1918,.1625,.1407,.1230,.1096,                3862
3863  91        !        .4323,.3582,.3109,.2889,.2803,.2706,.2410,.2224,                3863
3864  92        !        .4610,.4026,.3624,.3212,.2926,.2551,.2375,.2015/                3864
3865  93         DATA G5/.4199,.3837,.3401,.2979,.2623,.2318,.2108,.1854,               3865
3866  94        !        .3924,.3642,.3194,.2760,.2427,.2157,.1902,.1721,                3866
3867  95        !        .3794,.3479,.3025,.2673,.2311,.2019,.1842,.1613,                3867
3868  96        !        .3674,.3448,.2961,.2593,.2255,.1994,.1785,.1594,                3868
3869  97        !        .3573,.3443,.2910,.2517,.2293,.2006,.1843,.1679,                3869
3870  98        !        .3661,.3438,.2935,.2597,.2336,.2225,.2143,.2116,                3870
3871  99        !        .3674,.3435,.3080,.2728,.2606,.2577,.2573,.2573,                3871
3872 100        !        .3685,.3453,.3210,.3014,.2942,.2933,.2932,.2932,                3872
3873 101        !        .3814,.3612,.3341,.3276,.3257,.3253,.3252,.3252,                3873
3874 102        !        .3903,.3752,.3570,.3522,.3513,.3510,.3506,.3496,                3874
3875 103        !        .4012,.3899,.3782,.3751,.3743,.3741,.3734,.3713,                3875
3876 104        !        .4155,.4057,.3956,.3930,.3920,.3913,.3907,.3890,                3876
3877 105        !        .4290,.4205,.4118,.4092,.4077,.4065,.4059,.4047,                3877
3878 106        !        .5411,.5385,.5359,.5353,.5351,.5350,.5350,.5350/                3878
3879 107         DATA G6/.5823,.5812,.5801,.5797,.5796,.5797,.5797,.5797,               3879
3880 108        !        .6096,.6090,.6085,.6082,.6082,.6083,.6083,.6083,                3880
3881 109        !        .6308,.6306,.6305,.6303,.6303,.6305,.6305,.6305,                3881
3882 110        !        .6481,.6483,.6485,.6483,.6484,.6486,.6487,.6487,                3882
3883 111        !        .6627,.6632,.6637,.6636,.6637,.6640,.6640,.6640,                3883
3884 112        !        .6754,.6761,.6769,.6768,.6770,.6773,.6773,.6773,                3884
3885 113        !        .6866,.6875,.6885,.6884,.6886,.6890,.6890,.6890,                3885
3886 114        !        .6966,.6977,.6989,.6989,.6991,.6995,.6995,.6995,                3886
3887 115        !        .7056,.7070,.7083,.7083,.7085,.7090,.7090,.7090,                3887
3888 116        !        .7139,.7154,.7169,.7169,.7172,.7176,.7177,.7177,                3888
3889 117        !        .7214,.7231,.7248,.7248,.7251,.7256,.7256,.7256,                3889
3890 118        !        .7285,.7303,.7321,.7321,.7325,.7330,.7330,.7330,                3890
3891 119        !        .7350,.7370,.7390,.7390,.7393,.7398,.7399,.7399,                3891
3892 120        !        .7411,.7432,.7453,.7454,.7457,.7463,.7463,.7463/                3892
3893 121         DATA G7/.8069,.8103,.8138,.8139,.8145,.8152,.8153,.8153,               3893
3894 122        !        .8454,.8496,.8538,.8540,.8547,.8556,.8557,.8557,                3894
3895 123        !        .8727,.8774,.8822,.8825,.8832,.8842,.8843,.8843,                3895
3896 124        !        .8938,.8990,.9042,.9046,.9054,.9064,.9065,.9065,                3896
3897 125        !        .9111,.9166,.9222,.9226,.9235,.9246,.9247,.9247,                3897
```

```
3898    126       !       .9258,.9316,.9374,.9379,.9387,.9399,.9400,.9400,                3898
3899    127       !       .9384,.9445,.9506,.9511,.9520,.9532,.9533,.9533,                3899
3900    128       !       .9496,.9559,.9622,.9627,.9637,.9649,.9650,.9650,                3900
3901    129       !       .9596,.9661,.9727,.9731,.9741,.9754,.9755,.9755,                3901
3902    130       !       .9686,.9753,.9821,.9826,.9836,.9849,.9850,.9850,                3902
3903    131       !       .9769,.9837,.9906,.9912,.9922,.9936,.9937,.9937,                3903
3904    132       !       .9845,.9915,.9986,.9991,.9999,.9999,.9999,.9999,                3904
3905    133       !       .9915,.9987,.9999,.9999,.9999,.9999,.9999,.9999,                3905
3906    134       !       .9981,.9999,.9999,.9999,.9999,.9999,.9999,.9999/                3906
3907    135   C-------------------------------------------------------------              3907
3908    136   C     REAL AIR EOS, TABLE LOOKUP ON GILMORE DATA.  (NO TEMP. MODEL)         3908
3909    137   C     TO AVOID COSTLY LOGARITHMIC FUNCTIONS THE TABLE "G" IS STORED IN A     3909
3910    138   C     FORM SO THAT THE HEXADECIMAL WORD STRUCTURE OF A 32 BIT MACHINE       3910
3911    139   C     MAY BE EXPLOITED.                                                     3911
3912    140   C     THIS LOGIC MAY BE TRANSFERED TO OTHER MACHINES BY RECALCULATING       3912
3913    141   C     THE TABLE "G" APPROPRIATE TO THE WORD ARCITECTURE OF THAT MACHINE.     3913
3914    142   C     MACHINE DEPENDENT FUNCTIONS AND KEY NUMBERS MUST ALSO BE CHANGED.     3914
3915    143   C-------------------------------------------------------------              3915
3916    144         RL16E = 1./XL16E                                                      3916
3917    145         IST = 0                                                               3917
3918    146         NR  = N                                                               3918
3919    147   C                                                                           3919
3920    148     10  CONTINUE                                                            3920
3921    149         NST = MINO(NR,M)                                                      3921
3922    150   C                                                                           3922
3923    151         DO 20 IRE=1,NST                                                       3923
3924    152         RHO(IRE) = .774413*RRR(IST+IRE)                                       3924
3925    153         E(IRE) = AMAX1(3.e8,10000.*EEE(IST+IRE)/RRR(IST+IRE))                 3925
3926    154   C                                                                           3926
3927    155   C     CALCULATE MASS DENSITY VARIATION INDEX "I".                           3927
3928    156   C                                                                           3928
3929    157         TEM = ALOG(RHO(IRE))*RL16E + 500.0                                    3929
3930    158         I(IRE)   = AINT(TEM)                                                  3930
3931    159         OMP(IRE) = TEM - FLOAT(I(IRE))                                        3931
3932    160         I(IRE)   = 502 - I(IRE)                                               3932
3933    161         I(IRE)   = MAXO(I(IRE),1)                                             3933
3934    162   C                                                                           3934
3935    163   C     CALCULATE INTERNAL ENERGY VARIATION INDEX "J".                        3935
3936    164   C                                                                           3936
3937    165         TEM = ALOG(E(IRE))*RL16E                                              3937
3938    166         JCY = AINT(TEM)                                                       3938
3939    167         TEM = TEM - FLOAT(JCY)                                                3939
3940    168         TEM = EXP(XL16E*TEM)                                                  3940
3941    169         JCY = JCY - 7                                                         3941
3942    170         JS  = AINT(TEM)                                                       3942
3943    171         Q(IRE)   = TEM - FLOAT(JS)                                            3943
3944    172         J(IRE)   = JS + 15*JCY                                                3944
3945    173         J(IRE)   = MINO(J(IRE),104)                                           3945
3946    174         J(IRE)   = I(IRE) + 8*J(IRE)                                          3946
3947    175         I(IRE)   = J(IRE) - 8                                                 3947
3948    176     20  CONTINUE                                                            3948
3949    177   C                                                                           3949
3950    178         DO 30 IRE=1,NST                                                       3950
3951    179         T11(IRE) = GF(I(IRE))                                                 3951
3952    180         T21(IRE) = GF(I(IRE)+1)                                               3952
3953    181         T12(IRE) = GF(J(IRE))                                                 3953
3954    182         T22(IRE) = GF(J(IRE)+1)                                               3954
3955    183     30  CONTINUE                                                            3955
3956    184   C                                                                           3956
3957    185   C     CALCULATE GAMMA BY LINEAR INTERPOLATION.                              3957
3958    186   C                                                                           3958
3959    187         DO 40 IRE=1,NST                                                       3959
3960    188         T12(IRE) = T12(IRE) - T11(IRE)                                        3960
3961    189         T22(IRE) = T22(IRE) - T21(IRE)                                        3961
3962    190         GAMMA(IST+IRE) =       OMP(IRE) *(T11(IRE) + Q(IRE)*T12(IRE))         3962
3963    191        !                 + (1. - OMP(IRE))*(T21(IRE) + Q(IRE)*T22(IRE))     3963
3964    192        !                 +  1.                                              3964
3965    193     40  CONTINUE                                                            3965
3966    194   C                                                                           3966
3967    195         NR  = NR - NST                                                        3967
3968    196         IST = IST + NST                                                       3968
3969    197         IF(NR.GT.0) GO TO 10                                                  3969
3970    198   C                                                                           3970
3971    199   C --- EXIT POINT FROM SUBROUTINE ------------------------------------      3971
```

```
3972    200   C
3973    201   C     ------
3974    202         RETURN
3975    203   C     ------
3976    204   C
3977    205   C     ---
3978    206         END
```



```
3979      1         SUBROUTINE LIFTDR
3980      2   C
3981      3         include     'cmsh00.h'
3982      4         include     'chyd00.h'
3983      5         include     'cint00.h'
3984      6         include     'cphs10.h'
3985      7         include     'cphs20.h'
3986      8         REAL PRESS(1000),DYNPRS(1000),XLOCAT(1000),YLOCAT(1000)
3987      9   C
3988     10           XLIFT = 0.
3989     11           XDRAG = 0.
3990     12           XMOMN = 0.
3991     13           UINVR = 2. / UVIN / UVIN / RIN
3992     14           XYU = COS( ALPHA )
3993     15           XYV = SIN( ALPHA )
3994     16           NBB = 0
3995     17              DO 210 IE = 1 , NE
3996     18          IJE5 = JE( 5 , IE )
3997     19          IF( IJE5 . EQ . 5 ) THEN
3998     20              NBB = NBB + 1
3999     21              IV1 = JE( 1 , IE )
4000     22              IV2 = JE( 2 , IE )
4001     23              ISL = JE( 3 , IE )
4002     24              PRES = HYDV( ISL , 4 ) - PINL
4003     25              PRESS( NBB ) = PRES
4004     26              XLIFT = XLIFT + PRES * XE( 1 , IE ) *
4005     27         .                    ( - XN( IE ) * XYV + YN( IE ) * XYU )
4006     28              XDRAG = XDRAG + PRES * XE( 1 , IE ) *
4007     29         .                    ( XN( IE ) * XYU + YN( IE ) * XYV )
4008     30              XLOCAT( NBB ) = .5 * ( XV( 1 , IV1 ) + XV( 1 , IV2 ) )
4009     31              XXV = XLOCAT( NBB )
4010     32              YLOCAT( NBB ) = .5 * ( XV( 2 , IV1 ) + XV( 2 , IV2 ) )
4011     33              YYV = YLOCAT( NBB )
4012     34              XMOMN = XMOMN + PRES * XE( 1 , IE ) *
4013     35         .                    ( XN( IE ) * XXV - YN( IE ) * YYV )
4014     36   C
4015     37              END IF
4016     38   C
4017     39    210       CONTINUE
4018     40   C
4019     41           XLIFT = XLIFT * UINVR
4020     42           XDRAG = XDRAG * UINVR
4021     43           XMOMN = XMOMN * UINVR
4022     44           WRITE (4) NBB,(XLOCAT(KK),YLOCAT(KK),PRESS(KK),KK=1,NBB)
4023     45           WRITE (9) XLIFT,XDRAG,XMOMN,XMCHIN,ALFA
4024     46           PRINT *, XLIFT,XDRAG,XMOMN,XMCHIN,ALFA
4025     47   C
4026     48   C --- EXIT POINT FROM SUBROUTINE ------------------------------------
4027     49   C
4028     50   C     ------
4029     51         RETURN
4030     52   C     ------
4031     53   C
4032     54   C     ---
4033     55         END
```

```
      SUBROUTINE VERDELT( KSD , INDCTR , NIDUMP , JJTRIG , IITRIG )
C
C-----------------------------------------------------------------I
C                                                                 I
C     VERDEL FORCE DELETION OF CELL NUMBER KSD                    I
C                                                                 I
C-----------------------------------------------------------------I
C
      IMPLICIT REAL (A-H,O-Z)
C
      include     'cmsh00.h'
      include     'chyd00.h'
      include     'cint00.h'
      include     'cphs10.h'
      include     'cphs20.h'
C
        INTEGER JUV(MEM),JUE(MEM),JUS(MEM)
        INTEGER IUV(MEM),IUE(MEM),IUS(MEM)
        INTEGER IITRIG(200)
C
      EQUIVALENCE (PR,JUV)
      EQUIVALENCE (UR,JUE)
      EQUIVALENCE (VR,JUS)
      EQUIVALENCE (PL,IUV)
      EQUIVALENCE (UL,IUE)
      EQUIVALENCE (VL,IUS)
C
C   JUV( IVV ) >> NV
C   IUV( NV ) >> IVV
C
C         DO *** KI = 1 , JVDELT
C         IVM = NVDELT( KI )
C         JVM = IVDELT( KI )
C         JUV( IVM ) = JVM
C         IUV( JVM ) = IVM
C
C         DO *** KI= 1 , IETRIG
C         IEM = NECRSS( KI )
C         JEM = IECRSS( KI )
C         JUE( IEM ) = JEM
C         IUE( JEM ) = IEM
C
C         DO *** KI = 1 , ITRIG
C         ISM = NSCRSS( KI )
C         JSM = ISCRSS( KI )
C         JUS( ISM ) = JSM
C         IUS( JSM ) = ISM
C
          FLUXPP = .00001 * HYDMOM( 4 )
          FLUXUU = .00001 * HYDMOM( 2 )
          FLUXRR = .00001 * HYDMOM( 1 )
          AREVGG = AREDEL * SAREVG
          XYLONG = 0.
          XYSHRT = 10000000.
          XYLNGT = 0.
C
          KV1 = JS( 1 , KSD )
          KV2 = JS( 2 , KSD )
          KV3 = JS( 3 , KSD )
          JKV1 = JV( 2 , KV1 )
          JKV2 = JV( 2 , KV2 )
          JKV3 = JV( 2 , KV3 )
          KE1 = JS( 4 , KSD )
          KE2 = JS( 5 , KSD )
          KE3 = JS( 6 , KSD )
          IKE1 = IABS( KE1 )
          IKE2 = IABS( KE2 )
          IKE3 = IABS( KE3 )
          IJE51 = JE( 5 , IKE1 )
          IJE52 = JE( 5 , IKE2 )
          IJE53 = JE( 5 , IKE3 )
          IKKE = 0
          IF( IJE53 . NE . 0 . AND . JKV2 . LT . 0 ) THEN
```

```
 74   74            IKKE = 4                                                  74
 75   75            IEIN1 = - JKV1                                            75
 76   76            IEIN2 = - JKV2                                            76
 77   77            IKKE1 = IKE3                                              77
 78   78            KKE1 = KE3                                                78
 79   79            KKV1 = KV3                                                79
 80   80            IKKE2 = IKE1                                              80
 81   81            KKE2 = KE1                                                81
 82   82            KKV2 = KV1                                                82
 83   83            IKKE3 = IKE2                                              83
 84   84            KKE3 = KE2                                                84
 85   85            KKV3 = KV2                                                85
 86   86  C                                                                   86
 87   87            ELSE IF( IJE52 . NE . 0 . AND . JKV1 . LT . 0 ) THEN      87
 88   88            IKKE = 4                                                  88
 89   89            IEIN1 = - JKV3                                            89
 90   90            IEIN2 = - JKV1                                            90
 91   91            IKKE1 = IKE2                                              91
 92   92            KKE1 = KE2                                                92
 93   93            KKV1 = KV2                                                93
 94   94            IKKE2 = IKE3                                              94
 95   95            KKE2 = KE3                                                95
 96   96            KKV2 = KV3                                                96
 97   97            IKKE3 = IKE1                                              97
 98   98            KKE3 = KE1                                                98
 99   99            KKV3 = KV1                                                99
100  100  C                                                                   100
101  101            ELSE IF( IJE51 . NE . 0 . AND . JKV3 . LT . 0 ) THEN     101
102  102            IKKE = 4                                                 102
103  103            IEIN1 = - JKV2                                           103
104  104            IEIN2 = - JKV3                                           104
105  105            IKKE1 = IKE1                                             105
106  106            KKE1 = KE1                                               106
107  107            KKV1 = KV1                                               107
108  108            IKKE2 = IKE2                                             108
109  109            KKE2 = KE2                                               109
110  110            KKV2 = KV2                                               110
111  111            IKKE3 = IKE3                                             111
112  112            KKE3 = KE3                                               112
113  113            KKV3 = KV3                                               113
114  114  C                                                                  114
115  115            ELSE IF( IJE53 . EQ . 0 . AND . JKV3 . LT . 0 . AND .    115
116  116         .                                    JKV1 . LT . 0 ) THEN    116
117  117            IKKE = 3                                                 117
118  118            IEIN1 = - JKV3                                           118
119  119            IEIN2 = - JKV1                                           119
120  120            IKKE1 = IKE3                                             120
121  121            KKE1 = KE3                                               121
122  122            KKV1 = KV3                                               122
123  123            IKKE2 = IKE1                                             123
124  124            KKE2 = KE1                                               124
125  125            KKV2 = KV1                                               125
126  126            IKKE3 = IKE2                                             126
127  127            KKE3 = KE2                                               127
128  128            KKV3 = KV2                                               128
129  129  C                                                                  129
130  130            ELSE IF( IJE52 . EQ . 0 . AND . JKV2 . LT . 0 . AND .    130
131  131         .                                    JKV3 . LT . 0 ) THEN    131
132  132            IKKE = 3                                                 132
133  133            IEIN1 = - JKV2                                           133
134  134            IEIN2 = - JKV3                                           134
135  135            IKKE1 = IKE2                                             135
136  136            KKE1 = KE2                                               136
137  137            KKV1 = KV2                                               137
138  138            IKKE2 = IKE3                                             138
139  139            KKE2 = KE3                                               139
140  140            KKV2 = KV3                                               140
141  141            IKKE3 = IKE1                                             141
142  142            KKE3 = KE1                                               142
143  143            KKV3 = KV1                                               143
144  144  C                                                                  144
145  145            ELSE IF( IJE51 . EQ . 0 . AND . JKV1 . LT . 0 . AND .    145
146  146         .                                    JKV2 . LT . 0 ) THEN    146
147  147            IKKE = 3                                                 147
```

```
148  148            IEIN1 = - JKV1
149  149            IEIN2 = - JKV2
150  150            IKKE1 = IKE1
151  151            KKE1 = KE1
152  152            KKV1 = KV1
153  153            IKKE2 = IKE2
154  154            KKE2 = KE2
155  155            KKV2 = KV2
156  156            IKKE3 = IKE3
157  157            KKE3 = KE3
158  158            KKV3 = KV3
159  159   C
160  160            ELSE IF( IJE53 . NE . 0 ) THEN
161  161            IKKE = 1
162  162            IEIN = - JKV1
163  163            IKKE1 = IKE3
164  164            KKE1 = KE3
165  165            KKV1 = KV3
166  166            IKKE2 = IKE1
167  167            KKE2 = KE1
168  168            KKV2 = KV1
169  169            KKE3 = KE2
170  170            IKKE3 = IKE2
171  171            KKV3 = KV2
172  172   C
173  173            ELSE IF( IJE52 . NE . 0 ) THEN
174  174            IKKE = 1
175  175            IEIN = - JKV3
176  176            IKKE1 = IKE2
177  177            KKE1 = KE2
178  178            KKV1 = KV2
179  179            IKKE2 = IKE3
180  180            KKE2 = KE3
181  181            KKV2 = KV3
182  182            IKKE3 = IKE1
183  183            KKE3 = KE1
184  184            KKV3 = KV1
185  185   C
186  186            ELSE IF( IJE51 . NE . 0 ) THEN
187  187            IKKE = 1
188  188            IEIN = - JKV2
189  189            IKKE1 = IKE1
190  190            KKE1 = KE1
191  191            KKV1 = KV1
192  192            IKKE2 = IKE2
193  193            KKE2 = KE2
194  194            KKV2 = KV2
195  195            IKKE3 = IKE3
196  196            KKE3 = KE3
197  197            KKV3 = KV3
198  198   C
199  199            ELSE IF( JKV3 . LT . 0 ) THEN
200  200            IKKE = 2
201  201            IEIN = - JKV3
202  202            IKKE1 = IKE3
203  203            KKE1 = KE3
204  204            KKV1 = KV3
205  205            IKKE2 = IKE1
206  206            KKE2 = KE1
207  207            KKV2 = KV1
208  208            IKKE3 = IKE2
209  209            KKE3 = KE2
210  210            KKV3 = KV2
211  211   C
212  212            ELSE IF( JKV2 . LT . 0 ) THEN
213  213            IKKE = 2
214  214            IEIN = - JKV2
215  215            IKKE1 = IKE2
216  216            KKE1 = KE2
217  217            KKV1 = KV2
218  218            IKKE2 = IKE3
219  219            KKE2 = KE3
220  220            KKV2 = KV3
221  221            IKKE3 = IKE1
```

```
222     222             KKE3 = KE1                                                  222
223     223             KKV3 = KV1                                                  223
224     224     C                                                                   224
225     225             ELSE IF( JKV1 . LT . 0 ) THEN                               225
226     226             IKKE = 2                                                    226
227     227             IEIN = - JKV1                                               227
228     228             IKKE1 = IKE1                                                228
229     229             KKE1 = KE1                                                  229
230     230             KKV1 = KV1                                                  230
231     231             IKKE2 = IKE2                                                231
232     232             KKE2 = KE2                                                  232
233     233             KKV2 = KV2                                                  233
234     234             IKKE3 = IKE3                                                234
235     235             KKE3 = KE3                                                  235
236     236             KKV3 = KV3                                                  236
237     237             END IF                                                      237
238     238     C                                                                   238
239     239             IF( IKKE . EQ . 4 ) THEN                                    239
240     240             JV1 = JE( 1 , IEIN2 )                                       240
241     241             JV2 = JE( 2 , IEIN2 )                                       241
242     242             JJV3 = JE( 1 , IKKE3 )                                      242
243     243             JJV4 = JE( 2 , IKKE3 )                                      243
244     244             IF( JJV3 . EQ . JV1 ) THEN                                  244
245     245             JV3 = JJV3                                                  245
246     246             JV4 = JJV4                                                  246
247     247             ELSE                                                        247
248     248             JV3 = JJV4                                                  248
249     249             JV4 = JJV3                                                  249
250     250             END IF                                                      250
251     251             XA = XV( 1 , JV2 ) - XV( 1 , JV1 )                          251
252     252             YA = XV( 2 , JV2 ) - XV( 2 , JV1 )                          252
253     253             XB = XV( 1 , JV4 ) - XV( 1 , JV3 )                          253
254     254             YB = XV( 2 , JV4 ) - XV( 2 , JV3 )                          254
255     255             AB = XA * XB + YA * YB                                      255
256     256             IF( AB . GT . 0. ) IKKE = 5                                 256
257     257             END IF                                                      257
258     258     C                                                                   258
259     259     C   IJTRIG NUMBER OF CIRCUMFERENCE EDGES AROUND VOID                259
260     260     C   ITRIG NUMBER OF TRIANGLES TO BE DELETED                        260
261     261     C   IETRIG NUMBER OF EDGES TO BE DELETED                           261
262     262     C   JVDELT NUMBER OF VERTICES TO BE DELETED                        262
263     263     C                                                                   263
264     264     C   IVDELT(*) SEQUENCE OF VERTICES TO BE DELETED                    264
265     265     C   ISCRSS(*) SEQUENCE OF TRIANGLES TO BE DELETED                  265
266     266     C   IECRSS(*) SEQUENCE OF EDGES TO BE DELETED                      266
267     267     C                                                                   267
268     268             IF( JV( 1 , KV1 ) . EQ . 3 ) RETURN                         268
269     269             IF( JV( 1 , KV2 ) . EQ . 3 ) RETURN                         269
270     270             IF( JV( 1 , KV3 ) . EQ . 3 ) RETURN                         270
271     271             IJTRIG = 0                                                  271
272     272             ITRIG = 0                                                   272
273     273             IETRIG = 0                                                  273
274     274             JVDELT = 0                                                  274
275     275             JLOOP = 0                                                   275
276     276     C                                                                   276
277     277             IF( IKKE . EQ . 0 ) THEN                                    277
278     278     C                                                                   278
279     279     C    THE TRIANGLE TO BE DELETED IS INTIRELY IN THE DOMAIN OF COMPUTATION .  279
280     280     C    THE FIRST LOOP IS AROUND VERTEX KV1 .                          280
281     281     C                                                                   281
282     282             IVV = KV1                                                   282
283     283             IE = IKE3                                                   283
284     284             IV1 = JE( 1 , IE )                                          284
285     285             IF( IV1 . EQ . IVV ) THEN                                   285
286     286             ISI = JE( 3 , IE )                                          286
287     287             ELSE                                                        287
288     288             ISI = JE( 4 , IE )                                          288
289     289             END IF                                                      289
290     290             IS = ISI                                                    290
291     291     C                                                                   291
292     292     110     CONTINUE                                                    292
293     293     C                                                                   293
294     294             ITRIG = ITRIG + 1                                           294
295     295             ISCRSS( ITRIG ) = IS                                        295
```

```
296   296  C
297   297            IF( ITRIG . EQ . 2 ) THEN
298   298            IJTRIG = 0
299   299            IETRIG = IETRIG + 1
300   300            IECRSS( IETRIG ) = IEIB
301   301            END IF
302   302  C
303   303            IETRIG = IETRIG + 1
304   304            IECRSS( IETRIG ) = IE
305   305  C
306   306            IF(
307   307           .    HYDFLX( IS , 4 ) . GT . FLUXPP . OR .
308   308           .    HYDFLX( IS , 2 ) . GT . FLUXUU . OR .
309   309           .    HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
310   310           .    KSDELT( IS ) . GT . NIDUMP . OR .
311   311           .    XS( 3 , IS ) . GT . AREVGG ) THEN
312   312            INDCTR = 3
313   313            RETURN
314   314            END IF
315   315  C
316   316            DO 120 IR = 1 , 3
317   317            JR = MOD( IR , 3 ) + 1
318   318            IEA = IABS( JS( JR + 3 , IS ) )
319   319            IF( IEA . EQ . IE ) THEN
320   320            IIR = MOD( JR , 3 ) + 4
321   321            IEI = JS( IIR , IS )
322   322            IEIB = IABS( IEI )
323   323            XEIEB = XE( 1 , IEIB )
324   324            XYLNGT = XYLNGT + XEIEB
325   325            IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
326   326            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
327   327            IJTRIG = IJTRIG + 1
328   328            IICOLR( IJTRIG ) = IEI
329   329            JJR = MOD( JR + 1 , 3 ) + 4
330   330            IER = IABS( JS( JJR , IS ) )
331   331  C
332   332            IV1 = JE( 1 , IER )
333   333            IF( IV1 . EQ . IVV ) THEN
334   334            ISR = JE( 3 , IER )
335   335            ELSE
336   336            ISR = JE( 4 , IER )
337   337            END IF
338   338            END IF
339   339  C
340   340  120       CONTINUE
341   341  C
342   342            IF( ISR . NE . ISI ) THEN
343   343            IS = ISR
344   344            IE = IER
345   345            GO TO 110
346   346            END IF
347   347  C
348   348            IETRIG = IETRIG + 1
349   349            IECRSS( IETRIG ) = IKE2
350   350            IJTRIG = IJTRIG - 2
351   351  C
352   352  C    FIRST LOOP SUROUNDING KV1 IS DONE, SECOND LOOP OVER KV2 START .
353   353  C
354   354            IVV = KV2
355   355            IE = IABS( IICOLR( IJTRIG + 1 ) )
356   356            IV1 = JE( 1 , IE )
357   357            IF( IV1 . EQ . IVV ) THEN
358   358            ISI = JE( 3 , IE )
359   359            ELSE
360   360            ISI = JE( 4 , IE )
361   361            END IF
362   362            IS = ISI
363   363  C
364   364            ILOOP = 0
365   365  130       CONTINUE
366   366            JDOUBL = IABS( IICOLR( IJTRIG ) )
367   367  C
368   368            ITRIG = ITRIG + 1
369   369            ISCRSS( ITRIG ) = IS
```

```
370   370            IETRIG = IETRIG + 1                                    370
371   371            IECRSS( IETRIG ) = IE                                  371
372   372   C                                                               372
373   373            IF(                                                    373
374   374           .    HYDFLX( IS , 4 ) . GT . FLUXPP . OR .              374
375   375           .    HYDFLX( IS , 2 ) . GT . FLUXUU . OR .              375
376   376           .    HYDFLX( IS , 1 ) . GT . FLUXRR . OR .              376
377   377           .    KSDELT( IS ) . GT . NIDUMP . OR .                  377
378   378           .    XS( 3 , IS ) . GT . AREVGG ) THEN                  378
379   379            INDCTR = 3                                             379
380   380            RETURN                                                 380
381   381            END IF                                                 381
382   382   C                                                               382
383   383            DO 140 IR = 1 , 3                                      383
384   384            JR = MOD( IR , 3 ) + 1                                 384
385   385            IEA = IABS( JS( JR + 3 , IS ) )                        385
386   386            IF( IEA . EQ . IE ) THEN                               386
387   387            IIR = MOD( JR , 3 ) + 4                                387
388   388            IEI = JS( IIR , IS )                                   388
389   389            IEIB = IABS( IEI )                                     389
390   390            XEIEB = XE( 1 , IEIB )                                 390
391   391            XYLNGT = XYLNGT + XEIEB                                391
392   392            IF( XYLONG . LT . XEIEB ) XYLONG = XEIFB               392
393   393            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB               393
394   394            ILOOP = ILOOP + 1                                      394
395   395            IF( !LOOP . EQ . 1 . AND . JDOUBL . EQ . IEIB ) THEN   395
396   396            JLOOP = 1                                              396
397   397            IETRIG = IETRIG + 1                                    397
398   398            IECRSS( IETRIG ) = JDOUBL                              398
399   399            IJTRIG = IJTRIG - 1                                    399
400   400            IF( IEI . GT . 0 ) THEN                                400
401   401            JKVV = JE( 1 , IEIB )                                  401
402   402            ELSE                                                   402
403   403            JKVV = JE( 2 , IEIB )                                  403
404   404            END IF                                                 404
405   405            JVDELT = JVDELT + 1                                    405
406   406            IVDELT( JVDELT ) = JKVV                                406
407   407            ILOOP = 0                                              407
408   408            ELSE                                                   408
409   409            IJTRIG = IJTRIG + 1                                    409
410   410            IICOLR( IJTRIG ) = IEI                                 410
411   411            END IF                                                 411
412   412            JJR = MOD( JR + 1 , 3 ) + 4                            412
413   413            IER = IABS( JS( JJR , IS ) )                           413
414   414   C                                                               414
415   415            IV1 = JE( 1 , IER )                                    415
416   416            IF( IV1 . EQ . IVV ) THEN                              416
417   417            ISR = JE( 3 , IER )                                    417
418   418            ELSE                                                   418
419   419            ISR = JE( 4 , IER )                                    419
420   420            END IF                                                 420
421   421            END IF                                                 421
422   422   C                                                               422
423   423   140      CONTINUE                                               423
424   424   C                                                               424
425   425            IF( IER . NE . IKE2 ) THEN                             425
426   426            IS = ISR                                               426
427   427            IE = IER                                               427
428   428            GO TO 130                                              428
429   429            END IF                                                 429
430   430            IJTRIG = IJTRIG - 1                                    430
431   431   C                                                               431
432   432   C    SECOND LOOP SUROUNDING KV2 IS DONE, THIRD LOOP OVER KV3 START .  432
433   433   C                                                               433
434   434            KET = IECRSS( 2 )                                      434
435   435            IVV = KV3                                              435
436   436            IE = IABS( IICOLR( IJTRIG + 1 ) )                      436
437   437            IF( IE . EQ . KET ) THEN                               437
438   438            JLOOP = 2                                              438
439   439   C                                                               439
440   440   150      CONTINUE                                               440
441   441            IKET = IICOLR( 1 )                                     441
442   442            KKET = IABS( IKET )                                    442
443   443            JKET = IABS( IICOLR( IJTRIG ) )                        443
```

```
444   444             IF( JKET . EQ . KKET ) THEN                                    444
445   445             JLOOP = 3                                                      445
446   446             IF( IKET . GT . 0 ) THEN                                       446
447   447             JKVV = JE( 1 , KKET )                                          447
448   448             ELSE                                                           448
449   449             JKVV = JE( 2 , KKET )                                          449
450   450             END IF                                                         450
451   451             JVDELT = JVDELT + 1                                            451
452   452             IVDELT( JVDELT ) = JKVV                                        452
453   453             DO 160 KK = 2 , IJTRIG                                         453
454   454             IICOLR( KK - 1 ) = IICOLR( KK )                                454
455   455   160       CONTINUE                                                       455
456   456             IJTRIG = IJTRIG - 2                                            456
457   457             IETRIG = IETRIG + 1                                            457
458   458             IECRSS( IETRIG ) = KKET                                        458
459   459             GO TO 150                                                      459
460   460             END IF                                                         460
461   461             GO TO 170                                                      461
462   462             END IF                                                         462
463   463             IV1 = JE( 1 , IE )                                             463
464   464             IF( IV1 . EQ . IVV ) THEN                                      464
465   465             ISI = JE( 3 , IE )                                             465
466   466             ELSE                                                           466
467   467             ISI = JE( 4 , IE )                                             467
468   468             END IF                                                         468
469   469             IS = ISI                                                       469
470   470   C                                                                        470
471   471             ILOOP = 0                                                      471
472   472   180       CONTINUE                                                       472
473   473             KDOUBL = IABS( IICOLR( IJTRIG ) )                              473
474   474   C                                                                        474
475   475             ITRIG = ITRIG + 1                                              475
476   476             ISCRSS( ITRIG ) = IS                                           476
477   477             IETRIG = IETRIG + 1                                            477
478   478             IECRSS( IETRIG ) = IE                                          478
479   479   C                                                                        479
480   480             IF(                                                            480
481   481            .    HYDFLX( IS , 4 ) . GT . FLUXPP . OR .                      481
482   482            .    HYDFLX( IS , 2 ) . GT . FLUXUU . OR .                      482
483   483            .    HYDFLX( IS , 1 ) . GT . FLUXRR . OR .                      483
484   484            .    KSDELT( IS ) . GT . NIDUMP . OR .                          484
485   485            .    XS( 3 , IS ) . GT . AREVGG ) THEN                          485
486   486             INDCTR = 3                                                     486
487   487             RETURN                                                         487
488   488             END IF                                                         488
489   489   C                                                                        489
490   490             DO 190 IR = 1 , 3                                              490
491   491             JR = MOD( IR , 3 ) + 1                                         491
492   492             IEA = IABS( JS( JR + 3 , IS ) )                                492
493   493             IF( IEA . EQ . IE ) THEN                                       493
494   494             IIR = MOD( JR , 3 ) + 4                                        494
495   495             IEI = JS( IIR , IS )                                           495
496   496             IEIB = IABS( IEI )                                             496
497   497             XEIEB = XE( 1 , IEIB )                                         497
498   498             XYLNGT = XYLNGT + XEIEB                                        498
499   499             IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB                       499
500   500             IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB                       500
501   501             ILOOP = ILOOP + 1                                              501
502   502             IF( ILOOP . EQ . 1 . AND . KDOUBL . EQ . IEIB ) THEN           502
503   503             JLOOP = 4                                                      503
504   504             IETRIG = IETRIG + 1                                            504
505   505             IECRSS( IETRIG ) = KDOUBL                                      505
506   506             IJTRIG = IJTRIG - 1                                            506
507   507             IF( IEI . GT . 0 ) THEN                                        507
508   508             JKVV = JE( 1 , IEIB )                                          508
509   509             ELSE                                                           509
510   510             JKVV = JE( 2 , IEIB )                                          510
511   511             END IF                                                         511
512   512             JVDELT = JVDELT + 1                                            512
513   513             IVDELT( JVDELT ) = JKVV                                        513
514   514             ILOOP = 0                                                      514
515   515             ELSE                                                           515
516   516             IJTRIG = IJTRIG + 1                                            516
517   517             IICOLR( IJTRIG ) = IEI                                         517
```

```
518  518            END IF                                                    518
519  519            JJR = MOD( JR + 1 , 3 ) + 4                               519
520  520            IER = IABS( JS( JJR , IS ) )                              520
521  521  C                                                                   521
522  522            IV1 = JE( 1 , IER )                                       522
523  523            IF( IV1 . EQ . IVV ) THEN                                 523
524  524            ISR = JE( 3 , IER )                                       524
525  525            ELSE                                                      525
526  526            ISR = JE( 4 , IER )                                       526
527  527            END IF                                                    527
528  528            END IF                                                    528
529  529  C                                                                   529
530  530  190       CONTINUE                                                  530
531  531  C                                                                   531
532  532            IF( IER . NE . KET ) THEN                                 532
533  533            IS = ISR                                                  533
534  534            IE = IER                                                  534
535  535            GO TO 180                                                 535
536  536            END IF                                                    536
537  537  C                                                                   537
538  538  200       CONTINUE                                                  538
539  539            IKET = IICOLR( 1 )                                        539
540  540            KKET = IABS( IKET )                                       540
541  541            JKET = IABS( IICOLR( IJTRIG ) )                           541
542  542            IF( JKET . EQ . KKET ) THEN                               542
543  543            JLOOP = 5                                                 543
544  544            IF( IKET . GT . 0 ) THEN                                  544
545  545            JKVV = JE( 1 , KKET )                                     545
546  546            ELSE                                                      546
547  547            JKVV = JE( 2 , KKET )                                     547
548  548            END IF                                                    548
549  549            JVDELT = JVDELT + 1                                       549
550  550            IVDELT( JVDELT ) = JKVV                                   550
551  551            DO 210 KK = 2 , IJTRIG                                    551
552  552            IICOLR( KK - 1 ) = IICOLR( KK )                           552
553  553  210       CONTINUE                                                  553
554  554            IJTRIG = IJTRIG - 2                                       554
555  555            IETRIG = IETRIG + 1                                       555
556  556            IECRSS( IETRIG ) = KKET                                   556
557  557            GO TO 200                                                 557
558  558            END IF                                                    558
559  559  C                                                                   559
560  560  170       CONTINUE                                                  560
561  561  C                                                                   561
562  562            INDCTR = 2                                                562
563  563  C          IF( XYLONG / XYSHRT . GT . 10. . AND . JLOOP . EQ . 0 ) RETURN  563
564  564  C                                                                   564
565  565            ELSE IF( IKKE . EQ . 1 ) THEN                             565
566  566  C                                                                   566
567  567  C    BEGINING THE DELETION PROCESS IF KSD HAS AN EDGE ON THE BOUNDARY  567
568  568  C    THE FIRST LOOP IS AROUND VERTEX KKV2 .                         568
569  569  C                                                                   569
570  570            IVV = KKV2                                                570
571  571            IE = IEIN                                                 571
572  572            IVIN = JE( 2 , IE )                                       572
573  573            XXYY1B = XE( 1 , IE ) + XE( 1 , IKKE1 )                   573
574  574            IV1 = JE( 1 , IE )                                        574
575  575            IF( IV1 . EQ . IVV ) THEN                                 575
576  576            ISI = JE( 3 , IE )                                        576
577  577            ELSE                                                      577
578  578            ISI = JE( 4 , IE )                                        578
579  579            END IF                                                    579
580  580            IS = ISI                                                  580
581  581  C                                                                   581
582  582  220       CONTINUE                                                  582
583  583  C                                                                   583
584  584            ITRIG = ITRIG + 1                                         584
585  585            ISCRSS( ITRIG ) = IS                                      585
586  586  C                                                                   586
587  587            IETRIG = IETRIG + 1                                       587
588  588            IECRSS( IETRIG ) = IE                                     588
589  589  C                                                                   589
590  590            IF(                                                       590
591  591       .       HYDFLX( IS , 4 ) . GT . FLUXPP . OR .                  591
```

```
592  592          .       HYDFLX( IS , 2 ) . GT . FLUXUU . OR .
593  593          .       HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
594  594          .       KSDELT( IS ) . GT . NIDUMP . OR .
595  595          .       XS( 3 , IS ) . GT . AREVGG ) THEN
596  596               INDCTR = 3
597  597               RETURN
598  598               END IF
599  599     C
600  600               DO 230 IR = 1 , 3
601  601               JR = MOD( IR , 3 ) + 1
602  602               IEA = IABS( JS( JR + 3 , IS ) )
603  603               IF( IEA . EQ . IE ) THEN
604  604               IIR = MOD( JR , 3 ) + 4
605  605               IEI = JS( IIR , IS )
606  606               IEIB = IABS( IEI )
607  607               XEIEB = XE( 1 , IEIB )
608  608               XYLNGT = XYLNGT + XEIEB
609  609               IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
610  610               IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
611  611               IJTRIG = IJTRIG + 1
612  612               IICOLR( IJTRIG ) = IEI
613  613               JJR = MOD( JR + 1 , 3 ) + 4
614  614               IER = IABS( JS( JJR , IS ) )
615  615     C
616  616               IV1 = JE( 1 , IER )
617  617               IF( IV1 . EQ . IVV ) THEN
618  618               ISR = JE( 3 , IER )
619  619               ELSE
620  620               ISR = JE( 4 , IER )
621  621               END IF
622  622               END IF
623  623     C
624  624     230       CONTINUE
625  625     C
626  626               IF( IER . NE . IKKE1 ) THEN
627  627               IS = ISR
628  628               IE = IER
629  629               GO TO 220
630  630               END IF
631  631     C
632  632               IETRIG = IETRIG + 1
633  633               IECRSS( IETRIG ) = IKKE1
634  634               IJTRIG = IJTRIG - 2
635  635     C
636  636     C    FIRST LOOP SUROUNDING KKV2 IS DONE, SECOND LOOP OVER KKV3 START .
637  637     C
638  638               IVV = KKV3
639  639               IE = IABS( IICOLR( IJTRIG + 1 ) )
640  640               IV1 = JE( 1 , IE )
641  641               IF( IV1 . EQ . IVV ) THEN
642  642               ISI = JE( 3 , IE )
643  643               ELSE
644  644               ISI = JE( 4 , IE )
645  645               END IF
646  646               IS = ISI
647  647     C
648  648               ILOOP = 0
649  649     240       CONTINUE
650  650               JDOUBL = IABS( IICOLR( IJTRIG ) )
651  651     C
652  652               ITRIG = ITRIG + 1
653  653               ISCRSS( ITRIG ) = IS
654  654               IETRIG = IETRIG + 1
655  655               IECRSS( IETRIG ) = IE
656  656     C
657  657               IF(
658  658          .       HYDFLX( IS , 4 ) . GT . FLUXPP . OR .
659  659          .       HYDFLX( IS , 2 ) . GT . FLUXUU . OR .
660  660          .       HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
661  661          .       KSDELT( IS ) . GT . NIDUMP . OR .
662  662          .       XS( 3 , IS ) . GT . AREVGG ) THEN
663  663               INDCTR = 3
664  664               RETURN
665  665               END IF
```

```
      C
                DO 250 IR = 1 , 3
                JR = MOD( IR , 3 ) + 1
                IEA = IABS( JS( JR + 3 , IS ) )
                IF( IEA . EQ . IE ) THEN
                IIR = MOD( JR , 3 ) + 4
                IEI = JS( IIR , IS )
                IEIB = IABS( IEI )
                XEIEB = XE( 1 , IEIB )
                XYLNGT = XYLNGT + XEIEB
                IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
                IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
                ILOOP = ILOOP + 1
                IF( ILOOP . EQ . 1 . AND . JDOUBL . EQ . IEIB ) THEN
                JLOOP = 1
                IETRIG = IETRIG + 1
                IECRSS( IETRIG ) = JDOUBL
                IJTRIG = IJTRIG - 1
                IF( IEI . GT . 0 ) THEN
                JKVV = JE( 1 , IEIB )
                ELSE
                JKVV = JE( 2 , IEIB )
                END IF
                JVDELT = JVDELT + 1
                IVDELT( JVDELT ) = JKVV
                ILOOP = 0
                ELSE
                IJTRIG = IJTRIG + 1
                IICOLR( IJTRIG ) = IEI
                END IF
                JJR = MOD( JR + 1 , 3 ) + 4
                IER = IABS( JS( JJR , IS ) )
      C
                IV1 = JE( 1 , IER )
                IF( IV1 . EQ . IVV ) THEN
                ISR = JE( 3 , IER )
                ELSE
                ISR = JE( 4 , IER )
                END IF
                END IF
      C
      250       CONTINUE
      C
                IF( IER . NE . IKKE3 ) THEN
                IS = ISR
                IE = IER
                GO TO 240
                END IF
      C
                IETRIG = IETRIG + 1
                IECRSS( IETRIG ) = IKKE3
                IJTRIG = IJTRIG - 1
      C
      C     SECOND LOOP SUROUNDING KKV3 IS DONE, THIRD LOOP OVER KKV1 START .
      C
                IVV = KKV1
                IE = IABS( IICOLR( IJTRIG + 1 ) )
                IF( JE( 5 , IE ) . NE . 0 ) THEN
                IER = IE
                GO TO 260
                END IF
                IV1 = JE( 1 , IE )
                IF( IV1 . EQ . IVV ) THEN
                ISI = JE( 3 , IE )
                ELSE
                ISI = JE( 4 , IE )
                END IF
                IS = ISI
                ISI = 0
      C
                ILOOP = 0
      270       CONTINUE
                KDOUBL = IABS( IICOLR( IJTRIG ) )
      C
```

```
                ITRIG = ITRIG + 1
                ISCRSS( ITRIG ) = IS
                IETRIG = IETRIG + 1
                IECRSS( IETRIG ) = IE
C
                IF(
     .              HYDFLX( IS , 4 ) . GT . FLUXPP . OR .
     .              HYDFLX( IS , 2 ) . GT . FLUXUU . OR .
     .              HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
     .              KSDELT( IS ) . GT . NIDUMP . OR .
     .              XS( 3 , IS ) . GT . AREVGG ) THEN
                INDCTR = 3
                RETURN
                END IF
C
                DO 280 IR = 1 , 3
                JR = MOD( IR , 3 ) + 1
                IEA = IABS( JS( JR + 3 , IS ) )
                IF( IEA . EQ . IE ) THEN
                IIR = MOD( JR , 3 ) + 4
                IEI = JS( IIR , IS )
                IEIB = IABS( IEI )
                XEIEB = XE( 1 , IEIB )
                XYLNGT = XYLNGT + XEIEB
                IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
                IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
                ILOOP = ILOOP + 1
                IF( ILOOP . EQ . 1 . AND . KDOUBL . EQ . IEIB ) THEN
                JLOOP = 2
                IETRIG = IETRIG + 1
                IECRSS( IETRIG ) = KDOUBL
                IJTRIG = IJTRIG - 1
                IF( IEI . GT . 0 ) THEN
                JKVV = JE( 1 , IEIB )
                ELSE
                JKVV = JE( 2 , IEIB )
                END IF
                JVDELT = JVDELT + 1
                IVDELT( JVDELT ) = JKVV
                ILOOP = 0
                ELSE
                IJTRIG = IJTRIG + 1
                IICOLR( IJTRIG ) = IEI
                END IF
                JJR = MOD( JR + 1 , 3 ) + 4
                IER = IABS( JS( JJR , IS ) )
C
                IV1 = JE( 1 , IER )
                IF( IV1 . EQ . IVV ) THEN
                ISR = JE( 3 , IER )
                ELSE
                ISR = JE( 4 , IER )
                END IF
                END IF
C
280             CONTINUE
C
                IF( ISR . NE . ISI ) THEN
                IS = ISR
                IE = IER
                GO TO 270
                END IF
C
260             CONTINUE
C
                IETRIG = IETRIG + 1
                IECRSS( IETRIG ) = IER
C
                ITYPE = JE( 5 , IER )
C
                XEIEB = XE( 1 , IER )
                XEIEB = XXYYIB + XEIEB
                XYLNGT = XYLNGT + XEIEB
                IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
```

```
814  814            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB                    814
815  815  C                                                                     815
816  816            INDCTR = 2                                                  816
817  817  C          IF( XYLONG / XYSHRT . GT . 10. . AND . JLOOP . EQ . 0 ) RETURN 817
818  818  C                                                                     818
819  819            IV1 = IVIN                                                  819
820  820            IE1 = IICOLR( IJTRIG )                                      820
821  821            IF( IE1 . GT . 0 ) THEN                                     821
822  822            IV2 = JE( 2 , IE1 )                                         822
823  823            ELSE                                                        823
824  824            IV2 = JE( 1 , - IE1 )                                       824
825  825            END IF                                                      825
826  826  C                                                                     826
827  827            NEC = IECRSS( IETRIG )                                      827
828  828            IETRIG = IETRIG - 1                                         828
829  829  C                                                                     829
830  830            JV( 2 , IV2 ) = - NEC                                       830
831  831            JE( 1 , NEC ) = IV2                                         831
832  832            JE( 2 , NEC ) = IV1                                         832
833  833            JE( 4 , NEC ) = 0                                           833
834  834            JE( 5 , NEC ) = ITYPE                                       834
835  835  C                                                                     835
836  836            IJTRIG = IJTRIG + 1                                         836
837  837            IICOLR( IJTRIG ) = NEC                                      837
838  838  C                                                                     838
839  839            ELSE IF( IKKE . EQ . 2 ) THEN                               839
840  840  C                                                                     840
841  841  C    BEGINING THE DELETION PROCESS IF KSD HAS A VERTEX ON THE BOUNDARY 841
842  842  C    THE FIRST LOOP IS AROUND VERTEX KKV1 .                           842
843  843  C                                                                     843
844  844            IVV = KKV1                                                  844
845  845            IE = IEIN                                                   845
846  846            IVIN = JE( 2 , IE )                                         846
847  847            XXYYIB = XE( 1 , IE )                                       847
848  848            IV1 = JE( 1 , IE )                                          848
849  849            IF( IV1 . EQ . IVV ) THEN                                   849
850  850            ISI = JE( 3 , IE )                                          850
851  851            ELSE                                                        851
852  852            ISI = JE( 4 , IE )                                          852
853  853            END IF                                                      853
854  854            IS = ISI                                                    854
855  855  C                                                                     855
856  856  290       CONTINUE                                                    856
857  857  C                                                                     857
858  858            ITRIG = ITRIG + 1                                           858
859  859            ISCRSS( ITRIG ) = IS                                        859
860  860  C                                                                     860
861  861            IETRIG = IETRIG + 1                                         861
862  862            IECRSS( IETRIG ) = IE                                       862
863  863  C                                                                     863
864  864            IF(                                                         864
865  865       .       HYDFLX( IS , 4 ) . GT . FLUXPP . OR .                    865
866  866       .       HYDFLX( IS , 2 ) . GT . FLUXUU . OR .                    866
867  867       .       HYDFLX( IS , 1 ) . GT . FLUXRR . OR .                    867
868  868       .       KSDELT( IS ) . GT . NIOUMP . OR .                        868
869  869       .       XS( 3 , IS ) . GT . AREVGG ) THEN                        869
870  870            INDCTR = 3                                                  870
871  871            RETURN                                                      871
872  872            END IF                                                      872
873  873  C                                                                     873
874  874            DO 300 IR = 1 , 3                                           874
875  875            JR = MOD( IR , 3 ) + 1                                      875
876  876            IEA = IABS( JS( JR + 3 , IS ) )                             876
877  877            IF( IEA . EQ . IE ) THEN                                    877
878  878            IIR = MOD( JR , 3 ) + 4                                     878
879  879            IEI = JS( IIR , IS )                                        879
880  880            IEIB = IABS( IEI )                                          880
881  881            XEIEB = XE( 1 , IEIB )                                      881
882  882            XYLNGT = XYLNGT + XEIEB                                     882
883  883            IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB                    883
884  884            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB                    884
885  885            IJTRIG = IJTRIG + 1                                         885
886  886            IICOLR( IJTRIG ) = IEI                                      886
887  887            JJR = MOD( JR + 1 , 3 ) + 4                                 887
```

```
888  888            IER = IABS( JS( JJR , IS ) )
889  889  C
890  890            IV1 = JE( 1 , IER )
891  891            IF( IV1 . EQ . IVV ) THEN
892  892            ISR = JE( 3 , IER )
893  893            ELSE
894  894            ISR = JE( 4 , IER )
895  895            END IF
896  896            END IF
897  897  C
898  898  300       CONTINUE
899  899  C
900  900            IF( IER . NE . IKKE3 ) THEN
901  901            IS = ISR
902  902            IE = IER
903  903            GO TO 290
904  904            END IF
905  905            IJTRIG = IJTRIG - 2
906  906  C
907  907  C    FIRST LOOP SUROUNDING KKV1 IS DONE, SECOND LOOP OVER KKV2 START .
908  908  C
909  909            IVV = KKV2
910  910            IE = IABS( IICOLR( IJTRIG + 1 ) )
911  911            IV1 = JE( 1 , IE )
912  912            IF( IV1 . EQ . IVV ) THEN
913  913            ISI = JE( 3 , IE )
914  914            ELSE
915  915            ISI = JE( 4 , IE )
916  916            END IF
917  917            IS = ISI
918  918  C
919  919            ILOOP = 0
920  920  310       CONTINUE
921  921            IDOUBL = IABS( IICOLR( IJTRIG ) )
922  922  C
923  923            ITRIG = ITRIG + 1
924  924            ISCRSS( ITRIG ) = IS
925  925  C
926  926            IETRIG = IETRIG + 1
927  927            IECRSS( IETRIG ) = IE
928  928  C
929  929            IF(
930  930       .       HYDFLX( IS , 4 ) . GT . FLUXPP . OR .
931  931       .       HYDFLX( IS , 2 ) . GT . FLUXUU . OR .
932  932       .       HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
933  933       .       KSDELT( IS ) . GT . NIDUMP . OR .
934  934       .       XS( 3 , IS ) . GT . AREVGG ) THEN
935  935            INDCTR = 3
936  936            RETURN
937  937            END IF
938  938  C
939  939            DO 320 IR = 1 , 3
940  940            JR = MOD( IR , 3 ) + 1
941  941            IEA = IABS( JS( JR + 3 , IS ) )
942  942            IF( IEA . EQ . IE ) THEN
943  943            IIR = MOD( JR , 3 ) + 4
944  944            IEI = JS( IIR , IS )
945  945            IEIB = IABS( IEI )
946  946            XEIEB = XE( 1 , IEIB )
947  947            XYLNGT = XYLNGT + XEIEB
948  948            IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
949  949            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
950  950            ILOOP = ILOOP + 1
951  951            IF( ILOOP . EQ . 1 . AND . IDOUBL . EQ . IEIB ) THEN
952  952            JLOOP = 1
953  953            IETRIG = IETRIG + 1
954  954            IECRSS( IETRIG ) = IDOUBL
955  955            IJTRIG = IJTRIG - 1
956  956            IF( IEI . GT . 0 ) THEN
957  957            JKVV = JE( 1 , IEIB )
958  958            ELSE
959  959            JKVV = JE( 2 , IEIB )
960  960            END IF
961  961            JVDELT = JVDELT + 1
```

```
                IVDELT( JVDELT ) = JKVV
                ILOOP = 0
                ELSE
                IJTRIG = IJTRIG + 1
                IICOLR( IJTRIG ) = IEI
                END IF
                JJR = MOD( JR + 1 , 3 ) + 4
                IER = IABS( JS( JJR , IS ) )
C
                IV1 = JE( 1 , IER )
                IF( IV1 . EQ . IVV ) THEN
                ISR = JE( 3 , IER )
                ELSE
                ISR = JE( 4 , IER )
                END IF
                END IF
C
320             CONTINUE
C
                IF( IER . NE . IKKE2 ) THEN
                IS = ISR
                IE = IER
                GO TO 310
                END IF
C
                IJTRIG = IJTRIG - 1
C
C     SECOND LOOP SUROUNDING KKV2 IS DONE, THIRD LOOP OVER KKV3 START .
C
                IVV = KKV3
                IE = IABS( IICOLR( IJTRIG + 1 ) )
                IV1 = JE( 1 , IE )
                IF( IV1 . EQ . IVV ) THEN
                ISI = JE( 3 , IE )
                ELSE
                ISI = JE( 4 , IE )
                END IF
                IS = ISI
C
                ILOOP = 0
330             CONTINUE
                KDOUBL = IABS( IICOLR( IJTRIG ) )
C
                ITRIG = ITRIG + 1
                ISCRSS( ITRIG ) = IS
                IETRIG = IETRIG + 1
                IECRSS( IETRIG ) = IE
C
                IF(
     .              HYDFLX( IS , 4 ) . GT . FLUXPP . OR .
     .              HYDFLX( IS , 2 ) . GT . FLUXUU . OR .
     .              HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
     .              KSDELT( IS ) . GT . NIDUMP . OR .
     .              XS( 3 , IS ) . GT . AREVGG ) THEN
                INDCTR = 3
                RETURN
                END IF
C
                DO 340 IR = 1 , 3
                JR = MOD( IR , 3 ) + 1
                IEA = IABS( JS( JR + 3 , IS ) )
                IF( IEA . EQ . IE ) THEN
                IIR = MOD( JR , 3 ) + 4
                IEI = JS( IIR , IS )
                IEIB = IABS( IEI )
                XEIEB = XE( 1 , IEIB )
                XYLNGT = XYLNGT + XEIEB
                IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
                IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
                ILOOP = ILOOP + 1
                IF( ILOOP . EQ . 1 . AND . KDOUBL . EQ . IEIB ) THEN
                JLOOP = 2
                IETRIG = IETRIG + 1
                IECRSS( IETRIG ) = KDOUBL
```

```
1036    1036            IJTRIG = IJTRIG - 1
1037    1037            IF( IEI . GT . 0 ) THEN
1038    1038            JKVV = JE( 1 , IEIB )
1039    1039            ELSE
1040    1040            JKVV = JE( 2 , IEIB )
1041    1041            END IF
1042    1042            JVDELT = JVDELT + 1
1043    1043            IVDELT( JVDELT ) = JKVV
1044    1044            ILOOP = 0
1045    1045            ELSE
1046    1046            IJTRIG = IJTRIG + 1
1047    1047            IICOLR( IJTRIG ) = IEI
1048    1048            END IF
1049    1049            JJR = MOD( JR + 1 , 3 ) + 4
1050    1050            IER = IABS( JS( JJR , IS ) )
1051    1051    C
1052    1052            IV1 = JE( 1 , IER )
1053    1053            IF( IV1 . EQ . IVV ) THEN
1054    1054            ISR = JE( 3 , IER )
1055    1055            ELSE
1056    1056            ISR = JE( 4 , IER )
1057    1057            END IF
1058    1058            END IF
1059    1059    C
1060    1060    340     CONTINUE
1061    1061    C
1062    1062            IF( IER . NE . IKKE3 ) THEN
1063    1063            IS = ISR
1064    1064            IE = IER
1065    1065            GO TO 330
1066    1066            END IF
1067    1067    C
1068    1068            IETRIG = IETRIG + 1
1069    1069            IECRSS( IETRIG ) = IKKE3
1070    1070            IETRIG = IETRIG + 1
1071    1071            IECRSS( IETRIG ) = IKKE2
1072    1072    C
1073    1073            IJTRIG = IJTRIG - 1
1074    1074    C
1075    1075    C   THIRD LOOP SUROUNDING KKV3 IS DONE, FOURTH LOOP OVER KKV1 START .
1076    1076    C
1077    1077            IVV = KKV1
1078    1078            IE = IABS( IICOLR( IJTRIG + 1 ) )
1079    1079            IF( JE( 5 , IE ) . NE . 0 ) THEN
1080    1080            IER = IE
1081    1081            GO TO 350
1082    1082            END IF
1083    1083            IV1 = JE( 1 , IE )
1084    1084            IF( IV1 . EQ . IVV ) THEN
1085    1085            ISI = JE( 3 , IE )
1086    1086            ELSE
1087    1087            ISI = JE( 4 , IE )
1088    1088            END IF
1089    1089            IS = ISI
1090    1090            ISI = 0
1091    1091    C
1092    1092            ILOOP = 0
1093    1093    360     CONTINUE
1094    1094            JDOUBL = IABS( IICOLR( IJTRIG ) )
1095    1095    C
1096    1096            ITRIG = ITRIG + 1
1097    1097            ISCRSS( ITRIG ) = IS
1098    1098            IETRIG = IETRIG + 1
1099    1099            IECRSS( IETRIG ) = IE
1100    1100    C
1101    1101            IF(
1102    1102           .    HYDFLX( IS , 4 ) . GT . FLUXPP . OR .
1103    1103           .    HYDFLX( IS , 2 ) . GT . FLUXUU . OR .
1104    1104           .    HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
1105    1105           .    KSDELT( IS ) . GT . NIDUMP . OR .
1106    1106           .    XS( 3 , IS ) . GT . AREVGG ) THEN
1107    1107            INDCTR = 3
1108    1108            RETURN
1109    1109            END IF
```

```
1110  1110  C
1111  1111        DO 370 IR = 1 , 3
1112  1112        JR = MOD( IR , 3 ) + 1
1113  1113        IEA = IABS( JS( JR + 3 , IS ) )
1114  1114        IF( IEA . EQ . IE ) THEN
1115  1115        IIR = MOD( JR , 3 ) + 4
1116  1116        IEI = JS( IIR , IS )
1117  1117        IEIB = IABS( IEI )
1118  1118        XEIEB = XE( 1 , IEIB )
1119  1119        XYLNGT = XYLNGT + XEIEB
1120  1120        IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
1121  1121        IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
1122  1122        ILOOP = ILOOP + 1
1123  1123        IF( ILOOP . EQ . 1 . AND . JDOUBL . EQ . IEIB ) THEN
1124  1124        JLOOP = 3
1125  1125        IETRIG = IETRIG + 1
1126  1126        IECRSS( IETRIG ) = JDOUBL
1127  1127        IJTRIG = IJTRIG - 1
1128  1128        IF( IEI . GT . 0 ) THEN
1129  1129        JKVV = JE( 1 , IEIB )
1130  1130        ELSE
1131  1131        JKVV = JE( 2 , IEIB )
1132  1132        END IF
1133  1133        JVDELT = JVDELT + 1
1134  1134        IVDELT( JVDELT ) = JKVV
1135  1135        ILOOP = 0
1136  1136        ELSE
1137  1137        IJTRIG = IJTRIG + 1
1138  1138        IICOLR( IJTRIG ) = IEI
1139  1139        END IF
1140  1140        JJR = MOD( JR + 1 , 3 ) + 4
1141  1141        IER = IABS( JS( JJR , IS ) )
1142  1142  C
1143  1143        IV1 = JE( 1 , IER )
1144  1144        IF( IV1 . EQ . IVV ) THEN
1145  1145        ISR = JE( 3 , IER )
1146  1146        ELSE
1147  1147        ISR = JE( 4 , IER )
1148  1148        END IF
1149  1149        END IF
1150  1150  C
1151  1151  370   CONTINUE
1152  1152  C
1153  1153        IF( ISR . NE . ISI ) THEN
1154  1154        IS = ISR
1155  1155        IE = IER
1156  1156        GO TO 360
1157  1157        END IF
1158  1158  C
1159  1159  350   CONTINUE
1160  1160  C
1161  1161        IETRIG = IETRIG + 1
1162  1162        IECRSS( IETRIG ) = IER
1163  1163  C
1164  1164        ITYPE = JE( 5 , IER )
1165  1165  C
1166  1166        XEIEB = XE( 1 , IER )
1167  1167        XEIEB = XXYYIB + XEIEB
1168  1168        XYLNGT = XYLNGT + XEIEB
1169  1169        IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
1170  1170        IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
1171  1171  C
1172  1172        INDCTR = 2
1173  1173  C      IF( XYLONG / XYSHRT . GT . 10. . AND . JLOOP . EQ . 0 ) RETURN
1174  1174  C
1175  1175        IV1 = IVIN
1176  1176        IE1 = IICOLR( IJTRIG )
1177  1177        IF( IE1 . GT . 0 ) THEN
1178  1178        IV2 = JE( 2 , IE1 )
1179  1179        ELSE
1180  1180        IV2 = JE( 1 , - IE1 )
1181  1181        END IF
1182  1182  C
1183  1183        NEC = IECRSS( IETRIG )
```

```
1184  1184            IETRIG = IETRIG - 1
1185  1185  C
1186  1186            JV( 2 , IV2 ) = - NEC
1187  1187            JE( 1 , NEC ) = IV2
1188  1188            JE( 2 , NEC ) = IV1
1189  1189            JE( 4 , NEC ) = 0
1190  1190            JE( 5 , NEC ) = ITYPE
1191  1191  C
1192  1192            IJTRIG = IJTRIG + 1
1193  1193            IICOLR( IJTRIG ) = NEC
1194  1194  C
1195  1195            ELSE IF( IKKE . EQ . 3 ) THEN
1196  1196  C
1197  1197  C     BEGINING THE DELETION PROCESS IF KSD HAS TWO VERTECIS ON THE BOUNDARY
1198  1198  C     BUT THE EDGE THAT CONNECT THEM IS IN THE COMPUTATIONAL DOMAIN.
1199  1199  C     THE FIRST LOOP IS AROUND VERTEX KKV1 .
1200  1200  C
1201  1201            IVV = KKV1
1202  1202            IE = IEIN1
1203  1203            XXYYIB = XE( 1 , IE )
1204  1204            IV1 = JE( 1 , IE )
1205  1205            IVIN1 = JE( 2 , IE )
1206  1206            IF( IV1 . EQ . IVV ) THEN
1207  1207            ISI = JE( 3 , IE )
1208  1208            ELSE
1209  1209            ISI = JE( 4 , IE )
1210  1210            END IF
1211  1211            IS = ISI
1212  1212  C
1213  1213  380       CONTINUE
1214  1214  C
1215  1215            ITRIG = ITRIG + 1
1216  1216            ISCRSS( ITRIG ) = IS
1217  1217            IETRIG = IETRIG + 1
1218  1218            IECRSS( IETRIG ) = IE
1219  1219  C
1220  1220            IF(
1221  1221       .        HYDFLX( IS , 4 ) . GT . FLUXPP . OR .
1222  1222       .        HYDFLX( IS , 2 ) . GT . FLUXUU . OR .
1223  1223       .        HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
1224  1224       .        KSDELT( IS ) . GT . NIDUMP . OR .
1225  1225       .        XS( 3 , IS ) . GT . AREVGG ) THEN
1226  1226            INDCTR = 3
1227  1227            RETURN
1228  1228            END IF
1229  1229  C
1230  1230            DO 390 IR = 1 , 3
1231  1231            JR = MOD( IR , 3 ) + 1
1232  1232            IEA = IABS( JS( JR + 3 , IS ) )
1233  1233            IF( IEA . EQ . IE ) THEN
1234  1234            IIR = MOD( JR , 3 ) + 4
1235  1235            IEI = JS( IIR , IS )
1236  1236            IEIB = IABS( IEI )
1237  1237            XEIEB = XE( 1 , IEIB )
1238  1238            XYLNGT = XYLNGT + XEIEB
1239  1239            IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
1240  1240            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
1241  1241            IJTRIG = IJTRIG + 1
1242  1242            IICOLR( IJTRIG ) = IEI
1243  1243            JJR = MOD( JR + 1 , 3 ) + 4
1244  1244            IER = IABS( JS( JJR , IS ) )
1245  1245  C
1246  1246            IV1 = JE( 1 , IER )
1247  1247            IF( IV1 . EQ . IVV ) THEN
1248  1248            ISR = JE( 3 , IER )
1249  1249            ELSE
1250  1250            ISR = JE( 4 , IER )
1251  1251            END IF
1252  1252            END IF
1253  1253  C
1254  1254  390       CONTINUE
1255  1255  C
1256  1256            IF( IER . NE . IKKE3 ) THEN
1257  1257            IS = ISR
```

```
1258  1258            IE = IER                                                1258
1259  1259            GO TO 380                                               1259
1260  1260            END IF                                                  1260
1261  1261  C                                                                 1261
1262  1262  C     FIRST LOOP SUROUNDING KKV1 IS DONE, SECOND LOOP OVER KKV2 START .  1262
1263  1263  C                                                                 1263
1264  1264            IJTRIG = IJTRIG - 1                                     1264
1265  1265  400       CONTINUE                                                1265
1266  1266  C                                                                 1266
1267  1267            IEJK = IICOLR( IJTRIG )                                 1267
1268  1268            IF( IEJK . GT . 0 ) THEN                                1268
1269  1269            IVIEJK = JE( 1 , IEJK )                                 1269
1270  1270            IJEJK5 = JE( 5 , IEJK )                                 1270
1271  1271            ELSE                                                    1271
1272  1272            IVIEJK = JE( 2 , -IEJK )                                1272
1273  1273            IJEJK5 = JE( 5 , -IEJK )                                1273
1274  1274            END IF                                                  1274
1275  1275  C                                                                 1275
1276  1276            IF( IJEJK5 . EQ . 0 ) THEN                              1276
1277  1277            JLOOP = 1                                               1277
1278  1278  C                                                                 1278
1279  1279  C     INTERMEDIATE LOOP START .                                   1279
1280  1280  C                                                                 1280
1281  1281            IEJKI = IABS( IICOLR( IJTRIG - 1 ) )                    1281
1282  1282            IEJK2 = IABS( IEJK )                                    1282
1283  1283            IETRIG = IETRIG + 1                                     1283
1284  1284            IECRSS( IETRIG ) = IEJK2                                1284
1285  1285            IJTRIG = IJTRIG - 2                                     1285
1286  1286            IVV = IVIEJK                                            1286
1287  1287            JVDELT = JVDELT + 1                                     1287
1288  1288            IVDELT( JVDELT ) = IVV                                  1288
1289  1289            IE = IEJKI                                              1289
1290  1290            IV1 = JE( 1 , IE )                                      1290
1291  1291            IF( IV1 . EQ . IVV ) THEN                               1291
1292  1292            ISI = JE( 3 , IE )                                      1292
1293  1293            ELSE                                                    1293
1294  1294            ISI = JE( 4 , IE )                                      1294
1295  1295            END IF                                                  1295
1296  1296            IS = ISI                                                1296
1297  1297            IET = IEJK2                                             1297
1298  1298  C                                                                 1298
1299  1299  410       CONTINUE                                                1299
1300  1300  C                                                                 1300
1301  1301            ITRIG = ITRIG + 1                                       1301
1302  1302            ISCRSS( ITRIG ) = IS                                    1302
1303  1303  C                                                                 1303
1304  1304            IETRIG = IETRIG + 1                                     1304
1305  1305            IECRSS( IETRIG ) = IE                                   1305
1306  1306  C                                                                 1306
1307  1307            IF(                                                     1307
1308  1308           .    HYDFLX( IS , 4 ) . GT . FLUXPP . OR .               1308
1309  1309           .    HYDFLX( IS , 2 ) . GT . FLUXUU . OR .               1309
1310  1310           .    HYDFLX( IS , 1 ) . GT . FLUXRR . OR .               1310
1311  1311           .    KSDELT( IS ) . GT . NIDUMP . OR .                   1311
1312  1312           .    XS( 3 , IS ) . GT . AREVGG ) THEN                   1312
1313  1313            INDCTR = 3                                              1313
1314  1314            RETURN                                                  1314
1315  1315            END IF                                                  1315
1316  1316  C                                                                 1316
1317  1317            DO 420 IR = 1 , 3                                       1317
1318  1318            JR = MOD( IR , 3 ) + 1                                  1318
1319  1319            IEA = IABS( JS( JR + 3 , IS ) )                         1319
1320  1320            IF( IEA . EQ . IE ) THEN                                1320
1321  1321            IIR = MOD( JR , 3 ) + 4                                 1321
1322  1322            IEI = JS( IIR , IS )                                    1322
1323  1323            IEIB = IABS( IEI )                                      1323
1324  1324            XEIEB = XE( 1 , IEIB )                                  1324
1325  1325            XYLNGT = XYLNGT + XEIEB                                 1325
1326  1326            IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB                1326
1327  1327            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB                1327
1328  1328            IIKK = IABS( IICOLR( IJTRIG ) )                         1328
1329  1329            IF( IIKK . EQ . IEIB ) THEN                             1329
1330  1330            JLOOP = 2                                               1330
1331  1331            IETRIG = IETRIG + 1                                     1331
```

```
1332  1332            IECRSS( IETRIG ) = IEIB
1333  1333            IJTRIG = IJTRIG - 1
1334  1334            IF( IEI . GT . 0 ) THEN
1335  1335            JKVV = JE( 1 , IEIB )
1336  1336            ELSE
1337  1337            JKVV = JE( 2 , IEIB )
1338  1338            END IF
1339  1339            JVDELT = JVDELT + 1
1340  1340            IVDELT( JVDELT ) = JKVV
1341  1341            ELSE
1342  1342            IJTRIG = IJTRIG + 1
1343  1343            IICOLR( IJTRIG ) = IEI
1344  1344            END IF
1345  1345            JJR = MOD( JR + 1 , 3 ) + 4
1346  1346            IER = IABS( JS( JJR , IS ) )
1347  1347  C
1348  1348            IV1 = JE( 1 , IER )
1349  1349            IF( IV1 . EQ . IVV ) THEN
1350  1350            ISR = JE( 3 , IER )
1351  1351            ELSE
1352  1352            ISR = JE( 4 , IER )
1353  1353            END IF
1354  1354            END IF
1355  1355  C
1356  1356  420       CONTINUE
1357  1357  C
1358  1358            IF( IER . NE . IET ) THEN
1359  1359            IS = ISR
1360  1360            IE = IER
1361  1361            GO TO 410
1362  1362            END IF
1363  1363  C
1364  1364            GO TO 400
1365  1365            END IF
1366  1366  C
1367  1367  C     INTERMEDIATE LOOP IS DONE, SECOND LOOP OVER KKV2 START .
1368  1368  C
1369  1369            IVV = KKV2
1370  1370            IE = IEIN2
1371  1371            IVIN2 = JE( 2 , IE )
1372  1372            IEJKK = IICOLR( IJTRIG )
1373  1373            IV1 = JE( 1 , IE )
1374  1374            IF( IV1 . EQ . IVV ) THEN
1375  1375            ISI = JE( 3 , IE )
1376  1376            ELSE
1377  1377            ISI = JE( 4 , IE )
1378  1378            END IF
1379  1379            IS = ISI
1380  1380  C
1381  1381  430       CONTINUE
1382  1382  C
1383  1383            ITRIG = ITRIG + 1
1384  1384            ISCRSS( ITRIG ) = IS
1385  1385  C
1386  1386            IETRIG = IETRIG + 1
1387  1387            IECRSS( IETRIG ) = IE
1388  1388  C
1389  1389            IF(
1390  1390           .    HYDFLX( IS , 4 ) . GT . FLUXPP . OR .
1391  1391           .    HYDFLX( IS , 2 ) . GT . FLUXUU . OR .
1392  1392           .    HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
1393  1393           .    KSDELT( IS ) . GT . NIDUMP . OR .
1394  1394           .    XS( 3 , IS ) . GT . AREVGG ) THEN
1395  1395            INDCTR = 3
1396  1396            RETURN
1397  1397            END IF
1398  1398  C
1399  1399            DO 440 IR = 1 , 3
1400  1400            JR = MOD( IR , 3 ) + 1
1401  1401            IEA = IABS( JS( JR + 3 , IS ) )
1402  1402            IF( IEA . EQ . IE ) THEN
1403  1403            IIR = MOD( JR , 3 ) + 4
1404  1404            IEI = JS( IIR , IS )
1405  1405            IEIB = IABS( IEI )
```

```
1406  1406            XEIEB = XE( 1 , IEIB )                                  1406
1407  1407            XYLNGT = XYLNGT + XEIEB                                 1407
1408  1408            IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB                1408
1409  1409            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB                1409
1410  1410            IJTRIG = IJTRIG + 1                                     1410
1411  1411            IICOLR( IJTRIG ) = IEI                                  1411
1412  1412            JJR = MOD( JR + 1 , 3 ) + 4                             1412
1413  1413            IER = IABS( JS( JJR , IS ) )                            1413
1414  1414  C                                                                 1414
1415  1415            IV1 = JE( 1 , IER )                                     1415
1416  1416            IF( IV1 . EQ . IVV ) THEN                               1416
1417  1417            ISR = JE( 3 , IER )                                     1417
1418  1418            ELSE                                                    1418
1419  1419            ISR = JE( 4 , IER )                                     1419
1420  1420            END IF                                                  1420
1421  1421            END IF                                                  1421
1422  1422  C                                                                 1422
1423  1423  440       CONTINUE                                                1423
1424  1424  C                                                                 1424
1425  1425            IF( IER . NE . IKKE2 ) THEN                             1425
1426  1426            IS = ISR                                                1426
1427  1427            IE = IER                                                1427
1428  1428            GO TO 430                                               1428
1429  1429            END IF                                                  1429
1430  1430  C                                                                 1430
1431  1431            IJTRIG = IJTRIG - 1                                     1431
1432  1432  C                                                                 1432
1433  1433  C     SECOND LOOP SUROUNDING KKV2 IS DONE, THIRD LOOP OVER KKV3 START .  1433
1434  1434  C                                                                 1434
1435  1435            IVV = KKV3                                              1435
1436  1436            IE = IABS( IICOLR( IJTRIG + 1 ) )                       1436
1437  1437            IV1 = JE( 1 , IE )                                      1437
1438  1438            IF( IV1 . EQ . IVV ) THEN                               1438
1439  1439            ISI = JE( 3 , IE )                                      1439
1440  1440            ELSE                                                    1440
1441  1441            ISI = JE( 4 , IE )                                      1441
1442  1442            END IF                                                  1442
1443  1443            IS = ISI                                                1443
1444  1444  C                                                                 1444
1445  1445            ILOOP = 0                                               1445
1446  1446  450       CONTINUE                                                1446
1447  1447            IDOUBL = IABS( IICOLR( IJTRIG ) )                       1447
1448  1448  C                                                                 1448
1449  1449            ITRIG = ITRIG + 1                                       1449
1450  1450            ISCRSS( ITRIG ) = IS                                    1450
1451  1451            IETRIG = IETRIG + 1                                     1451
1452  1452            IECRSS( IETRIG ) = IE                                   1452
1453  1453  C                                                                 1453
1454  1454            IF(                                                     1454
1455  1455     .          HYDFLX( IS , 4 ) . GT . FLUXPP . OR .               1455
1456  1456     .          HYDFLX( IS , 2 ) . GT . FLUXUU . OR .               1456
1457  1457     .          HYDFLX( IS , 1 ) . GT . FLUXRR . OR .               1457
1458  1458     .          KSDELT( IS ) . GT . NIDUMP . OR .                   1458
1459  1459     .          XS( 3 , IS ) . GT . AREVGG ) THEN                   1459
1460  1460            INDCTR = 3                                              1460
1461  1461            RETURN                                                  1461
1462  1462            END IF                                                  1462
1463  1463  C                                                                 1463
1464  1464            DO 460 IR = 1 , 3                                       1464
1465  1465            JR = MOD( IR , 3 ) + 1                                  1465
1466  1466            IEA = IABS( JS( JR + 3 , IS ) )                         1466
1467  1467            IF( IEA . EQ . IE ) THEN                                1467
1468  1468            IIR = MOD( JR , 3 ) + 4                                 1468
1469  1469            IEI = JS( IIR , IS )                                    1469
1470  1470            IEIB = IABS( IEI )                                      1470
1471  1471            XEIEB = XE( 1 , IEIB )                                  1471
1472  1472            XYLNGT = XYLNGT + XEIEB                                 1472
1473  1473            IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB                1473
1474  1474            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB                1474
1475  1475            ILOOP = ILOOP + 1                                       1475
1476  1476            IF( ILOOP . EQ . 1 . AND . IDOUBL . EQ . IEIB ) THEN    1476
1477  1477            JLOOP = 3                                               1477
1478  1478            IETRIG = IETRIG + 1                                     1478
1479  1479            IECRSS( IETRIG ) = IDOUBL                               1479
```

```
1480  1480            IJTRIG = IJTRIG - 1
1481  1481            IF( IEI . GT . 0 ) THEN
1482  1482            JKVV = JE( 1 , IEIB )
1483  1483            ELSE
1484  1484            JKVV = JE( 2 , IEIB )
1485  1485            END IF
1486  1486            JVDELT = JVDELT + 1
1487  1487            IVDELT( JVDELT ) = JKVV
1488  1488            ILOOP = 0
1489  1489            ELSE
1490  1490            IJTRIG = IJTRIG + 1
1491  1491            IICOLR( IJTRIG ) = IEI
1492  1492            END IF
1493  1493            JJR = MOD( JR + 1 , 3 ) + 4
1494  1494            IER = IABS( JS( JJR , IS ) )
1495  1495  C
1496  1496            IV1 = JE( 1 , IER )
1497  1497            IF( IV1 . EQ . IVV ) THEN
1498  1498            ISR = JE( 3 , IER )
1499  1499            ELSE
1500  1500            ISR = JE( 4 , IER )
1501  1501            END IF
1502  1502            END IF
1503  1503  C
1504  1504  460       CONTINUE
1505  1505  C
1506  1506            IF( IER . NE . IKKE3 ) THEN
1507  1507            IS = ISR
1508  1508            IE = IER
1509  1509            GO TO 450
1510  1510            END IF
1511  1511  C
1512  1512            IETRIG = IETRIG + 1
1513  1513            IECRSS( IETRIG ) = IKKE3
1514  1514            IETRIG = IETRIG + 1
1515  1515            IECRSS( IETRIG ) = IKKE2
1516  1516  C
1517  1517            IJTRIG = IJTRIG - 1
1518  1518  C
1519  1519  C    THIRD LOOP SUROUNDING KKV3 IS DONE, FOURTH LOOP OVER KKV1 START .
1520  1520  C
1521  1521            IVV = KKV1
1522  1522            IE = IABS( IICOLR( IJTRIG + 1 ) )
1523  1523            IF( JE( 5 , IE ) . NE . 0 ) THEN
1524  1524            IER = IE
1525  1525            GO TO 470
1526  1526            END IF
1527  1527            IV1 = JE( 1 , IE )
1528  1528            IF( IV1 . EQ . IVV ) THEN
1529  1529            ISI = JE( 3 , IE )
1530  1530            ELSE
1531  1531            ISI = JE( 4 , IE )
1532  1532            END IF
1533  1533            IS = ISI
1534  1534            ISI = 0
1535  1535  C
1536  1536            ILOOP = 0
1537  1537  480       CONTINUE
1538  1538            JDOUBL = IABS( IICOLR( IJTRIG ) )
1539  1539  C
1540  1540            ITRIG = ITRIG + 1
1541  1541            ISCRSS( ITRIG ) = IS
1542  1542            IETRIG = IETRIG + 1
1543  1543            IECRSS( IETRIG ) = IE
1544  1544  C
1545  1545            IF(
1546  1546           .       HYDFLX( IS , 4 ) . GT . FLUXPP . OR .
1547  1547           .       HYDFLX( IS , 2 ) . GT . FLUXUU . OR .
1548  1548           .       HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
1549  1549           .       KSDELT( IS ) . GT . NIDUMP . OR .
1550  1550           .       XS( 3 , IS ) . GT . AREVGG ) THEN
1551  1551            INDCTR = 3
1552  1552            RETURN
1553  1553            END IF
```

```
1554  1554  C
1555  1555        DO 490 IR = 1 , 3
1556  1556        JR = MOD( IR , 3 ) + 1
1557  1557        IEA = IABS( JS( JR + 3 , IS ) )
1558  1558        IF( IEA . EQ . IE ) THEN
1559  1559        IIR = MOD( JR , 3 ) + 4
1560  1560        IEI = JS( IIR , IS )
1561  1561        IEIB = IABS( IEI )
1562  1562        XEIEB = XE( 1 , IEIB )
1563  1563        XYLNGT = XYLNGT + XEIEB
1564  1564        IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
1565  1565        IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
1566  1566        ILOOP = ILOOP + 1
1567  1567        IF( ILOOP . EQ . 1 . AND . JDOUBL . EQ . IEIB ) THEN
1568  1568        JLOOP = 4
1569  1569        IETRIG = IETRIG + 1
1570  1570        IECRSS( IETRIG ) = JDOUBL
1571  1571        IJTRIG = IJTRIG - 1
1572  1572        IF( IEI . GT . 0 ) THEN
1573  1573        JKVV = JE( 1 , IEIB )
1574  1574        ELSE
1575  1575        JKVV = JE( 2 , IEIB )
1576  1576        END IF
1577  1577        JVDELT = JVDELT + 1
1578  1578        IVDELT( JVDELT ) = JKVV
1579  1579        ILOOP = 0
1580  1580        ELSE
1581  1581        IJTRIG = IJTRIG + 1
1582  1582        IICOLR( IJTRIG ) = IEI
1583  1583        END IF
1584  1584        JJR = MOD( JR + 1 , 3 ) + 4
1585  1585        IER = IABS( JS( JJR , IS ) )
1586  1586  C
1587  1587        IV1 = JE( 1 , IER )
1588  1588        IF( IV1 . EQ . IVV ) THEN
1589  1589        ISR = JE( 3 , IER )
1590  1590        ELSE
1591  1591        ISR = JE( 4 , IER )
1592  1592        END IF
1593  1593        END IF
1594  1594  C
1595  1595  490   CONTINUE
1596  1596  C
1597  1597        IF( ISR . NE . ISI ) THEN
1598  1598        IS = ISR
1599  1599        IE = IER
1600  1600        GO TO 480
1601  1601        END IF
1602  1602  C
1603  1603  470   CONTINUE
1604  1604  C
1605  1605        IETRIG = IETRIG + 1
1606  1606        IECRSS( IETRIG ) = IER
1607  1607  C
1608  1608        ITYPE = JE( 5 , IER )
1609  1609  C
1610  1610        XEIEB = XE( 1 , IER )
1611  1611        XEIEB = XXYYIB + XEIEB
1612  1612        XYLNGT = XYLNGT + XEIEB
1613  1613        IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
1614  1614        IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
1615  1615  C
1616  1616        INDCTR = 2
1617  1617  C      IF( XYLONG / XYSHRT . GT . 10. . AND . JLOOP . EQ . 0 ) RETURN
1618  1618  C
1619  1619        JE( 2 , IEJKK ) = IVIN2
1620  1620  C
1621  1621        IV1 = IVIN1
1622  1622        IE1 = IICOLR( IJTRIG )
1623  1623        IF( IE1 . GT . 0 ) THEN
1624  1624        IV2 = JE( 2 , IE1 )
1625  1625        ELSE
1626  1626        IV2 = JE( 1 , - IE1 )
1627  1627        END IF
```

```
1628  1628  C
1629  1629              NEC = IECRSS( IETRIG )
1630  1630              IETRIG = IETRIG - 1
1631  1631  C
1632  1632              JV( 2 , IV2 ) = - NEC
1633  1633              JE( 1 , NEC ) = IV2
1634  1634              JE( 2 , NEC ) = IV1
1635  1635              JE( 4 , NEC ) = 0
1636  1636              JE( 5 , NEC ) = ITYPE
1637  1637  C
1638  1638              IJTRIG = IJTRIG + 1
1639  1639              IICOLR( IJTRIG ) = NEC
1640  1640  C
1641  1641              ELSE IF( IKKE . EQ . 4 ) THEN
1642  1642                print*,'ikke=4',ksd,ikke
1643  1643  C
1644  1644  C     BEGINING THE DELETION PROCESS IF KSD HAS AN EDGE ON THE BOUNDARY
1645  1645  C     AND THE THIRD VERTEX IS OLSO ON THE BOUNDARY.
1646  1646  C     THE FIRST LOOP IS AROUND VERTEX KKV2 .
1647  1647  C
1648  1648                IVV = KKV2
1649  1649                IE = IEIN1
1650  1650                XXYYIB = XE( 1 , IE ) + XE( 1 , IKKE1 )
1651  1651                IV1 = JE( 1 , IE )
1652  1652                IVIN1 = JE( 2 , IE )
1653  1653                IF( IV1 . EQ . IVV ) THEN
1654  1654                ISI = JE( 3 , IE )
1655  1655                ELSE
1656  1656                ISI = JE( 4 , IE )
1657  1657                END IF
1658  1658                IS = ISI
1659  1659  C
1660  1660  500           CONTINUE
1661  1661  C
1662  1662                ITRIG = ITRIG + 1
1663  1663                ISCRSS( ITRIG ) = IS
1664  1664                IETRIG = IETRIG + 1
1665  1665                IECRSS( IETRIG ) = IE
1666  1666  C
1667  1667                IF(
1668  1668           .        HYDFLX( IS , 4 ) . GT . FLUXPP . OR .
1669  1669           .        HYDFLX( IS , 2 ) . GT . FLUXUU . OR .
1670  1670           .        HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
1671  1671           .        KSDELT( IS ) . GT . NIDUMP . OR .
1672  1672           .        XS( 3 , IS ) . GT . AREVGG ) THEN
1673  1673                INDCTR = 3
1674  1674                RETURN
1675  1675                END IF
1676  1676  C
1677  1677                DO 510 IR = 1 , 3
1678  1678                JR = MOD( IR , 3 ) + 1
1679  1679                IEA = IABS( JS( JR + 3 , IS ) )
1680  1680                IF( IEA . EQ . IE ) THEN
1681  1681                IIR = MOD( JR , 3 ) + 4
1682  1682                IEI = JS( IIR , IS )
1683  1683                IEIB = IABS( IEI )
1684  1684                XEIEB = XE( 1 , IEIB )
1685  1685                XYLNGT = XYLNGT + XEIEB
1686  1686                IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
1687  1687                IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
1688  1688                IJTRIG = IJTRIG + 1
1689  1689                IICOLR( IJTRIG ) = IEI
1690  1690                JJR = MOD( JR + 1 , 3 ) + 4
1691  1691                IER = IABS( JS( JJR , IS ) )
1692  1692  C
1693  1693                IV1 = JE( 1 , IER )
1694  1694                IF( IV1 . EQ . IVV ) THEN
1695  1695                ISR = JE( 3 , IER )
1696  1696                ELSE
1697  1697                ISR = JE( 4 , IER )
1698  1698                END IF
1699  1699                END IF
1700  1700  C
1701  1701  510           CONTINUE
```

```
1702  1702  C
1703  1703            IF( IER . NE . IKKE1 ) THEN
1704  1704            IS = ISR
1705  1705            IE = IER
1706  1706            GO TO 500
1707  1707            END IF
1708  1708  C
1709  1709  C     FIRST LOOP SUROUNDING KKV2 IS DONE, SECOND LOOP OVER KKV3 START .
1710  1710  C
1711  1711            IJTRIG = IJTRIG - 1
1712  1712  520       CONTINUE
1713  1713  C
1714  1714            IEJK = IICOLR( IJTRIG )
1715  1715            IF( IEJK . GT . 0 ) THEN
1716  1716            IVIEJK = JE( 1 , IEJK )
1717  1717            IJEJK5 = JE( 5 , IEJK )
1718  1718            ELSE
1719  1719            IVIEJK = JE( 2 , -IEJK )
1720  1720            IJEJK5 = JE( 5 , -IEJK )
1721  1721            END IF
1722  1722  C
1723  1723            IF( IJEJK5 . EQ . 0 ) THEN
1724  1724  C
1725  1725  C     INTERMEDIATE LOOP START .
1726  1726  C
1727  1727            JLOOP = 1
1728  1728            IEJKI = IABS( IICOLR( IJTRIG - 1 ) )
1729  1729            IEJK2 = IABS( IEJK )
1730  1730            IETRIG = IETRIG + 1
1731  1731            IECRSS( IETRIG ) = IEJK2
1732  1732            IJTRIG = IJTRIG - 2
1733  1733            IVV = IVIEJK
1734  1734            JVDELT = JVDELT + 1
1735  1735            IVDELT( JVDELT ) = IVV
1736  1736            IE = IEJKI
1737  1737            IV1 = JE( 1 , IE )
1738  1738            IF( IV1 . EQ . IVV ) THEN
1739  1739            ISI = JE( 3 , IE )
1740  1740            ELSE
1741  1741            ISI = JE( 4 , IE )
1742  1742            END IF
1743  1743            IS = ISI
1744  1744            IET = IEJK2
1745  1745  C
1746  1746  530       CONTINUE
1747  1747  C
1748  1748            ITRIG = ITRIG + 1
1749  1749            ISCRSS( ITRIG ) = IS
1750  1750  C
1751  1751            IETRIG = IETRIG + 1
1752  1752            IECRSS( IETRIG ) = IE
1753  1753  C
1754  1754            IF(
1755  1755      .        HYDFLX( IS , 4 ) . GT . FLUXPP . OR .
1756  1756      .        HYDFLX( IS , 2 ) . GT . FLUXUU . OR .
1757  1757      .        HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
1758  1758      .        KSDFLT( IS ) . GT . NIDUMP . OR .
1759  1759      .        XS( 3 , IS ) . GT . AREVGG ) THEN
1760  1760            INDCTR = 3
1761  1761            RETURN
1762  1762            END IF
1763  1763  C
1764  1764            DO 540 IR = 1 , 3
1765  1765            JR = MOD( IR , 3 ) + 1
1766  1766            IEA = IABS( JS( JR + 3 , IS ) )
1767  1767            IF( IEA . EQ . IE ) THEN
1768  1768            IIR = MOD( JR , 3 ) + 4
1769  1769            IEI = JS( IIR , IS )
1770  1770            IEIB = IABS( IEI )
1771  1771            XEIEB = XE( 1 , IEIB )
1772  1772            XYLNGT = XYLNGT + XEIEB
1773  1773            IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
1774  1774            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
1775  1775            IIKK = IABS( IICOLR( IJTRIG ) )
```

```
1776  1776            IF( IIKK . EQ . IEIB ) THEN
1777  1777            JLOOP = 2
1778  1778            IETRIG = IETRIG + 1
1779  1779            IECRSS( IETRIG ) = IEIB
1780  1780            IJTRIG = IJTRIG - 1
1781  1781            IF( IEI . GT . 0 ) THEN
1782  1782            JKVV = JE( 1 , IEIB )
1783  1783            ELSE
1784  1784            JKVV = JE( 2 , IEIB )
1785  1785            END IF
1786  1786            JVDELT = JVDELT + 1
1787  1787            IVDELT( JVDELT ) = JKVV
1788  1788            ELSE
1789  1789            IJTRIG = IJTRIG + 1
1790  1790            IICOLR( IJTRIG ) = IEI
1791  1791            END IF
1792  1792            JJR = MOD( JR + 1 , 3 ) + 4
1793  1793            IER = IABS( JS( JJR , IS ) )
1794  1794  C
1795  1795            IV1 = JE( 1 , IER )
1796  1796            IF( IV1 . EQ . IVV ) THEN
1797  1797            ISR = JE( 3 , IER )
1798  1798            ELSE
1799  1799            ISR = JE( 4 , IER )
1800  1800            END IF
1801  1801            END IF
1802  1802  C
1803  1803  540       CONTINUE
1804  1804  C
1805  1805            IF( IER . NE . IET ) THEN
1806  1806            IS = ISR
1807  1807            IE = IER
1808  1808            GO TO 530
1809  1809            END IF
1810  1810  C
1811  1811            GO TO 520
1812  1812            END IF
1813  1813  C
1814  1814  C    INTERMEDIATE LOOP IS DONE, SECOND LOOP OVER KKV3 START .
1815  1815  C
1816  1816            IVV = KKV3
1817  1817            IE = IEIN2
1818  1818            IVIN2 = JE( 2 , IE )
1819  1819            IEJKK = IICOLR( IJTRIG )
1820  1820            IV1 = JE( 1 , IE )
1821  1821            IF( IV1 . EQ . IVV ) THEN
1822  1822            ISI = JE( 3 , IE )
1823  1823            ELSE
1824  1824            ISI = JE( 4 , IE )
1825  1825            END IF
1826  1826            IS = ISI
1827  1827  C
1828  1828  550       CONTINUE
1829  1829  C
1830  1830            ITRIG = ITRIG + 1
1831  1831            ISCRSS( ITRIG ) = IS
1832  1832  C
1833  1833            IETRIG = IETRIG + 1
1834  1834            IECRSS( IETRIG ) = IE
1835  1835  C
1836  1836            IF(
1837  1837       .        HYDFLX( IS , 4 ) . GT . FLUXPP . OR .
1838  1838       .        HYDFLX( IS , 2 ) . GT . FLUXUU . OR .
1839  1839       .        HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
1840  1840       .        KSDELT( IS ) . GT . NIDUMP . OR .
1841  1841       .        XS( 3 , IS ) . GT . AREVGG ) THEN
1842  1842            INDCTR = 3
1843  1843            RETURN
1844  1844            END IF
1845  1845  C
1846  1846            DO 560 IR = 1 , 3
1847  1847            JR = MOD( IR , 3 ) + 1
1848  1848            IEA = IABS( JS( JR + 3 , IS ) )
1849  1849            IF( IEA . EQ . IE ) THEN
```

```
1850  1850            IIR = MOD( JR , 3 ) + 4                                  1850
1851  1851            IEI = JS( IIR , IS )                                     1851
1852  1852            IEIB = IABS( IEI )                                       1852
1853  1853            XEIEB = XE( 1 , IEIB )                                   1853
1854  1854            XYLNGT = XYLNGT + XEIEB                                  1854
1855  1855            IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB                 1855
1856  1856            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB                 1856
1857  1857            IJTRIG = IJTRIG + 1                                      1857
1858  1858            IICOLR( IJTRIG ) = IEI                                   1858
1859  1859            JJR = MOD( JR + 1 , 3 ) + 4                              1859
1860  1860            IER = IABS( JS( JJR , IS ) )                             1860
1861  1861  C                                                                  1861
1862  1862            IV1 = JE( 1 , IER )                                      1862
1863  1863            IF( IV1 . EQ . IVV ) THEN                                1863
1864  1864            ISR = JE( 3 , IER )                                      1864
1865  1865            ELSE                                                     1865
1866  1866            ISR = JE( 4 , IER )                                      1866
1867  1867            END IF                                                   1867
1868  1868            END IF                                                   1868
1869  1869  C                                                                  1869
1870  1870  560       CONTINUE                                                 1870
1871  1871  C                                                                  1871
1872  1872            IF( IER . NE . IKKE3 ) THEN                              1872
1873  1873            IS = ISR                                                 1873
1874  1874            IE = IER                                                 1874
1875  1875            GO TO 550                                                1875
1876  1876            END IF                                                   1876
1877  1877  C                                                                  1877
1878  1878            IJTRIG = IJTRIG - 1                                      1878
1879  1879            IETRIG = IETRIG + 1                                      1879
1880  1880            IECRSS( IETRIG ) = IKKE3                                 1880
1881  1881            IETRIG = IETRIG + 1                                      1881
1882  1882            IECRSS( IETRIG ) = IKKE1                                 1882
1883  1883  C                                                                  1883
1884  1884  C    SECOND LOOP SUROUNDING KKV3 IS DONE, THIRD LOOP OVER KKV1 START .  1884
1885  1885  C                                                                  1885
1886  1886            IVV = KKV1                                               1886
1887  1887            IE = IABS( IICOLR( IJTRIG + 1 ) )                        1887
1888  1888            IF( JE( 5 , IE ) . NE . 0 ) THEN                         1888
1889  1889            IER = IE                                                 1889
1890  1890            GO TO 570                                                1890
1891  1891            END IF                                                   1891
1892  1892            IV1 = JE( 1 , IE )                                       1892
1893  1893            IF( IV1 . EQ . IVV ) THEN                                1893
1894  1894            ISI = JE( 3 , IE )                                       1894
1895  1895            ELSE                                                     1895
1896  1896            ISI = JE( 4 , IE )                                       1896
1897  1897            END IF                                                   1897
1898  1898            IS = ISI                                                 1898
1899  1899            ISI = 0                                                  1899
1900  1900  C                                                                  1900
1901  1901  580       CONTINUE                                                 1901
1902  1902  C                                                                  1902
1903  1903            ITRIG = ITRIG + 1                                        1903
1904  1904            ISCRSS( ITRIG ) = IS                                     1904
1905  1905            IETRIG = IETRIG + 1                                      1905
1906  1906            IECRSS( IETRIG ) = IE                                    1906
1907  1907  C                                                                  1907
1908  1908            IF(                                                      1908
1909  1909     .          HYDFLX( IS , 4 ) . GT . FLUXPP . OR .                 1909
1910  1910     .          HYDFLX( IS , 2 ) . GT . FLUXUU . OR .                 1910
1911  1911     .          HYDFLX( IS , 1 ) . GT . FLUXRR . OR .                 1911
1912  1912     .          KSDELT( IS ) . GT . NIDUMP . OR .                     1912
1913  1913     .          XS( 3 , IS ) . GT . AREVGG ) THEN                     1913
1914  1914            INDCTR = 3                                               1914
1915  1915            RETURN                                                   1915
1916  1916            END IF                                                   1916
1917  1917  C                                                                  1917
1918  1918            DO 590 IR = 1 , 3                                        1918
1919  1919            JR = MOD( IR , 3 ) + 1                                   1919
1920  1920            IEA = IABS( JS( JR + 3 , IS ) )                          1920
1921  1921            IF( IEA . EQ . IE ) THEN                                 1921
1922  1922            IIR = MOD( JR , 3 ) + 4                                  1922
1923  1923            IEI = JS( IIR , IS )                                     1923
```

```
1924  1924            IEIB = IABS( IEI )                                        1924
1925  1925            XEIEB = XE( 1 , IEIB )                                    1925
1926  1926            XYLNGT = XYLNGT + XEIEB                                   1926
1927  1927            IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB                  1927
1928  1928            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB                  1928
1929  1929            IJTRIG = IJTRIG + 1                                       1929
1930  1930            IICOLR( IJTRIG ) = IEI                                    1930
1931  1931            JJR = MOD( JR + 1 , 3 ) + 4                               1931
1932  1932            IER = IABS( JS( JJR , IS ) )                              1932
1933  1933  C                                                                   1933
1934  1934            IV1 = JE( 1 , IER )                                       1934
1935  1935            IF( IV1 . EQ . IVV ) THEN                                 1935
1936  1936            ISR = JE( 3 , IER )                                       1936
1937  1937            ELSE                                                      1937
1938  1938            ISR = JE( 4 , IER )                                       1938
1939  1939            END IF                                                    1939
1940  1940            END IF                                                    1940
1941  1941  C                                                                   1941
1942  1942  590       CONTINUE                                                  1942
1943  1943  C                                                                   1943
1944  1944            IF( ISR . NE . ISI ) THEN                                 1944
1945  1945            IS = ISR                                                  1945
1946  1946            IE = IER                                                  1946
1947  1947            GO TO 580                                                 1947
1948  1948            END IF                                                    1948
1949  1949  C                                                                   1949
1950  1950  570       CONTINUE                                                  1950
1951  1951  C                                                                   1951
1952  1952            IETRIG = IETRIG + 1                                       1952
1953  1953            IECRSS( IETRIG ) = IER                                    1953
1954  1954  C                                                                   1954
1955  1955            ITYPE = JE( 5 , IER )                                     1955
1956  1956  C                                                                   1956
1957  1957            XEIEB = XE( 1 , IER )                                     1957
1958  1958            XEIEB = XXYYIB + XEIEB                                    1958
1959  1959            XYLNGT = XYLNGT + XEIEB                                   1959
1960  1960            IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB                  1960
1961  1961            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB                  1961
1962  1962  C                                                                   1962
1963  1963            INDCTR = 2                                                1963
1964  1964  C          IF( XYLONG / XYSHRT . GT . 10. . AND . JLOOP . EQ . 0 ) RETURN 1964
1965  1965  C                                                                   1965
1966  1966            JE( 2 , IEJKK ) = IVIN2                                   1966
1967  1967  C                                                                   1967
1968  1968            IV1 = IVIN1                                               1968
1969  1969            IE1 = IICOLR( IJTRIG )                                    1969
1970  1970            IF( IE1 . GT . 0 ) THEN                                   1970
1971  1971            IV2 = JE( 2 , IE1 )                                       1971
1972  1972            ELSE                                                      1972
1973  1973            IV2 = JE( 1 , - IE1 )                                     1973
1974  1974            END IF                                                    1974
1975  1975  C                                                                   1975
1976  1976            NEC = IECRSS( IETRIG )                                    1976
1977  1977            IETRIG = IETRIG - 1                                       1977
1978  1978  C                                                                   1978
1979  1979            JV( 2 , IV2 ) = - NEC                                     1979
1980  1980            JE( 1 , NEC ) = IV2                                       1980
1981  1981            JE( 2 , NEC ) = IV1                                       1981
1982  1982            JE( 4 , NEC ) = 0                                         1982
1983  1983            JE( 5 , NEC ) = ITYPE                                     1983
1984  1984  C                                                                   1984
1985  1985            IJTRIG = IJTRIG + 1                                       1985
1986  1986            IICOLR( IJTRIG ) = NEC                                    1986
1987  1987  C                                                                   1987
1988  1988            ELSE IF( IKKE . EQ . 5 ) THEN                             1988
1989  1989              print*,'ikke=5',ksd,ikke                                1989
1990  1990  C                                                                   1990
1991  1991  C    BEGINING THE DELETION PROCESS IF KSD HAS AN EDGE ON THE BOUNDARY 1991
1992  1992  C    AND THE THIRD VERTEX IS OLSO ON THE BOUNDARY.                   1992
1993  1993  C    THE FIRST LOOP IS AROUND VERTEX KKV3 .                          1993
1994  1994  C                                                                   1994
1995  1995            IVV = KKV3                                                1995
1996  1996            IE = IEIN2                                                1996
1997  1997            XXYYIB = XE( 1 , IE )                                     1997
```

```
1998 1998            IV1 = JE( 1 , IE )
1999 1999            IVIN1 = JE( 2 , IE )
2000 2000            IF( IV1 . EQ . IVV ) THEN
2001 2001            ISI = JE( 3 , IE )
2002 2002            ELSE
2003 2003            ISI = JE( 4 , IE )
2004 2004            END IF
2005 2005            IS = ISI
2006 2006   C
2007 2007   600      CONTINUE
2008 2008   C
2009 2009            ITRIG = ITRIG + 1
2010 2010            ISCRSS( ITRIG ) = IS
2011 2011            IETRIG = IETRIG + 1
2012 2012            IECRSS( IETRIG ) = IE
2013 2013   C
2014 2014            IF(
2015 2015     .         HYDFLX( IS , 4 ) . GT . FLUXPP . OR .
2016 2016     .         HYDFLX( IS , 2 ) . GT . FLUXUU . OR .
2017 2017     .         HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
2018 2018     .         KSDELT( IS ) . GT . NIDUMP . OR .
2019 2019     .         XS( 3 , IS ) . GT . AREVGG ) THEN
2020 2020            INDCTR = 3
2021 2021            RETURN
2022 2022            END IF
2023 2023   C
2024 2024            DO 610 IR = 1 , 3
2025 2025            JR = MOD( IR , 3 ) + 1
2026 2026            IEA = IABS( JS( JR + 3 , IS ) )
2027 2027            IF( IEA . EQ . IE ) THEN
2028 2028            IIR = MOD( JR , 3 ) + 4
2029 2029            IEI = JS( IIR , IS )
2030 2030            IEIB = IABS( IEI )
2031 2031            XEIEB = XE( 1 , IEIB )
2032 2032            XYLNGT = XYLNGT + XEIEB
2033 2033            IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
2034 2034            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
2035 2035            IJTRIG = IJTRIG + 1
2036 2036            IICOLR( IJTRIG ) = IEI
2037 2037            JJR = MOD( JR + 1 , 3 ) + 4
2038 2038            IER = IABS( JS( JJR , IS ) )
2039 2039   C
2040 2040            IV1 = JE( 1 , IER )
2041 2041            IF( IV1 . EQ . IVV ) THEN
2042 2042            ISR = JE( 3 , IER )
2043 2043            ELSE
2044 2044            ISR = JE( 4 , IER )
2045 2045            END IF
2046 2046            END IF
2047 2047   C
2048 2048   610      CONTINUE
2049 2049   C
2050 2050            IF( IER . NE . IKKE2 ) THEN
2051 2051            IS = ISR
2052 2052            IE = IER
2053 2053            GO TO 600
2054 2054            END IF
2055 2055   C
2056 205?   C    FIRST LOOP SUROUNDING KKV3 IS DONE, SECOND LOOP OVER KKV2 START .
2057 20?    C
2058 2?              IJTRIG = IJTRIG - 1
2059 ?      620      CONTINUE
2060    J   C
2061  ?61            IEJK = IICOLR( IJTRIG )
2062  ?062           IF( IEJK . GT . 0 ) THEN
2063  ?063           IVIEJK = JE( 1 , IEJK )
2064 2064            IJEJK5 = JE( 5 , IEJK )
2065 2065            ELSE
2066 2066            IVIEJK = JE( 2 , -IEJK )
2067 2067            IJEJK5 = JE( 5 , -IEJK )
2068 2068            END IF
2069 2069   C
2070 2070            IF( IJEJK5 . EQ . 0 ) THEN
2071 2071   C
```

```
2072    2072  C     INTERMEDIATE LOOP START .                                  2072
2073    2073  C                                                                2073
2074    2074              JLOOP = 1                                            2074
2075    2075              IEJKI = IABS( IICOLR( IJTRIG - 1 ) )                 2075
2076    2076              IEJK2 = IABS( IEJK )                                 2076
2077    2077              IETRIG = IETRIG + 1                                  2077
2078    2078              IECRSS( IETRIG ) = IEJK2                             2078
2079    2079              IJTRIG = IJTRIG - 2                                  2079
2080    2080              IVV = IVIEJK                                         2080
2081    2081              JVDELT = JVDELT + 1                                  2081
2082    2082              IVDELT( JVDELT ) = IVV                               2082
2083    2083              IE = IEJKI                                           2083
2084    2084              IV1 = JE( 1 , IE )                                   2084
2085    2085              IF( IV1 . EQ  IVV ) THEN                             2085
2086    2086              ISI = JE( 3 , IE )                                   2086
2087    2087              ELSE                                                 2087
2088    2088              ISI = JE( 4 , IE )                                   2088
2089    2089              END IF                                               2089
2090    2090              IS = ISI                                             2090
2091    2091              IET = IEJK2                                          2091
2092    2092  C                                                                2092
2093    2093  630         CONTINUE                                             2093
2094    2094  C                                                                2094
2095    2095              ITRIG = ITRIG + 1                                    2095
2096    2096              ISCRSS( ITRIG ) = IS                                 2096
2097    2097  C                                                                2097
2098    2098              IETRIG = IETRIG + 1                                  2098
2099    2099              IECRSS( IETRIG ) = IE                                2099
2100    2100  C                                                                2100
2101    2101              IF(                                                  2101
2102    2102         .       HYDFLX( IS , 4 ) . GT . FLUXPP . OR .             2102
2103    2103         .       HYDFLX( IS , 2 ) . GT . FLUXUU . OR .             2103
2104    2104         .       HYDFLX( IS , 1 ) . GT . FLUXRR . OR .             2104
2105    2105         .       KSDELT( IS ) . GT . NIDUMP . OR .                 2105
2106    2106         .       XS( 3 , IS ) . GT . AREVGG ) THEN                 2106
2107    2107              INDCTR = 3                                           2107
2108    2108              RETURN                                               2108
2109    2109              END IF                                               2109
2110    2110  C                                                                2110
2111    2111              DO 640 IR = 1 , 3                                    2111
2112    2112              JR = MOD( IR , 3 ) + 1                               2112
2113    2113              IEA = IABS( JS( JR + 3 , IS ) )                      2113
2114    2114              IF( IEA . EQ . IE ) THEN                             2114
2115    2115              IIR = MOD( JR , 3 ) + 4                              2115
2116    2116              IEI = JS( IIR , IS )                                 2116
2117    2117              IEIB = IABS( IEI )                                   2117
2118    2118              XEIEB = XE( 1 , IEIB )                               2118
2119    2119              XYLNGT = XYLNGT + XEIEB                              2119
2120    2120              IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB             2120
2121    2121              IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB             2121
2122    2122              IIKK = IABS( IICOLR( IJTRIG ) )                      2122
2123    2123              IF( IIKK . EQ . IEIB ) THEN                          2123
2124    2124              JLOOP = 2                                            2124
2125    2125              IETRIG = IETRIG + 1                                  2125
2126    2126              IECRSS( IETRIG ) = IEIB                              2126
2127    2127              IJTRIG = IJTRIG - 1                                  2127
2128    2128              IF( IEI . GT . 0 ) THEN                              2128
2129    2129              JKVV = JE( 1 , IEIB )                                2129
2130    2130              ELSE                                                 2130
2131    2131              JKVV = JE( 2 , IEIB )                                2131
2132    2132              END IF                                               2132
2133    2133              JVDELT = JVDELT + 1                                  2133
2134    2134              IVDELT( JVDELT ) = JKVV                              2134
2135    2135              ELSE                                                 2135
2136    2136              IJTRIG = IJTRIG + 1                                  2136
2137    2137              IICOLR( IJTRIG ) = IEI                               2137
2138    2138              END IF                                               2138
2139    2139              JJR = MOD( JR + 1 , 3 ) + 4                          2139
2140    2140              IER = IABS( JS( JJR , IS ) )                         2140
2141    2141  C                                                                2141
2142    2142              IV1 = JE( 1 , IER )                                  2142
2143    2143              IF( IV1 . EQ . IVV ) THEN                            2143
2144    2144              ISR = JE( 3 , IER )                                  2144
2145    2145              ELSE                                                 2145
```

```
2146  2146            ISR = JE( 4 , IER )                                          2146
2147  2147            END IF                                                       2147
2148  2148            END IF                                                       2148
2149  2149  C                                                                      2149
2150  2150  640       CONTINUE                                                     2150
2151  2151  C                                                                      2151
2152  2152            IF( IER . NE . IET ) THEN                                    2152
2153  2153            IS = ISR                                                     2153
2154  2154            IE = IER                                                     2154
2155  2155            GO TO 630                                                    2155
2156  2156            END IF                                                       2156
2157  2157  C                                                                      2157
2158  2158            GO TO 620                                                    2158
2159  2159            END IF                                                       2159
2160  2160  C                                                                      2160
2161  2161  C     INTERMEDIATE LOOP IS DONE, SECOND LOOP OVER KKV2 START .         2161
2162  2162  C                                                                      2162
2163  2163            IVV = KKV2                                                   2163
2164  2164            IE = IEIN1                                                   2164
2165  2165            XXYYIC = XE( 1 , IE ) + XE( 1 , IKKE1 ) + XE( 1 , IEIB )     2165
2166  2166            XYLNGT = XYLNGT + XXYYIC - XE( 1 , IEIB )                    2166
2167  2167            IF( XYLONG . LT . XXYYIC ) XYLONG = XXYYIC                   2167
2168  2168            IF( XYSHRT . GT . XXYYIC ) XYSHRT = XXYYIC                   2168
2169  2169            IVIN2 = JE( 2 , IE )                                         2169
2170  2170            IEJKK = IICOLR( IJTRIG )                                     2170
2171  2171            IV1 = JE( 1 , IE )                                           2171
2172  2172            IF( IV1 . EQ . IVV ) THEN                                    2172
2173  2173            ISI = JE( 3 , IE )                                           2173
2174  2174            ELSE                                                         2174
2175  2175            ISI = JE( 4 , IE )                                           2175
2176  2176            END IF                                                       2176
2177  2177            IS = ISI                                                     2177
2178  2178  C                                                                      2178
2179  2179  650       CONTINUE                                                     2179
2180  2180  C                                                                      2180
2181  2181            ITRIG = ITRIG + 1                                            2181
2182  2182            ISCRSS( ITRIG ) = IS                                         2182
2183  2183  C                                                                      2183
2184  2184            IETRIG = IETRIG + 1                                          2184
2185  2185            IECRSS( IETRIG ) = IE                                        2185
2186  2186  C                                                                      2186
2187  2187            IF(                                                          2187
2188  2188           .    HYDFLX( IS , 4 ) . GT . FLUXPP . OR .                    2188
2189  2189           .    HYDFLX( IS , 2 ) . GT . FLUXUU . OR .                    2189
2190  2190           .    HYDFLX( IS , 1 ) . GT . FLUXRR . OR .                    2190
2191  2191           .    KSDELT( IS ) . GT . NIDUMP . OR .                        2191
2192  2192           .    XS( 3 , IS ) . GT . AREVGG ) THEN                        2192
2193  2193            INDCTR = 3                                                   2193
2194  2194            RETURN                                                       2194
2195  2195            END IF                                                       2195
2196  2196  C                                                                      2196
2197  2197            DO 660 IR = 1 , 3                                            2197
2198  2198            JR = MOD( IR , 3 ) + 1                                       2198
2199  2199            IEA = IABS( JS( JR + 3 , IS ) )                              2199
2200  2200            IF( IEA . EQ . IE ) THEN                                     2200
2201  2201            IIR = MOD( JR , 3 ) + 4                                      2201
2202  2202            IEI = JS( IIR , IS )                                         2202
2203  2203            IEIB = IABS( IEI )                                           2203
2204  2204            XEIEB = XE( 1 , IEIB )                                       2204
2205  2205            XYLNGT = XYLNGT + XEIEB                                      2205
2206  2206            IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB                     2206
2207  2207            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB                     2207
2208  2208            IJTRIG = IJTRIG + 1                                          2208
2209  2209            IICOLR( IJTRIG ) = IEI                                       2209
2210  2210            JJR = MOD( JR + 1 , 3 ) + 4                                  2210
2211  2211            IER = IABS( JS( JJR , IS ) )                                 2211
2212  2212  C                                                                      2212
2213  2213            IV1 = JE( 1 , IER )                                          2213
2214  2214            IF( IV1 . EQ . IVV ) THEN                                    2214
2215  2215            ISR = JE( 3 , IER )                                          2215
2216  2216            ELSE                                                         2216
2217  2217            ISR = JE( 4 , IER )                                          2217
2218  2218            END IF                                                       2218
2219  2219            END IF                                                       2219
```

```
2220  2220  C
2221  2221  660       CONTINUE
2222  2222  C
2223  2223            IF( IER . NE . IKKE2 ) THEN
2224  2224            IS = ISR
2225  2225            IE = IER
2226  2226            GO TO 650
2227  2227            END IF
2228  2228  C
2229  2229            IJTRIG = IJTRIG - 1
2230  2230            IETRIG = IETRIG + 1
2231  2231            IECRSS( IETRIG ) = IKKE2
2232  2232            IETRIG = IETRIG + 1
2233  2233            IECRSS( IETRIG ) = IKKE1
2234  2234  C
2235  2235  C     SECOND LOOP SUROUNDING KKV2 IS DONE, THIRD LOOP OVER KKV3 START .
2236  2236  C
2237  2237            IVV = KKV3
2238  2238            IE = IABS( IICOLR( IJTRIG + 1 ) )
2239  2239            IF( JE( 5 , IE ) . NE . 0 ) THEN
2240  2240            IER = IE
2241  2241            GO TO 670
2242  2242            END IF
2243  2243            IV1 = JE( 1 , IE )
2244  2244            IF( IV1 . EQ . IVV ) THEN
2245  2245            ISI = JE( 3 , IE )
2246  2246            ELSE
2247  2247            ISI = JE( 4 , IE )
2248  2248            END IF
2249  2249            IS = ISI
2250  2250            ISI = 0
2251  2251  C
2252  2252  680       CONTINUE
2253  2253  C
2254  2254            ITRIG = ITRIG + 1
2255  2255            ISCRSS( ITRIG ) = IS
2256  2256            IETRIG = IETRIG + 1
2257  2257            IECRSS( IETRIG ) = IE
2258  2258  C
2259  2259            IF(
2260  2260           .    HYDFLX( IS , 4 ) . GT . FLUXPP . OR .
2261  2261           .    HYDFLX( IS , 2 ) . GT . FLUXJU . OR .
2262  2262           .    HYDFLX( IS , 1 ) . GT . FLUXRR . OR .
2263  2263           .    KSDELT( IS ) . GT . NIDUMP . OR .
2264  2264           .    XS( 3 , IS ) . GT . AREVGG ) THEN
2265  2265            INDCTR = 3
2266  2266            RETURN
2267  2267            END IF
2268  2268  C
2269  2269            DO 690 IR = 1 , 3
2270  2270            JR = MOD( IR , 3 ) + 1
2271  2271            IEA = IABS( JS( JR + 3 , IS ) )
2272  2272            IF( IEA . EQ . IE ) THEN
2273  2273            IIR = MOD( JR , 3 ) + 4
2274  2274            IEI = JS( IIR , IS )
2275  2275            IEIB = IABS( IEI )
2276  2276            XEIEB = XE( 1 , IEIB )
2277  2277            XYLNGT = XYLNGT + XEIEB
2278  2278            IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
2279  2279            IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
2280  2280            IJTRIG = IJTRIG + 1
2281  2281            IICOLR( IJTRIG ) = IEI
2282  2282            JJR = MOD( JR + 1 , 3 ) + 4
2283  2283            IER = IABS( JS( JJR , IS ) )
2284  2284  C
2285  2285            IV1 = JE( 1 , IER )
2286  2286            IF( IV1 . EQ . IVV ) THEN
2287  2287            ISR = JE( 3 , IER )
2288  2288            ELSE
2289  2289            ISR = JE( 4 , IER )
2290  2290            END IF
2291  2291            END IF
2292  2292  C
2293  2293  690       CONTINUE
```

```
2294  2294  C
2295  2295              IF( ISR . NE . ISI ) THEN
2296  2296              IS = ISR
2297  2297              IE = IER
2298  2298              GO TO 680
2299  2299              END IF
2300  2300  C
2301  2301  670         CONTINUE
2302  2302  C
2303  2303              IETRIG = IETRIG + 1
2304  2304              IECRSS( IETRIG ) = IER
2305  2305  C
2306  2306              ITYPE = JE( 5 , IER )
2307  2307  C
2308  2308              XEIEB = XE( 1 , IER )
2309  2309              XEIEB = XXYYIB + XEIEB
2310  2310              XYLNGT = XYLNGT + XEIEB
2311  2311              IF( XYLONG . LT . XEIEB ) XYLONG = XEIEB
2312  2312              IF( XYSHRT . GT . XEIEB ) XYSHRT = XEIEB
2313  2313  C
2314  2314              INDCTR = 2
2315  2315  C           IF( XYLONG / XYSHRT . GT . 10. . AND . JLOOP . EQ . 0 ) RETURN
2316  2316  C
2317  2317              JE( 2 , IEJKK ) = IVIN2
2318  2318  C
2319  2319              IV1 = IVIN1
2320  2320              IE1 = IICOLR( IJTRIG )
2321  2321              IF( IE1 . GT . 0 ) THEN
2322  2322              IV2 = JE( 2 , IE1 )
2323  2323              ELSE
2324  2324              IV2 = JE( 1 , - IE1 )
2325  2325              END IF
2326  2326  C
2327  2327              NEC = IECRSS( IETRIG )
2328  2328              IETRIG = IETRIG - 1
2329  2329  C
2330  2330              JV( 2 , IV2 ) = - NEC
2331  2331              JE( 1 , NEC ) = IV2
2332  2332              JE( 2 , NEC ) = IV1
2333  2333              JE( 4 , NEC ) = 0
2334  2334              JE( 5 , NEC ) = ITYPE
2335  2335  C
2336  2336              IJTRIG = IJTRIG + 1
2337  2337              IICOLR( IJTRIG ) = NEC
2338  2338  C
2339  2339              END IF
2340  2340  C
2341  2341  C     LOOP OVER TRIANGLE KSD IS DONE
2342  2342  C
2343  2343  C     ELIMINATING THE DELETED TRIANGLES FROM JSDELT ARRAY
2344  2344  C
2345  2345              LSDELT = 0
2346  2346              DO 1520 IS = 1 , ISDELT
2347  2347              JSP = JSDELT( IS )
2348  2348              ILOOP = 0
2349  2349              IF( JSP . EQ . 0 ) THEN
2350  2350              ILOOP = 1
2351  2351              ELSE
2352  2352              DO 1525 IKS = 1 , ITRIG
2353  2353              ISP = ISCRSS( IKS )
2354  2354              IF( JSP . EQ . ISP ) ILOOP = 1
2355  2355  1525        CONTINUE
2356  2356              END IF
2357  2357              IF( ILOOP . EQ . 0 ) THEN
2358  2358              LSDELT = LSDELT + 1
2359  2359              JSDELT( LSDELT ) = JSP
2360  2360              END IF
2361  2361  1520        CONTINUE
2362  2362              ISDELT = LSDELT
2363  2363  C
2364  2364              JVDELT = JVDELT + 1
2365  2365              IVDELT( JVDELT ) = KV1
2366  2366              JVDELT = JVDELT + 1
2367  2367              IVDELT( JVDELT ) = KV2
```

```
2368  2368            JVDELT = JVDELT + 1                                                    2368
2369  2369            IVDELT( JVDELT ) = KV3                                                 2369
2370  2370  C                                                                                2370
2371  2371            DO 700 IE = 1 , IJTRIG                                                 2371
2372  2372            IEM = IABS( IICOLR( IE ) )                                             2372
2373  2373            JUE( IE ) = IEM                                                        2373
2374  2374            IV1 = JE( 1 , IEM )                                                    2374
2375  2375            IV2 = JE( 2 , IEM )                                                    2375
2376  2376            IEE1 = JV( 2 , IV1 )                                                   2376
2377  2377            IEE2 = JV( 2 , IV2 )                                                   2377
2378  2378            IF( IEE1 . GT . 0 ) JV( 2 , IV1 ) = IEM                                2378
2379  2379            IF( IEE2 . GT . 0 ) JV( 2 , IV2 ) = IEM                                2379
2380  2380  700       CONTINUE                                                               2380
2381  2381  C                                                                                2381
2382  2382            JTRIG = IJTRIG                                                         2382
2383  2383            ISTOP = 0                                                              2383
2384  2384            NSINTL = 0                                                             2384
2385  2385  C                                                                                2385
2386  2386            JJTRIG = IJTRIG                                                        2386
2387  2387            DO 710 IE = 1 , JTRIG                                                  2387
2388  2388            IEM = IICOLR( IE )                                                     2388
2389  2389            IF( IEM . GT . 0 ) THEN                                                2389
2390  2390            JUV( IE ) = JE( 1 , IEM )                                              2390
2391  2391            ELSE                                                                   2391
2392  2392            JUV( IE ) = JE( 2 , - IEM )                                            2392
2393  2393            END IF                                                                 2393
2394  2394            IITRIG( IE ) = JUV( IE )                                               2394
2395  2395  710       CONTINUE                                                               2395
2396  2396  C                                                                                2396
2397  2397  720       CONTINUE                                                               2397
2398  2398  C                                                                                2398
2399  2399            JTRIGP = JTRIG + 1                                                     2399
2400  2400            DO 730 IE = 1 , JTRIG                                                  2400
2401  2401            IEM = IICOLR( IE )                                                     2401
2402  2402            IF( IEM . GT . 0 ) THEN                                                2402
2403  2403            JUV( IE ) = JE( 1 , IEM )                                              2403
2404  2404            ELSE                                                                   2404
2405  2405            JUV( IE ) = JE( 2 , - IEM )                                            2405
2406  2406            END IF                                                                 2406
2407  2407  730       CONTINUE                                                               2407
2408  2408  C                                                                                2408
2409  2409            AREMIN = 1000000.                                                      2409
2410  2410            IEMIN = 1                                                              2410
2411  2411            DO 740 IE = 1 , JTRIG                                                  2411
2412  2412  C                                                                                2412
2413  2413            IEM = MOD( IE - 1 , JTRIG ) + 1                                        2413
2414  2414            IEP = MOD( IE , JTRIG ) + 1                                            2414
2415  2415            IEI = MOD( IE + 1 , JTRIG ) + 1                                        2415
2416  2416  C                                                                                2416
2417  2417            IV1 = JUV( IEM )                                                       2417
2418  2418            IV2 = JUV( IEP )                                                       2418
2419  2419            IV3 = JUV( IEI )                                                       2419
2420  2420  C                                                                                2420
2421  2421            X1 = XV( 1 , IV1 ) - XV( 1 , IV2 )                                     2421
2422  2422            Y1 = XV( 2 , IV1 ) - XV( 2 , IV2 )                                     2422
2423  2423            X2 = XV( 1 , IV3 ) - XV( 1 , IV2 )                                     2423
2424  2424            Y2 = XV( 2 , IV3 ) - XV( 2 , IV2 )                                     2424
2425  2425            XSIN = ( X2 * Y1 - X1 * Y2 )                                           2425
2426  2426            XCOS = ( X1 * X2 + Y1 * Y2 )                                           2426
2427  2427            XCOT = XCOS / ( XSIN + 1.E-8 )                                         2427
2428  2428            IF( XSIN . LT . 0. . AND . XCOT . LT . AREMIN ) THEN                   2428
2429  2429            AREMIN = XCOT                                                          2429
2430  2430            IEMIN = IE                                                             2430
2431  2431            END IF                                                                 2431
2432  2432            ANGLE( IE ) = XSIN / ( ABS( XCOS ) + 1.E-7 )                           2432
2433  2433  C                                                                                2433
2434  2434  740       CONTINUE                                                               2434
2435  2435  C                                                                                2435
2436  2436            DO 750 IE = 1 , JTRIG                                                  2436
2437  2437            IEP = MOD( IE - IEMIN + JTRIG , JTRIG ) + 1                            2437
2438  2438            JEN( IEP ) = IICOLR( IE )                                              2438
2439  2439            ANGLER( IEP ) = ANGLE( IE )                                            2439
2440  2440  750       CONTINUE                                                               2440
2441  2441  C                                                                                2441
```

```
2442   2442            DO 760 IE = 1 , JTRIG                                    2442
2443   2443            IICOLR( IE ) = JEN( IE )                                 2443
2444   2444            ANGLE( IE ) = ANGLER( IE )                               2444
2445   2445   760      CONTINUE                                                 2445
2446   2446   C                                                                 2446
2447   2447            IFINAL = 0                                               2447
2448   2448            IEI = 1                                                  2448
2449   2449            DO 770 IE = 1 , JTRIG                                    2449
2450   2450            SANGLE = ANGLE( IE )                                     2450
2451   2451            IANGLE( IE ) = - 1                                       2451
2452   2452            IF( SANGLE . GT . 1.E-2 ) IANGLE( IE ) = 1               2452
2453   2453   770      CONTINUE                                                 2453
2454   2454   C                                                                 2454
2455   2455            DO 780 IE = 1 , JTRIG                                    2455
2456   2456            IEM = MOD( IE - 1 , JTRIG ) + 1                          2456
2457   2457            IEP = MOD( IE , JTRIG ) + 1                              2457
2458   2458            IKM = MOD( IE + 1 , JTRIG ) + 1                          2458
2459   2459            KEM = IANGLE( IEM )                                      2459
2460   2460            KEP = IANGLE( IEP )                                      2460
2461   2461            KKM = IANGLE( IKM )                                      2461
2462   2462            IF( KEM . EQ . - 1 . AND .                               2462
2463   2463         .      KEP . EQ . 1 . AND .                                 2463
2464   2464         .      KKM . EQ . - 1 . AND . IFINAL . EQ . 0 ) THEN        2464
2465   2465            IEI = IKM                                                2465
2466   2466            IFINAL = 1                                               2466
2467   2467            END IF                                                   2467
2468   2468   780      CONTINUE                                                 2468
2469   2469   C                                                                 2469
2470   2470            IF( IFINAL . EQ .  0 ) THEN                              2470
2471   2471            DO 790 IE = 1 , JTRIG                                    2471
2472   2472            IEM = MOD( IE - 1 , JTRIG ) + 1                          2472
2473   2473            IEP = MOD( IE , JTRIG ) + 1                              2473
2474   2474            KEM = IANGLE( IEM )                                      2474
2475   2475            KEP = IANGLE( IEP )                                      2475
2476   2476            IF( KEM . EQ . - 1 . AND . KEP . EQ . 1 . AND .          2476
2477   2477         .                              IFINAL . EQ . 0 ) THEN       2477
2478   2478            IEI = MOD( IE + 1 , JTRIG ) + 1                          2478
2479   2479            IFINAL = 1                                               2479
2480   2480            END IF                                                   2480
2481   2481   790      CONTINUE                                                 2481
2482   2482            END IF                                                   2482
2483   2483   C                                                                 2483
2484   2484            IF( IFINAL . EQ .  0 ) THEN                              2484
2485   2485            ANGMIN = 10000000.                                       2485
2486   2486            DO 800 IE = 1 , JTRIG                                    2486
2487   2487            XANGLE = ANGLE( IE )                                     2487
2488   2488            SANGLE = ABS( XANGLE - 1. )                              2488
2489   2489            IF( XANGLE . GT . 0. . AND . SANGLE . LT . ANGMIN ) THEN 2489
2490   2490            IEI = MOD( IE , JTRIG ) + 1                              2490
2491   2491            ANGMIN = SANGLE                                          2491
2492   2492            END IF                                                   2492
2493   2493   800      CONTINUE                                                 2493
2494   2494            END IF                                                   2494
2495   2495   C                                                                 2495
2496   2496            DO 810 IE = 1 , JTRIG                                    2496
2497   2497            IEP = MOD( IE - IEI + JTRIGP , JTRIG ) + 1               2497
2498   2498            JEN( IEP ) = IICOLR( IE )                                2498
2499   2499            ANGLER( IEP ) = ANGLE( IE )                              2499
2500   2500   810      CONTINUE                                                 2500
2501   2501   C                                                                 2501
2502   2502            DO 820 IE = 1 , JTRIG                                    2502
2503   2503            ANGLE( IE ) = ANGLER( IE )                               2503
2504   2504            IICOLR( IE ) = JEN( IE )                                 2504
2505   2505   820      CONTINUE                                                 2505
2506   2506   C                                                                 2506
2507   2507            DO 830 IE = 1 , JTRIG                                    2507
2508   2508            IEM = JEN( IE )                                          2508
2509   2509            IF( IEM . GT . 0 ) THEN                                  2509
2510   2510            JUV( IE ) = JE( 1 , IEM )                                2510
2511   2511            ELSE                                                     2511
2512   2512            JUV( IE ) = JE( 2 , - IEM )                              2512
2513   2513            END IF                                                   2513
2514   2514   830      CONTINUE                                                 2514
2515   2515   C                                                                 2515
```

```
2516  2516            IF( JTRIG . EQ . 3 ) THEN
2517  2517  C
2518  2518            NSC = ISCRSS( ITRIG )
2519  2519            ITRIG = ITRIG - 1
2520  2520            NSINTL = NSINTL + 1
2521  2521            INVTRG( NSINTL ) = NSC
2522  2522            JS( 1 , NSC ) = JUV( 1 )
2523  2523            JS( 2 , NSC ) = JUV( 2 )
2524  2524            JS( 3 , NSC ) = JUV( 3 )
2525  2525            JS( 4 , NSC ) = JEN( 1 )
2526  2526            JS( 5 , NSC ) = JEN( 2 )
2527  2527            JS( 6 , NSC ) = JEN( 3 )
2528  2528  C
2529  2529            IV1 = JS( 1 , NSC )
2530  2530            IV2 = JS( 2 , NSC )
2531  2531            IV3 = JS( 3 , NSC )
2532  2532            AX = XV( 1 , IV2 ) - XV( 1 , IV1 )
2533  2533            AY = XV( 2 , IV2 ) - XV( 2 , IV1 )
2534  2534            BX = XV( 1 , IV3 ) - XV( 1 , IV1 )
2535  2535            BY = XV( 2 , IV3 ) - XV( 2 , IV1 )
2536  2536            XS( 3 , NSC ) = 0.5 * ( AX * BY - AY * BX )
2537  2537  C
2538  2538            SAREA( NSC ) = 1. / XS( 3 , NSC )
2539  2539            XXC = ( XV( 1 , IV1 ) + XV( 1 , IV2 ) + XV( 1 , IV3 ) ) *
2540  2540           .        THIRD
2541  2541            YYC = ( XV( 2 , IV1 ) + XV( 2 , IV2 ) + XV( 2 , IV3 ) ) *
2542  2542           .        THIRD
2543  2543            XS( 1 , NSC ) = XXC
2544  2544            XS( 2 , NSC ) = YYC
2545  2545            HYDFLX( NSC , 4 ) = 0.
2546  2546            HYDFLX( NSC , 1 ) = 0.
2547  2547            HYDFLX( NSC , 2 ) = 0.
2548  2548            KSDELT( NSC ) = 1
2549  2549  C
2550  2550            DO 840 IR = 1 , MHQ
2551  2551            HYDV( NSC , IR ) = ( HYDVVV( IV1 , IR ) +
2552  2552           .                     HYDVVV( IV2 , IR ) +
2553  2553           .                     HYDVVV( IV3 , IR ) ) * THIRD
2554  2554  840       CONTINUE
2555  2555  C
2556  2556            HDUM          = 1. / ( HYDV( NSC , 1 ) + 1.E-12 )
2557  2557            HYDV( NSC , 2 ) = HYDV( NSC , 2 ) * HDUM
2558  2558            HYDV( NSC , 3 ) = HYDV( NSC , 3 ) * HDUM
2559  2559            HYDV( NSC , 4 ) = ( HYDV( NSC , 4 )  -
2560  2560           .                  .5 * HYDV( NSC , 1 ) *
2561  2561           . ( HYDV( NSC , 2 ) * HYDV( NSC , 2 ) +
2562  2562           .   HYDV( NSC , 3 ) * HYDV( NSC , 3 ) ) ) *
2563  2563           .                     ( HYDV( NSC , 5 ) - 1. )
2564  2564  C
2565  2565            ISTOP = 1
2566  2566  C
2567  2567            ELSE IF( JTRIG . EQ . 4 ) THEN
2568  2568  C
2569  2569            NSC = ISCRSS( ITRIG )
2570  2570            ITRIG = ITRIG - 1
2571  2571            NSINTL = NSINTL + 1
2572  2572            INVTRG( NSINTL ) = NSC
2573  2573            NEC = IECRSS( IETRIG )
2574  2574            IETRIG = IETRIG - 1
2575  2575  C
2576  2576            IJTRIG = IJTRIG + 1
2577  2577            JUE( IJTRIG ) = NEC
2578  2578  C
2579  2579            JE( 1 , NEC ) = JUV( 1 )
2580  2580            JE( 2 , NEC ) = JUV( 3 )
2581  2581            JE( 5 , NEC ) = 0
2582  2582  C
2583  2583            JS( 1 , NSC ) = JUV( 1 )
2584  2584            JS( 2 , NSC ) = JUV( 2 )
2585  2585            JS( 3 , NSC ) = JUV( 3 )
2586  2586            JS( 4 , NSC ) = JEN( 1 )
2587  2587            JS( 5 , NSC ) = JEN( 2 )
2588  2588            JS( 6 , NSC ) = - NEC
2589  2589  C
```

```
2590  2590            NSC = ISCRSS( ITRIG )                                    2590
2591  2591            ITRIG = ITRIG - 1                                        2591
2592  2592            NSINTL = NSINTL + 1                                      2592
2593  2593            INVTRG( NSINTL ) = NSC                                   2593
2594  2594  C                                                                  2594
2595  2595            JS( 1 , NSC ) = JUV( 1 )                                 2595
2596  2596            JS( 2 , NSC ) = JUV( 3 )                                 2596
2597  2597            JS( 3 , NSC ) = JUV( 4 )                                 2597
2598  2598            JS( 4 , NSC ) = NEC                                      2598
2599  2599            JS( 5 , NSC ) = JEN( 3 )                                 2599
2600  2600            JS( 6 , NSC ) = JEN( 4 )                                 2600
2601  2601  C                                                                  2601
2602  2602            DO 850 IKR = 1 , 2                                       2602
2603  2603            NSS = INVTRG( NSINTL + 1 - IKR )                         2603
2604  2604            IV1 = JS( 1 , NSS )                                      2604
2605  2605            IV2 = JS( 2 , NSS )                                      2605
2606  2606            IV3 = JS( 3 , NSS )                                      2606
2607  2607            AX = XV( 1 , IV2 ) - XV( 1 , IV1 )                       2607
2608  2608            AY = XV( 2 , IV2 ) - XV( 2 , IV1 )                       2608
2609  2609            BX = XV( 1 , IV3 ) - XV( 1 , IV1 )                       2609
2610  2610            BY = XV( 2 , IV3 ) - XV( 2 , IV1 )                       2610
2611  2611            XS( 3 , NSS ) = 0.5 * ( AX * BY - AY * BX )              2611
2612  2612  C                                                                  2612
2613  2613            SAREA( NSS ) = 1. / XS( 3 , NSS )                        2613
2614  2614            XXC = ( XV( 1 , IV1 ) + XV( 1 , IV2 ) + XV( 1 , IV3 ) ) *2614
2615  2615       .          THIRD                                              2615
2616  2616            YYC = ( XV( 2 , IV1 ) + XV( 2 , IV2 ) + XV( 2 , IV3 ) ) *2616
2617  2617       .          THIRD                                              2617
2618  2618            XS( 1 , NSS ) = XXC                                      2618
2619  2619            XS( 2 , NSS ) = YYC                                      2619
2620  2620            HYDFLX( NSS , 4 ) = 0.                                   2620
2621  2621            HYDFLX( NSS , 1 ) = 0.                                   2621
2622  2622            HYDFLX( NSS , 2 ) = 0.                                   2622
2623  2623            KSDELT( NSS ) = 1                                        2623
2624  2624  C                                                                  2624
2625  2625            DO 860 IR = 1 , MHQ                                      2625
2626  2626            HYDV( NSS , IR ) = ( HYDVVV( IV1 , IR ) +                2626
2627  2627       .                         HYDVVV( IV2 , IR ) +                2627
2628  2628       .                         HYDVVV( IV3 , IR ) ) * THIRD        2628
2629  2629  860     CONTINUE                                                   2629
2630  2630  C                                                                  2630
2631  2631            HDUM          = 1. / ( HYDV( NSS , 1 ) + 1.E-12 )        2631
2632  2632            HYDV( NSS , 2 ) = HYDV( NSS , 2 ) * HDUM                 2632
2633  2633            HYDV( NSS , 3 ) = HYDV( NSS , 3 ) * HDUM                 2633
2634  2634            HYDV( NSS , 4 ) = ( HYDV( NSS , 4 )  -                   2634
2635  2635       .                      .5 * HYDV( NSS , 1 ) *                2635
2636  2636       .    ( HYDV( NSS , 2 ) * HYDV( NSS , 2 ) +                    2636
2637  2637       .      HYDV( NSS , 3 ) * HYDV( NSS , 3 ) ) ) *                 2637
2638  2638       .                        ( HYDV( NSS , 5 ) - 1. )            2638
2639  2639  C                                                                  2639
2640  2640  850     CONTINUE                                                   2640
2641  2641            ISTOP = 1                                                2641
2642  2642  C                                                                  2642
2643  2643            ELSE                                                     2643
2644  2644  C                                                                  2644
2645  2645            NSC = ISCRSS( ITRIG )                                    2645
2646  2646            ITRIG = ITRIG - 1                                        2646
2647  2647            NSINTL = NSINTL + 1                                      2647
2648  2648            INVTRG( NSINTL ) = NSC                                   2648
2649  2649            NEC = IECRSS( IETRIG )                                   2649
2650  2650            IETRIG = IETRIG - 1                                      2650
2651  2651  C                                                                  2651
2652  2652            IJTRIG = IJTRIG + 1                                      2652
2653  2653            JUE( IJTRIG ) = NEC                                      2653
2654  2654  C                                                                  2654
2655  2655            JE( 1 , NEC ) = JUV( 1 )                                 2655
2656  2656            JE( 2 , NEC ) = JUV( 3 )                                 2656
2657  2657            JE( 5 , NEC ) = 0                                        2657
2658  2658  C                                                                  2658
2659  2659            JS( 1 , NSC ) = JUV( 1 )                                 2659
2660  2660            JS( 2 , NSC ) = JUV( 2 )                                 2660
2661  2661            JS( 3 , NSC ) = JUV( 3 )                                 2661
2662  2662            JS( 4 , NSC ) = JEN( 1 )                                 2662
2663  2663            JS( 5 , NSC ) = JEN( 2 )                                 2663
```

```
2664  2664            JS( 6 , NSC ) = - NEC
2665  2665  C
2666  2666            IICOLR( 1 ) = NEC
2667  2667            JTRIG = JTRIG - 1
2668  2668            DO 870 IEE = 2 , JTRIG
2669  2669            IICOLR( IEE ) = JEN( IEE + 1 )
2670  2670  870       CONTINUE
2671  2671  C
2672  2672            IV1 = JS( 1 , NSC )
2673  2673            IV2 = JS( 2 , NSC )
2674  2674            IV3 = JS( 3 , NSC )
2675  2675            AX = XV( 1 , IV2 ) - XV( 1 , IV1 )
2676  2676            AY = XV( 2 , IV2 ) - XV( 2 , IV1 )
2677  2677            BX = XV( 1 , IV3 ) - XV( 1 , IV1 )
2678  2678            BY = XV( 2 , IV3 ) - XV( 2 , IV1 )
2679  2679            XS( 3 , NSC ) = 0.5 * ( AX * BY - AY * BX )
2680  2680  C
2681  2681            SAREA( NSC ) = 1. / XS( 3 , NSC )
2682  2682            XXC = ( XV( 1 , IV1 ) + XV( 1 , IV2 ) + XV( 1 , IV3 ) ) *
2683  2683           .        THIRD
2684  2684            YYC = ( XV( 2 , IV1 ) + XV( 2 , IV2 ) + XV( 2 , IV3 ) ) *
2685  2685           .        THIRD
2686  2686            XS( 1 , NSC ) = XXC
2687  2687            XS( 2 , NSC ) = YYC
2688  2688            HYDFLX( NSC , 4 ) = 0.
2689  2689            HYDFLX( NSC , 1 ) = 0.
2690  2690            HYDFLX( NSC , 2 ) = 0.
2691  2691            KSDELT( NSC ) = 1
2692  2692  C
2693  2693            DO 880 IR = 1 , MHQ
2694  2694            HYDV( NSC , IR ) = ( HYDVVV( IV1 , IR ) +
2695  2695           .                    HYDVVV( IV2 , IR ) +
2696  2696           .                    HYDVVV( IV3 , IR ) ) * THIRD
2697  2697  880       CONTINUE
2698  2698  C
2699  2699            HDUM          = 1. / ( HYDV( NSC , 1 ) + 1.E-12 )
2700  2700            HYDV( NSC , 2 ) = HYDV( NSC , 2 ) * HDUM
2701  2701            HYDV( NSC , 3 ) = HYDV( NSC , 3 ) * HDUM
2702  2702            HYDV( NSC , 4 ) = ( HYDV( NSC , 4 )  -
2703  2703           .                   .5 * HYDV( NSC , 1 ) *
2704  2704           .  ( HYDV( NSC , 2 ) * HYDV( NSC , 2 ) +
2705  2705           .    HYDV( NSC , 3 ) * HYDV( NSC , 3 ) ) ) *
2706  2706           .                     ( HYDV( NSC , 5 ) - 1. )
2707  2707  C
2708  2708            END IF
2709  2709            IF( ISTOP . EQ . 0 ) GO TO 720
2710  2710  C
2711  2711            DO 890 ISS = 1 , NSINTL
2712  2712            IS = INVTRG( ISS )
2713  2713            DO 890 IR = 4 , 6
2714  2714            IE = JS( IR , IS )
2715  2715            IF( IE . GT . 0 ) THEN
2716  2716            JE( 3 , IE ) = IS
2717  2717            ELSE
2718  2718            JE( 4 , - IE ) = IS
2719  2719            END IF
2720  2720  890       CONTINUE
2721  2721  C
2722  2722            DO 900 IENN = 1 , IJTRIG
2723  2723            IEN = JUE( IENN )
2724  2724            JV1 = JE( 1 , IEN )
2725  2725            JV2 = JE( 2 , IEN )
2726  2726            AX = XV( 1 , JV2 ) - XV( 1 , JV1 )
2727  2727            AY = XV( 2 , JV2 ) - XV( 2 , JV1 )
2728  2728            XE( 1 , IEN ) = SQRT( AX * AX + AY * AY )
2729  2729            XEREV = 1. / XE( 1 , IEN )
2730  2730            XN( IEN ) = AY * XEREV
2731  2731            YN( IEN ) = - AX * XEREV
2732  2732            ISSR = JE( 4 , IEN )
2733  2733            ISSL = JE( 3 , IEN )
2734  2734  C
2735  2735            IF( JE( 5 , IEN ) . NE . 0 ) THEN
2736  2736  C
2737  2737            AA = XV( 1 , JV2 ) - XV( 1 , JV1 )
```

```
2738  2738            BB = XV( 2 , JV2 ) - XV( 2 , JV1 )                                  2738
2739  2739            XEL = XS( 1 , ISSL )                                                2739
2740  2740            YEL = XS( 2 , ISSL )                                                2740
2741  2741            CC = XEL - XV( 1 , JV1 )                                            2741
2742  2742            DD = YEL - XV( 2 , JV1 )                                            2742
2743  2743            EE = ( AA * CC + BB * DD ) * XEREV * XEREV                          2743
2744  2744            XER = XV( 1 , JV1 ) + AA * EE                                       2744
2745  2745            YER = XV( 2 , JV1 ) + BB * EE                                       2745
2746  2746            AX = XER - XEL                                                      2746
2747  2747            AY = YER - YEL                                                      2747
2748  2748            XE( 2 , IEN ) = SQRT( AX * AX + AY * AY )                           2748
2749  2749            XEREV = 1. / XE( 2 , IEN )                                          2749
2750  2750            XXN( IEN ) = AX * XEREV                                             2750
2751  2751            YYN( IEN ) = AY * XEREV                                             2751
2752  2752            XE( 2 , IEN ) = 2. * XE( 2 , IEN )                                  2752
2753  2753            XYMIDL( IEN ) = .5                                                  2753
2754  2754            XMIDL( IEN ) = XER                                                  2754
2755  2755            YMIDL( IEN ) = YER                                                  2755
2756  2756  C                                                                             2756
2757  2757            ELSE                                                                2757
2758  2758  C                                                                             2758
2759  2759            XER = XS( 1 , ISSR )                                                2759
2760  2760            YER = XS( 2 , ISSR )                                                2760
2761  2761            XEL = XS( 1 , ISSL )                                                2761
2762  2762            YEL = XS( 2 , ISSL )                                                2762
2763  2763  C                                                                             2763
2764  2764            AA = XV( 1 , JV2 ) - XV( 1 , JV1 )                                  2764
2765  2765            BB = XV( 2 , JV2 ) - XV( 2 , JV1 )                                  2765
2766  2766            CC = XEL - XER                                                      2766
2767  2767            DD = YEL - YER                                                      2767
2768  2768            ACA = XER - XV( 1 , JV1 )                                           2768
2769  2769            DBD = YER - XV( 2 , JV1 )                                           2769
2770  2770            EE = ( ACA * DD - DBD * CC ) / ( AA * DD - BB * CC )                2770
2771  2771            XMIDL( IEN ) = XV( 1 , JV1 ) + AA * EE                              2771
2772  2772            YMIDL( IEN ) = XV( 2 , JV1 ) + BB * EE                              2772
2773  2773  C                                                                             2773
2774  2774            XEMID = XMIDL( IEN ) - XEL                                          2774
2775  2775            YEMID = YMIDL( IEN ) - YEL                                          2775
2776  2776  C                                                                             2776
2777  2777            AX = XER - XEL                                                      2777
2778  2778            AY = YER - YEL                                                      2778
2779  2779            XE( 2 , IEN ) = SQRT( AX * AX + AY * AY )                           2779
2780  2780            XEREV = 1. / XE( 2 , IEN )                                          2780
2781  2781            XXN( IEN ) = AX * XEREV                                             2781
2782  2782            YYN( IEN ) = AY * XEREV                                             2782
2783  2783  C                                                                             2783
2784  2784            XYMIDL( IEN ) = SQRT( XEMID * XEMID + YEMID * YEMID ) * XEREV       2784
2785  2785  C                                                                             2785
2786  2786            END IF                                                              2786
2787  2787  C                                                                             2787
2788  2788  900       CONTINUE                                                            2788
2789  2789  C                                                                             2789
2790  2790  C     ORDER THE DELETED VERTECIS IN A DECENDED ORDER IN AN ARRAY              2790
2791  2791  C     NVDELT                                                                  2791
2792  2792  C                                                                             2792
2793  2793            KFLIP = JVDELT                                                      2793
2794  2794            DO 910 KK = 1 ,  JVDELT                                             2794
2795  2795            IFLIP = 1                                                           2795
2796  2796            NVDELT( KK ) = IVDELT( 1 )                                          2796
2797  2797            DO 920 KI = 1 , KFLIP                                               2797
2798  2798            IF( IVDELT( KI ) . GT . NVDELT( KK ) ) THEN                         2798
2799  2799            NVDELT( KK ) = IVDELT( KI )                                         2799
2800  2800            IFLIP = KI                                                          2800
2801  2801            END IF                                                              2801
2802  2802  920       CONTINUE                                                            2802
2803  2803            ISS = 0                                                             2803
2804  2804            DO 930 KI = 1 , KFLIP                                               2804
2805  2805            IF( KI . NE . IFLIP ) THEN                                          2805
2806  2806            ISS = ISS + 1                                                       2806
2807  2807            IVDELT( ISS ) = IVDELT( KI )                                        2807
2808  2808            END IF                                                              2808
2809  2809  930       CONTINUE                                                            2809
2810  2810            KFLIP = KFLIP - 1                                                   2810
2811  2811  910       CONTINUE                                                            2811
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```
2812    2812    C
2813    2813    C    ORDER THE DELETED EDGES IN A DECENDED ORDER IN AN ARRAY
2814    2814    C    NECRSS
2815    2815    C
2816    2816              KFLIP = IETRIG
2817    2817              DO 940 KK = 1 , IETRIG
2818    2818              IFLIP = 1
2819    2819              NECRSS( KK ) = IECRSS( 1 )
2820    2820              DO 950 KI = 1 , KFLIP
2821    2821              IF( IECRSS( KI ) . GT . NECRSS( KK ) ) THEN
2822    2822              NECRSS( KK ) = IECRSS( KI )
2823    2823              IFLIP = KI
2824    2824              END IF
2825    2825    950       CONTINUE
2826    2826              ISS = 0
2827    2827              DO 960 KI = 1 , KFLIP
2828    2828              IF( KI . NE . IFLIP ) THEN
2829    2829              ISS = ISS + 1
2830    2830              IECRSS( ISS ) = IECRSS( KI )
2831    2831              END IF
2832    2832    960       CONTINUE
2833    2833              KFLIP = KFLIP - 1
2834    2834    940       CONTINUE
2835    2835    C
2836    2836    C    ORDER THE DELETED CELLS IN A DECENDED ORDER IN AN ARRAY
2837    2837    C    NSCRSS
2838    2838    C
2839    2839              KFLIP = ITRIG
2840    2840              DO 970 KK = 1 , ITRIG
2841    2841              IFLIP = 1
2842    2842              NSCRSS( KK ) = ISCRSS( 1 )
2843    2843              DO 980 KI = 1 , KFLIP
2844    2844              IF( ISCRSS( KI ) . GT . NSCRSS( KK ) ) THEN
2845    2845              NSCRSS( KK ) = ISCRSS( KI )
2846    2846              IFLIP = KI
2847    2847              END IF
2848    2848    980       CONTINUE
2849    2849              ISS = 0
2850    2850              DO 990 KI = 1 , KFLIP
2851    2851              IF( KI . NE . IFLIP ) THEN
2852    2852              ISS = ISS + 1
2853    2853              ISCRSS( ISS ) = ISCRSS( KI )
2854    2854              END IF
2855    2855    990       CONTINUE
2856    2856              KFLIP = KFLIP - 1
2857    2857    970       CONTINUE
2858    2858    C
2859    2859              DO 1000 KI = 1 , JVDELT
2860    2860              IVDELT( KI ) = NV + 1 - KI
2861    2861    1000      CONTINUE
2862    2862    C
2863    2863              DO 1010 KI = 1 , IETRIG
2864    2864              IECRSS( KI ) = NE + 1 - KI
2865    2865    1010      CONTINUE
2866    2866    C
2867    2867              DO 1020 KI = 1 , ITRIG
2868    2868              ISCRSS( KI ) = NS + 1 - KI
2869    2869    1020      CONTINUE
2870    2870    C
2871    2871    C    IT MAKE SURE THAT VERTICES THAT ARE TO BE DELETED ARE NOT
2872    2872    C    REPLACED BY VERTICES THAS ARE TO BE DELETED ALSO
2873    2873    C
2874    2874              DO 1030 KI = 1 , JVDELT
2875    2875              IVM = NVDELT( KI )
2876    2876              DO 1030 KK = 1 , JVDELT
2877    2877              JVM = IVDELT( KK )
2878    2878              IF( IVM . EQ . JVM . AND . KK . NE . KI ) THEN
2879    2879              IVDUM = IVDELT( KI )
2880    2880              IVDELT( KI ) = IVM
2881    2881              IVDELT( KK ) = IVDUM
2882    2882              END IF
2883    2883    1030      CONTINUE
2884    2884    C
2885    2885    C    IT MAKE SURE THAT EDGES THAT ARE TO BE DELETED ARE NOT
```

```
2886  2886  C     REPLACED BY EDGES THAS ARE TO BE DELETED ALSO                2886
2887  2887  C                                                                  2887
2888  2888              DO 1040 KI = 1 , IETRIG                                2888
2889  2889              IEM = NECRSS( KI )                                     2889
2890  2890              DO 1040 KK = 1 , IETRIG                                2890
2891  2891              JEM = IECRSS( KK )                                     2891
2892  2892              IF( IEM . EQ . JEM . AND . KK . NE . KI ) THEN         2892
2893  2893              IEDUM = IECRSS( KI )                                   2893
2894  2894              IECRSS( KI ) = IEM                                     2894
2895  2895              IECRSS( KK ) = IEDUM                                   2895
2896  2896              END IF                                                 2896
2897  2897  1040        CONTINUE                                               2897
2898  2898  C                                                                  2898
2899  2899  C     IT MAKE SURE THAT CELLS THAT ARE TO BE DELETED ARE NOT       2899
2900  2900  C     REPLACED BY CELLS THAS ARE TO BE DELETED ALSO                2900
2901  2901  C                                                                  2901
2902  2902              DO 1050 KI = 1 , ITRIG                                 2902
2903  2903              ISM = NSCRSS( KI )                                     2903
2904  2904              DO 1050 KK = 1 , ITRIG                                 2904
2905  2905              JSM = ISCRSS( KK )                                     2905
2906  2906              IF( ISM . EQ . JSM . AND . KK . NE . KI ) THEN         2906
2907  2907              ISDUM = ISCRSS( KI )                                   2907
2908  2908              ISCRSS( KI ) = ISM                                     2908
2909  2909              ISCRSS( KK ) = ISDUM                                   2909
2910  2910              END IF                                                 2910
2911  2911  1050        CONTINUE                                               2911
2912  2912  C                                                                  2912
2913  2913  C   IVDELT(*) SEQUENCE OF VERTICES TO BE DELETED END OF LIST       2913
2914  2914  C   NVDELT(*) SEQUENCE OF VERTICES TO BE REPLACED CURRENT IN LIST  2914
2915  2915  C   ISCRSS(*) SEQUENCE OF TRIANGLES TO BE DELETED END OF LIST      2915
2916  2916  C   NSCRSS(*) SEQUENCE OF TRIANGLES TO BE REPLACED CURRENT IN LIST 2916
2917  2917  C   IECRSS(*) SEQUENCE OF EDGES TO BE DELETED END OF LIST          2917
2918  2918  C   NECRSS(*) SEQUENCE OF EDGES TO BE REPLACED CURRENT IN LIST     2918
2919  2919  C                                                                  2919
2920  2920              DO 1060 KI = 1 , JVDELT                                2920
2921  2921              IVM = NVDELT( KI )                                     2921
2922  2922              JVM = IVDELT( KI )                                     2922
2923  2923  C                                                                  2923
2924  2924              XV( 1 , IVM ) = XV( 1 , JVM )                          2924
2925  2925              XV( 2 , IVM ) = XV( 2 , JVM )                          2925
2926  2926              JV( 1 , IVM ) = JV( 1 , JVM )                          2926
2927  2927  C                                                                  2927
2928  2928              DO 1060 IR = 1 , MHQ                                   2928
2929  2929              HYDVVV( IVM , IR ) = HYDVVV( JVM , IR )                2929
2930  2930  1060        CONTINUE                                               2930
2931  2931  C                                                                  2931
2932  2932              NVM = NV - JVDELT                                      2932
2933  2933              NEM = NE - IETRIG                                      2933
2934  2934              NSM = NS - ITRIG                                       2934
2935  2935  C                                                                  2935
2936  2936  C     UPDATE THE EDGES AND CELLS THAT ARE CONNECTED TO THE DELETED 2936
2937  2937  C     VERTICES                                                     2937
2938  2938  C                                                                  2938
2939  2939              JNVEDG = 0                                             2939
2940  2940              JNVTRG = 0                                             2940
2941  2941              DO 1070 JVDL = 1 , JVDELT                              2941
2942  2942              IVDL = NVDELT( JVDL )                                  2942
2943  2943              NVDL = IVDELT( JVDL )                                  2943
2944  2944              IF( IVDL . NE . NVDL ) THEN                            2944
2945  2945              IE = JV( 2 , NVDL )                                    2945
2946  2946              IF( IE . GT . 0 ) THEN                                 2946
2947  2947  C                                                                  2947
2948  2948              IV1 = JE( 1 , IE )                                     2948
2949  2949              IF( IV1 . EQ . NVDL ) THEN                             2949
2950  2950              ISI = JE( 3 , IE )                                     2950
2951  2951              ELSE                                                   2951
2952  2952              ISI = JE( 4 , IE )                                     2952
2953  2953              END IF                                                 2953
2954  2954              IS = ISI                                               2954
2955  2955  C                                                                  2955
2956  2956              JNVEDG = JNVEDG + 1                                    2956
2957  2957              INVEDG( JNVEDG ) = IE                                  2957
2958  2958              JNVTRG = JNVTRG + 1                                    2958
2959  2959              INVTRG( JNVTRG ) = IS                                  2959
```

```
2960  2960  C
2961  2961  1090      CONTINUE
2962  2962  C
2963  2963            DO 1080 IR = 1 , 3
2964  2964            JR = MOD( IR , 3 ) + 1
2965  2965            IEA = IABS( JS( JR + 3 , IS ) )
2966  2966            IF( IEA . EQ . IE ) THEN
2967  2967            JJR = MOD( JR + 1 , 3 ) + 4
2968  2968            IER = IABS( JS( JJR , IS ) )
2969  2969  C
2970  2970            IV1 = JE( 1 , IER )
2971  2971            IF( IV1 . EQ . NVDL ) THEN
2972  2972            ISR = JE( 3 , IER )
2973  2973            ELSE
2974  2974            ISR = JE( 4 , IER )
2975  2975            END IF
2976  2976            END IF
2977  2977  C
2978  2978  1080      CONTINUE
2979  2979  C
2980  2980            IF( ISR . NE . ISI ) THEN
2981  2981            IS = ISR
2982  2982            IE = IER
2983  2983  C
2984  2984            JNVEDG = JNVEDG + 1
2985  2985            INVEDG( JNVEDG ) = IE
2986  2986            JNVTRG = JNVTRG + 1
2987  2987            INVTRG( JNVTRG ) = IS
2988  2988  C
2989  2989            GO TO 1090
2990  2990            END IF
2991  2991  C
2992  2992            ELSE
2993  2993  C
2994  2994            IE = - IE
2995  2995            IV1 = JE( 1 , IE )
2996  2996            IF( IV1 . EQ . NVDL ) THEN
2997  2997            ISI = JE( 3 , IE )
2998  2998            ELSE
2999  2999            ISI = JE( 4 , IE )
3000  3000            END IF
3001  3001            IS = ISI
3002  3002            ISI = 0
3003  3003  C
3004  3004            JNVEDG = JNVEDG + 1
3005  3005            INVEDG( JNVEDG ) = IE
3006  3006            JNVTRG = JNVTRG + 1
3007  3007            INVTRG( JNVTRG ) = IS
3008  3008  C
3009  3009  1100      CONTINUE
3010  3010  C
3011  3011            DO 1110 IR = 1 , 3
3012  3012            JR = MOD( IR , 3 ) + 1
3013  3013            IEA = IABS( JS( JR + 3 , IS ) )
3014  3014            IF( IEA . EQ . IE ) THEN
3015  3015            JJR = MOD( JR + 1 , 3 ) + 4
3016  3016            IER = IABS( JS( JJR , IS ) )
3017  3017  C
3018  3018            IV1 = JE( 1 , IER )
3019  3019            IF( IV1 . EQ . NVDL ) THEN
3020  3020            ISR = JE( 3 , IER )
3021  3021            ELSE
3022  3022            ISR = JE( 4 , IER )
3023  3023            END IF
3024  3024            END IF
3025  3025  C
3026  3026  1110      CONTINUE
3027  3027  C
3028  3028            IF( ISR . NE . IS1 ) THEN
3029  3029            IS = ISR
3030  3030            IE = IER
3031  3031  C
3032  3032            JNVEDG = JNVEDG + 1
3033  3033            INVEDG( JNVEDG ) = IE
```

```
3034  3034            JNVTRG = JNVTRG + 1                                    3034
3035  3035            INVTRG( JNVTRG ) = IS                                  3035
3036  3036  C                                                                3036
3037  3037            GO TO 1100                                             3037
3038  3038            END IF                                                 3038
3039  3039  C                                                                3039
3040  3040            JNVEDG = JNVEDG + 1                                    3040
3041  3041            INVEDG( JNVEDG ) = IER                                 3041
3042  3042  C                                                                3042
3043  3043            END IF                                                 3043
3044  3044            END IF                                                 3044
3045  3045  1070      CONTINUE                                               3045
3046  3046  C                                                                3046
3047  3047            NSMNPT = INVTRG( 1 )                                   3047
3048  3048  C                                                                3048
3049  3049            DO 1120 IE = 1 , JNVEDG                                3049
3050  3050            IEE = INVEDG( IE )                                     3050
3051  3051            DO 1120 IIDG = IE + 1 , JNVEDG                         3051
3052  3052            IF( INVEDG( IIDG ) . EQ . IEE ) THEN                   3052
3053  3053            INVEDG( IIDG ) = 0                                     3053
3054  3054            END IF                                                 3054
3055  3055  1120      CONTINUE                                               3055
3056  3056  C                                                                3056
3057  3057            IEDUM = 0                                              3057
3058  3058            DO 1130 IIDG = 1 , JNVEDG                              3058
3059  3059            IF( INVEDG( IIDG ) . NE . 0 ) THEN                     3059
3060  3060            IEDUM = IEDUM + 1                                      3060
3061  3061            INVEDG( IEDUM ) = INVEDG( IIDG )                       3061
3062  3062            END IF                                                 3062
3063  3063  1130      CONTINUE                                               3063
3064  3064            JNVEDG = IEDUM                                         3064
3065  3065  C                                                                3065
3066  3066            DO 1140 IS = 1 , JNVTRG                                3066
3067  3067            ISS = INVTRG( IS )                                     3067
3068  3068            DO 1140 IITG = IS + 1 , JNVTRG                         3068
3069  3069            IF( INVTRG( IITG ) . EQ . ISS ) THEN                   3069
3070  3070            INVTRG( IITG ) = 0                                     3070
3071  3071            END IF                                                 3071
3072  3072  1140      CONTINUE                                               3072
3073  3073  C                                                                3073
3074  3074            ISDUM = 0                                              3074
3075  3075            DO 1150 IITG = 1 , JNVTRG                              3075
3076  3076            IF( INVTRG( IITG ) . NE . 0 ) THEN                     3076
3077  3077            ISDUM = ISDUM + 1                                      3077
3078  3078            INVTRG( ISDUM ) = INVTRG( IITG )                       3078
3079  3079            END IF                                                 3079
3080  3080  1150      CONTINUE                                               3080
3081  3081            JNVTRG = ISDUM                                         3081
3082  3082  C                                                                3082
3083  3083  C     UPDATE THE VERTECIS AND CELLS THAT ARE CONNECTED TO THE DELETED 3083
3084  3084  C     EDGES                                                      3084
3085  3085  C                                                                3085
3086  3086            DO 1160 IE = 1 , IETRIG                                3086
3087  3087            IES = IECRSS( IE )                                     3087
3088  3088  C                                                                3088
3089  3089            IV = JE( 1 , IES )                                     3089
3090  3090            IER = JV( 2 , IV )                                     3090
3091  3091            IIN = ISIGN( 1 , IER )                                 3091
3092  3092            IEE = IABS( IER )                                      3092
3093  3093            IEM = IEE                                              3093
3094  3094            DO 1170 KK = 1 , IETRIG                                3094
3095  3095            JEM = IECRSS( KK )                                     3095
3096  3096            IF( IEE . EQ . JEM ) IEM = NECRSS( KK )                3096
3097  3097  1170      CONTINUE                                               3097
3098  3098            JV( 2 , IV ) = IIN * IEM                               3098
3099  3099  C                                                                3099
3100  3100            IV = JE( 2 , IES )                                     3100
3101  3101            IER = JV( 2 , IV )                                     3101
3102  3102            IIN = ISIGN( 1 , IER )                                 3102
3103  3103            IEE = IABS( IER )                                      3103
3104  3104            IEM = IEE                                              3104
3105  3105            DO 1180 KK = 1 , IETRIG                                3105
3106  3106            JEM = IECRSS( KK )                                     3106
3107  3107            IF( IEE . EQ . JEM ) IEM = NECRSS( KK )                3107
```

```
3108  3108  1180      CONTINUE                                                  3108
3109  3109            JV( 2 , IV ) = IIN * IEM                                  3109
3110  3110  C                                                                   3110
3111  3111  1160      CONTINUE                                                  3111
3112  3112  C                                                                   3112
3113  3113            DO 1190 KK = 1 , JJTRIG                                   3113
3114  3114            IVV = IITRIG( KK )                                        3114
3115  3115            DO 1190 JVDL = 1 , JVDELT                                 3115
3116  3116            IVDL = NVDELT( JVDL )                                     3116
3117  3117            NVDL = IVDELT( JVDL )                                     3117
3118  3118            IF( IVV . EQ . NVDL ) IITRIG( KK ) = IVDL                 3118
3119  3119  1190      CONTINUE                                                  3119
3120  3120  C                                                                   3120
3121  3121            DO 1200 JVDL = 1 , JVDELT                                 3121
3122  3122            IVDL = NVDELT( JVDL )                                     3122
3123  3123            NVDL = IVDELT( JVDL )                                     3123
3124  3124            JV( 2 , IVDL ) = JV( 2 , NVDL )                           3124
3125  3125  1200      CONTINUE                                                  3125
3126  3126  C                                                                   3126
3127  3127            DO 1210 IS = 1 , JNVTRG                                   3127
3128  3128            ISS = INVTRG( IS )                                        3128
3129  3129  C                                                                   3129
3130  3130            IV = JS( 1 , ISS )                                        3130
3131  3131            IVM = IV                                                  3131
3132  3132            DO 1220 KI = 1 , JVDELT                                   3132
3133  3133            JVM = IVDELT( KI )                                        3133
3134  3134            IF( IV . EQ . JVM ) IVM = NVDELT( KI )                    3134
3135  3135  1220      CONTINUE                                                  3135
3136  3136            JS( 1 , ISS ) = IVM                                       3136
3137  3137  C                                                                   3137
3138  3138            IV = JS( 2 , ISS )                                        3138
3139  3139            IVM = IV                                                  3139
3140  3140            DO 1230 KI = 1 , JVDELT                                   3140
3141  3141            JVM = IVDELT( KI )                                        3141
3142  3142            IF( IV . EQ . JVM ) IVM = NVDELT( KI )                    3142
3143  3143  1230      CONTINUE                                                  3143
3144  3144            JS( 2 , ISS ) = IVM                                       3144
3145  3145  C                                                                   3145
3146  3146            IV = JS( 3 , ISS )                                        3146
3147  3147            IVM = IV                                                  3147
3148  3148            DO 1240 KI = 1 , JVDELT                                   3148
3149  3149            JVM = IVDELT( KI )                                        3149
3150  3150            IF( IV . EQ . JVM ) IVM = NVDELT( KI )                    3150
3151  3151  1240      CONTINUE                                                  3151
3152  3152            JS( 3 , ISS ) = IVM                                       3152
3153  3153  C                                                                   3153
3154  3154  1210      CONTINUE                                                  3154
3155  3155  C                                                                   3155
3156  3156            DO 1250 IE = 1 , JNVEDG                                   3156
3157  3157            IEE = INVEDG( IE )                                        3157
3158  3158  C                                                                   3158
3159  3159            IV = JE( 1 , IEE )                                        3159
3160  3160            IVM = IV                                                  3160
3161  3161            DO 1260 KI = 1 , JVDELT                                   3161
3162  3162            JVM = IVDELT( KI )                                        3162
3163  3163            IF( IV . EQ . JVM ) IVM = NVDELT( KI )                    3163
3164  3164  1260      CONTINUE                                                  3164
3165  3165            JE( 1 , IEE ) = IVM                                       3165
3166  3166  C                                                                   3166
3167  3167            IV = JE( 2 , IEE )                                        3167
3168  3168            IVM = IV                                                  3168
3169  3169            DO 1270 KI = 1 , JVDELT                                   3169
3170  3170            JVM = IVDELT( KI )                                        3170
3171  3171            IF( IV . EQ . JVM ) IVM = NVDELT( KI )                    3171
3172  3172  1270      CONTINUE                                                  3172
3173  3173            JE( 2 , IEE ) = IVM                                       3173
3174  3174  C                                                                   3174
3175  3175  1250      CONTINUE                                                  3175
3176  3176  C                                                                   3176
3177  3177  C     UPDATE THE VERTECIS AND EDGES THAT ARE CONNECTED TO THE DELETED 3177
3178  3178  C     CELSS                                                         3178
3179  3179  C                                                                   3179
3180  3180            DO 1280 IS = 1 , ITRIG                                    3180
3181  3181  C                                                                   3181
```

```
3182  3182            ISE = ISCRSS( IS )                                      3182
3183  3183  C                                                                 3183
3184  3184            IE = IABS( JS( 4 , ISE ) )                              3184
3185  3185            ISS = JE( 3 , IE )                                      3185
3186  3186            ISM = ISS                                               3186
3187  3187            DO 1290 KI = 1 , ITRIG                                  3187
3188  3188            JSM = ISCRSS( KI )                                      3188
3189  3189            IF( ISS . EQ . JSM ) ISM = NSCRSS( KI )                 3189
3190  3190  1290      CONTINUE                                                3190
3191  3191            JE( 3 , IE ) = ISM                                      3191
3192  3192  C                                                                 3192
3193  3193            ISS = JE( 4 , IE )                                      3193
3194  3194            ISM = ISS                                               3194
3195  3195            DO 1300 KI = 1 , ITRIG                                  3195
3196  3196            JSM = ISCRSS( KI )                                      3196
3197  3197            IF( ISS . EQ . JSM ) ISM = NSCRSS( KI )                 3197
3198  3198  1300      CONTINUE                                                3198
3199  3199            JE( 4 , IE ) = ISM                                      3199
3200  3200  C                                                                 3200
3201  3201            IE = IABS( JS( 5 , ISE ) )                              3201
3202  3202            ISS = JE( 3 , IE )                                      3202
3203  3203            ISM = ISS                                               3203
3204  3204            DO 1310 KI = 1 , ITRIG                                  3204
3205  3205            JSM = ISCRSS( KI )                                      3205
3206  3206            IF( ISS . EQ . JSM ) ISM = NSCRSS( KI )                 3206
3207  3207  1310      CONTINUE                                                3207
3208  3208            JE( 3 , IE ) = ISM                                      3208
3209  3209  C                                                                 3209
3210  3210            ISS = JE( 4 , IE )                                      3210
3211  3211            ISM = ISS                                               3211
3212  3212            DO 1320 KI = 1 , ITRIG                                  3212
3213  3213            JSM = ISCRSS( KI )                                      3213
3214  3214            IF( ISS . EQ . JSM ) ISM = NSCRSS( KI )                 3214
3215  3215  1320      CONTINUE                                                3215
3216  3216            JE( 4 , IE ) = ISM                                      3216
3217  3217  C                                                                 3217
3218  3218            IE = IABS( JS( 6 , ISE ) )                              3218
3219  3219            ISS = JE( 3 , IE )                                      3219
3220  3220            ISM = ISS                                               3220
3221  3221            DO 1330 KI = 1 , ITRIG                                  3221
3222  3222            JSM = ISCRSS( KI )                                      3222
3223  3223            IF( ISS . EQ . JSM ) ISM = NSCRSS( KI )                 3223
3224  3224  1330      CONTINUE                                                3224
3225  3225            JE( 3 , IE ) = ISM                                      3225
3226  3226  C                                                                 3226
3227  3227            ISS = JE( 4 , IE )                                      3227
3228  3228            ISM = ISS                                               3228
3229  3229            DO 1340 KI = 1 , ITRIG                                  3229
3230  3230            JSM = ISCRSS( KI )                                      3230
3231  3231            IF( ISS . EQ . JSM ) ISM = NSCRSS( KI )                 3231
3232  3232  1340      CONTINUE                                                3232
3233  3233            JE( 4 , IE ) = ISM                                      3233
3234  3234  C                                                                 3234
3235  3235  1280      CONTINUE                                                3235
3236  3236  C                                                                 3236
3237  3237            DO 1350 IE = 1 , IETRIG                                 3237
3238  3238            IES = IECRSS( IE )                                      3238
3239  3239  C                                                                 3239
3240  3240            IS = JE( 3 , IES )                                      3240
3241  3241            ISS = IS                                                3241
3242  3242            DO 1360 KI = 1 , ITRIG                                  3242
3243  3243            ISM = NSCRSS( KI )                                      3243
3244  3244            IF( IS . EQ . ISM ) ISS = ISCRSS( KI )                  3244
3245  3245  1360      CONTINUE                                                3245
3246  3246  C                                                                 3246
3247  3247            IF( ISS . NE . 0 ) THEN                                 3247
3248  3248  C                                                                 3248
3249  3249            IER = JS( 4 , ISS )                                     3249
3250  3250            IEE = IABS( IER )                                       3250
3251  3251            IEM = IEE                                               3251
3252  3252            DO 1370 KI = 1 , IETRIG                                 3252
3253  3253            JEM = IECRSS( KI )                                      3253
3254  3254            IF( IEE . EQ . JEM ) IEM = NECRSS( KI )                 3254
3255  3255  1370      CONTINUE                                                3255
```

```
3256   3256            JS( 4 , ISS ) = ISIGN( 1 , IER ) * IEM                  3256
3257   3257   C                                                                3257
3258   3258            IER = JS( 5 , ISS )                                     3258
3259   3259            IEE = IABS( IER )                                       3259
3260   3260            IEM = IEE                                               3260
3261   3261            DO 1380 KI = 1 , IETRIG                                 3261
3262   3262            JEM = IECRSS( KI )                                      3262
3263   3263            IF( IEE . EQ . JEM ) IEM = NECRSS( KI )                 3263
3264   3264   1380     CONTINUE                                                3264
3265   3265            JS( 5 , ISS ) = ISIGN( 1 , IER ) * IEM                  3265
3266   3266   C                                                                3266
3267   3267            IER = JS( 6 , ISS )                                     3267
3268   3268            IEE = IABS( IER )                                       3268
3269   3269            IEM = IEE                                               3269
3270   3270            DO 1390 KI = 1 , IETRIG                                 3270
3271   3271            JEM = IECRSS( KI )                                      3271
3272   3272            IF( IEE . EQ . JEM ) IEM = NECRSS( KI )                 3272
3273   3273   1390     CONTINUE                                                3273
3274   3274            JS( 6 , ISS ) = ISIGN( 1 , IER ) * IEM                  3274
3275   3275   C                                                                3275
3276   3276            END IF                                                  3276
3277   3277   C                                                                3277
3278   3278            IS = JE( 4 , IES )                                      3278
3279   3279            ISS = IS                                                3279
3280   3280            DO 1400 KI = 1 , ITRIG                                  3280
3281   3281            ISM = NSCRSS( KI )                                      3281
3282   3282            IF( IS . EQ . ISM ) ISS = ISCRSS( KI )                  3282
3283   3283   1400     CONTINUE                                                3283
3284   3284   C                                                                3284
3285   3285            IF( ISS . NE . 0 ) THEN                                 3285
3286   3286   C                                                                3286
3287   3287            IER = JS( 4 , ISS )                                     3287
3288   3288            IEE = IABS( IER )                                       3288
3289   3289            IEM = IEE                                               3289
3290   3290            DO 1410 KI = 1 , IETRIG                                 3290
3291   3291            JEM = IECRSS( KI )                                      3291
3292   3292            IF( IEE . EQ . JEM ) IEM = NECRSS( KI )                 3292
3293   3293   1410     CONTINUE                                                3293
3294   3294            JS( 4 , ISS ) = ISIGN( 1 , IER ) * IEM                  3294
3295   3295   C                                                                3295
3296   3296            IER = JS( 5 , ISS )                                     3296
3297   3297            IEE = IABS( IER )                                       3297
3298   3298            IEM = IEE                                               3298
3299   3299            DO 1420 KI = 1 , IETRIG                                 3299
3300   3300            JEM = IECRSS( KI )                                      3300
3301   3301            IF( IEE . EQ . JEM ) IEM = NECRSS( KI )                 3301
3302   3302   1420     CONTINUE                                                3302
3303   3303            JS( 5 , ISS ) = ISIGN( 1 , IER ) * IEM                  3303
3304   3304   C                                                                3304
3305   3305            IER = JS( 6 , ISS )                                     3305
3306   3306            IEE = IABS( IER )                                       3306
3307   3307            IEM = IEE                                               3307
3308   3308            DO 1430 KI = 1 , IETRIG                                 3308
3309   3309            JEM = IECRSS( KI )                                      3309
3310   3310            IF( IEE . EQ . JEM ) IEM = NECRSS( KI )                 3310
3311   3311   1430     CONTINUE                                                3311
3312   3312            JS( 6 , ISS ) = ISIGN( 1 , IER ) * IEM                  3312
3313   3313   C                                                                3313
3314   3314            END IF                                                  3314
3315   3315   C                                                                3315
3316   3316   1350     CONTINUE                                                3316
3317   3317   C                                                                3317
3318   3318            DO 1440 IE = 1 , IETRIG                                 3318
3319   3319            IEM = NECRSS( IE )                                      3319
3320   3320            JEM = IECRSS( IE )                                      3320
3321   3321   C                                                                3321
3322   3322            DO 1450 IK = 1 , 5                                      3322
3323   3323            JE( IK , IEM ) = JE( IK , JEM )                         3323
3324   3324   1450     CONTINUE                                                3324
3325   3325   C                                                                3325
3326   3326            XE( 1 , IEM ) = XE( 1 , JEM )                           3326
3327   3327            XE( 2 , IEM ) = XE( 2 , JEM )                           3327
3328   3328   C                                                                3328
3329   3329            XN( IEM ) = XN( JEM )                                   3329
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3330  3330            YN( IEM ) = YN( JEM )                                    3330
3331  3331            XXN( IEM ) = XXN( JEM )                                  3331
3332  3332            YYN( IEM ) = YYN( JEM )                                  3332
3333  3333            XMIDL( IEM ) = XMIDL( JEM )                              3333
3334  3334            YMIDL( IEM ) = YMIDL( JEM )                              3334
3335  3335            XYMIDL( IEM ) = XYMIDL( JEM )                            3335
3336  3336  1440      CONTINUE                                                 3336
3337  3337  C                                                                  3337
3338  3338            DO 1460 IS = 1 , ITRIG                                   3338
3339  3339            ISM = NSCRSS( IS )                                       3339
3340  3340            JSM = ISCRSS( IS )                                       3340
3341  3341  C                                                                  3341
3342  3342            DO 1470 IK = 1 , 6                                       3342
3343  3343            JS( IK , ISM ) = JS( IK , JSM )                          3343
3344  3344  1470      CONTINUE                                                 3344
3345  3345  C                                                                  3345
3346  3346            XS( 1 , ISM ) = XS( 1 , JSM )                            3346
3347  3347            XS( 2 , ISM ) = XS( 2 , JSM )                            3347
3348  3348            XS( 3 , ISM ) = XS( 3 , JSM )                            3348
3349  3349  C                                                                  3349
3350  3350            SAREA( ISM ) = SAREA( JSM )                              3350
3351  3351            KSDELT( ISM ) = KSDELT( JSM )                            3351
3352  3352  C                                                                  3352
3353  3353            DO 1480 IK = 1 , MHQ                                     3353
3354  3354            HYDV( ISM , IK ) = HYDV( JSM , IK )                      3354
3355  3355  1480      CONTINUE                                                 3355
3356  3356  C                                                                  3356
3357  3357            HYDFLX( ISM , 4 ) = HYDFLX( JSM , 4 )                    3357
3358  3358            HYDFLX( ISM , 1 ) = HYDFLX( JSM , 1 )                    3358
3359  3359            HYDFLX( ISM , 2 ) = HYDFLX( JSM , 2 )                    3359
3360  3360  C                                                                  3360
3361  3361  1460      CONTINUE                                                 3361
3362  3362  C                                                                  3362
3363  3363            NV = NVM                                                 3363
3364  3364            NE = NEM                                                 3364
3365  3365            NS = NSM                                                 3365
3366  3366  C                                                                  3366
3367  3367            DO 1490 IENN = 1 , IJTRIG                                3367
3368  3368            IE = JUE( IENN )                                         3368
3369  3369            DO 1490 KI = 1 , IETRIG                                  3369
3370  3370            JEM = IECRSS( KI )                                       3370
3371  3371            IF( IE . EQ . JEM ) JUE( IENN ) = NECRSS( KI )           3371
3372  3372  1490      CONTINUE                                                 3372
3373  3373  C                                                                  3373
3374  3374            DO 1540 IENN = 1 , JJTRIG                                3374
3375  3375            IVV = IITRIG( IENN )                                     3375
3376  3376            IF( JV( 1 , IVV ) . NE . 3 ) CALL RELAXY( IVV )          3376
3377  3377  1540      CONTINUE                                                 3377
3378  3378  C                                                                  3378
3379  3379            DO 1500 IENN = 1 , IJTRIG                                3379
3380  3380            IE = JUE( IENN )                                         3380
3381  3381            CALL RECNC( IE , IDONE , ITL , ITR , JA , JB , JC , JD )                3381
3382  3382            CALL RECNC( JA , JADONE , ITL , ITR , JAA , JAB , JAC , JAD )           3382
3383  3383            CALL RECNC( JB , JBDONE , ITL , ITR , JBA , JBB , JBC , JBD )           3383
3384  3384            CALL RECNC( JC , JCDONE , ITL , ITR , JCA , JCB , JCC , JCD )           3384
3385  3385            CALL RECNC( JD , JDDONE , ITL , ITR , JDA , JDB , JDC , JDD )           3385
3386  3386  1500      CONTINUE                                                 3386
3387  3387  C                                                                  3387
3388  3388            DO 1510 IPRTCL = 1 , NPT                                 3388
3389  3389            ISM = IJKPRT( IPRTCL )                                   3389
3390  3390            DO 1510 KI = 1 , ITRIG                                   3390
3391  3391            JSM = NSCRSS( KI )                                       3391
3392  3392            IF( ISM . EQ . JSM ) IJKPRT( IPRTCL ) = NSMNPT           3392
3393  3393  1510      CONTINUE                                                 3393
3394  3394  C                                                                  3394
3395  3395  C     UPDATE THE JSDELT ARRAY                                      3395
3396  3396  C                                                                  3396
3397  3397            DO 1530 IS = 1 , ISDELT                                  3397
3398  3398            JSP = JSDELT( IS )                                       3398
3399  3399            DO 1530 KI = 1 , ITRIG                                   3399
3400  3400            JSM = ISCRSS( KI )                                       3400
3401  3401            IF( JSP . EQ . JSM ) JSDELT( IS ) = NSCRSS( KI )         3401
3402  3402  1530      CONTINUE                                                 3402
3403  3403  C                                                                  3403
```

```
3404   3404              INOCTR = 1                                                    3404
3405   3405   C                                                                      3405
3406   3406   C --- EXIT POINT FROM SUBROUTINE ----------------------------------    3406
3407   3407   C                                                                      3407
3408   3408   C     ------                                                           3408
3409   3409         RETURN                                                           3409
3410   3410   C     ------                                                           3410
3411   3411   C                                                                      3411
3412   3412   C     ---                                                              3412
3413   3413         END                                                              3413
```

APPENDIX C

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A REVIEW OF PROPULSION APPLICATIONS OF THE PULSED DETONATION ENGINE CONCEPT

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A REVIEW OF PROPULSION APPLICATIONS OF THE PULSED DETONATION ENGINE CONCEPT

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Introduction

The early development leading to practical propulsion engines was almost completely associated with steady state engine concepts. Unsteady concepts, which initially appeared promising, never evolved from the conceptual state and have remained for the most part unexplored. The early work in unsteady propulsion suffered from a lack of appropriate analytical and design tools, a condition which seriously impeded the advancement of the unsteady concepts to a practical stage.

In this paper we review the historical development of unsteady propulsion by concentrating on one particular concept, the intermittent detonation engine, and discuss current research activities in this area. A review of the literature[1-24] reveals that a significant body of experimental and theoretical research exists in the area of unsteady propulsion. However, this research has not been extended to the point where a conclusive quantitative comparison can be made between impulsive engine concepts and steady state concepts. For example, the analysis given in References 8-11 of the performance of a detonation engine concept does not include frequency dependence, nor any analysis of losses due to multi-cycle operation. A new generation of analytical and computational tools exists today and allows us to revisit and analyse such issues with a high degree of confidence. Numerical simulation has developed to the state where it can now provide time dependent two and three dimensional modeling of complex internal flow processes[20,24,25] and will eventually result in tools for systematically analysing and optimising engineering design. In addition to a review of applications of the Pulsed Detonation Engine Concept here we will report results of a numerical study of the gasdynamics of a model of an air-breathing detonation engine with detailed analysis of the nonsteady flow pattern. This study was performed using new unsteady CFD tools which we will also describe.

Our paper is structured as follows: 1) historical review of the pulsed detonation development efforts; 2) description of the basic phenomenology of the air-breathing Pulsed Detonation Engine concept; 3) description of the mathematical formulation and new numerical scheme used to simulated the problem; 4) discussion of the simulation results; and 5) conclusions.

Historical Review

Constant Volume Combustion

From the very early development of jet-propulsion engines it was known that an engine based on a constant volume combustion process achieves higher efficiency than a constant pressure engine. This follows from a thermodynamic analysis of the engine cycle.[1]

Constant volume combustion was used in gas turbine engines at the beginning of this century, and the first gas turbine engines in commercial use were based on the constant volume cycle. Jet-propulsion engines were one of the applications of the constant volume cycle (or explosion cycle) which was explored in the late 1940s.[2] Although the explosion cycle operates at a larger pressure variation in the combustion chamber than in a pulse-jet[3,4], the cycle actually realised in these engines was not a fully constant volume one since the combustion chamber was open ended[2]. In Reference 2 the maximum pressure ratio measured in an explosion cycle engine was 3:1, whereas the pressure ratio for the same mixture under the assumption of a constant volume cycle would be 8:1. Also, this engine was limited by the available frequency of cycles, which in turn is limited by the reaction rate. A simple calculation [2] showed that if the combustion time could be reduced in this engine from 0.006 sec to 0.003 sec, the thrust per pound of mixture would increase 100%. Thus the explosion-cycle engine has two main disadvantages:

- Constrained volume combustion (as distinguished from constant volume combustion) does not take full advantage of the pressure rise characteristic of the constant volume combustion process.
- The frequency of the explosion cycle is limited by the reaction rate, which is only slightly higher than the deflagrative combustion rate.

The main advantage of the constant pressure cycle is that it leads to engine configurations with steady state

processes of injection of the fuel and oxidiser, combustion of the mixture, and expansion of the combustion products. These stages can be easily identified and the engine designer can optimize them on the basis of relatively simple steady state considerations.

At the same time an engine based on constant volume combustion will have an intermittent mode of operation, which may complicate its design and optimisation. We are interested in the question of whether this complication is worth the potential gains in engine efficiency.

Pulsed Detonation Engine as an Ultimate Constant Volume Combustion Concept

The detonation process, due to the very high rate of reaction, permits construction of a propulsion engine in which the constant volume process can be fully realised. In detonative combustion, the strong shock wave, which is part of the detonation wave, acts like a valve between the detonation products and the fresh charge. The speed of the detonation wave is about two orders of magnitude higher than the speed of a typical deflagration. This allows the design of propulsion engines with a very high power density. Usually, each detonation is initiated separately by a fully controlled ignition device, and the cycle frequency can be changed over a wide range of values. This also means that a device based on a detonative combustion cycle can be scaled and its operating parameters can be modified for a range of required output conditions. There have been numerous attempts to take advantage of detonative combustion for engine applications. In the following we give a description of the most relevant past experimental and analytical studies of the detonation engine concept.

Hoffmann's Report.

The first reported work on intermittent detonation is attributed to Hoffmann [5] in 1940. He operated an intermittent detonation test stand with acetylene-oxygen and bensine-oxygen mixtures. The addition of water vapor was used to prevent the highly sensitive acetylene-oxygen mixture from premature detonation. Hoffmann[5] indicated the importance of the spark plug location in reference to tube length and diffuser length. It was found that a continuous injection of the combustible mixture leads to only a narrow range of ignition frequencies which will produce an intermittent detonation cycle. These frequencies are governed by the time required for the mixture to reach the igniter, time of transition from deflagration to detonation, and time of expansion of the detonation products. Hoffmann attempted to find the optimum cycle frequency experimentally. It was discovered that detonation-tube firing occurred at lower frequencies than the spark-plug energising frequencies indicating that the injection flow rate and ignition were out of phase. Events prevented further work by Hoffmann and co-workers.

Nicholls Experiments.

A substantial effort in intermittent detonation engine research was done by a group headed by J. A. Nicholls[6-10] of The University of Michigan beginning in the early 50's. The most relevant work concerns a set of experiments carried out in a six foot long detonation tube[6]. The detonation tube was constructed from a one inch internal diameter stainless steel tube. The fuel and oxidiser were injected under pressure from the left end of the tube and ignited at the some distance down stream. The tube was mounted on a pendulum platform, suspended by support wires. Thrust for single detonations was measured by detecting tube (platform) movement relative to a stationary pointer. For multi-cycle detonations thrust measurement was achieved by mounting the thrust end of the tube to the free end of the cantilever beam. In addition to direct thrust measurements the temperature on the inner wall of the detonation tube was measured.

Fuel mixtures of hydrogen/oxygen, hydrogen/air, acetylene-oxygen and acetylene-air mixtures were used. The gaseous oxidiser and fuel were continuously injected at the closed end wall of the detonation tube and three fixed flow rates were used. Under these conditions the only parameters which could be varied were the fuel/oxidiser ratio and frequency of ignition. A maximum gross thrust of $\approx 3.2lb$ was measured in hydrogen/air mixture at the frequency of ≈ 30 detonations per second. The most promising results were demonstrated for the H_2/Air mixture, where a fuel specific impulse of $I_{sp} = 2100$ sec was reached. The maximum frequency of detonations obtained in all experiments was 35 Hs. The temperature measurements on the inner wall showed that for the highest frequency of detonations the temperature did not exceed 800° F.

In their later work,[8,9,10] the University of Michigan group concentrated on development of the Rotating Detonation Wave Rocket Motor. No further work on the pulsed detonation cycle was pursued.

Krzycki Experiments

In a setup somewhat similar to Nicholl's, L. J. Krzycki[11] performed an experimental investigation of intermittent detonations with frequencies up to 60 cps. An attempt was also made to analyze the basic phenomena using unsteady gas dynamic theory. Krzycki's attempt to analyse the basic phenomena relied on wave diagrams to trace characteristics, assumptions of isentropic flow for detonation and expansion, and incompressible flow for mixture injection processes. The most convincing

data from the experiments is the measurement of thrust for a range of initiation frequencies and mixture flow rates. Unfortunately no direct pressure measurement in the device are reported so that only indirect evidence exists of the nature of the process observed.

The basic test stand used by Krzycki is very similar to that used by Nicholls et al.[6] The length of the detonation tube and internal diameter were exactly the same as those in Nicholl's experiments. A Propane/Air mixture was continuously injected through a reversed-flow diffuser for better mixing, and ignited at the some distance from the injection point by an automobile spark plug. The spark frequency was varied from 1 to 60 cps. The spark plug power output was varied inversely with the initiation frequency and at the frequency of 60 cps was only 0.65 Joule. This fact alone eliminated the possibility of direct initiation of the detonation wave by the spark and consequently all of the experiments must have been based on transition from deflagration to detonation. According to experimental data and theory,[12] for direct initiation of a mixture of propane-air at the detonability limits, an energy release on the order of 10^6 Joules is required. Thus, the required deflagration-detonation transition region length would have been prohibitively large for the propane-air mixture. It follows that in all of the experiments a substantial part of the process was deflagrative. This resulted in low efficiency, and negligible thrust. Krzycki repeated the experiments of Nicholls using exactly the same size detonation tube and basically the same rates of injection of the detonable mixture. Krzycki's experimental results are very well documented, allowing a clear picture of the physical processes occurring in the tube to be deduced. A conclusion, arrived at by the author, was that thrust was possible from such a device but practical applications did not appear promising. It is unfortunate that, possibly based on Krzycki's extensive but misleading results, all experimental work related to the pulsed detonation engine concept stopped at this time.

Work Reported in Russian sources on Pulse Detonation Devices

A review of the Russian literature has not uncovered work concerning applications of pulsed detonation devices to propulsion. However there are numerous reports of applications of such devices for producing nitrogen oxide[13] (an old Zeldovich idea to bind nitrogen directly from air to produce fertilisers) and as rock crushing devices[14].

Korovin et al.[15] provide a most interesting account of the operation of a commercial detonation reactor. The main objective of this study was to examine the efficiency of thermal oxidation of nitrogen in an intermittent detonative process as well as an assessment of such technological issues as the fatigue of the reactor parts exposed to the intermittent detonation waves over a prolonged time. The reactor consisted of a tube with an inner diameter of 16 mm and length 1.3 m joined by a conical diffuser to a second tube with an inner diameter of 70 mm and length 3 m. The entire detonation reactor was submerged in running water. The detonation mixture was introduced at the end wall of the small tube. CH_4, O_2 and N_2 comprised the mixture composition and the mixture ratios were varied during the continuous operation of the reactor. The detonation wave velocity was measured directly by piezoelectric sensors placed in the small and large tubes. The detonation initiation frequency in the reactor was 2-16 Hz. It is reported that the apparatus operated without significant changes for 2000 hours.

Smirnov and Boichenko[14] studied intermittent detonations of gasoline-air mixtures in a 3 m long and 22 mm inner diameter tube operating in the 6-8 Hz ignition frequency range. The main motivation of this work was to improve the efficiency of a commercial rock crushing apparatus based on intermittent detonations of the gasoline-air mixtures.[15] The authors investigated the dependence of the length of the transitional region from deflagration to detonation on the initial temperature of the mixture.

As a result of the information contained in the Soviet reports, it can be concluded that reliable commercial devices based on intermittent detonations can be constructed and operated.

Development of the Blast Propulsion System at JPL

Work at the Jet Propulsion Laboratory (JPL) by Back, Varsi and others[16–19] concerned an experimental and theoretical study of the feasibility of a rocket thruster using intermittent detonations of solid explosive useful for propulsion in dense or high-pressure atmospheres of certain solar system planets. The JPL work was directed at very specific applications; however, the studies[17–19] addressed some key issues of devices using unsteady process such as propulsion efficiency. The JPL studies have important implications to pulsed detonation propulsion systems.

Reference 19 gives the basic description of the test stand used. In this work a Deta sheet type C explosive was detonated inside a small detonation chamber attached to nozzles of various length and geometry. The nozzles, complete with firing plug, were mounted in a containment vessel which could be pressurised with the mixture of various inert gases from vacuum to 70 atm. The apparatus measured directly the thrust generated by single detonations of a small amount of solid explosive charge expanding into conical or straight nozzles.

Thrust and specific impulse was measured by a pendulum balance system.

Results obtained from an extensive experimental study of the explosively driven rocket have lead to the following conclusions. First, rockets with long nozzles show increasing specific impulse with increasing ambient pressure in CO_2 and N_2. Short nozzles, on the other hand, show that specific impulse is independent of ambient pressure. Most importantly, most of the experiments obtained a relatively high specific impulse of 250 seconds and larger. This result is all the more striking since the detonation of a solid explosive yields a relatively low energy release of approximately 1000 cal/gm compared with 3000 cal/gm obtained in hydrogen oxygen combustion. Thus, it can be concluded that the total losses in a thruster based on unsteady expansion are not prohibitive and, in principle, very efficient propulsion systems operating on intermittent detonations are possible.

Detonation Engine Studies at Naval Postgraduate School

A modest exploratory study of a propulsion device utilising detonation phenomena was conducted at the Naval Postgraduate School.[20–23] During this study, several fundamentally new elements were introduced to the concept distinguishing the new device from previous ones.

First, it is important to note that the experimental apparatus constructed by Helman et al.[21] was the first successful self aspirating air breathing detonation device. Intermittent detonation frequencies of 25 Hz were obtained. This frequency was in phase with the fuel mixture injection through timed fuel valve opening and spark discharge. The feasibility of intermittent injection was established. Pressure measurements showed conclusively that a detonation process occurred at the frequency chosen for fuel injection. Further, self aspiration was shown to be effective. Finally, the effectiveness of a primary detonation as a driver for the main detonation was clearly demonstrated. Although the NPS studies were abbreviated, many of the technical issues considered to be essential for efficient intermittent detonation propulsion were addressed with positive results.

Simulations of Pulsed Detonation Engine Cycle at NASA-Ames Center

Recently Cambier and Adelman [24] carried out numerical simulations of a pulsed detonation engine cycle taking into account finite rate chemistry. Unfortunately, the simulations were restricted to a quasi-one dimensional model. The configuration considered had a 6 cm inner diameter 50 cm long main chamber which was attached to a 43 cm diverging nozzle. It was assumed that a stoichiometric mixture of hydrogen/air at 3.0 atmospheres is injected from an inlet on the closed end wall of the detonation chamber. At such conditions Cambier and Adelman estimated a large range of possible detonation frequencies of engine operation up to 667 Hz. The origin of this estimate is not clear from their work, since according to their simulations, the detonation, expansion and fresh charge fill requires 2.5 msec. This value leads to a maximum frequency of 400 Hz. The simulated engine performance yielded a large average thrust of 893 lb and an unusually high specific impulse of 6507 sec. These simulations were the first to demonstrate the use of modern CFD methods to address the technical issues associated with unsteady pulsed detonation concepts.

In the remaining sections we discuss a particular propulsion concept based on the results of the experiments of Helman et al.[22] and describe a computational study of its performance characteristics. The unsteady numerical scheme used for the study made use of unique simulation techniques; the key ingredients of these techniques are also described.

A Generic Pulsed Detonation Engine

The generic device we consider here is a small engine 15 cm long and 15 cm in diameter. The combustible gas mixture is injected at the closed end of the detonation chamber and a detonation wave propagates through the mixture. The size of the engine suggests a small payload, but the concept can be extended to larger payloads simply by scaling up the size of the detonation chamber and possibly combining a number of engines into one large propulsion engine. A key issue in the pulsed detonation engine concept is the design of the main detonation chamber. The detonation chamber geometry determines the propulsion efficiency and the duration of the cycle (frequency of detonations). Since the fresh charge for the generic engine is supplied from the external flow field, the efficiency of the engine depends on the interaction of the surrounding flow with the internal flow dynamics. The range of the physical processes requiring simulation in order to model the complex flow phenomena associated with the detonation engine performance is very broad. A partial list is:

1. Initiation and propagation of the detonation wave inside the chamber,
2. Expansion of the detonation products from the chamber into the air stream around the chamber at flight Mach numbers.
3. Reverse flow from the surrounding air into the chamber resulting from over expansion of the detonation products,
4. Pressure buildup in the chamber due to reverse flow. The flow pattern inside the chamber during post-exhaust pressure buildup determines the strategy

for mixing the next detonation charge,

5. Strong mutual interaction between the flow processes inside the chamber and flow around the engine.

All of these processes are interdependent and their timing is crucial to the engine efficiency. Thus, unlike simulations of steady state engines, the phenomena described above can not be evaluated independently.

The need to resolve the flow regime inside the chamber accounting for nozzles, air inlets etc., and at the same time resolve the flow around the engine, where the flow regime varies from high subsonic, locally transonic and supersonic, makes it a challenging computational problem.

The main issue is to determine the timing of the air intake for the fresh gas charge. It is sufficient to assume invicid flow for the purpose of simulating the expansion of the detonation products and fresh gas intake. In the following we present the first results of an invicid simulation of the detonation cycle in a cylindrical chamber. First, we describe our computational method for solving the time dependent Euler equations used in the study.

The Unsteady Euler Solver

A new second order algorithm for solving the Euler equations on an unstructured grid was used in our study of the detonation concept. The approach is based on first and second order Godunov methods. The method leads to an extremely efficient and fast Flow Solver which is fully vectorised and easily lends itself to parallelisation. The low memory requirements and speed of the method are due to the use of a unique data structure.

Until recently most CFD simulations were carried out with logically structured grids. Vectorisation and/or parallelisation did not present a problem. The increased need for simulation of flow phenomena in the vicinity of complex geometrical bodies and surfaces has led to the development of CFD codes for logically unstructured grids. The most successful of these unstructured grid codes are based on finite elements or finite volume methods. For an unstructured grid in two-dimensions, the computational domain is usually covered by triangles and the indices of the arrays containing the values of the hydrodynamic flow quantities are not related directly to the actual geometric location of a node. The calculations performed on unstructured grids evolve around the elemental grid shape (e.g. the triangle for two-dimensional problems) and there is no obvious pattern to the order in which the local integrations should be performed. Explicit integration of hydrodynamic problems on an unstructured grid requires that a logical substructure should be created which identifies the locations in the global arrays of all the local quantities necessary for the integration of one element. This usually results in a large price in computational efficiency, in memory requirements, and in code complexity. As a consequence, vectorisation for the conventional unstructured grid methods has concentrated on rearrangement of the data structure in a manner such that these locally centered data structures appear as global arrays. This can be done to some extent using machine dependent Gather-Scatter operations.[25,26] Additional optimisation can be achieved using localisation and search algorithms. However, these methods are complex and result in marginal improvement. Most optimised unstructured codes to date run considerably slower and require an order of magnitude more memory per grid cell then their structured counterparts. Parallelisation of the conventional unstructured codes is even more difficult, there is very little experience with unstructured codes on massively parallel computers.

The method we have developed overcomes these difficulties and results in code with speed and memory requirements comparable to those found in structured grid codes. Moreover, the ability to construct grids with arbitrary resolution leads to a flexibility in dealing with complex geometries not attainable with structured grids. The essence of the method is based on independent flux calculation across the edges of a dual baricentric grid, followed by node integration. This approach is order independent. Below we give the essential details of our algorithm; a complete description follows later.

Basic Integration Algorithm.

We begin by describing the first order Godunov method for the system of two-dimensional (axi-symmetric) Euler equations written in conservation law form as

$$\frac{\partial \vec{Q}}{\partial t} + \frac{\partial \vec{F}}{\partial x} + \frac{\partial \vec{G}}{\partial r} = -\frac{1}{r}\vec{C} \ , \qquad (1)$$

where,

$$\vec{Q} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ e \end{pmatrix}, \ \vec{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (e+p)u \end{pmatrix}, \ \vec{G} = \begin{pmatrix} \rho v \\ \rho vu \\ \rho v^2 + p \\ (e+p)v \end{pmatrix},$$

$$\vec{C} = \begin{pmatrix} \rho v \\ \rho vu \\ \rho v^2 \\ (e+p)v \end{pmatrix}.$$

Here u and v are the x and r velocity vector components, p is the pressure, ρ is the density and e is the total energy of the fluid per unit volume. It is assumed that a mixed (initial conditions, boundary conditions) problem is properly posed for the set of equations (1)

and that an initial distribution of the fluid parameters is given at $t = 0$ and some boundary conditions defining a unique solution are specified on the boundary of the computational domain.

We look for a solution of the system of equations represented by Eq. 1 in the computational domain covered by an unstructured grid. As an example, Fig. 1a shows the unstructured triangular grid used in the pulsed detonation engine simulation. Here most of the computational effort is committed to the resolution of the flow inside the engine detonation chamber and in the immediate vicinity of the nozzle. In Figure 1b an enlargement of the nozzle region is shown, illustrating the ability to represent geometry of arbitrary complexity and with localized resolution.

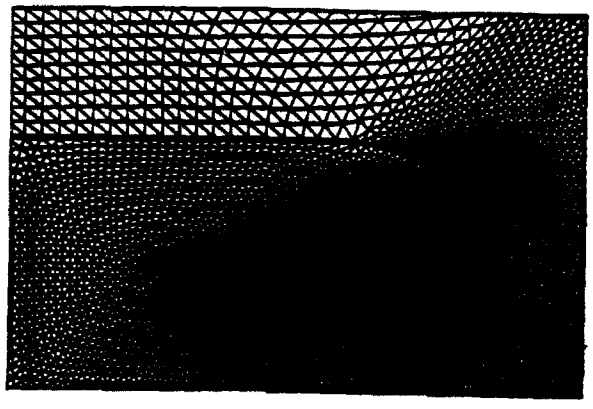


Figure 1a Computational domain and grid used in simulation of PDE operation.

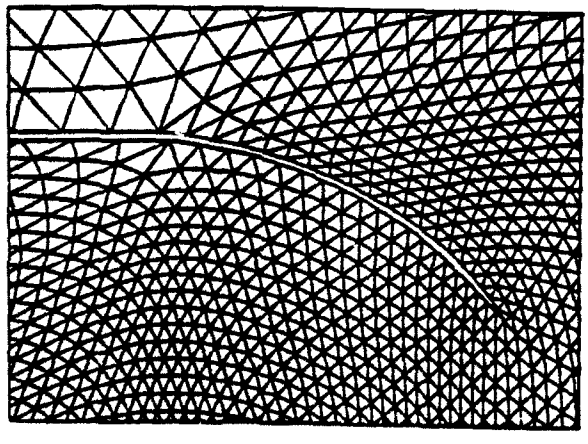


Figure 1b Enlargment of computational grid in the vicinity of the PDE nozzle.

Fig. 2 displays a fragment of the computational domain with the corresponding dual grid. The secondary or dual grid is formed by connecting the baricenters of the primary mesh, thus forming finite polygons around the primary vertices.

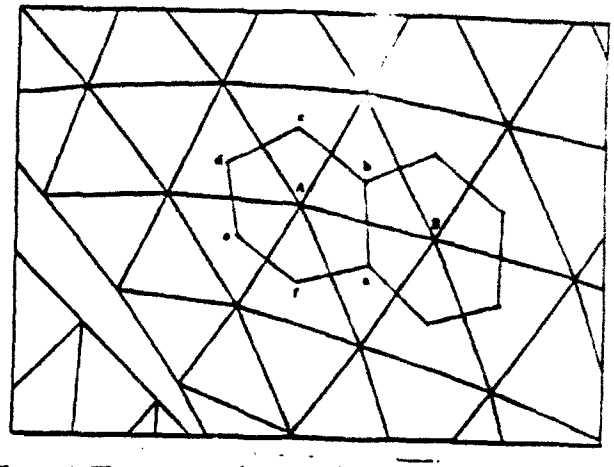


Figure 2 The primary (triangles) and secondary (polygons) unstructured grids.

We have found, as have others,[27] that the best practical representation of the integration volume is obtained when the dual grid is formed by connecting baricenters of the triangles. Integration by the Godunov method[28] can be divided into two basic steps: 1. Calculation of the fluxes at the edges of the secondary grid using solutions of a set of one dimensional Riemann problems; 2. Integration of the system of partial differential equations which amounts to addition of all the fluxes for every polygon at a particular time step.

To define the fluxes for the grid shown in Fig. 2 at every edge of the main grid it is necessary to solve the corresponding Riemann problem. For example, to define the flux at the edge ab, we solve the Riemann problem between points A and B. The solution of this problem is in coordinates local to the edge of the dual grid ab so that the tangential component of velocity will be directed along this edge (ab). Implementation of our approach requires maintaining strict consistency when defining the "left" and "right" states for the Riemann problems at the edges ab, bc, cd, de, ef, and fa. For this reason we define not only the location of the vertices and lengths of the edges but also the direction of the edges with respect to the primary grid. For the clockwise integration pattern in the same Polygon, point A will be the "right" state for all the Riemann problems related to this point and the neighbor will represent the "left" side of the diaphragm.

It is easy to see that the flux calculation is based on information at only two nodes and requires single geometrical parameters defining the edge of the secondary

grid that dissects the line connecting the two points. Thus, we can calculate all the values needed for flux calculation in one loop over all edges of the primary grid without any details related to the geometrical structures which these edges form. This in turn assures parallelisation or vectorisation of the algorithm for the bulk of the calculations involving the Riemann solver that provides the first order flux. The only procedure not readily parallelisable is the integration of the fluxes for the flow variables at the vertices of the grid. Here we use the "edge coloring" technique which allows us to split the flux addition loop into 7 or 8 loops for edges of different color. Each of these loops is usually large enough not to impair vectorisation. At this stage all the fluxes are added with their correct sign corresponding to the chosen direction of integration within the cell. The amount of calculation required here is minimal since the fluxes are known and need only to be multiplied at each time step by a simple factor and added to the vertex quantity.

Second Order Integration Algorithm

The second order solver is constructed along lines similar to that from the first-order method. At each cell edge the Riemann problem is solved for some specified pair of left and right conditions. The solution to this Riemann problem is then used in the calculation of fluxes which are added later to advance to the next integration step. The extension to second order is achieved by using extrapolation in space and time to obtain time-centered left and right limiting values as inputs for the Riemann problem. The basic implementation of the method of calculation of second order accurate fluxes is fundamentally the same as for one dimensional cases. The only difference is in the method of obtaining linear extrapolation of the flow variables as a first guess of their value at the edges of the dual grid. To obtain the first guess we need to know the gradient of some gasdynamical parameter U at the vertices of the primary mesh. The value of ∇ U can be evaluated by using a linear path integral along the edges which delineates the finite volume associated with the vertex. For vertex A in Figure 2 :

$$\int_A \nabla U dA = \oint_l U n \, dl \qquad (2)$$

where integration along the path l in this case is equivalent to integration along the edges ab, bc, cd, de, ef, fa. Knowing the gradient of the gasdynamic parameter in the volume related to vertex A will allow us to extrapolate the values of this parameter at any location within the volume. This permits us to evaluate the first guess for U at the edges of the dual grid. The final four steps of the implementation of the second order algorithm has been described previously.[28]

A schematic flow chart of the basic steps of the second order algorithm implementation is shown in Figure 3.

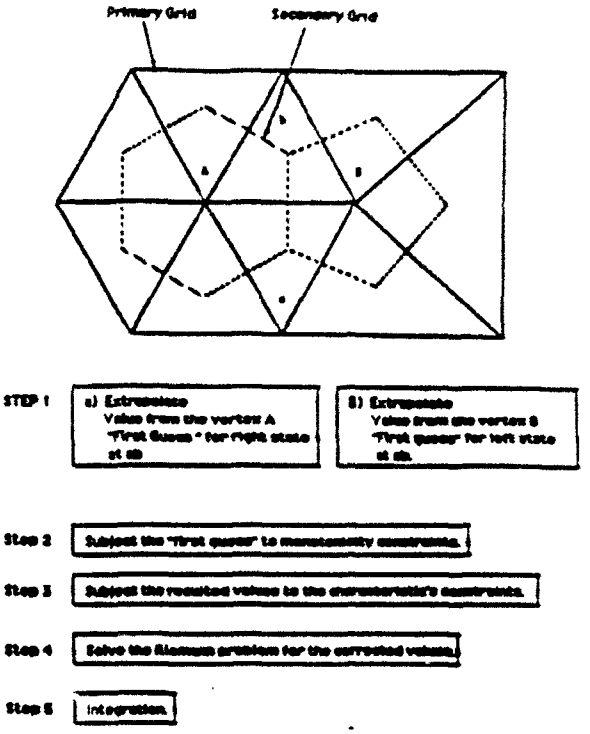


Figure 3 Grid schematic and outline of steps for second order Godunov method.

Simulations of the Generic Pulsed Detonation Engine

In this section we present sample results of simulations of the generic PDE device using the numerical code described in the preceding section. In Figure 1a the computational domain containing the PDE main detonation chamber is shown covered with the unstructured grid. In our sample simulation we have chosen a small ≈ 15 cm long and ≈ 15 cm internal diameter cylindrical chamber with a small converging nozzle. This geometry is one of a number of the geometries we have analyzed in a parametric study whose goal is to evaluate and optimise a typical PDE device. The device shown in Figure 1a does not represent the optimum and is given here to illustrate our methodology. We consider a situation when the PDE serves as a main thruster for a vehicle traveling in air with the velocity of M = 0.9 and located at the aft end of the vehicle. The main objectives of the simulations presented here are:

1. To find the maximum cycle frequency. This is determined by the time required from detonation, exhaust of combustion products and intake of fresh charge for the next detonation.

2. To calculate the thrust produced during each cycle and the integrated thrust as a function of time.

The simulation begins at $t = 0$ when a strong detonation wave is initiated inside the detonation chamber. Initially the detonation wave travels from the open aft end of the chamber towards the interior with a maximum velocity of 1800 $\frac{m}{sec}$ and maximum pressure of $20 * 10^5 Pa$. The distribution of pressure, velocity, and density of the detonation wave is defined through the *selfsimilar* solution for a planar detonation wave. The wave was directed towards the interior of the chamber to capture the kinetic energy of the wave and to prolong exposure of the inner chamber walls to the high pressure. In Figure 4a simulation results are shown at time $t = 0.19$ *msec* in the form of pressure contours and particle paths from different locations inside and outside the detonation chamber. From the pressure contour plots we observe that the shock reflection from the inner wall has taken place and detonation products are expanding into the ambient airstream. The flow inside the chamber is choked due to the converging nozzle and the maximum pressure behind the shock is $\approx 8atm$. The pressure inside the chamber is less than 3 atm. The strong expansion of the detonation products into the ambient airstream produces a shock wave with a spherical like front rapidly decaying in strength. As a result of the interaction of the expanding detonation products with the external flow a large toroidal vortex is created. The vortex is carried away quickly from the chamber by the external flow and by its own flow momentum.

In Figure 4a we also show particle paths for the particles introduced inside the chamber and outside just above the nozzle. Examination of these trajectories allows us to follow the dynamics of the chamber evacuation and refill. In order to track the detonation products we initially place marker particles inside the chamber at three cross sections in clusters of four distributed equally normal to the detonation chamber axis. Each particle has a different color; however, particles in the same cluster have the same shade of color. At the three chosen cross sections we have designated shades of red, yellow, and blue for the particles located correspondingly at the left end, center and beginning of the nozzle cross sections of the chamber. The movement of these particles is shown by connecting them with a continuous line beginning with particle location at $t = 0$ to the present time. In Figure 4a we observe that at time $t = 0.19 * 10^{-3}$ sec all particles originally in the nozzle cross section and three of the particles originally in the mid section have left the detonation chamber. However, particles originally introduced on the inner wall of the chamber have only advanced to the nozzle region.

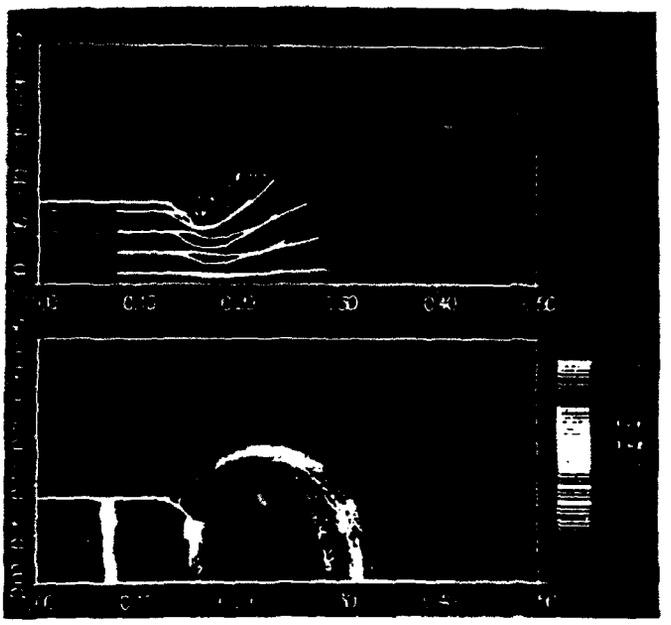
We use a different technique for observing the motion of the ambient gas outside the chamber. Here a cluster of seven particles is introduced every $0.5 * 10^{-4}$ seconds in the external flow above the nozzle. All such particles are traced as they move with the flow until they leave the computational domain. At any given time only the current location of the particle is displayed, and since the particles are introduced periodically with time there is a large number of particles to trace. We assign a color to every cluster of external particles to keep track of the time when they were introduced in the calculation. The colors vary from magenta for those particles introduced early in calculation, to blue for those introduced shortly at the time before the end of a detonation cycle. In Figure 4a corresponding to very early times, only one cluster of external particles is visible. This cluster was introduced at $t = 0$ and is tracking the expanding flow of the detonation products.

In Figure 4b the simulation results are shown for $t = 1.7 * 10^{-3}$ sec. The pressure contours show that a shock wave develops at the external edge of the nozzle as a result of a strong expansion of the Mach 0.9 external flow. A result of overexpansion of the detonation products is that the pressure inside the detonation chamber is lower than the ambient pressure, causing the shock to be located lower on the external surface of the nozzle. The external flow about the chamber has a stagnation point on the axis of symmetry downstream at $\approx 25cm$. At this time as it is evident from the particle trajectories that most of the detonation products have left the chamber. Figure 4b shows one continuous trace of the particles originating at the back wall of the detonation chamber having advanced well ahead of the stagnation point in the external flow.

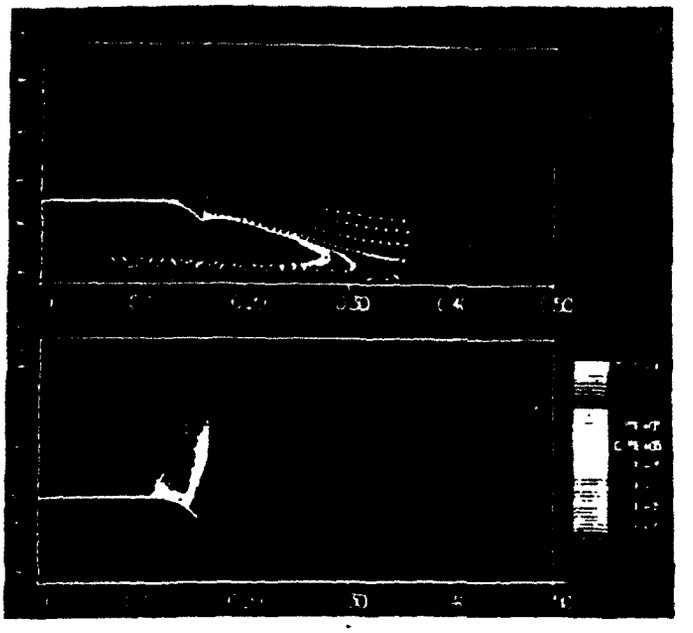
The marker particles released outside and just above the nozzles exit show two distinct flow paths. One path takes the flow past the stagnation point to the right of the detonation chamber; this flow path is marked by the four upper particle traces. Another flow path, marked by three lower particle released close to the nozzle surface is deflected towards the detonation chamber exit. Figure 4b shows this deflected stream approaching the detonation chamber nozzle. The magenta color of these particles indicates they were released at $\approx 0.5 * 10^{-3}$ sec.

Figure 4c corresponds to the simulation time $t = 0.47 * 10^{-3}$ sec. The pressure inside the chamber has risen $\approx 1atm$. Higher pressure at the chamber exit has caused the shock standing on the external surface of the nozzle to move upwards. The particles marking the movement of fresh air into the chamber show these to be well inside with some reflecting from the end wall giving a second stagnation point for the reversed fresh airflow.

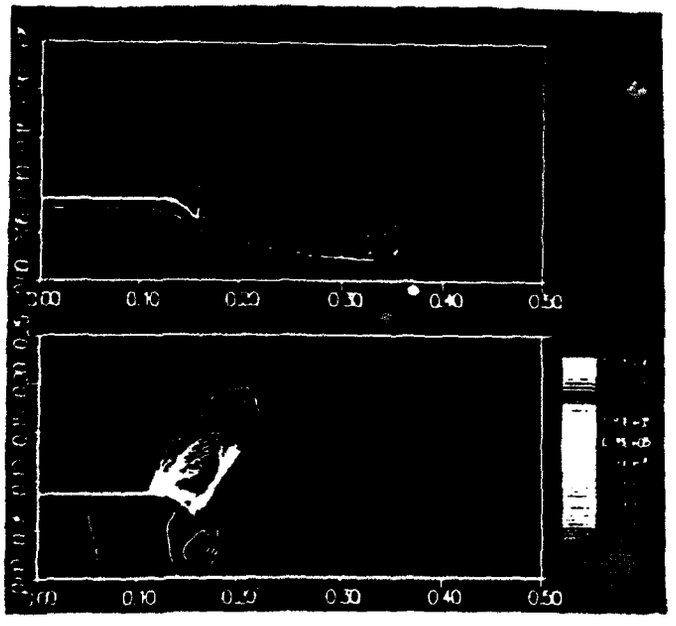
Figure 4d corresponds to the end of the first cycle when the detonation chamber should be filled with fresh charge and ready for the next detonation. In this figure the particle paths indicate that the chamber refills in a



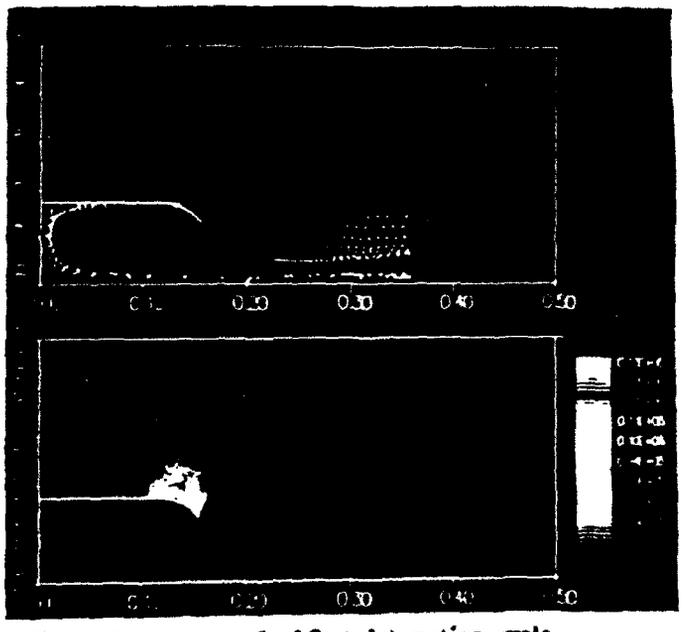
a) t = 0.19 msec,



c) t = 4.7 msec,



b) t = 1.7 msec,



d) t = 7.4 msec, end of first detonation cycle.

Figure 4 Pressure contours and particle paths for various times during the PDE simulation;
a) t = 0.19 msec, b) t = 1.7 msec,
c) t = 4.7 msec, d) t = 7.4 msec, end of first detonation cycle.

pattern suitable for fast mixing of the fuel-air mixture. We conjecture that fuel injection along the chamber axis will promote fast fuel-air mixing. We can see in Figure 4d that the farther injection of the external air flow inside the chamber stopped, and from that point on the mixture composition in the chamber will be fixed.

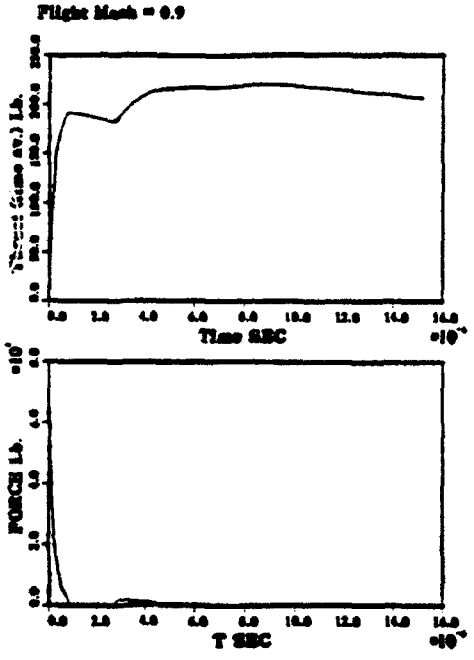


Figure 5 Thrust and force generated by PDE as function of time.

In Figure 5 total force and time averaged thrust generated by the device in the simulations discussed previously are shown as a function of time. The time averaged thrust is based on the total time for one cycle. As seen in Figure 5, initially a very large force of $\approx 7 * 10^4 lb$ is felt on the end wall of the detonation chamber. This is a result of the inwardly moving detonation wave used in our simulation. Very early during the sequence, this wave reflects from the left wall of the detonation chamber generating briefly a large force. This force rapidly decays and at $t \approx 1.0 * 10^{-4}$ sec changes sign due to interaction of the strong shock wave with the converging nozzle. This effect is noticeable in the thrust data; the average thrust decreases somewhat after reaching levels of $\approx 200 lbs$. The shock partially reflects from the converging nozzle walls and generates a wave moving to the left wall. The reflected wave thereafter generates positive thrust from $t \approx 3.0 * 10^{-4}$ sec. Finally thrust levels reach the maximum of 225 lbs. and then decays slowly as a result of the cross sectional drag force. The simulations predict that to sustain this level of thrust will require a detonation frequency of about 150 Hz.

Conclusions

The main intent of the present study was to carry out a review of the relevant literature in the area of detonation propulsion, to assess the state-of-the-art, and to recommend future research based on our findings. We have reviewed the literature and presented our summary in first section of this paper. Our initial conclusion from the review is that there is a substantial body of evidence leading toward the possibility of producing propulsion engines with significant thrust levels based on an intermittent detonation.

Most of the historical attempts at producing thrust based on the intermittent detonation cycle were carried out with the same basic experimental setup; namely, a long straight detonation tube employing forced fuel injection at the closed tube end. We have discussed the many reasons why such a device cannot take proper advantage of the physical processes associated with detonation.

The experiments performed at the Naval Postgraduate School using a self-aspirating mode of operation for pulsed detonation thruster produced very useful results which, upon further examination, provide us with a route towards practical propulsion engines of variable thrust levels which are both controllable and scalable.

We have explored some of the implications of the possible applications of the self aspirating detonation engine concept and have developed a suitable numerical simulation code to be used as a design, analysis and evaluation tool. In fact, the preliminary analysis of a candidate detonation chamber flow properties was shown to be dominated completely by unsteady gasdynamics. An attempt to understand the flow properties based on any steady state model or one-dimensional unsteady analytical model will miss such important aspects as fuel-air mixing and, shock reflelction from internal geometrical obstacle such as the converging nozzle. The unsteady simlation code developed during the course of our study is a necessary tool that we plan to use in a study leading to a feasible prototype engine design realising the full potential of the intermittent detonation process.

Acknowledgements

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COMPUTATIONAL ANALYSIS OF PULSED DETONATION ENGINES AND APPLICATIONS

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1. Introduction

This paper presents the results of a computational fluid dynamic simulation/ parameter study of the SAIC Pulsed Detonation Engine (PDE) concept. Results from computer simulations of generic PDE geometries over a wide range of subsonic and supersonic flight Mach numbers indicate that potentially practical detonation engines can now be conceptualized and optimized for specific flight requirements and missions. Specifically, the study shows that primary propulsion for aerodynamic vehicles of the PENAID variety may be possible at Mach numbers $0.5 < M < 0.8$, thrust levels on the order of 100 pounds and a specific fuel consumption of the order of 1 lb./(lb.hr.). The predicted performance places the PDE propulsion concept in a strongly competitive position compared with present day small turbojets. The PDE concept has the added attractiveness of rapid variable thrust control, no moving parts and the potential for low cost manufacturing. Finally, the PDE concept is scalable over a wide range of engine sizes and thrust levels. For example, it is theoretically possible to produce PDE engines on the order of one to several inches in diameter and thrusts on the order of pounds, as well as devices which provide thousands of pounds thrust.

A literature search of past research on related concepts and devices uncovered important information which proved useful in pursuing our present study. A review of the literature[1-24] reveals that a significant body of experimental and theoretical research exists in the area of unsteady propulsion. However, this research was not sufficiently extensive to provide a conclusive quantitative comparison between impulsive engine concepts and steady state concepts. In addition, the computational and analytical techniques were not sufficiently developed in the past to treat the inherently unsteady flows of pulsed engines. A new generation of analytical and computational tools exists today, allowing us to revisit and analyze these devices with a high degree of confidence.

Our paper is organized into the following sections: 2) description of the basic phenomenology of the air-breathing Pulsed Detonation Engine concept; 3) discussion of the numerical simulation results; and 4) conclusions. Details of the mathematical formulation of the simulation and a discussion of the numerical code used in the present study are given elsewhere.[25,26]

2. The Generic Pulsed Detonation Engine

A detonation process, due to the very high rate of reaction, leads to a propulsion concept in which the constant volume process can be fully realized. In detonative combustion, the strong shock wave, which is part of the detonation wave, acts like a valve between the detonation products and fresh charge. The speed of the detonation wave is about two orders of magnitude higher than the speed of a typical deflagration. This allows the design of propulsion engines with a very high power density. Each detonation has to be initiated separately by a fully controlled ignition device, with a wide range of variable cycle frequencies. There is no theoretical restriction on the range of operating frequencies; they are uncoupled from acoustical chamber resonancies. This is very important feature of the constant volume detonation process that differentiates it from the process occurring in a pulse-jet;[3-4] the pulse jet cycle is tuned to the acoustical resonances of the combustion chamber. This leads to a lack of scalability for the pulse jet concept.

A physical restriction dictating the range of detonation frequency arises from the rate at which the fuel/air mixture can be introduced into the detonation chamber. This also means that a device based on a detonative combustion cycle can be scaled and its operating parameters can be modified for a range of required output conditions. There have been numerous attempts to take advantage of detonative combustion for engine applications. The most recent and successful of these attempts was carried out at the Naval Postgraduate School (NPS) by Helman et al.[22] During this study, several fundamentally new elements were introduced to the concept distinguishing the NPS research device from previous studies. First, it is important to note that the NPS experimental apparatus was the first successful self aspirating air breathing detonation device. Intermittent detonation frequencies of 25 Hz were obtained. This frequency

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was in phase with the fuel mixture injection through timed fuel valve opening and spark ignition. The feasibility of intermittent injection was established. Pressure measurements showed conclusively that a detonation process occurred at the frequency chosen for fuel injection. Further, self aspiration was shown to be effective. Finally, the effectiveness of a primary detonation as a driver for the main detonation was clearly demonstrated. Although the NPS studies were abbreviated, many of the technical issues considered to be essential for efficient intermittent detonation propulsion were addressed with positive results.

As a result of the survey of past research on intermittent detonation devices, we have focussed our attention on the NPS experiments of Helman et al.[22] The remainder of this paper is concerned with a computer simulation of performance characteristics of such a device. We have chosen a generic geometry, applicable to certain present day vehicle and mission requirements, and have parametrically varied key features which affect performance and assessed the effects of these variations.

The generic device we consider here is a small engine 15 cm long and 15 cm in diameter. Figure 1 shows a schematic of the basic detonation chamber attached to the aft end of a generic aerodynamic vehicle. The combustible gas mixture is injected at the closed end of the detonation chamber and a detonation wave propagates through the mixture. The size of the engine suggests a small payload or aerodynamic vehicle, but the concept can be extended to larger payloads simply by scaling up the size of the detonation chamber and possibly combining a number of chambers into one larger engine. As an example, a PENAID vehicle has been conceptualized requiring an engine with a diameter of roughly 15 cm and a useful continuous thrust at Mach 0.8 approximately 60-90 pounds. Such an engine should have a specific fuel consumption in the range of 1.7 to 1.9 lb. fuel/hr per pound and an endurance on the order of 10-30 minutes. These specifications are met by present day small turbojets. Hence, in order to be competitive, a PDE must at least meet these requirements. Should this prove to be the case, a PDE with no moving parts would be a very attractive engine from the point of view of performance, ease of manufacturing and cost.

A key issue in the pulsed detonation engine concept is the design of the main detonation chamber. The detonation chamber geometry determines the propulsion efficiency and the duration of the cycle (frequency of detonations). Since the fresh charge for the generic engine is supplied from the external flow field, the efficiency of the engine depends on the interaction of the surrounding flow with the internal flow dynamics. The range of the physical process requiring simulation in order to model the complex flow phenomena associated with the detonation engine performance is very broad. A partial list is:

1. Initiation and propagation of the detonation wave inside the chamber,
2. Expansion of the detonation products from the chamber into the air stream around the chamber at flight Mach numbers,
3. Fresh air intake from the surrounding air into the chamber.
4. The flow pattern inside the chamber during post-exhaust pressure buildup which determines the strategy for mixing the next detonation charge,
5. Strong mutual interaction between the flow inside the chamber and surrounding the engine.

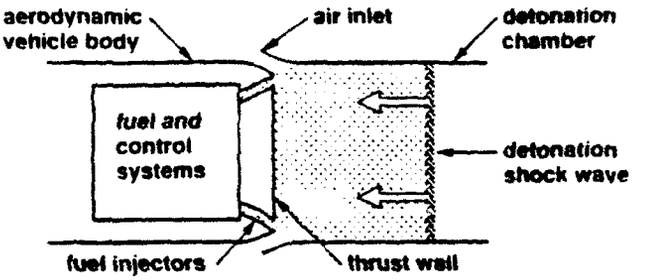

Figure 1. Schematic of the generic PDE showing detonation chamber, inlet, detonation wave, fuel injectors and position relative to an aerodynamic vehicle.

All of these processes are interdependent, and interaction and timing are crucial to engine efficiency. Thus, unlike simulations of steady state engines, the phenomena described above can not be evaluated independently.

The need to resolve the flow regime inside the chamber accounting for nozzles, air inlets etc., and at the same time resolve the flow outside and surrounding the engine, where the flow regime varies from high subsonic, locally transonic and supersonic, makes it a challenging computational problem.

The single most important issue is to determine the timing of the air intake for the fresh charge leading to repetitive detonations. It is sufficient to assume inviscid flow for the purpose of simulating the expansion of the detonation products and fresh air intake. The assumption of inviscid flow makes the task of numerically simulating the PDE flow phenomena somewhat easier than if a fully viscous flow model were employed. For the size of the generic device studied in this work the effects of viscous boundary layers are negligible with the exception of possible boundary layer effects on the valve and inlet geometries discussed subsequently. Boundary layer effects on the present results are discussed later.

3. Results of Simulationnal Parameter Study

As mentioned, and as shown in Figure 1, we have chosen a small $\approx$ 15 cm long and $\approx$ 15 cm internal diameter cylindrical chamber as the basic device. In the figure, the detonation chamber including detonation wave and inlet valves are shown schematically. The PDE, as envisioned in the present study, would most naturally be applicable for a class of aerodynamic vehicles such as target drones and PENAID missiles among others. The exact details of this basic chamber geometry were modified during the course of the study in order to obtain the required aerodynamic or propulsion effects; however, these modifications did not significantly change the total internal volume of the chamber. Thus, the performance results for the different cases can be compared holding the chamber volume constant. The schematic shown in Figure 1 does not represent an optimum configuration and is given here mainly to illustrate our methodology. We consider a situation where the PDE serves as the main thruster for an aerodynamic vehicle traveling in air with Mach numbers between M = 0.2 and M = 5.0, and is located at the aft end of the vehicle. The main objectives of our study are:

1. To calculate the thrust produced during each cycle and the integrated thrust as a function of time,
2. To find the maximum cycle frequency. This is determined by the time required from detonation to the final exhaust of combustion products and intake of fresh charge for the next detonation,
3. To evaluate the parametric dependence of the thrust and detonation frequency on the flight Mach number and detonation chamber geometry details.

In addition to the technical objectives outlined above, we have set another goal for our study. We require that the best, but by no means optimum, configuration produce a minimum of 60 pounds thrust at an operating frequency of 140 cycles per second. The definition of best is that configuration which satisfies the technical objectives outlined above and meets the operational goal of 60 pounds thrust and 140 Hz frequency over the flight regimes from M=.2 to M=0.9. (The Mach number range corresponds to that of a PENAID missile mission profile.)

To achieve these objectives we have conducted a comprehensive parametric simulational study of the PDE performance. We have studied PDE engine performance for a range of Mach numbers with two separate initial detonation locations in the chamber and for various geometry modifications. In addition to the range of subsonic Mach numbers we have examined PDE performance in the supersonic regime, 2 < M < 5. The geometry modifications included converging exhaust nozzles, inlets and dynamic valves. A computer simulation code was developed and optimized for a Stellar graphics workstation to carry out the analysis. In addition, a particle-tracing package was developed and implemented in the code. This allowed us to analyze the flow pattern inside and outside the detonation chamber, the main sources creating this pattern as a function of time, and the composition of the resulting gas mixture (air/detonation products).

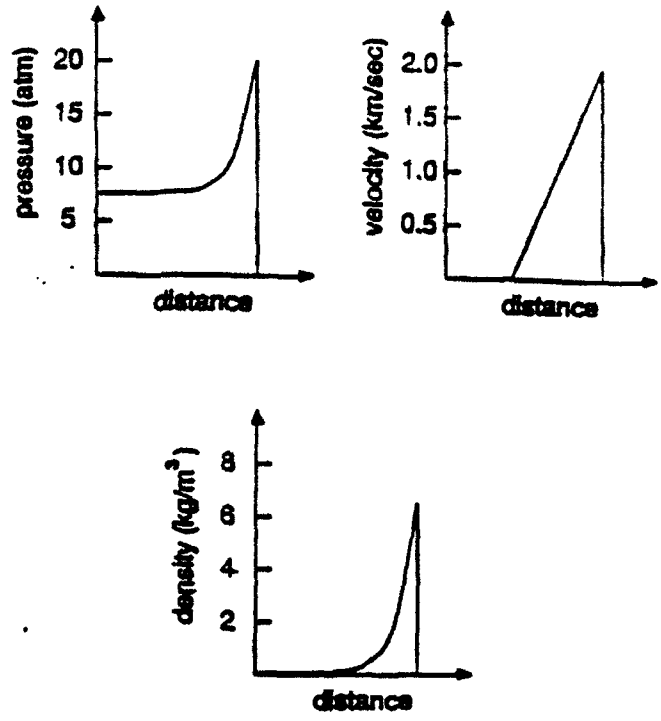

Figure 2. Distribution of gasdynamic parameters behind the detonation wave according to a 1-D self-similar solution.

First we will describe in detail the results for a typical simulation, Case 1, and illustrate the main features of our analysis.

Case 1. The simulation begins at $t = 0$ when a strong detonation wave is initiated inside the detonation chamber. The detonation chamber for this case includes a simple annular inlet which remains open during operation. The external freestream Mach number is 0.8. The specific fuel chosen for the present simulations is ethylene. The chemical reaction occurring in the ethylene/air detonation process is given by:

$$C_2H_4 + 3O_2 + 11.24N_2 \longrightarrow 2H_2O + 2CO_2 + 11.24N_2$$

The detonability limits of ethylene in air range from 4 to 12% by volume and depend somewhat on temperature and pressure. We assume for the sake of simplicity that

the fuel/air ratio is 6% by volume. Because the detonation initiation and propagation (detonative combustion) takes place several orders of magnitude faster than any of the other flow processes in or surrounding the device, finite rate chemistry is not included in the simulations. Instead the equation of state for the flow in the chamber immediately after detonative combustion was adjusted to represent the correct physical state of the combustion products. Initially the detonation wave travels from the closed end of the chamber towards the open aft end with a maximum velocity of 1800 m/sec and maximum pressure of $20 * 10^5 Pa$. The initiation of the main detonation wave is assumed to take place via a device proposed and successfully implemented by Helman, *et al.*;[22] namely, a primary detonation is established in a small tube containing an oxygen rich mixture. This mixture requires a low initiation energy but will sustain a detonation which, in turn, is used to trigger the main detonation wave. We do not model the detonation tube; but, we assume that such a device is present to trigger the main detonation at $t = 0$. The distribution of pressure, velocity, and density of the detonation wave is defined through the selfsimilar solution for a planar detonation wave. A schematic of the detonation wave distribution in space in Figure 2 shows pressure, temperature and velocity as a function of the spatial extent of the detonation wave.

In Figure 3a simulation results are shown at time $t = 0.64$ m/sec in the form of pressure contours and particle paths from different locations inside and outside the detonation chamber. The free stream Mach Number is 0.8. From the pressure contour plots we observe that the detonation shock wave has left the chamber and is freely expanding outwardly in the external flow. The strong expansion of the detonation products into the ambient airstream produces a shock wave with a spherical-like front that rapidly decays in strength away from the source. A large toroidal vortex is created as a result of the interaction of the expanding detonation products with the external flow. The vortex is carried away quickly from the chamber by the external flow and by its own momentum. At the time shown in Figure 3a, the detonation products are almost fully expanded into the ambient air and the maximum pressure at the front of the shock wave is 1.2 atm. As a result of this expansion the detonation products inside the detonation chamber are overexpanded and their pressure is 0.45 atm.

In the upper frame of Figure 3a we show particle paths for the marker particles introduced inside the chamber and outside just above the nozzle exit. Examination of these trajectories allows us to follow the dynamics of the chamber evacuation and subsequent refill. In order to track the detonation products we initially place marker particles inside the chamber at three separate cross sections in clusters of four. Each particle has a different color; however, particles in the same cluster have the same shade of color. At the three chosen cross sections we have designated shades of red, yellow, and blue for the particles located correspondingly at the left chamber end, center and aft end of the nozzle cross section. The movement of these particles is shown by connecting them with a continuous line beginning with particle location at $t = 0$ to the present time. In Figure 3a we observe that at time $t = 0.64 * 10^{-3}$ sec all particles originally in the nozzle cross section (the cross section at the aft end) and three of the particles originally in the mid section have left the detonation chamber. However, particles originally introduced at the inner end wall of the chamber (red traces) have only advanced to the nozzle region.

We use a different particle technique for observing the motion of the ambient gas outside the chamber. Here a cluster of seven particles is introduced every $0.5 * 10^{-4}$ seconds in the external flow above the nozzle. All such particles are traced as they move with the flow until they leave the computational domain. At any given time only the current location of the particle is displayed, and since the particles are introduced periodically with time, there are many particles to trace. We assign a color to every cluster of external particles to keep track of the time when they were introduced in the calculation. The colors vary from magenta for those particles introduced early in the calculation, to blue for those introduced near the end of a detonation cycle. In Figure 3a, which corresponds to early times, only 12 clusters of external particles are visible. These clusters were introduced from $t = 0$ to $0.6 * 10^{-3}$ second, vary from magenta to red in color, and are tracking the expanding flow of the detonation products.

In Figure 3b the simulation results for the same case are shown for $t = 1.4 * 10^{-3}$ sec. The pressure contours show that a strong stagnation point develops on the axis of symmetry downstream at $\approx$ 25 cm as a result of a strong expansion of the Mach 0.8 external flow around the engine. At this time it is evident from the particle trajectories that most of the detonation products have left the chamber. Figure 3b also shows that only traces of the particles originating at the back wall of the detonation chamber are left in the computational domain. These particles advanced to the aft end of the chamber and then following the contraction of the over expanded detonation products, reversed their flow direction. The pressure contour plots in Figure 3b show the formation of an additional stagnation point at the closed end wall of the detonation chamber resulting from the inverse flow of the detonation products. The average pressure in the chamber is below ambient and is $\approx$ 0.55 atm.

The marker particles released outside and just above the nozzle exit show two distinct flow paths. One path

takes the flow past the stagnation point to the far right of the detonation chamber; this flow path is marked by the four upper particle traces. Another flow path, marked by three lower particles released close to the external wall of the chamber, are deflected from the stagnation region towards the detonation chamber exit. The magenta color of these particles indicates they were released at $t \approx 0.6 * 10^{-3}$ sec.

Figure 3c corresponds to the simulation time $t = 2.2 * 10^{-3}$ sec. The pressure inside the chamber has risen to ≈ 0.8 atm. The stagnation region at the closed end of the detonation chamber continues to develop and has produced a compression wave moving toward the open end of the chamber. The particles marking the movement of fresh air into the chamber show these to be well inside the chamber, with some reflecting from the end wall and contributing to the pressure at the second stagnation point. The circular motion of a few of the detonation products particles (red solid lines), indicates that the detonation products which did not expand with the first shock wave are now "trapped" inside the detonation chamber.

Figures 3d and 3e correspond to the end of the first cycle when the detonation chamber should be filled with fresh charge and ready for the next detonation. However, these figures indicate that the fresh air refill is not totally satisfactory for this chamber configuration. The marker particle paths indicate that the chamber refill is incomplete and at a time of $t = 4.7 * 10^{-3}$ sec the refill process has essentially stopped. As a result, only about a third of the detonation chamber volume has enough fresh air for the next detonation cycle.

In Figure 4 the total force and time averaged thrust generated by the device in the simulations just discussed, are shown as a function of time. The time averaged thrust is based on the total time for one cycle defined as $7.0 * 10^{-3}$ sec. This time is equivalent to a detonation frequency of 140 Hz. As seen in the figure, initially a very large force of $\approx 3.2 * 10^3$lb is felt on the end wall of the detonation chamber. This force is a result of the high pressure behind the detonation wave. It rapidly decays and at $t \approx 0.5 * 10^{-3}$ sec changes sign due to over expansion and dynamic pressure of the external flow. This effect is noticeable in the thrust data; the average thrust increases rapidly but decreases after reaching levels of ≈ 55 lbs. At the end of the simulation the thrust is actually negative ≈ -20 lbs. The average thrust for one cycle in this case will be ≈ 10 lbs.

The simulation just described has served to illustrate the information generated with the numerical simulations. For the remaining simulations, emphasis was placed on determining the effects of propagation direction of the main detonation wave, effects of inlet and valve geometry, detonation chamber geometry and Mach number. Many of the simulations produced unsatisfactory results from the point of view of ineffective fresh air refill and hence either not enough fresh charge for repetitive detonations or too slow a refill resulting in low detonation frequency. We give below examples of successful simulations at Mach 0.8, Case 2 and Mach 2, Case 3.

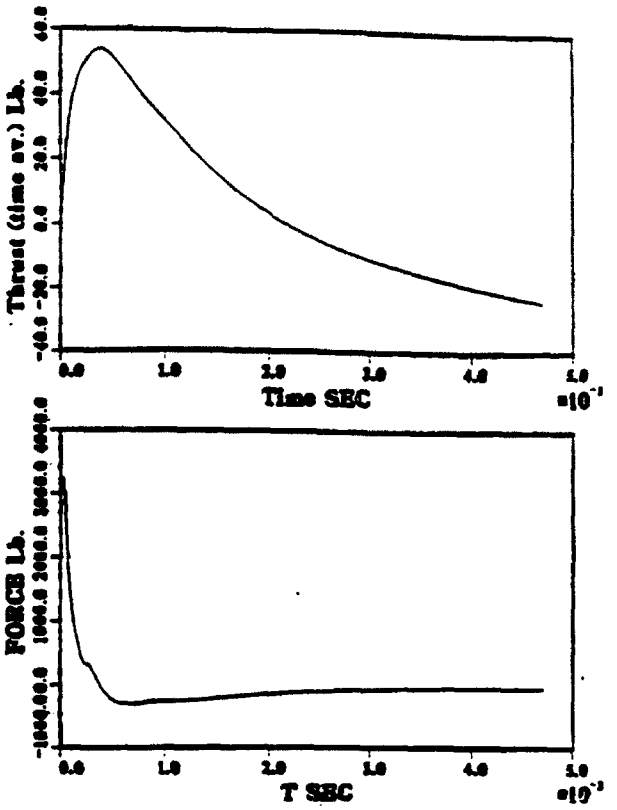

Figure 4. Time averaged thrust and force data from simulation of Case 1.

Case 2. The results from all simulations show that, irrespective of the inlet geometry, but with a straight nozzle and initial detonation position at the nozzle exit plane, sufficient thrust levels can be produced. A remaining problem in view of the objectives is to demonstrate that enough fresh air can be injected into the chamber to produce the required conditions for intermittent detonation at a frequency of 140 Hz. To accomplish this, we have considered a contoured inlet in the periphery of the end wall of the detonation chamber. The details of this inlet geometry and the computational grid are shown in Figure 5.

For the initial tests with this inlet no attempt was made to optimize the inlet geometry for a given flow regime. Figures 6a-f present results for the simulation of the chamber geometry shown in Figure 5.

The flight Mach number in this case is 0.8. The initial detonation wave is launched inwards and its energy parameters are the same as in all previous cases. In Figure 6a we see two distinct shock waves expanding into ambient air: one generated by expansion from the aft of the chamber and another produced by the expansion through the inlet. We also notice some particles tracing the motion of the detonation products flowing out through the inlet. In Figure 6b, at time $t = 0.7 * 10^{-3}$ sec., fresh air is noted entering the chamber through the inlet. At this time the dominant pressure in the chamber is 0.77 atm. Figure 6c shows that at the time $t = 1.4 * 10^{-3}$ sec, 3/4 of the detonation chamber is filled with fresh air. The strong air jet entering the chamber impinges the axis of symmetry, creating two large vortices which rotate in opposite directions. Such vortical motion would promote effective fuel-air mixing in the chamber. In Figure 6d, $t = 2.4 * 10^{-3}$ sec., the fresh air stream begins to exit the chamber. At this point the mixture inside the chamber has achieved the required conditions for the next detonation. This result translates to a sustained detonation frequency of $\approx$ 400 Hz. In Figures 6e-f we follow the later evolution of the flow pattern inside and outside the chamber. We observe strong air flow through the inlet with a strong recirculation pattern, which will assure fuel air mixing even if the fuel is injected into the chamber with a delay to sustain intermittent detonation at a lower frequency. In Figure 7 thrust and force simulated for the last case are shown as a function of time. First we notice that the maximum thrust for this case is $\approx$ 70 lbs., somewhat lower than for the cases with a very simple annular inlet and completely flat end walls.

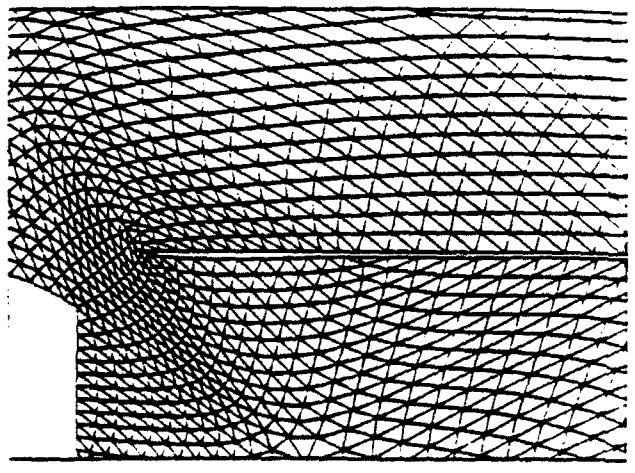

Figure 5. Computational grid for the inlet geometry used in simulation of Case 2.

This results from a reduction of the area normal to the propagation direction of the detonation wave due to the inlet geometry. It is surprising that the case with the inlet results in a reduction of the average thrust as a function of time that is almost the same as for a case without inlet at the same Mach number ($\approx$ 90 lb reduction without the inlet and 100 lb reduction with the inlet). This strongly indicates that the generic inlet we have just considered will not contribute significantly to the drag produced by the chamber dynamics and interaction with the ambient flow. The cycle average thrust generated by the PDE based on 150 Hz operation frequency in this case is $\approx$ 100 lbs. This value is somewhat larger than the thrust targeted for this study.

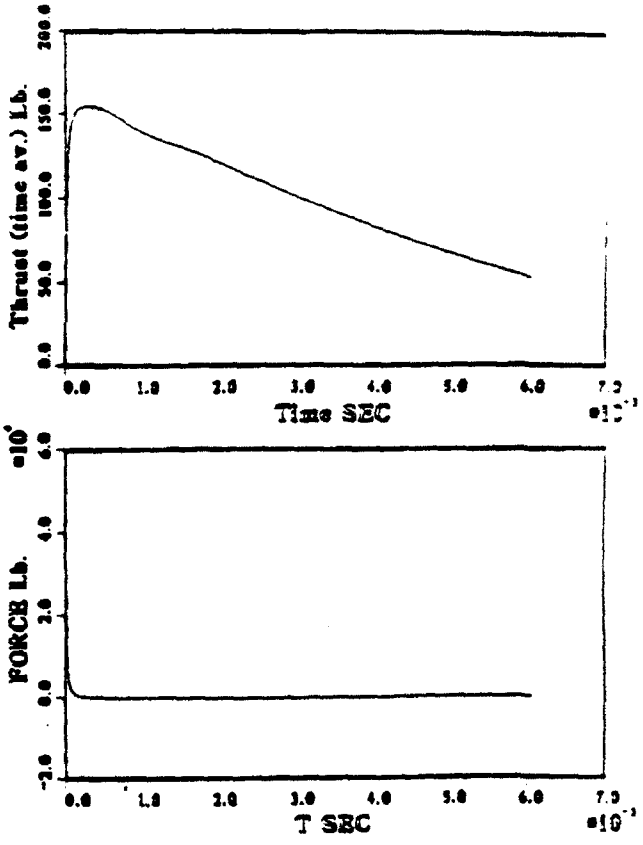

Figure 7. Time averaged thrust and force data from simulation of Case 2.

Case 3. Results for a Mach 2.0 simulation of the same geometry as in the previous simulation; but with a more geometrically complex inlet are shown in Figures 8a-b. The inlet geometry for this case was determined from near choked flow conditions in the throat region of the inlet. In addition to the pressure contours and particle paths, in this case we also show velocity vectors.

We observe in these figures that the detonation chamber is quickly filled with fresh air at the time $t = 1.3 * 10^{-3}$ sec., which corresponds to a detonation frequency of 700 Hz. In practice this high frequency will be difficult to realize, because of the mixing and initiation problems. In Figure 9 we show thrust and force results for this simulation. We observe that after $3.0 * 10^{-3}$ sec. the net average thrust is still 50 lbs.

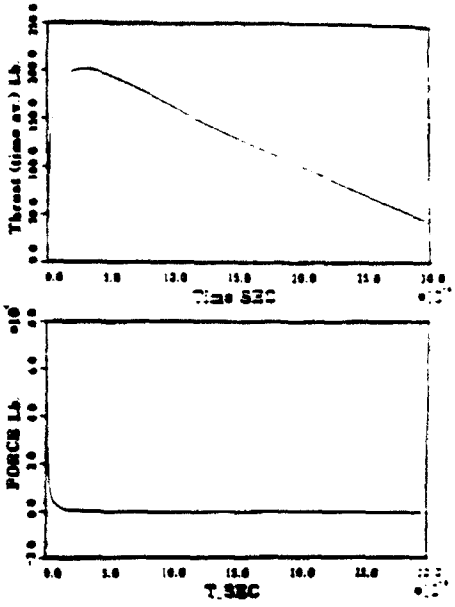

Figure 9. Time averaged thrust and force data from simulation of Case 3, 140 Hz detonation frequency.

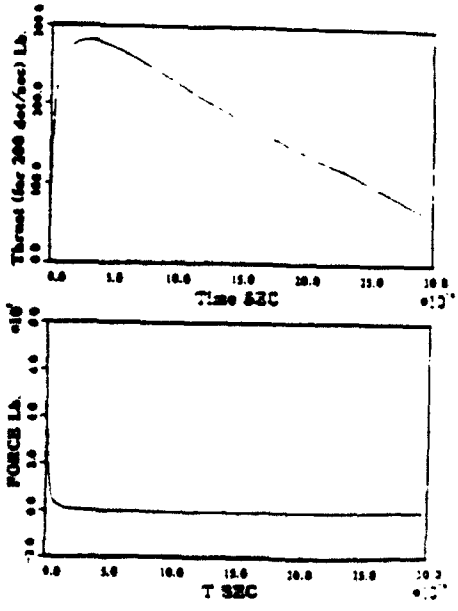

Figure 10. Time averaged thrust and force data from simulation of Case 3, 200 Hz detonation frequency.

The cycle averaged thrust based on 140 Hz detonation frequency, for this simulation is $\approx$ 70 lbs. However, as previously mentioned the fresh air refill time allows a much higher frequency of detonations. Figure 10 shows the same results as Figure 9, but calculated for a 200 Hz cycle frequency. In this case the maximum average thrust is $\approx$ 280 lbs. and the net cycle averaged thrust is $\approx$ 100 lbs. This result indicates the promising potential of the PDE concept for supersonic propulsion.

4. Conclusions

In this section we present our conclusions reached after carrying out a review of past research on detonative propulsion and a detailed numerical simulation of a generic pulsed detonation engine (PDE) device. The primary conclusion is that the PDE shows promising potential in providing primary propulsion for a range of present day aerodynamic vehicles such as target drones, PENAID missiles and other smart missiles that require loitering and throttling capability. The operating flight regimes of such a propulsion engine may extend from the low subsonic to supersonic regimes.

Most of the past attempts at producing thrust based on an intermittent detonation cycle were carried out with the same basic experimental set-up; namely, a long straight detonation tube employing forced fuel injection at the closed tube end. We have pointed out the reasons[25] why such a device cannot take proper advantage of the physical processes associated with detonative combustion. We have also indicated that, because of the conclusions reached during experiments with such devices, the development of intermittent detonative propulsion was adversely prejudiced and stalled at an early stage.

The experiments performed at the Naval Postgraduate School based on a self-aspirating mode of operation for a pulsed detonation thruster produced very useful results which, upon further examination, provide us with a route towards practical detonation engines of variable thrust levels that are both controllable and scalable. A generic PDE device based on the NPS experiments was conceptualized and served as the basic model for a comprehensive series of numerical simulations. The goal of the simulations was to understand the parametric dependence of the PDE device variables on propulsion performance such as thrust and detonation cycle frequency.

The principle conclusions drawn from the simulation results are as follows. First, the target thrust and cycle frequency of 60-90 pounds and 140 Hz, respectively, have been realized in the simulations. These target values were dictated by knowledge of present day requirements for planned aerodynamic vehicles such as PENAID devices. Before proceeding, it is appropriate to mention again that the performance of the PDE device is governed entirely by unsteady flow processes. None of the wave averaging effects which had been predicted

by previous studies were found and, it was shown dramatically that the internal (detonation, expansion, refill and mixing) flow processes are directly coupled to the external (shock formation, stagnation point formation, vortex shedding, etc.) flow processes. These two flows must be simultaneously analyzed if a reliable estimate of performance is to be determined. The present study is the first fully unsteady computational analysis of an intermittent detonation scheme with realistic geometry and external flow computed self-consistently.

The simulations further showed that the best thrust performance was realized when the full kinetic energy of the detonation wave was captured on the thrust surface (the closed end wall of the detonation chamber). This indicates that the detonation initiation must be controlled; the ignition must take place in the vicinity of the exit plane of the chamber resulting in initial propagation of the wave towards the chamber wall. The magnitude of the total and time averaged thrust is a strong function of the strength of the wave, the cross-sectional area of the end wall normal to the wave direction, and a weak function of the specific geometrical details of such variables as valve or inlet shape. The simulations also showed that for most situations involving simple inlets (flat cylindrically symmetric openings in the chamber external wall) the thrust data was independent of whether the valve intermittently opens or remains open during the full cycle. This leads to the possibility of a permanently open valve and a no moving parts manifestation of a PDE device. The thrust data indicates a dependence on the external flight conditions, e.g. Mach number. The Mach number plays a role in the wave drag that the geometry of the PDE will incur; the details of the valve and inlet configurations figure prominently in the total wave drag.

On the other hand the simulations showed that the timing of the fresh air refilling required to recharge the chamber for subsequent detonations is a strong function of the details of the valve and inlet geometry, the expansion of the combustion products, the resulting over-expansion of the chamber flow and, the external flow regime and interaction of the external flow with the internal flow. For subsonic flight, Mach 0.2-0.9, the fresh air entering the chamber comes from two separate principal flow processes; one comes from the flow through any valve or inlet and the other comes from the self-aspiration or reverse flow from the aft end of the chamber due to strong over-expansion. All these processes are interdependent, as reported in Section 3, and, in order to search for a given performance in a given device requires variation of many parameters. The simulation results obtained to date provide an understanding of the effects caused by variation of the above mentioned parameters, and with the information available we are able to conclude that a PDE propulsion unit can be optimized (although no optimization studies were carried out) for a given flight regime. In order to find an optimum configuration satisfying given performance over a wide flight regime a more extensive simulation study will be required. It was mentioned earlier that the simulations presented here were carried out under the assumption of inviscid flow; boundary layer effects were not included. The addition of boundary layers to the PDE engine inlets and valves, the only components where boundary layers will be significant, will lead to increased performance. Roughly the same amount of fresh air will flow into the over expanded detonation chamber but at a somewhat slower rate and in a pattern that will promote enhanced circulation and hence fuel/air mixing. We return to the issue of optimization below.

We give now results from sample performance calculations of the application of the PDE device to proposed aerodynamic vehicles such as a PENAID missile based on the results from our simulations. These predictions are based on point design data for an inlet geometry which has not been optimized. We believe that increased performance can be found through a systematic optimization of the PDE device characteristics. First we consider the Mach 0.8 case and the inlet described in Case 2.

The maximum operation frequency for the device is 400 Hz. The following performance is a consequence of the simulation data:

For a frequency of 100 Hz.:

Thrust	.79 lb.
Fuel flow rate	.0.025 lb./sec.
Fuel weight for 12 min.	.18 lb.
Oxygen weight	.1.8 lb.
Fuel for detonation tube	.0.6 lb.
Total oxygen and fuel weight	.20.4 lb.
Total engine weight	.30.2 lb.
Specific fuel consumption	.1.14 lb./(lb.*hr.)

Assuming the PDE device geometry is kept fixed, a higher detonation frequency will result in a linear increase in thrust and fuel flow rate at the same specific fuel consumption. For example, if the detonation frequency is increased to 200 Hz., the performance data are:

Thrust	.157 lb.
Fuel flow rate	.0.05 lb./sec.
Fuel weight for 12 min	.36 lb.
Oxygen weight	.3.6 lb.
Fuel for detonation tube	.1.2 lb.
Total oxygen and fuel weight	40.8 lb.
Total engine weight	54.4 lb.
Specific fuel consumption	.1.14 lb./(lb.*hr.)

At lower Mach numbers, M=0.5, the maximum operating frequencies will be lower since the external dynamic pressure responsible for supplying fresh air to the chamber is also lower. For the device under considera-

tion here the maximum frequency is 250 Hz.

For a frequency of 100 Hz.:

Thrust	100 lb.
Fuel flow rate	0.025 lb./sec.
Fuel weight for 12 min	.18 lb.
Oxygen weight	.1.8 lb.
Fuel for detonation tube	.0.6 lb.
Total oxygen and fuel weight	.20.4 lb.
Total engine weight	30.2 lb.
Specific fuel consumption	.0.9 lb./(lb.*hr.)

Again, if the frequency is increased the thrust will increase linearly; operation at 200 Hz. yields:

Thrust	.200 lb.
Fuel flow rate	0.05 lb./sec.
Fuel weight for 12 min	.36 lb.
Oxygen weight	3.6 lb.
Fuel for detonation tube	1.2 lb.
Total oxygen and fuel weight	40.8 lb.
Total engine weight	.54.2 lb.
Specific fuel consumption	.0.9 lb./(lb.*hr.)

The examples of performance of PDE devices given above are based on point design conditions arising from the simulations discussed in Section 3 of this report. They cannot be extrapolated with any degree of reliability to other conditions or configurations. We conclude however, that the performance computed for the indicated device is encouraging from the point of view of thrust, thrust control, simplicity of the device (no moving parts) and specific fuel consumption (SFC). The specific fuel consumption computed above is competitive with present day small turbojet engines. The SFC for a PDE could be signficantly lower than for small turbojets (SFC's for small turbojets are in the range of 1.8-2.0 lb./(lb.*hr.)). Thus, for a given mission and vehicle, a PDE propulsion unit would be more fuel efficient resulting in increased range. Moreover, if the expected thrust control in PDE's is realizable, it may be possible to produce propulsion units that can slow down, loiter and maneuver and finally accelerate to full thrust again rapidly.

A final conclusion can be made concerning the application of PDE's to supersonic vehicles. As shown in the simulations the ability to refill the detonation chamber with fresh air charge is a very strong function of valve and inlet geometry. Refilling may also be somewhat enhanced by the self-aspiration effect, but; to a much less extent than in the subsonic case. The example of supersonic operation discussed in Section 3 shows that care must be taken in design of the inlet or valve configuration. The flow in the chamber must allow for refill and fuel/air mixing. More than likely choked flow conditions will be required at the inlet entrance to the chamber. This could lead to complications in the design of a PDE with simple geometry; choked flow conditions are a function of the external Mach number and a fixed inlet will be optimal only for a small range of the operating envelope. On the other hand, if a given vehicle is to fly at supersonic speeds and is launched at supersonic speeds, this problem may not appear. Further, if the given vehicle is launched at subsonic speeds and a booster is used to bring it up to the required supersonic operating speed, the problem may again not appear. We conclude that the PDE has potential for the supersonic flight regime and it is not excluded that a configuration can be found which will operate over the flight regimes $0.2 <$ Mach number < 3 in a fuel efficient manner.

Finally it is appropriate to speculate that the PDE concept is a candidiate for a hybrid propulsion device. Consider the following scenario. At low altitudes, up to 30-50 km, and at speeds ranging from low supersonic to hypersonic ($2 <$ Mach number < 10) an air breathing engine can operate. Above these conditions air breathing is not effective and rocket propulsion is required. A PDE can operate in an air breathing mode as long as the external conditions allow it, and when no longer possible, the detonation chamber may be considered a rocket chamber in which detonation occurs with the fuel and oxygen supplied from on-board storage. Similar considerations have been made for NASP propulsion; serious penalties are made in that large quantities of fuel must be carried. However, for vehicles such as the current Pegasus, a PDE propulsion device may be attractive from the point of view of thrust control over a large portion of the flight envelope.

Acknowledgements

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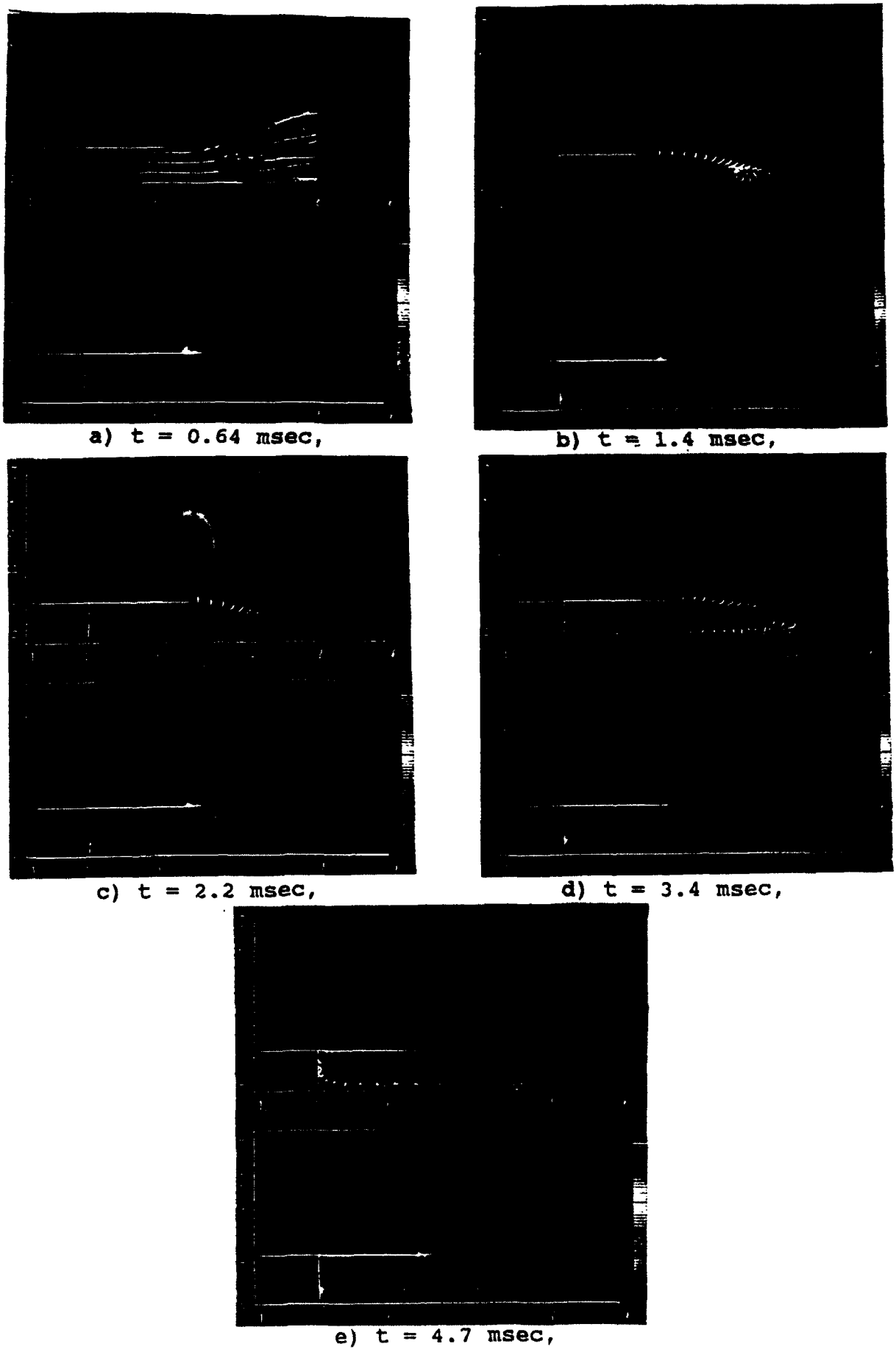
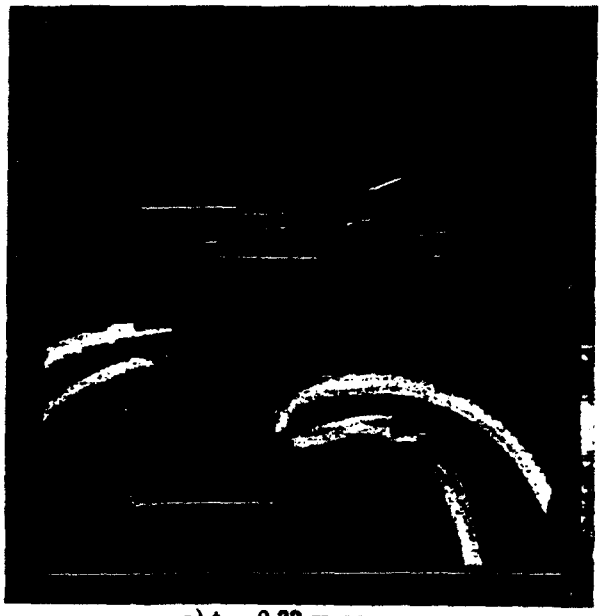
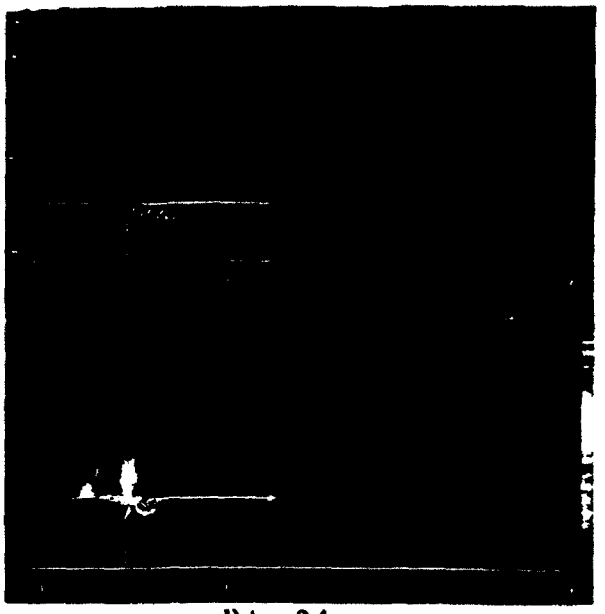


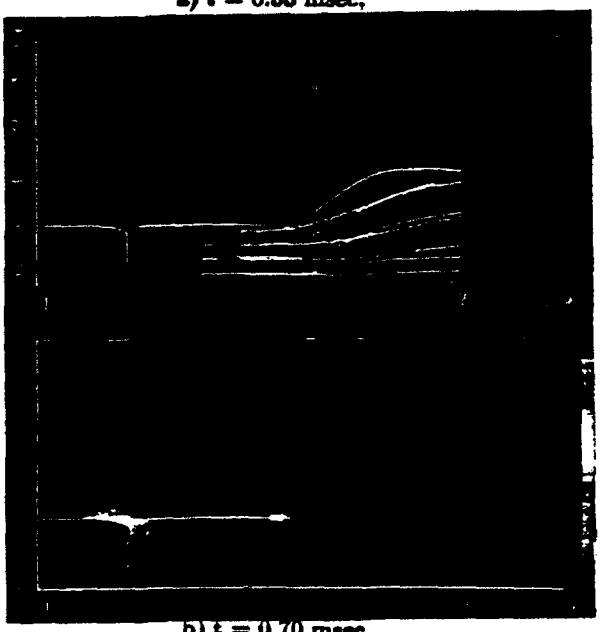
Figure 3 Pressure contours and marker particle paths for Case 1, M = 0.8, no inlet, inward initial detonation location.



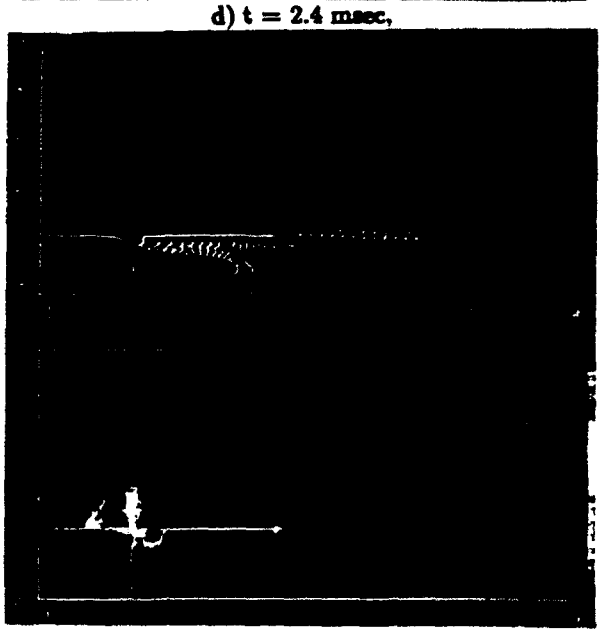
a) t = 0.33 msec,



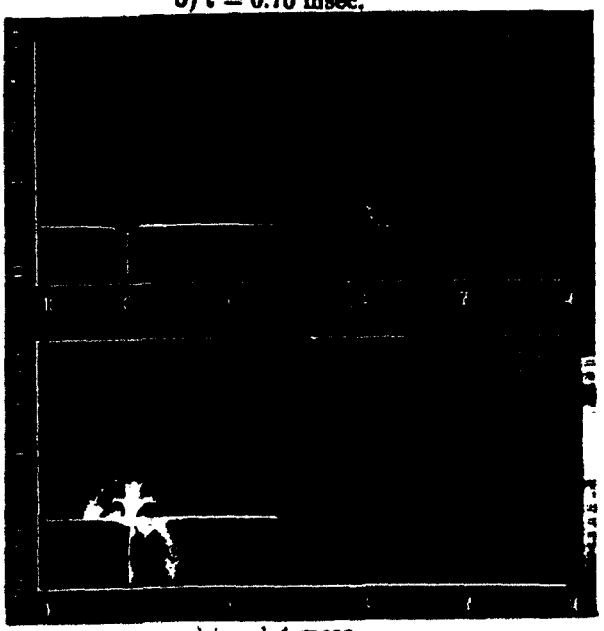
d) t = 2.4 msec,



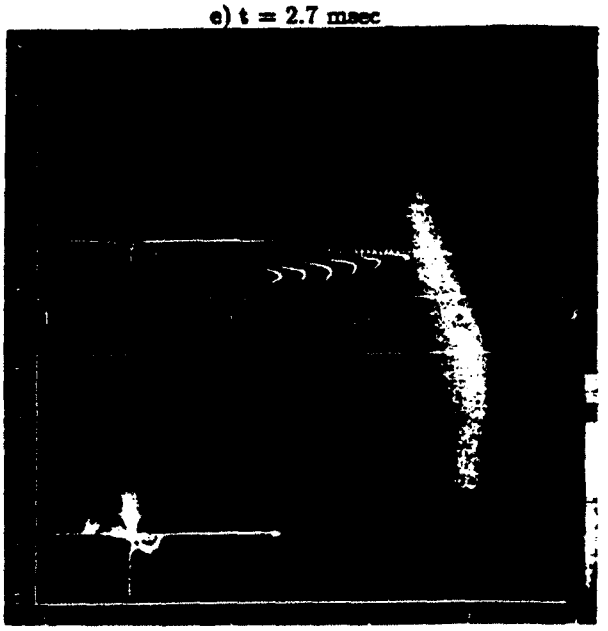
b) t = 0.70 msec,



e) t = 2.7 msec

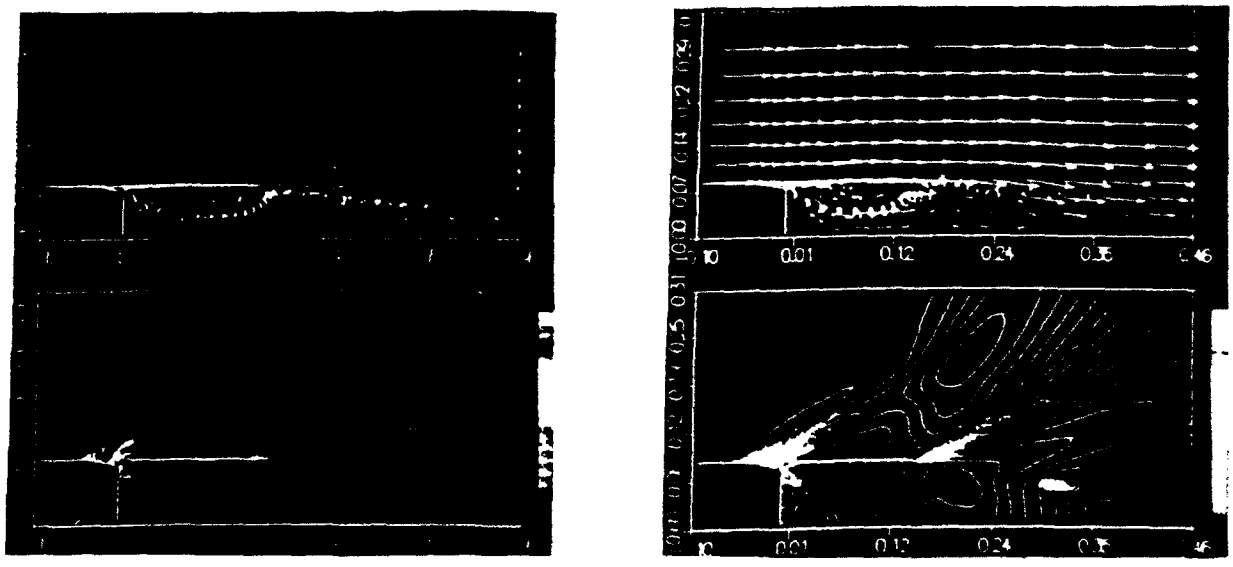


c) t = 1.4 msec,



f) t = 4.1 msec

Figure 6 Pressure contours and marker particle paths for Case 2, M = 0.8, inlet geometry of Figure 5, outward initial detonation location.



a) t = 1.3 msec,

b) t = 2.1 msec,

Figure 8 Pressure contours and marker particle paths for Case 3, M = 2.0, sculptured inlet, outward initial detonation location.

AIAA-90-0699

A FAST UNSTRUCTURED GRID SECOND ORDER GODUNOV SOLVER (FUGGS)

Itzhak Lottati, Shmuel Eidelman, and Adam Drobot
Science Applications International Corporation
McLean, VA

28th Aerospace Sciences Meeting
January 8-11, 1990/Reno, Nevada

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ABSTRACT

We describe a new technique for solving Euler's equations on an unstructured triangular grid with arbitrary connectivity. The formulation is based on Godunov methods and is second order accurate. The use of a unique data structure leads to an easily vectorized and parallelized code with speed and memory requirements comparable to those found with logically structured grids. The new algorithm has been tested for a wide range of flow conditions ranging from low speed subsonic flow to hypersonic flow with Mach number 32. The results obtained are comparable to or better than those obtained with leading flow solvers in all of the regimes tested. The code contains no free parameters and can be used in complex flow problems where a variety of flow conditions may be encountered.

INTRODUCTION

This paper introduces a new second order algorithm for solving the Euler equations on an unstructured grid, using an approach based on first and second order Godunov methods. The formulation presented here leads to an extremely efficient and fast Flow Solver which is fully vectorized and easily lends itself to parallelization. The low memory requirements and speed of the method are due to the use of a unique data structure.

Explicit hydrodynamic numerical algorithms are easily adapted to Massively Parallel Computers (MPC) for logically structured grids. This is a consequence of the fact that the calculation of the flow quantities are locally determined. For logically structured quadrilateral grids, the integration algorithm or Flow Solver computes the new flow values at the grid cell nodes (or centers) using the values of the flow parameters from the previous timestep employing four or more of the adjacent nodes. Higher order structured solvers are usually more computationally intensive, but retain the ability of the solver algorithm to be separated into several distinct steps, each of which can easily be vectorized and parallelized.

Until recently, most CFD simulations were carried out with logically structured grids and consequently vectorization and/or parallelization did not present a problem. The increased need for simulation of flow phenomena in the vicinity of complex geometrical bodies and surfaces has led to the emergence of CFD codes based on logically unstructured grids. The most successful of these unstructured grid codes are based on finite elements [1-6] or finite volume [7-12] methods.

Unstructured grid CFD computations in two-dimensions usually decompose the simulation domain into triangular elements. The physical location of the triangular elements and the accompanying list of vertices and edges is random with respect to the element index, making it necessary to maintain an indirect addressing system containing the connectivity information.

Calculations performed on unstructured grids evolve around the elemental grid shape (e.g. the triangle for two-dimensional problems); there is no obvious pattern to the order in which the local integrations should be performed. Explicit integration of hydrodynamic problems on an unstructured grid requires that a logical substructure be created identifing the locations in the global arrays of all the local quantities necessary for the integration of one element. As a result, there is usually a significant cost in computational efficiency, memory requirement, and code complexity. Approaches to vectorization for the conventional unstructured grid methods have concentrated on rearrangement of the data structure in a manner such that these locally centered data structures appear as global arrays. This can be done to some extent using machine dependent Gather-Scatter operations. Additional optimization can be achieved using localization and search algorithms [13]. However, these methods are complex and result in marginal performance. To date, most optimized unstructured codes have run considerably slower and require an order of magnitude more memory per grid cell than their structured counterparts. Parallelization of the conventional unstructured codes is even more difficult, and there is very little experience with unstructured codes on Massively Parallel Computers.

The method we describe in this paper overcomes these difficulties and results in code with speed and memory requirements comparable to those found in structured grid codes. Moreover, the ability to construct grids with arbitrary resolution leads to a flexibility in dealing with complex geometries which is not attainable with structured grids. The essence of the method is based on independent flux calculation across the edges of a dual baricentric grid, followed by node integration. This approach allows the flux and integration calculations to be performed on global arrays, coded as large vector loops, and is independent of element position on the unstructured grid.

In this paper we discuss our choice for data structure, the numerical algorithm (for first and second order solvers), and the results of test calculations. In realistic CFD

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problems the physical domain may contain regions that span all flow regimes. It is very important that the numerical code be able to perform well over the full range of flow parameters with no a priori code "refinement." This is especially true of complex problems where flow conditions cannot be easily assessed in all subdomains. A robust code has clear advantages if it is possible to apply it with confidence under such circumstances. We have chosen four test problems to benchmark and validate the FUGGS code. These include: i) a subsonic flow case for steady flow with M = 0.2; ii) supersonic steady flow with M = 2.0; iii) hypersonic steady flow with M = 32.0; and iv) transit supersonic flow in a shock tube and over a wedge. For all of the test cases the method developed resulted in accurate solutions comparable to or better than reported in the literature by other leading CFD researchers. At the same time, the combination of using unstructured methods and our specific implementation yielded the lowest utilization of computer time and memory needed to achieve a given level of accuracy.

DATA STRUCTURE

On an unstructured grid, the data that describes the connectivity of a grid and the associated geometrical coefficients can represent a considerable overhead on memory usage. We have implemented a rather simple data structure which permits efficient finite difference integration of fluid quantities with only one level of indirection. For two dimensions, the data consists of lists of vertices, edges, and triangles. The physical quantities are stored at vertex locations. The vertex list consists of: the vertex positions (x,y), the fluid variables, the vertex volume, and workspace. The edge data is composed of: the addresses of the two vertices which form an edge, a vector which indicates the normal to the face that crosses an edge, the face area, and storage for the fluxes. The face is formed by joining the baricenters of the adjoining triangles which lie along the edge. This is the only data required in performing an iteration step. For convenience and ease of diagnostics, we have also maintained a list of triangles, including the positions of the baricenters, and the addresses of both the vertices and edges which form a triangle.

The data structure is compatible with algorithms which decompose the solution of the Euler equations into two steps. The first is determination of the fluxes. This can be realized by a loop over edges where the fluid quantities along the edge can be fetched through the indirect addressing of vertex data. The second step is to integrate the fluxes which contribute to the vertex. There are two options here: one is to maintain a list of flux elements at each vertex and to perform a loop over vertices and then fluxes to each vertex; the other is to again have a loop over edges where each contribution to the vertex is done as a random fetch and store using the appropriate vertex addresses stored by each edge.

BASIC INTEGRATION ALGORITHM

We begin by describing the first order Godunov method for a system of two-dimensional Euler equations written in conservation law form as

$$\frac{\partial \vec{Q}}{\partial t} + \frac{\partial \vec{F}}{\partial x} + \frac{\partial \vec{G}}{\partial y} = 0 , \qquad (1)$$

where,

$$\vec{Q} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ e \end{pmatrix}, \quad \vec{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (e + p)u \end{pmatrix}, \quad \vec{G} = \begin{pmatrix} \rho \\ \rho vu \\ \rho v^2 + p \\ (e + p)v \end{pmatrix} .$$

Here u and v are the x and y velocity vector components, p is the pressure, ρ is the density and e is the total energy of the fluid per unit volume. It is assumed that a mixed (initial conditions, boundary conditions) problem is properly posed for the set of equations (1), and that an initial distribution of the fluid parameters is given at t = 0, and the boundary conditions defining a unique solution are specified for the computational domain.

We seek a solution of the system of equations represented by Eq. (1) on a computational domain which is decomposed into triangles with arbitrary connectivity. An overwhelming advantage of using this method of domain decomposition is the ability to resolve extremely complicated geometries where the characteristic dimensions of subdomain features can vary over many orders of magnitude.

As an example, Figure 1 shows an unstructured triangular grid used in the simulation of flow for a new generation of the wide body tennis rackets with 21 cross string rows represented as solid circles and a tennis ball. In Figure 1a a blowup of the region near the racket surface is shown. This example illustrates the ability of the unstructured grids to represent geometry of arbitrary complexity and with localized resolution.

There are several options possible for storing physical information on an unstructured triangular grid: i) vertex centered; and ii) triangle centered on either a baricentric or Voronoi node. The selection of a specific grid structure offers two contrasting approaches. The first is to place the effort on creating an optimal grid, as is the case with Voronoi - Delauney meshes, while the second is to rely on the robustness of the integration algorithm. For complex configurations it is more difficult to achieve an optimum Voronoi-Delauney mesh and we have therefore opted for a simple baricentric grid.

This grid can always be constructed for a set of arbitrary triangles. The integration algorithm we have constructed can easily be implemented for both vertex and baricentered control volumes. Figure 2 displays a fragment of such a computational domain with the corresponding dual grid. The secondary or dual grid is formed by connecting the baricenters of the primary mesh, thus forming finite polygons around the primary vertices. Independent of the remarks made in Ref. 17 concerning usefulness of Dirichlet tessellation, we have confirmed that the best practical representation of the integration volume is obtained when the dual grid is formed by connecting baricenters of the triangles.

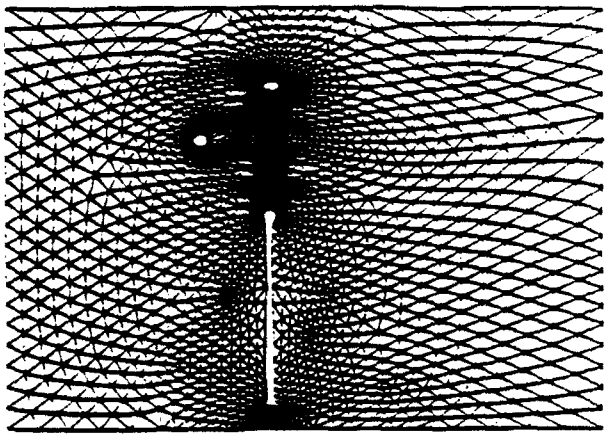

Figure 1 An illustration of the ability of a triangular grid to efficiently resolve the geometric complexity and features of objects with disparte spatial scales.

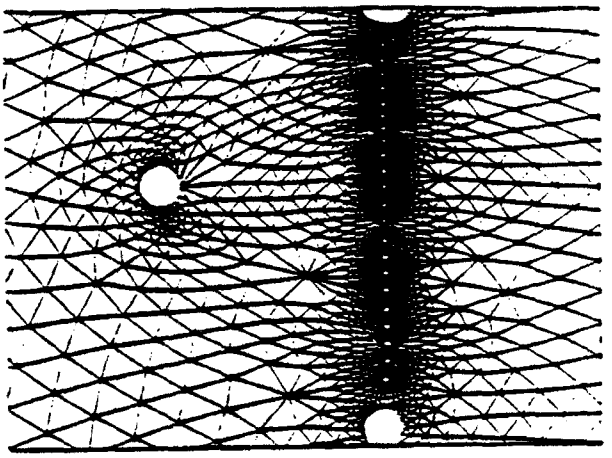

Figure 1a Detail showing the features of a wide body tennis racket simulation including 22 strings and a tennis ball.

In keeping with the philosophy that the overall scheme should be able to perform in all flow regimes with no prior tuning of "free" parameters, we have chosen Godunov methods for performing the numerical integration of the Euler equations in the control volume. These schemes are self consistent and do not contain any adjustable knobs. The superior performance of Godunov type schemes for logically structured grids is well documented and the advantages can be readily realized on triangular grids. Integration by the Godunov method consists of two basic steps: i) determination of the fluxes on the faces of the dual grid, which defines the control volume. This is accomplished by solving a set of one-dimensional Riemann problems along triangle edges; and ii) integration of the system of partial differential equations, which now amounts to a summation of all the fluxes for the vertex-centered control volume at each timestep.

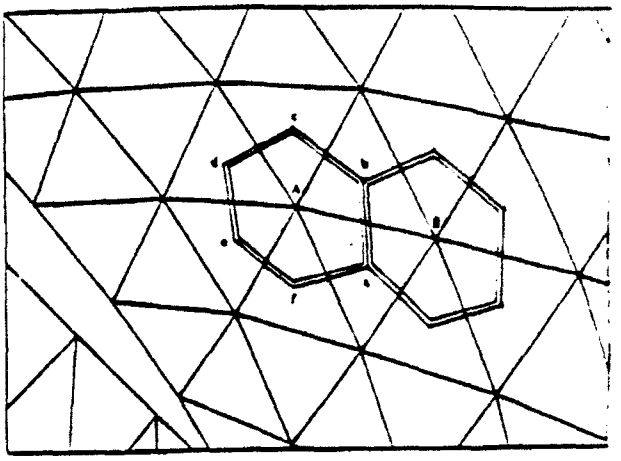

Figure 2 A triangular grid and the baricentered dual grid which defines the control volume. The fluxes are found on the faces of the control volume on each edge joining adjacent vertex points.

To define the fluxes flowing into the control volume shown in Figure 2, it is necessary to solve the Riemann problem along every edge of the primary grid and transverse to the faces of the dual grid. For example, to define the flux through the face **ab**, we solve the Riemann problem between vertices **A** and **B**. The solution of this problem is in coordinates local to the face of the dual grid **ab** so that the tangential component of velocity will be directed along **ab**. Implementation of our approach requires maintaining strict consistency when defining the "left" and "right" states for the Riemann problem at the faces **ab**, **bc**, **cd**, **de**, **ef**, and **fa**. For this reason we define not only the location of the vertices and areas of the faces but also the direction of the areas with respect to the primary grid edges. For the clockwise integration pattern in a polygon, vertex **A** will be the "left" state for all the Riemann problems related to this point and the neighbors will represent the "right" sides of the diaphragm.

It is easy to see that the flux calculation is based on information at only two nodes and requires simple geometrical parameters defining the face of the secondary grid which dissects the line connecting the two points. Thus, we can find all the values needed for the flux calculation in one vector loop over all edges of the primary grid without requiring any details related to the geometrical structures which these edges form. This in turn assures parallelization or vectorization of the algorithm for the bulk of the calculations involving the Riemann solver, which provides the first order fluxes.

The only procedure not obviously parallelizable is the integration of the fluxes for the flow variables at the vertices of the grid.

This operation requires a random fetch and store which can lead to conflicts that impair both parallelization and vectorization. Several common methods have been developed to deal with this difficulty. A practical approach is to split the integration of the fluxes into a small number of independent loops through the use of "edge" coloring. The number of loops necessary is determined by the maximum connectivity of any vertex in the domain and is

usually 7 or 8. Each of these loops is usually large enough not to impair vectorization. At this stage all the fluxes are added with their correct sign corresponding to the chosen direction of integration within the cell. The amount of computation required here is minimal since the fluxes are known and need only to be multiplied at each time step by a simple factor and added to the vertex quantity. This simple procedure results in a first order solver which is fully vectorized.

SECOND ORDER INEGRATION ALGORITHM

The second order solver is constructed along lines similar to that of the first-order method. At each cell face the Riemann problem is solved for the appropriate pair of left and right conditions. The solution to the Riemann problem is then used in calculation of fluxes, which are to be integrated later to advance to the next integration step. The extension to second order is achieved by using extrapolation in space and time to obtain time-centered left and right limiting values as inputs for the Riemann problem. The basic implementation of the method for finding the second order accurate fluxes is the same as for the one dimensional case and can be found in Refs. 14 and 16. The difference is the method of obtaining linear extrapolations for the flow variables as a first guess of their value on the faces of the dual grid. To obtain the initial guess we need to know the gradient of each gasdynamical parameter U at the vertices of the primary mesh. The value $\bar{\nabla}$ U can be evaluated by using the linear path integral around the *finite* volume associated with the vertex. For vertex A in Figure 2:

$$\int_A \bar{\nabla} U dA = \oint_l U \hat{n} dl$$

where integration along the path l in this case is equivalent to integration along the lines **ab, bc, cd, de, ef, fa,** and where n is a unit vector pointing outward from the control volume centered at A and normal to the integration path l. Knowing the gradient of the gasdynamic parameter in the volume related to vertex A allows us to extrapolate the values of this parameter at any location within the volume. This permits us to evaluate the first guess for U at the edges of the dual grid. The rest of the implementation of the second order algorithm is the same as described in Refs. 8 and 9. This includes monotonicity constraints similar to those introduced by VanLeer [15] and characteristic constraints described in Refs. 14 and 16.

A schematic of the basic steps for the second order algorithm is shown in Figure 3. This consists of five steps. They are: i) the calculation of the linearly extrapolated values at each side of the control volume faces using the left and right adjacent vertices and the values for each quantity and its gradient; ii) limiting the quantities obtained based on a monotonicity constraint; iii) a further limiter based on the solution of a one dimensional characteristic equation, which assures that the extrapolation does not violate the characteristics; iv) solution of the Riemann problem for the final extrapolated values with the limiters applied; and v) integration over the control volume.

The advantages of the method described will be demonstrated in the following section. The inclusion of the characteristic limiter has significantly improved the treatment of contact discontinuities and is the first such implementation on a triangular mesh.

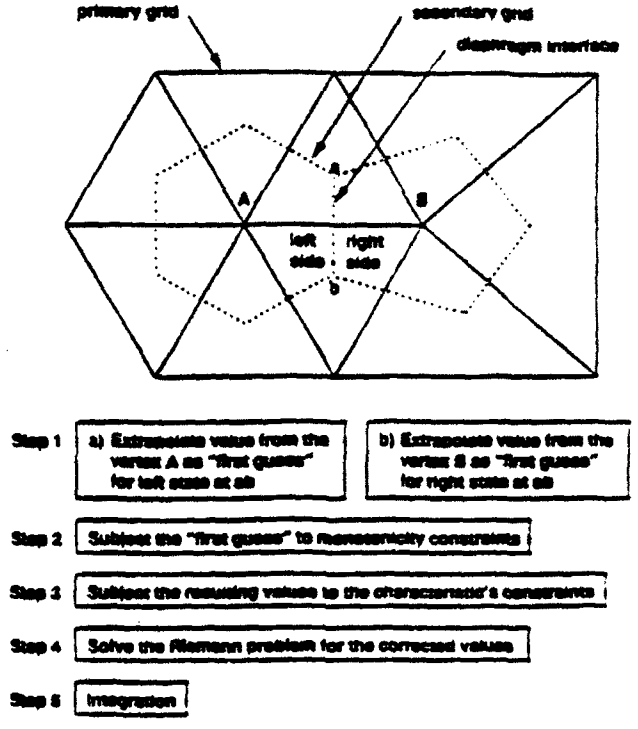

Figure 3 Schematic for stepwise implementation of the second order Godunov method on an unstructured grid.

RESULTS FOR TEST PROBLEMS

We have picked a set of test problems to demonstrate the performance of the FUGGS code for unsteady shock wave problems, and for subsonic, supersonic and hypersonic steady state flows. The cases in the chosen examples have analytical solutions that can be used to quantify the accuracy of the code and to validate the performance. This set of problems is frequently used by other CFD researchers and forms a basis for comparing FUGGS with other techniques.

a. Unsteady Shock Problem

As a first test we have chosen a case of planar shock wave propagation in a channel.

A section of the grid used for this test problem is shown in Figure 4. The total grid contained ~ 2000 vertices with a resolution of 100 points in the direction of propagation. We simulated a simple shock tube problem on

this grid where the gasdynamic parameters to the left and right of the diaphragm have the following values:

$P_l = 1.0$; $\rho_l = 1.0$; $U_l = 0$;
$V_l = 0$; $\gamma_l = 1.4$;
$P_r = 0.1$; $\rho_r = 0.125$; $U_r = 0$;
$V_r = 0$; $\gamma_r = 1.4$.

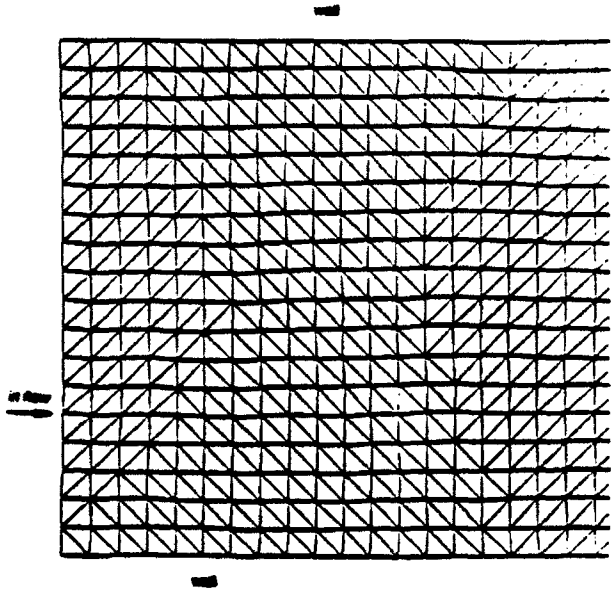

Figure 4 Section of grid from the unsteady shock problem.

This one dimensional problem was simulated on a rather ill formed grid (from the viewpoint of connectivity). Consequently the quality of the solution depended on the flow solver for accuracy. For the triangular shape of the elementary cell, planar shock and rarefaction waves generated by the solution always propagate at conflicting angles with respect to four out of the six edges of the control volume. The triangular grid chosen for this simple test problem therefore indicates the accuracy of FUGGS for shock waves of arbitrary shape and orientation moving through the computational domain. The density distribution found from three different versions of FUGGS is shown in Figure 5 as a function of x along the median cross section of the grid. The three cases are: i) first order Godunov method; ii) second order Godunov; and iii) second order Godunov with the characteristic limiter. The data displayed in the figure represents a loss of resolution due to interpolation of the actual grid values to the projected midsectional line. It is clear from Figure 5 that the final implementation of FUGGS with characteristic constraints yields the best results for contact discontinuities. The code also maintains the one dimensional structure for the shock in all three cases described above. The accurate representation of the density is also typical for all the other gasdynamic parameters.

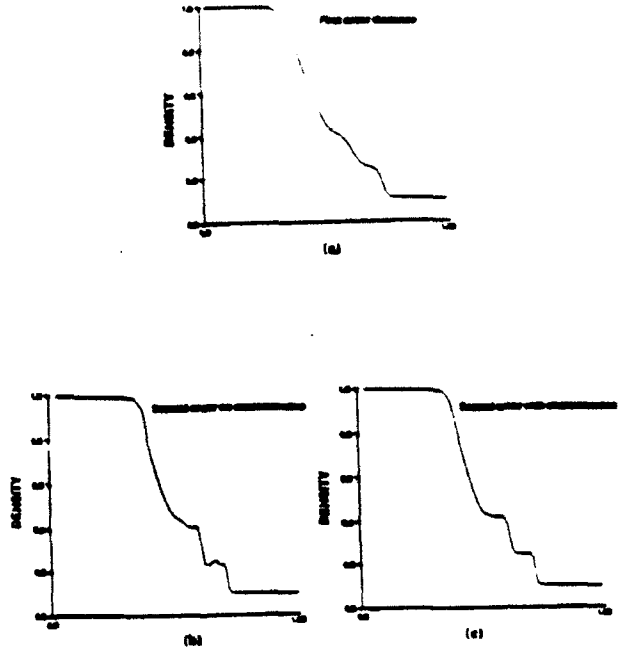

Figure 5 Solution to the density distribution of shock problem with three different versions of FUGGS: a) First Order Godunov, b) Second Order Godunov without characteristics and c) Second Order Godunov with characteristics.

b. Shock on Wedge

Here we demonstrate the performance of the methods for steady supersonic flow simulations. An analytical solution from oblique shock wave theory exists and can serve as an unambiguous comparison with the numerical simulation.

The initial grid for the shock on wedge problem is shown in Figure 6. This gridding results in ~ 500 vertices and ~ 800 triangles. The wedge angle in Figure 6 is 10°. The incoming flow enters the computational domain normal to the left boundary at Mach number M=2. Figures 7a and 7b show isomach lines for the steady flow solution from the first and second order Godunov solvers on the original grid. Comparing these two solutions we can see that the second order solution substantially improves the shock resolution. However, it is obvious that the grid density is too small to adequately resolve the oblique shock wave in both cases.

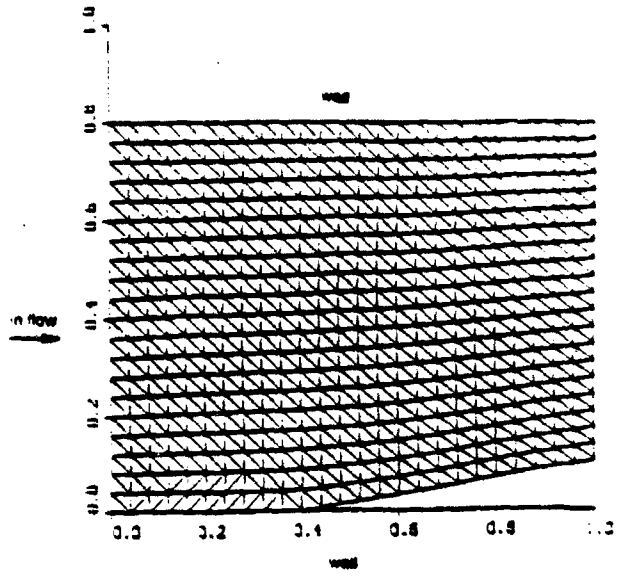

Figure 6 Coarse grid for shock on wedge problem.

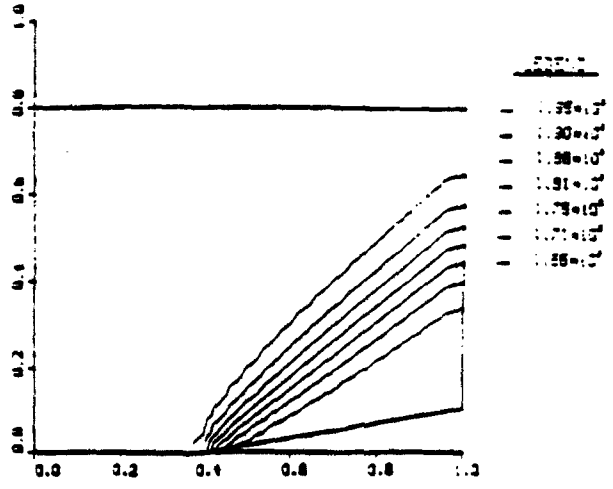

Figure 7a First order Godunov solution for the coarse grid shown in Figure 6.

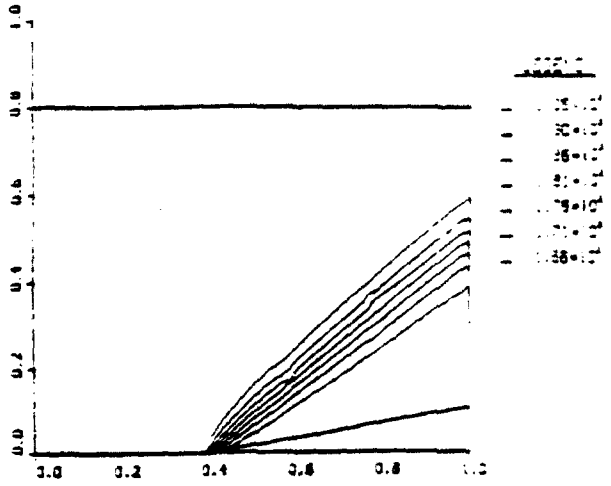

Figure 7b Second order Godunov solution for the grid shown in Figure 6.

To improve the accuracy a higher grid density is required in the region of discontinuity. This is achieved by subdividing the original elements of the grid in regions of large changes in flow parameters.

A variety of criteria can be devised to identify regions which require mesh refinement. An example is given in Ref. 2 where a preset condition is imposed on the resolution from local derivatives of the flow parameters. The implementation of this criteria in FUGGS would have led to a significant loss of computational efficiency because the stencil for the Laplacian is nonlocal and would require more than one level of indirectness. Instead we used a simple parameter variation criteria based on the local variation in pressure or density to select the grid regions needing refinement. Figure 8 shows an enhanced grid derived from the mesh shown in Figure 6 by two levels of subdivision. The number of triangles in this case increase from 800 to 1200. Figure 9 shows isomach lines of the solution using the second order method for the same shock on wedge problem as in Figures 7a and 7b. The improvement in shock resolution is dramatically noticeable. This problem also illustrates the ability of unstructured grid methods to provide local resolution for important flow features, without requiring excessive overhead for other regions of the computational domain.

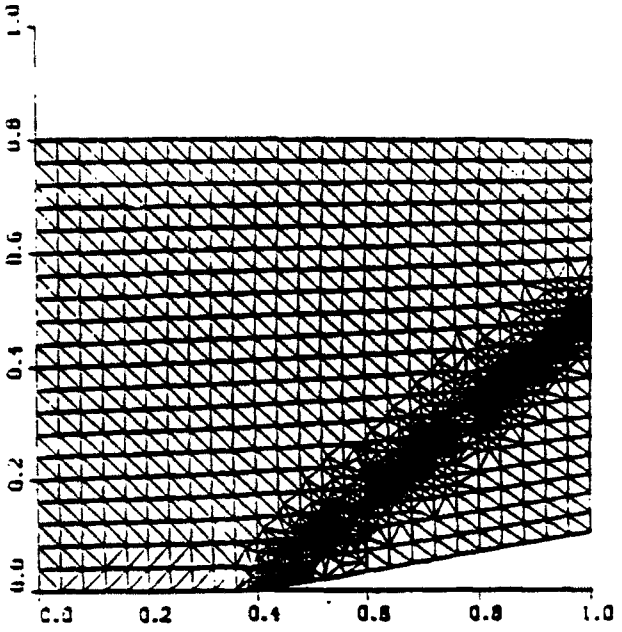

Figure 8 Improved grid for the shock on wedge problem with two levels of refinement based on 5% variation in local value.

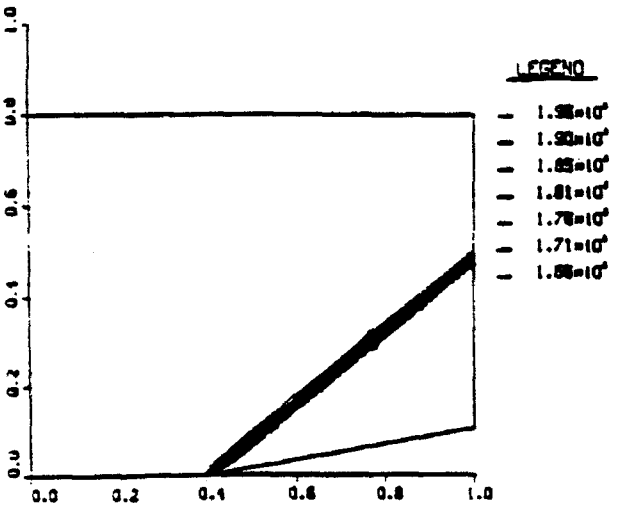

Figure 9 Second order Godunov solution for the shock on wedge problem using a grid with two levels of refinement.

c. Subsonic Flow

A challenging test problem to assess the performance of Euler codes for subsonic flow has been suggested by Pulliam [19]. He has computationally simulated a steady subsonic flow over an ellipse with major to minor axis ratio of 6:1. The numerical solution of Euler equations reported for this case at $M_\infty = 0.2$ with angle of attack $\alpha = 5°$ produced a lift coefficient of $C_L = 1.545$. As is well known from D'Alembert's Paradox, inviscid flow at low Mach numbers should yield $C_L = 0$ and have zero drag for a profile of an arbitrary shape. For this reason the problem posed by Pulliam is a good indicator of the accuracy and amount of artificial dissipation introduced by a numerical algorithm. Moreover, while a Euler solver is not meant to treat potential flow, a general purpose solver should be capable of simulating such flow conditions if they occur in a portion of a given problem without resorting to a different algorithm. In making a transition to full Navier-Stokes treatment, the use of a Euler solver is an essential step; it is important to have confidence that the artificial viscosity introduced does not dominate the solution.

For the case under consideration, it is very important to understand in detail the potential flow solution over an ellipse. Fortunately, the analytical solution is available and is relatively simple. The complex potential for the flow over a cylindrical ellipse is given by the following [20]:

$$F(z) = -\frac{1}{2} M_\infty (a+b) e^{-i\alpha} \left[\frac{z + \sqrt{z^2 - (a^2 - b^2)}}{a+b} + \frac{z - \sqrt{z^2 - (a^2 - b^2)}}{a-b} \right]$$

where $Z = x+iy$ and M_∞ is the Mach number. By taking the gradient of the potential we can find the velocity flow field explicitly:

$$\frac{U}{U_\infty} = \frac{(1+\lambda)\sin(\theta+\alpha)\sin\theta}{\lambda^2\cos^2\theta + \sin^2\theta}, \qquad \frac{V}{U_\infty} = \frac{(1+\lambda)\lambda\sin(\theta+\alpha)\cos\theta}{\lambda^2\cos^2\theta + \sin^2\theta}, \tag{3}$$

where $\lambda = b/a$ is the ratio of minor to major axis, θ is the angle in polar coordinates from the center of the ellipse, and α is the angle of attack.

In examining this equation, we find that the maximum value of velocity is a strong function of λ. For an ellipse with $\lambda = 1/6$, the maximum value V/U_∞ occurs at $\theta = 0$ or π and where $V_{MAX}/U_\infty = 7\sin\alpha$. For a flat plate where $\lambda \to 0$ the maximum velocity is infinite. The angle α defines the distance between the stagnation point where the velocity is zero (at $\theta = -\alpha$ and $\pi-\alpha$) and the point where the velocity is maximum (at $\theta = 0$ and π). For the case selected by Pulliam the distance between the point with minimum and maximum velocity is 0.19% of the length of the major axis.

This means that the gradient of velocity along the major axis of the ellipse in the vicinity of stagnation points is extremely high. With ~ 1000 points uniformly distributed on the surface of the ellipse, only one grid spacing is available to resolve both the stagnation point and the point at which maximum velocity occurs. Even though one would normally construct a nonuniform grid in the vicinity of the stagnation point, we estimate that enormous computational resources would be required to resolve the characteristic scale length for this problem. Traditional methods encounter difficulties in this situation because spatial splitting leads to a poor estimate of the gradient and

the low connectivity of the mesh introduces spurious vorticity.

We performed two simulations for the conditions described by Pulliam. The number of nodes used on the surface of the ellipse is the same as in Ref. [19]. The grid is shown in Figure 10 for these simulations in the region immediately proximate to the ellipse. This grid is of poor quality and highly distorted; contains ~ 6000 vertices and ~ 130 points on the surface of the ellipse. The results are shown in the form of pressure contours in Figures 11 and 12 for the first order and second order solvers respectively. In the case of the first order algorithm, we obtained a lift coefficient of C_L = 0.29. The pressure contours for this simulation are not smooth, attributable to the low level of accuracy of the solver. The same situation resulted in C_L = 0.252 when computed with the second order solver, and as can be seen in Figure 12 the pressure contours are considerably smoother. The result presented by Pulliam was $C_L \cong 1.55$, almost an order of magnitude higher than achieved with FUGGS. This highlights an important quality of our approach: the low generation of artificial viscosity. In comparison the lift obtained by Pulliam is as high as one would expect from thin profile theory and hence would mask real viscosity effects if they were added to the algorithm.

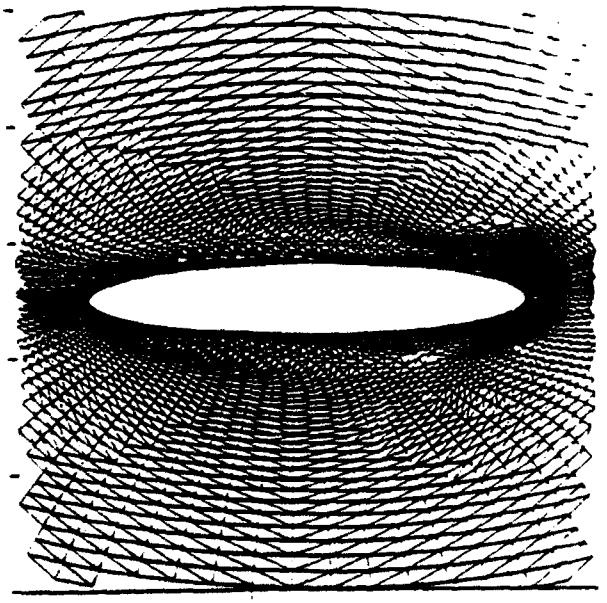

Figure 10 Section of the grid used in simulation of subsonic flow over an ellipse for conditions suggested by Pulliam [19].

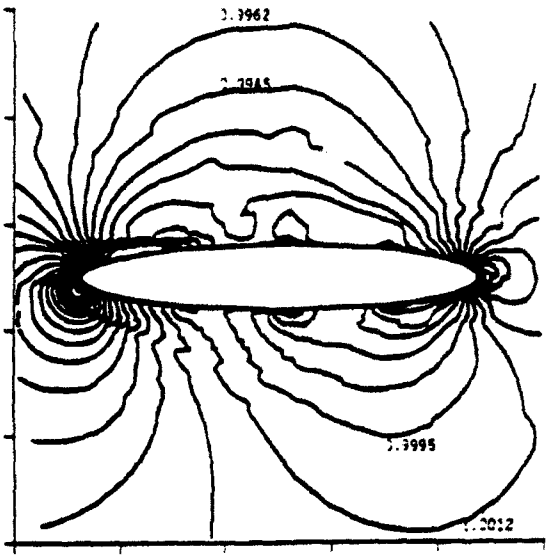

Figure 11 First Order Euler Solution for 6:1 Ellipse. Pressure contours. α = 5°; Mach = 0.2; 6065 vertices; C_L = 0.381; C_D = 0.101.

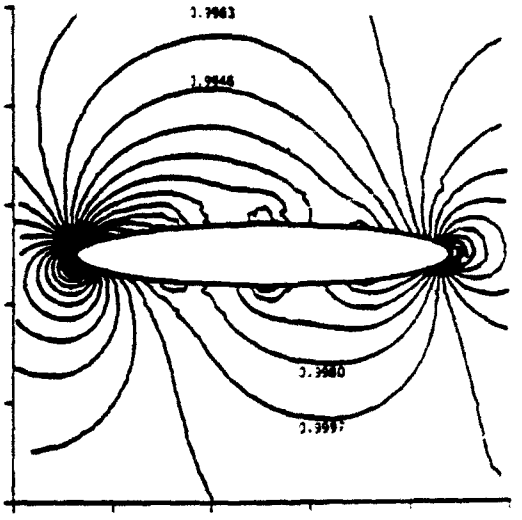

Figure 12 Second Order Euler Solution for 6:1 Ellipse. Pressure Contours. α = 5°; Mach = 0.2; 6065 vertices; C_L = 0.252; C_D = 0.004.

We also simulated flow over a cylinder at M = 0.2. The grid for this case is shown in Figure 13. We examined the numerically produced lift with inflow conditions at various angles with respect to the x - axis (0°, 5° , 20°, 45°). The lift coefficient was angle independent and had a value C_L = 0.76, almost 20 times smaller than reported by Pulliam, whose results are angle sensitive. With the first order scheme we achieved a lift coefficient of C_L = 0.47 with the drag coefficient $C_D \cong 1.49$. For the second order scheme, shown in Figure 14, the drag coefficient was reduced to C_D = 0.19 but the lift coefficient increased somewhat to the

value cited above. We also investigated the effects of grid refinement and found that a simple one level of refinement (adding ~ 400 vertices) led to a modest reduction in lift coefficient of about 20%. To reinforce a point made earlier, all of the results were achieved with no "free" parameters to adjust. These parameters are present in many CFD codes in the form of coefficient for artificial viscosity terms present the practitioner with a practical problem of how they should be selected for different flow conditions.

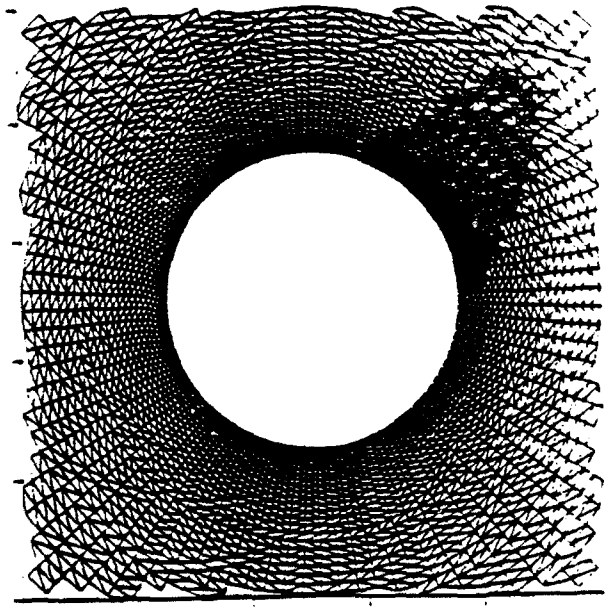

Figure 13 Grid for simulation of flow over a cylinder at varying inflow angles with respect to the mesh.

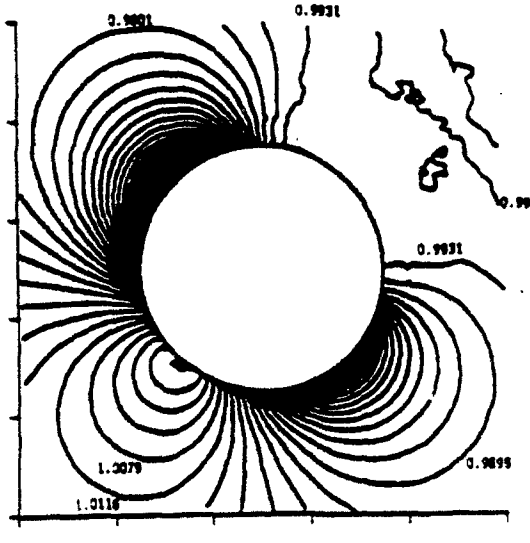

Figure 14 Second Order Euler Solution for a circular cylinder: $\alpha = 45°$; Mach = 0.2; 6311 vertices; $C_L = 0.761$; $C_D = 0.196$.

d. Hypersonic Flow

To demonstrate the versatility of the method for the entire range of flow regimes we have simulated a hypersonic flow test problem. One of the advantages of the Godunov type methods is that for the whole range of calculations performed (from low subsonic flow, supersonic flow, unsteady flow with strong shock, or hypersonic flow at Mach number M=32) it is unnecessary to change or adjust the numerical algorithm. In Ref. 21 performance of first and second order Godunov methods has been analyzed for hypersonic flow regimes. There, as a test problem, an analytical solution was used for a hypersonic flow around a flat plate of finite thickness. This solution was obtained based on the analogy between hypersonic flow over a flat plate of finite thickness and a strong planar explosion. Here we will use one expression from Ref. 21 which defines the shape of the shock wave as a function of plate thickness d, γ the adiabatic coefficient, and α a nondimensional scale factor related to the energy released at the stagnation point.

$$Y_{SHOCK} = \left(\frac{1}{2} D_f \frac{dx^2}{2}\right)^{1/3}$$

where D_f is a coefficient of order unity,

$$a = k_1 (\gamma-1)^{k_2+k_3 \ln(\gamma-1)}$$

while $k_1 = 0.36011$, $k_2 = -1.2537$, and $k_3 = -0.1847$.

As a direct comparison we solved the hypersonic flow problem for the same set of conditions as in Ref. 21:

$$U_\infty = 10011 \text{ meters/sec}, \; p = 98.72 \text{ Pa},$$
$$\rho = 1.24 \times 10^{-3} \text{kg/m}^3 \text{ and } \gamma = 1.2.$$

The grid used for this simulation is shown in Figure 15. This grid has ~ 5500 vertices and it's spatial resolution at the leading edge of the plate is of the same order as that of a 300 x 60 rectangular grid used in Ref. 12.

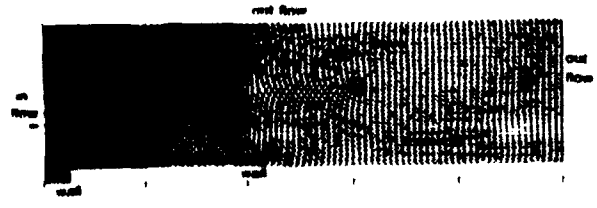

Figure 15 Grid for simulation of hypersonic flow over a flate plate.

In Figure 16 results for this simulation are shown in the form of pressure contours. Figure 16 also shows the location of the analytically calculated shock front by a discrete line (squares). The shock resolution and accuracy of its location are comparable to that obtained in Ref. 21, even

though our triangular grid has less than 1/3 the nodes than the rectangular grid used in Ref. 21. This is due to the fact that in constructing the triangular grid we had the flexibility to place the highest concentration of nodes in the area of the leading edge where the main properties of the flow are established.

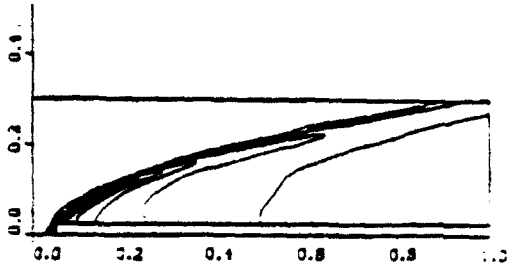

Figure 16 Second order solution for a flat plate. Pressure Contours. Mach = 32; 5509 grid vertices; $P_{max} = 5.0 \times 10^4$; $P_{min} = 98.7\ P_a$.

CODES COMPUTATIONAL EFFICIENCY

During the code development effort, great attention was paid to the code data structure, its efficiency and extendability to three dimensional calculations. In fact, the two dimensional version of the code has all the data structures required for the three dimensional simulations. That fact should be factored in comparing our storage overhead figures to those in other codes. Also while developing FUGGS we made a decision not to rely on machine-dependent functions, in order to assure portability. This feature is very important in the current supercomputing environment where a host of powerful parallel supercomputers and super workstations with diverse architecture are available and useful for different aspects of design.

The following performance characteristics have been achieved for the latest version of the FUGGS code:

1. First Order Godunov version:

Memory Requirement	36 places per triangle includes 5 physical quantities integer indexing arrays all geometric parameters
CPU Performance CRAY XMP-24 STELLAR 1000	 15 μsec/vertex/timestep 79 μsec/vertex/timestep

2. Second Order Godunov version:

Memory Requirement	39 places per triangle
CPU Performance CRAY XMP-24	45 μsec/vertex/timestep Monotonicity step 50% Characteristic limiter 15% Riemann Solver 30% Integration 5%
STELLAR 1000	214 μsec/vertex/timestep

These numbers are provisional since the code is still under development. We feel that further improvements in code performance will be achieved with respect to both timing and storage requirements.

CONCLUSION AND DISCUSSION

We have presented a method for the numerical solution of Euler equations on an unstructured triangular grid. The method was tested for a wide range of flow conditions,from low subsonic flow and unsteady flow with strong shock waves to hypersonic flow with Mach 32. For all these regimes, the method performed extremely well both in terms of solution accuracy and computational efficiency. The method is very robust and does not resort to adjustable computational parameters for the tested range of flow conditions. This is due to the fact that the numerical algorithm in FUGGS is based on Second Order Godunov schemes adapted to triangular grids. The method appears natural for unstructured triangular grids because the greater connectivity intuitively should lead to greater accuracy in eliminating errors introduced by splitting. In a typical hexagonal (or greater) control volume the contribution of fluxes is available from all six adjacent directions as opposed to just two in the case of a rectangular grid. Since the FUGGS method has been implemented on unstructured grids, it is possible to simulate flows over bodies of arbitrary geometry where the grid density can be concentrated in a region of flow discontinuity.

Especially interesting is the code's superior performance for the simulations of subsonic flow. For the test cases calculated here, our method appears to perform better than the leading industry codes like ARC2D and SYMTVD. We think that the two main reasons for the better performance are multidirectional splitting (to distinguish from two directional splitting typical for logically structured quadrilateral grids) and finite volume integration, more should be done to investigate this important aspect of the code's performance.

Historically, Euler solvers were developed to simulate nonisoentropic flows for which potential flow assumptions are incorrect. From the original development of numerical methods for the solution of Euler's equations, great effort has been devoted to resolving shocks and contact discontinuities, producing in dramatically improved results for shock wave hydrodynamics. At the same time, attention to the accurate solution of the velocity gradients has been neglected. While these gradients are more difficult to discern than shock waves, they are more prevalent in practical flow

problems and could lead to very significant errors in such important parameters as lift and drag coefficients. In addition, all vorticity and viscosity dominated phenomena depend on accurate solution of the velocity gradients. In view of the performed numerical simulations for subsonic flow over the ellipse and cylinder it is clear that unless these features are resolved, the numerical solution of Euler equations can introduce spurious vorticity, making the results from a full Navier-Stokes implementation impossible.

Acknowledgment

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Reflection of the Triple Point of the Mach Reflection in a Planar and Axisymmetric Converging Channels

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9th Mach Reflection Symposium
Freiburg
June 1990

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Introduction

Depending on their parameters, the encounter between a planar shock wave and a wedge can produce a classic case of the Mach Reflection. The Mach Reflection has a characteristic triple point, where three shocks and the contact discontinuity coalesce. In a shock tube or in a channel, a developed Mach Reflection can reflect further from the walls opposite the wedge. In this case, the Mach shock of the Mach Reflection will start reflecting when its triple point reaches the wall opposite the wedge. Upon reflection of this shock wave, a secondary Mach Reflection can form. Although the primary Mach Reflection has received considerable attention in scientific literature (Refs. 1,2,3), the phenomenology of the subsequent reflections was gone virtually unnoticed. In our literature review, we found only a short qualitative description of the phenomena by Bazhenova and Gvozdeva (Ref. 4). This omission is unfortunate, since it is a very practical case for propagation of the shock waves in channels of variable cross sections.

The direct simulation of the various cases of Mach Reflection has only become possible in the last decade. This problem is a challenging test for the numerical methods used in Computational Fluid Dynamics (CFD). An impressive demonstration of the capabilities of the direct numerical simulations of Mach Reflection phenomena is given by Glaz et al. (Ref. 5). They demonstrate that all the important phenomenology of the Mach Reflection, including slip line vortex and Mach shock wave bulging, can be simulated directly. This was achieved by using the Second Order Godunov method, numerical technique, developed in 80th, which is extremely robust and allows very accurate simulation of flow discontinuities.

The Second Order Godunov method was implemented on rectangular grids (Ref. 6) and in a few cases on general quadrilateral grids (Ref. 7). This approach has limited application, since the structured quadrilateral grids have great difficulty describing a complicated computational domain with multiple bodies of different geometries and scales. Recently, we have implemented the Second Order Godunov for unstructured triangular grids (Ref. 8). This enables us to combine the robust and accurate numerical algorithm with a griding technique, allowing us to describe very complex domains with ease and efficiency. In addition, we have developed a novel Dynamic Grid Adaptation methodology which allocates a dense computational grid only to regions where

enhanced resolution is needed to resolve strong gradients in flow parameters. As demonstrated in our paper, this enables an extremely economical allocation of computational resources and accurate simulation of a complicated phenomena like Mach Reflection.

In our study, we numerically simulate the formation of a Double Mach Reflection on a sloped wall of a converging channel, with subsequent reflection of the reflected wave at the straight wall of the channel. Presented here numerical results were obtained with the new numerical technique and we will describe in detail all the important new elements which we have introduced.

The Problem

Figure 1 shows a converging channel with a sloped wall at 27°. The figure illustrates our assumption that a Mach 8.7 shock wave travelling normally to the parallel walls enters the channel at the left hand side. According to analysis presented in Reference 9, this shock will have a Complex Mach Reflection when it encounters the converging wall of the channel. At some stage of the reflection process, the triple point will reach the opposite wall of the channel. Here the Mach stem shock wave will become incident, moving at an angle to the channel wall, as illustrated in Figure 2. The shock and wedge parameters chosen in our problem will cause formation of a secondary Mach reflection. The question is: What form will this secondary reflection take? Bazhenova and Gvozdeva offer a very general description of the anticipated effect, illustrated in Figure 3 (Ref. 4). In this reference, a system of secondary reflections shows the incident and Mach shocks are interchanging their positions with every new reflection, and the strength of the shock waves is increasing. It is not clear from Reference 4 what type of Mach Reflection will form, or how the secondary reflected wave, which expands in already perturbed gas, will be affected by the interactions with the strong slip surfaces located behind the original Mach shock.

We will directly simulate formation of the Mach Reflection at the channel oblique wall, as well as all secondary reflections which will occur according to the conditions outlined above for the channel geometry shown in Figure 1. In addition we will consider cases in which the channel shown in Figure 1 is axisymmetric and will study the same problem for this case. The motivation is further study of the phenomenology of shock wave focusing when a three-dimensional contraction occurs.

In our study we will consider an ideal, invisid gas which can lead to some distortion of our results compared with experimental data. However, we believe that this simplification will still capture the main phenomenology of wave formation and reflection, and will be of general value to the Mach Reflection Theory.

Numerical Method

In Reference 8 we introduced a new numerical algorithm: FUGGS (Fast Unstructured Second Order Godunov Solver), for solving Euler's equations of gasdynamics on unstructured triangular grids. The algorithm formulated and tested in Reference 8 is vertex-based. Here we will describe a new volume based version of the FUGGS method. The new version of the algorithm as illustrated in our paper, produces considerably more accurate solutions and it is more efficient. This contradicts published results (Ref. 10,11) on implementation of the triangle-based TVD schemes for unstructured triangular grids. The new algorithm has been validated for the range of subsonic, supersonic and hypersonic steady state and transient problems. Here we show only results for Mach Reflection in planar and axisymmetric channels..

The new triangle-based version of the FUGGS algorithm was extended to allow dynamic adaptive grid refinement for transient problems. We will give a description of the dynamic grid adaptation methodology used in FUGGS code.

A three dimensional version of the FUGGS algorithm was developed in an extremely short period of time. This was made possible by the simple structure of the basic algorithm. We will not present simulation results for the three dimensional FUGGS, however, the main elements of the FUGGS algorithm implementation in the three dimensions will be illustrated.

Vertex-Based and Triangle-Based Integration Algorithms

We consider a system of Euler equations written in conservation law form in three dimensions as:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} + \frac{\partial \mathbf{g}}{\partial y} + \frac{\partial \mathbf{h}}{\partial z} = 0 \tag{1}$$

where

$$\mathbf{U} = \begin{vmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{vmatrix}, \ \mathbf{f} = \begin{vmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ \rho uH \end{vmatrix}, \ \mathbf{g} = \begin{vmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ \rho vH \end{vmatrix}, \ \mathbf{h} = \begin{vmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ \rho wH \end{vmatrix}$$

Here u, v, and w are the x, y, and z velocity vector components, p is the pressure, ρ is the density and H is the total enthalpy and E is total energy of the fluid. It is assumed that a mixed (initial conditions, boundary conditions) problem is properly posed for the set of equations (1), that an initial distribution of the fluid parameters is given at t=0, and the boundary conditions defining a unique solution are specified for the computational domain.

We seek a solution of the system of equations (1) on the computational domain which is decomposed into tetrahedrons (triangles in two dimensions) with arbitrary connectivity. An overwhelming advantage of this method of domain decomposition is the ability to resolve extremely complicated geometries and flow regimes accurately and efficiently. This has been demonstrated in numerous publications on this topic (Ref. 12, 13, 14).

There are several options possible for storing natural physical parameters of the problem on an unstructured tetrahedral or triangular grid. In particular, we have examined: i) vertex centered; and ii) tetrahedron (or triangle) centered. These two approaches, while equivalent from the point of view of the formal numerical representation of the governing equations, lead to different algorithms. As shown below, this will have important consequences not only on data structure and algorithm efficiency, but moreover the different connectivity will affect the overall accuracy of the numerical solution.

In Figure 4, a fragment of the two-dimensional computational domain is shown. Here, together with the original triangular grid (solid lines), the secondary grid (broken line) is shown. This secondary grid is formed by connecting the barycenters of the primary grid. If a vertex based grid is used, the physical parameters of the problem are stored at vertices A, B, C..., and the integration is done for the volumes delineated by the polygons of the secondary grid. For instance, integration volume associated with vertex A is defined by the edges ab, bc, cd, de, ef, fa. For a triangle-based grid the physical parameters will be stored at the nodes of the secondary grid, and integration volume will be the triangle itself. We have shown (Ref. 15) that these two approaches lead to numerical algorithms with different connectivity, accuracy and efficiency. The fundamental algorithm of the second order Godunov method implemented in FUGGS can be illustrated in two dimensions for an edge of the grids control volume shown in Figure 5. The algorithmic steps of the second order Godunov method can be defined as follows:

1. Find the value of the gradient at the vertex point (or at the baricenter of the triangle for the triangle-based version) for the gasdynamic Parameter U;

2. Using the gradient values, find the interpolated values of U at the edges defining the control volume (sides of the triangle for the triangle-based scheme)

3. Limit these interpolated values based on a monotonicity condition (Ref. 16)

4. Subject the resulting values to the characteristic's constraints (Ref. 6)

5. Solve the Riemann problem for the corrected values.

This last step completes the definition of the fluxes at the edges of the control

volume. The flux values can be stored at the edges and the flux calculation loop will be arranged for the list of edges, which is the largest vector in the system. If the algorithm is vertex-based to calculate U^{n+1} values, we will integrate the fluxes at the edges of the secondary grid which define the control volume for the vertex. For the triangle-based algorithm U^{n+1}, value is obtained by integrating the fluxes at the sides of the triangles.

Implementation of the algorithm in three dimensions will have the same basic steps in flux calculation 1-5. To illustrate that point, Figure 6 shows a tetrahedral element of the grid. Here the fluxes are defined on the faces of the tetrahedral at the edge points. At step 1 the gradient is caluclated at the barycenter cell point for the tetrahedral. All the rest of the steps are identical to those described above. To find the value of U^{n+1} in the three dimensional case, we will add fluxes defined at the faces of the tethraletral. Most elements developed for the two dimensional code are applicable to this implementation of the three dimensional algorithm.

Direct Dynamic Refinement Method (DDRM)

Practical numerical simulations of the fluid dynamic problems call for modeling flows over complicated shapes. In addition, important flow features such as shed vortices, shock waves, slip lines and boundary layers usually have widely varied lengths and time scales and need to be resolved. Accurate solution of these problems require computational grids dynamically adapted to the evolving flow feature, and with full control over solution accuracy in the key regions of the computational domain. It is commonly accepted that only unstructured grids can provide full flexibility in obtaining the local grid resolution sufficient to accurately resolve subscale flow features. The five years since the introduction of these grids and methods in CFD research have produced landmark simulations clearly demonstrating their advantages (Ref. 12, 14, 17).

Although a number of research groups have demonstrated application of unstructured grids to simulations of steady state problems (Ref. 14, 17, 18), simulations of time-dependent problems were accomplished by a significantly smaller group (Ref. 19, 20). An adaptive refinement method developed by Lohner (Ref. 20) is based on a hierarchical system of grid refinement/coarsening in which each level of refinement has six possible cases and coarsening three cases of triangular cells formation. Every layer of refinement has a father/son relation with the previous layer, and all these layers of refined mesh move on the basic predefined grid. This technique has the demonstrated capability of carrying out simulations of extremely complex flow regimes. However, its rigid hierarchic approach to generating grid results in some implicit limitations. For example, a dynamically evolving grid will not have an element larger than the cell of the initial grid, or it will be impossible to reduce the cell volume abruptly in some areas without passing through all the necessary level of refinement.

In our paper we will report a new method of dynamic grid adaptation. This method is based on direct refinement and reconnection in the areas of monotonic flow preceding the regions with strong flow gradients. In Figure 7 we have illustrated the basic process of refinement accomplished in the DDRM method. The original grid is shown in Figure 7a. Figure 7b illustrates a one step grid refinement in which a new vertex is introduced into a triangular cell forming three new cells. This is followed by reconnection which modifies the grid in a manner demonstrated in Figure 7c. The process of refinement and reconnection can be continued until the necessaary grid resolution is achieved, as illustrated in Figures 7d and 7e. This direct approach to the grid refinement grants extreme flexibility in resolving local flow features. A similar simple method is applied to grid coarsening. In the first step of coarsening the marked vertices, all associated elements of the grid are simply removed, as shown in Figure 8a. During the second step, this void in the grid is filled with new larger triangles (Figure 8b), and then reconnected as shown in Figure 8c.

The Direct Dynamic Refinement Method (DDRM) was implemented for the second order-Godunov method (FUGGS algorithm Ref. 7, 15). Here we demonstrate its performance for a classical Mach Reflection problem.

Results

In Figures 8a, 8b, and 8c, simulation results are shown in the form of density contours for different stages of Mach Reflection in a planar channel. To illustrate the dynamics adaptation of the computational grid to the solution in the same figures, we show the grid as it evolves in time. The numerical solution develops as a classical case of Mach Reflection. Because we have assumed that the gas is ideal with $\gamma = 1.4$, according to Ben-Dor and Glass (Ref. 9) for the shock wave and wedge angle conditions chosen we should have a case of Complex Mach Reflection (CMR). We can observe in Figures 8a, 8b and 8c that the density contours definitely display the pattern of discontinuities attributed to CMR. In these figures we observe a well defined slip line vortex, slip line, triple point and the kink. For real gas, in this case, the Double Mach Reflection should occur. The slip line and slip line vortex will be located close to the Mach shock and will cause the Mach shock bulging (Ref. 5). However the perfect gas assumption will lead to CMR and extensive bulging will not arise, as is accurately predicted in our simulations. It is striking to observe in Figures 8a, 8b, and 8c that the numerical grid closely follows the evolving system of waves, and the high density grid is only observed in the areas of shock waves, slip lines and other flow discontinuities. The result is tremendous savings in both CPU and storage. For example, the grid shown in Figure 8c has only 6000 points (an equivalent of a grid 60x100 in the case of a structured rectangular grid).

Reflection of Mach shock from the wall opposite the wedge will start immediately after the stage shown in Figure 8c. This reflection results in formation of the secondary Mach Reflection which expands towards the channel's oblique wall. In Figure 9a, this secondary Mach Reflection can be clearly identified. In Figure 9b, the blow up of the region of the secondary Mach Reflection is shown. All the distinguishing characteristics of the Mach Reflection can be identified in this figure, including triple point, Mach shock. reflected shock and slip line. In addition to all these features, the secondary Mach Reflection has an additional kink, resulting from interaction of the reflected shock with the slip surface. It is clear that this interaction will affect significantly the dynamics of the secondary reflection.

In Figures 10a, 10b, and 10c, simulation results are shown for the Mach Reflection in an axisymmetric channel which has the same cross section as the planar channel. For direct comparison here the simulation results are presented in the same format as in Figures 8a, 8b, and 8c for the case of a Mach Reflection in a planar channel. The Mach Reflection in Figure 10a is analogous to its planar counterpart in Figures 8a and 8b. In Figure 10b it can be observed that the area of the shock between the triple point and the kink in the reflected shock tilts towards the axis of symmetry of the channel. This is even more pronounced in Figure 10c where the density contours are shown before the secondary reflection starts. It is apparent that the secondary reflection of the Mach shock will occur earlier in the axisymmetric channel than in its planar counterpart. Contraction in the radial direction results in a significant jump in density upon reflection. In Figure 11a we see that at the initial stages of the axisymmetric reflection, maximum density increased three-fold compared with the values observed in the initial reflection. This increase in density affects the increment between the contour levels displayed in Figure 11a and causes the slip line not to show. In Figure 11c a more advanced stage of the secondary reflection is shown. To examine in more detail the features of the secondary reflection in Figures 11b and 11d, we show an enlarged view of the secondary reflection region corresponding to Figures 11a and 11c. In these figures, we can observe the formation of a distinct reflected wave pattern with a characteristic double kink of the reflected wave similar to that seen in the secondary reflection in a planar channel. In the axisymmetric case, the secondary reflection is significantly stronger than in the case of a planar channel. Since this reflected wave propagates along the radius of the channel, it will expand rapidly. This can be observed in Figure 11c where the maximum value of density dropped 30% compared with the maximum in Figure 11a. For the same reason the triple point of the secondary Mach Reflection has advanced much farther towards the oblique wall in Figure 11d than in Figure 9b.

Conclusions

A computer code has been developed for Euler's equations of gas dynamics. This code uses unstructured grids for computational domain decomposition and its integration algorithm is based on the Second Order Godunov method. The code uses the Dynamic Grid Adaptation methodology, allowing economical allocation of computer resources to evolving flow features. In turn, it is then possible to carry out accurate simulations of complicated gas dynamic phenomena with affordable computer resources. Here the code has been demonstrated to produce an accurate simulation of Complex Mach Reflection in planar and axisymmetric channels. We also have simulated the initial stages of the secondary Mach Reflection from the channel wall opposite the oblique wall. In this case we observed new wave structures with a characteristic double kink. The formation of the second kink was a result of the interaction between the secondary reflected wave and the original slip line. It was noted that the dynamics of the secondary reflection is different in the planar and axisymmetric cases. In the axisymmetric case reflection in significantly stronger than in the planar case.

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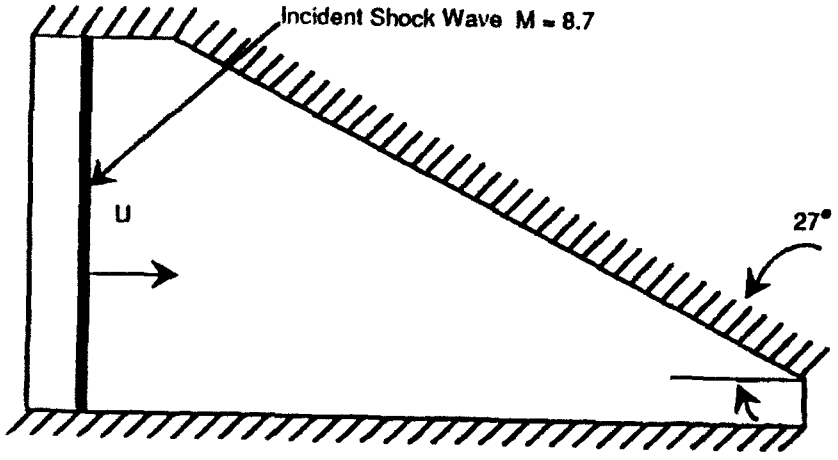


Figure 1. Channel Geometry and Initial Shock Location.

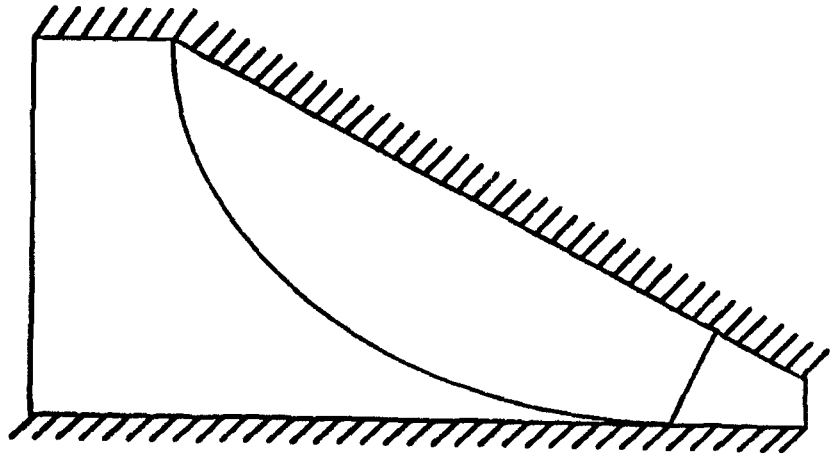


Figure 2. Reflected and Mach Stem Shock Waves at the Start of the Secondary Reflection.

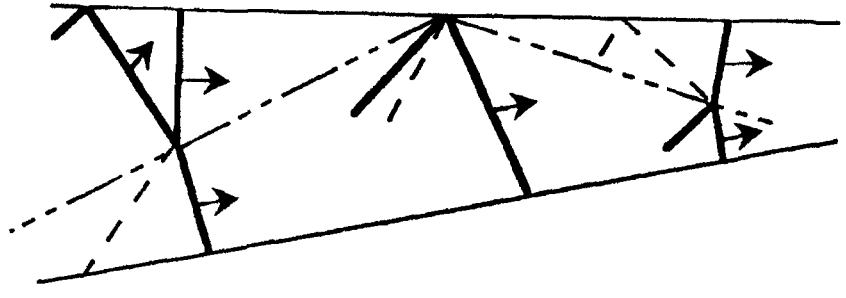


Figure 3. Schematics of Wave Propagation in a converging channel accoding to Bazhenova and Gvozdeva.

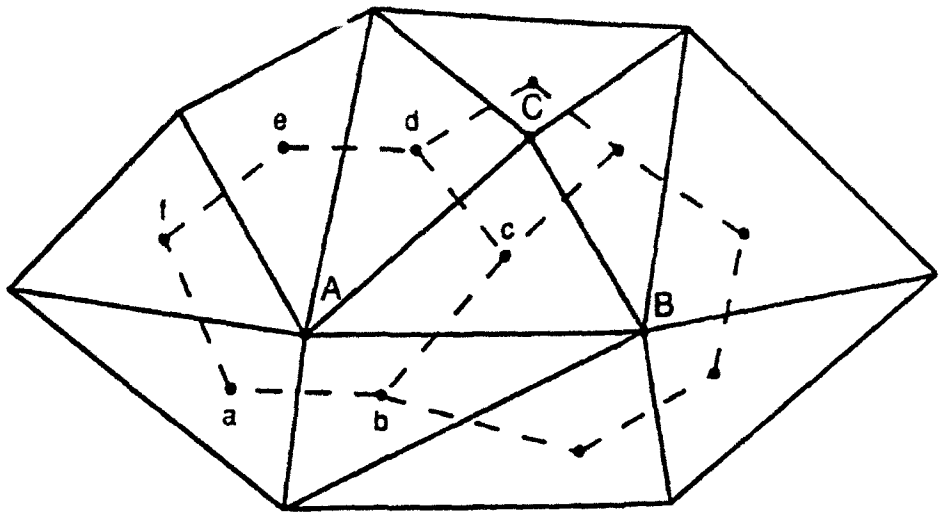
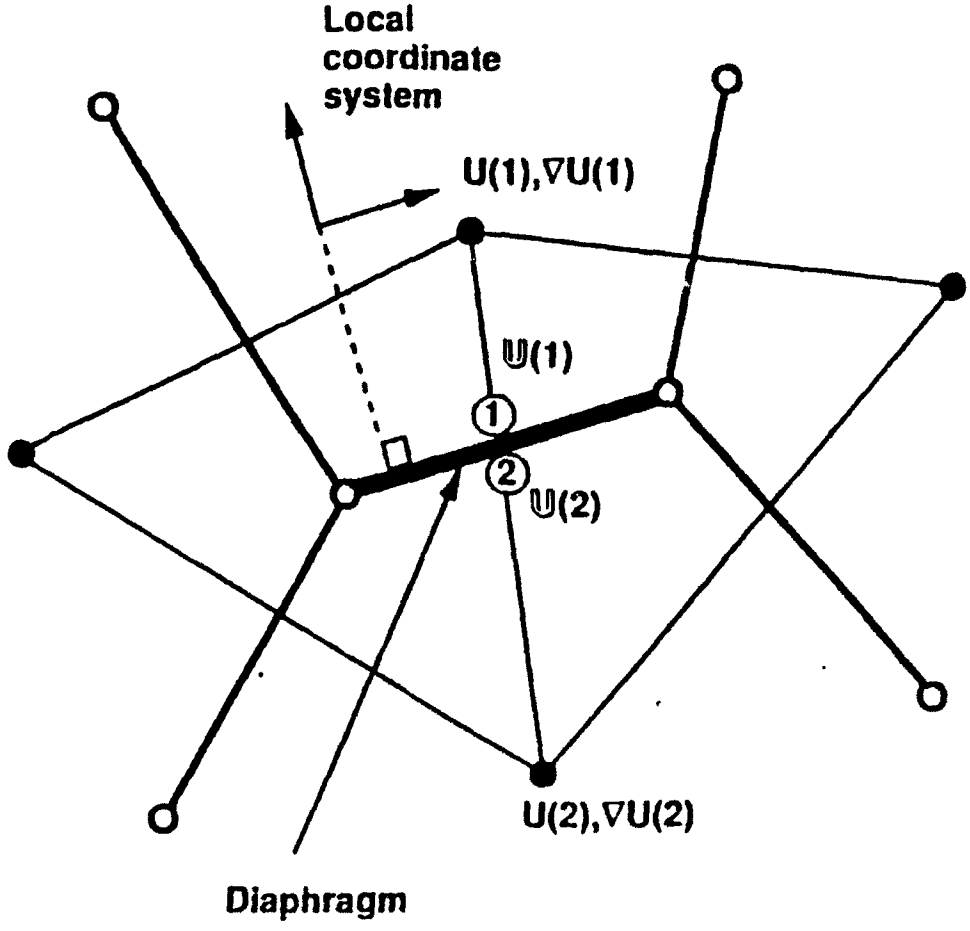
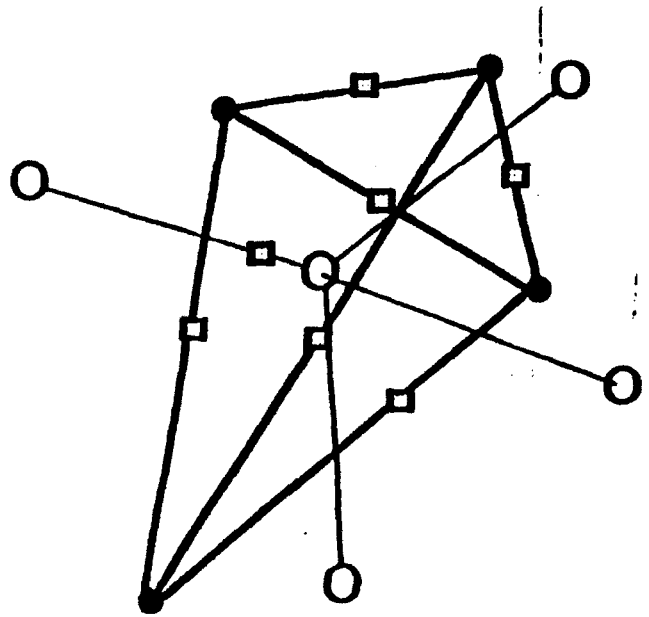


Figure 4.



Second Order Edge Based Flux Calculation

Figure 5.



Tetrahedral Element
Defined by four Vertices
and Baricentric Cell Point

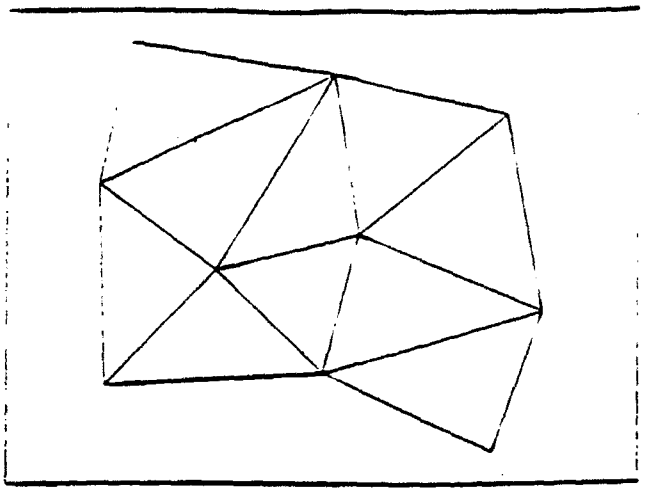
● Vertex Point

Cell Point
O at Tetrahedral
Baricenter

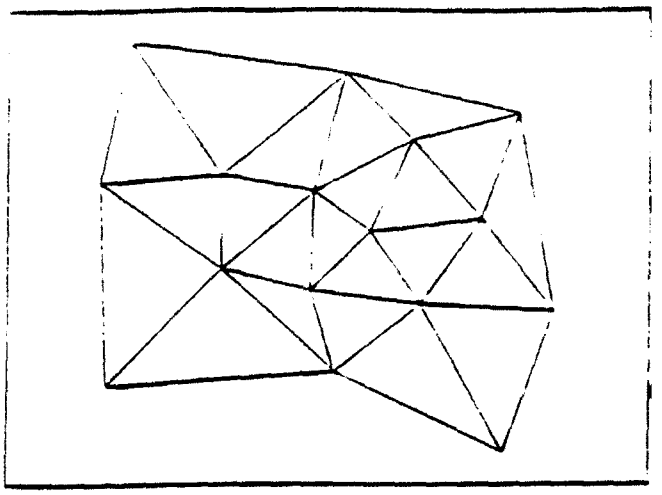
Edge Point
□ equidistant from
defining
Vertices

Scheme for Baricentric Three Dimensional Integration

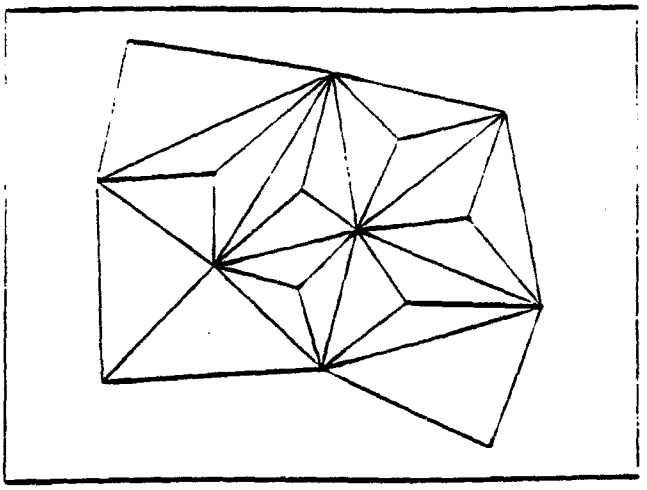
Figure 6.



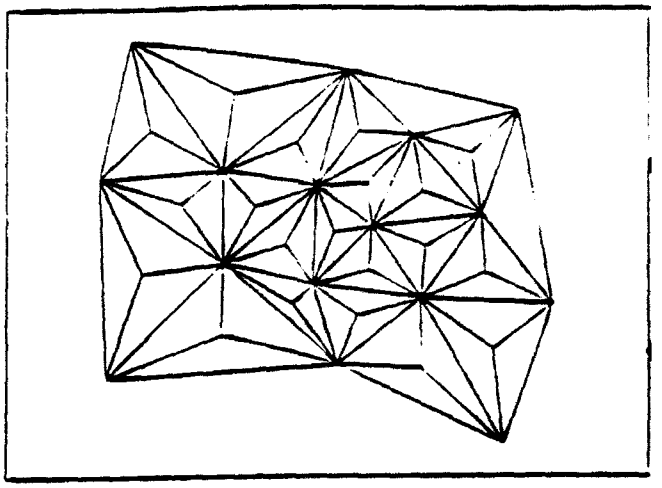
a. Original grid.



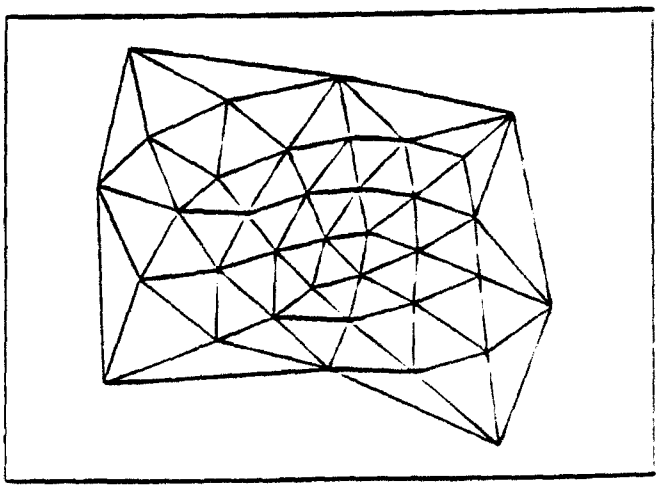
c. Grid after one refinement and one reconnection.



b. Grid after one refinement.

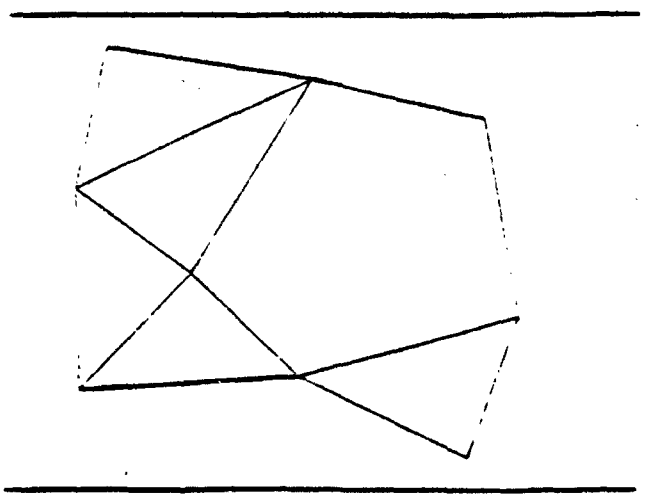


d. Second refinement.

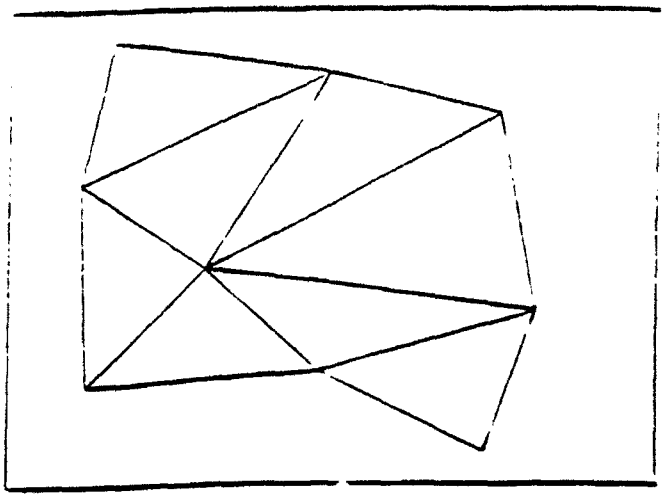


e. Second reconnection.

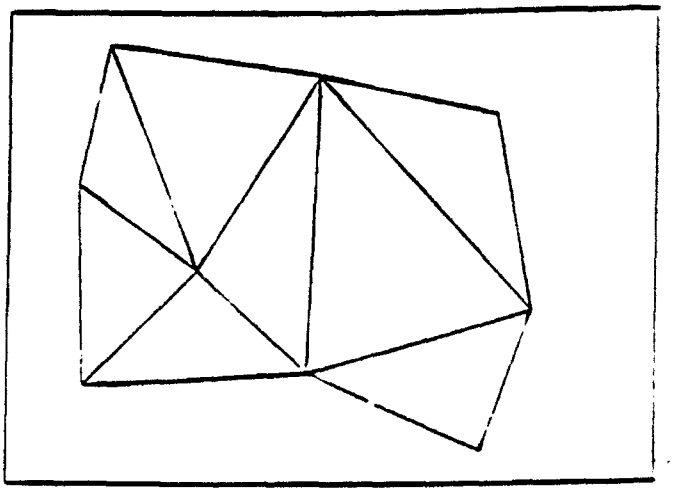
Figure 7. Illustration of the grid refinement process.



a. Point removal.

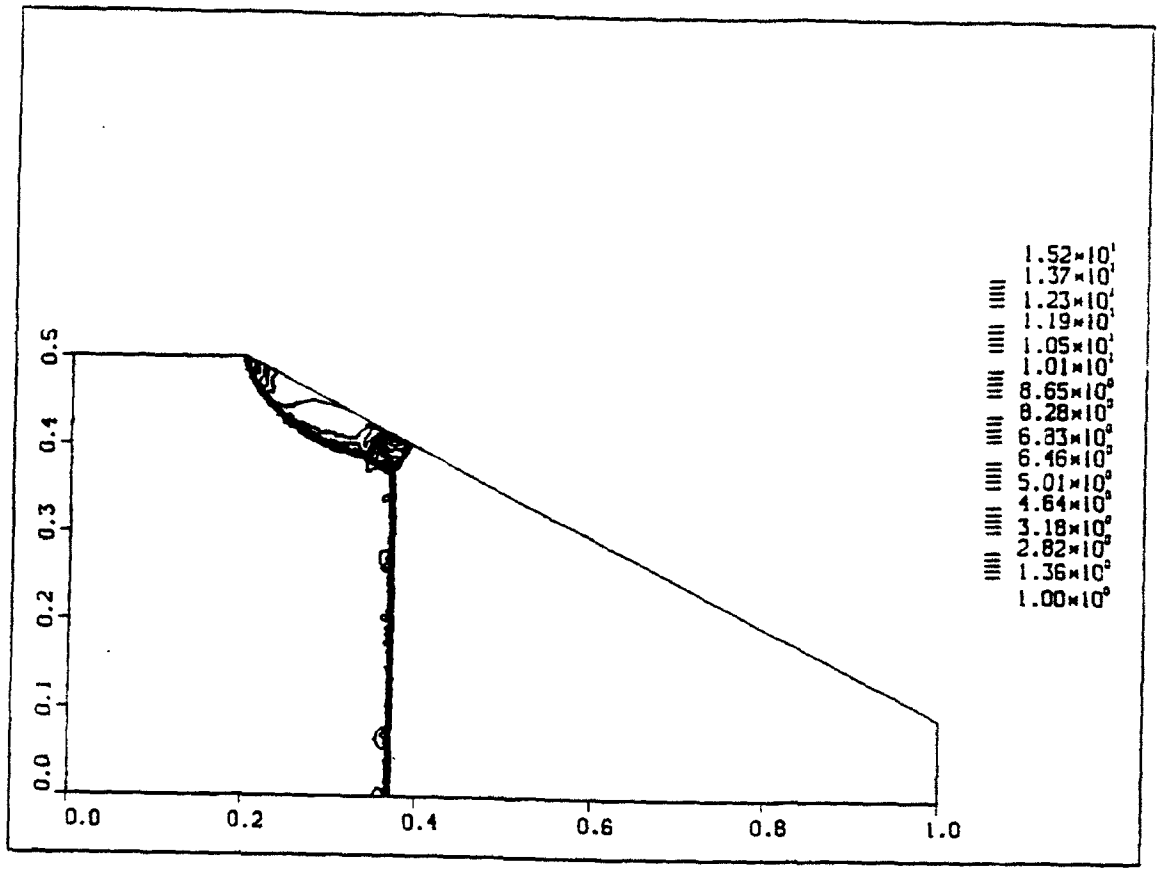


b. Construction of new cells.

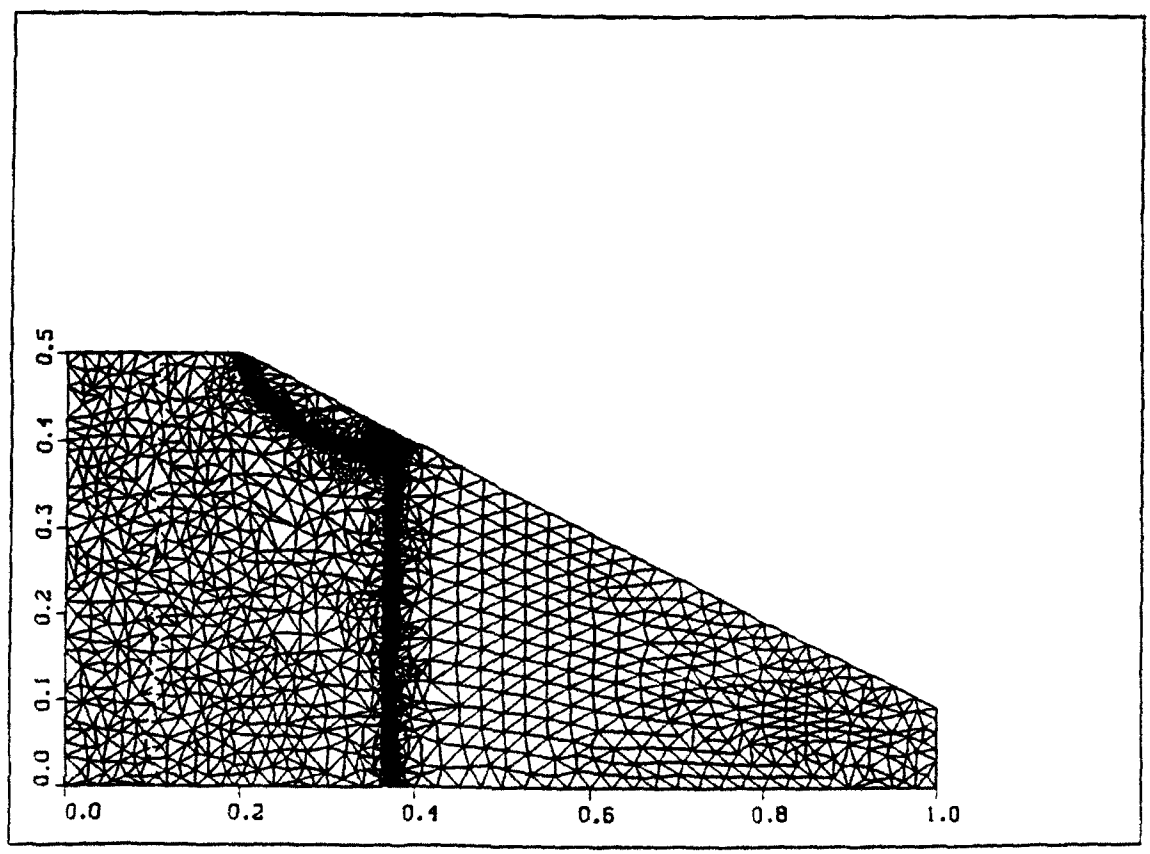


c. Final coarse grid after reconnection.

Figure 8. Illustration of the grid coarsening process.

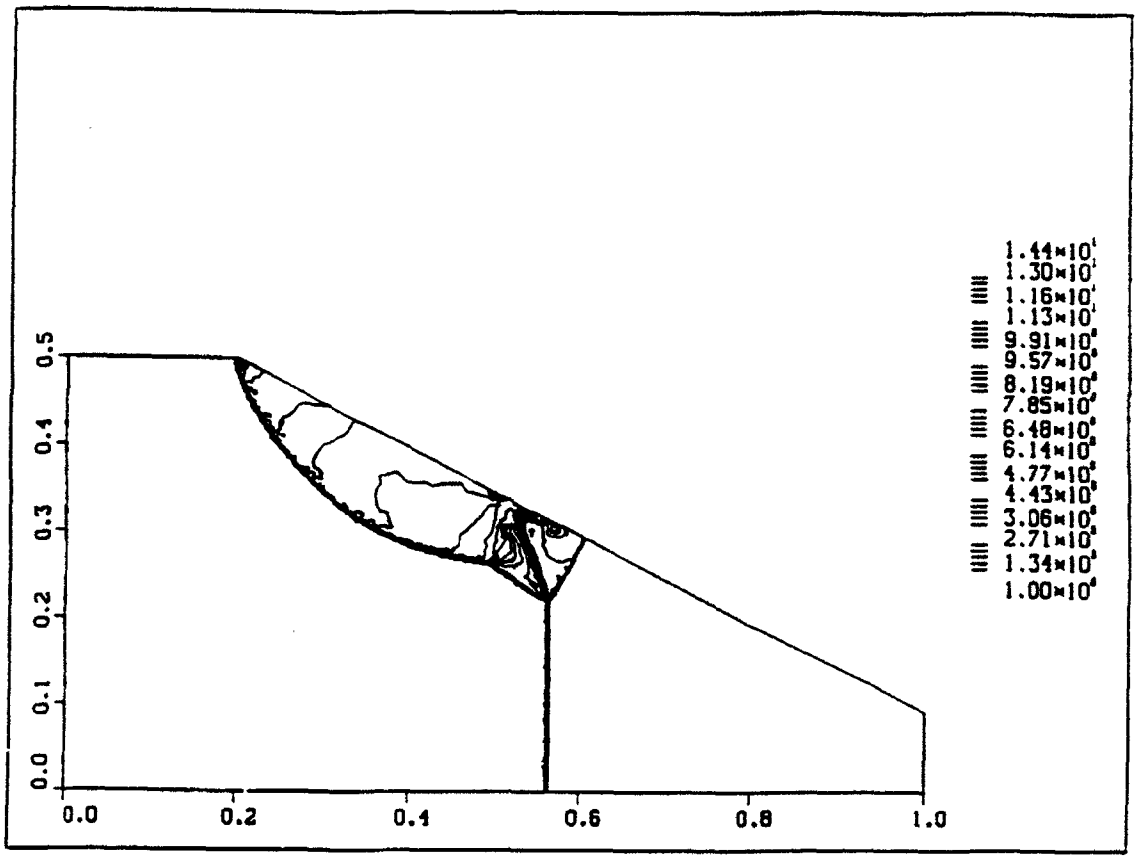


Density contours

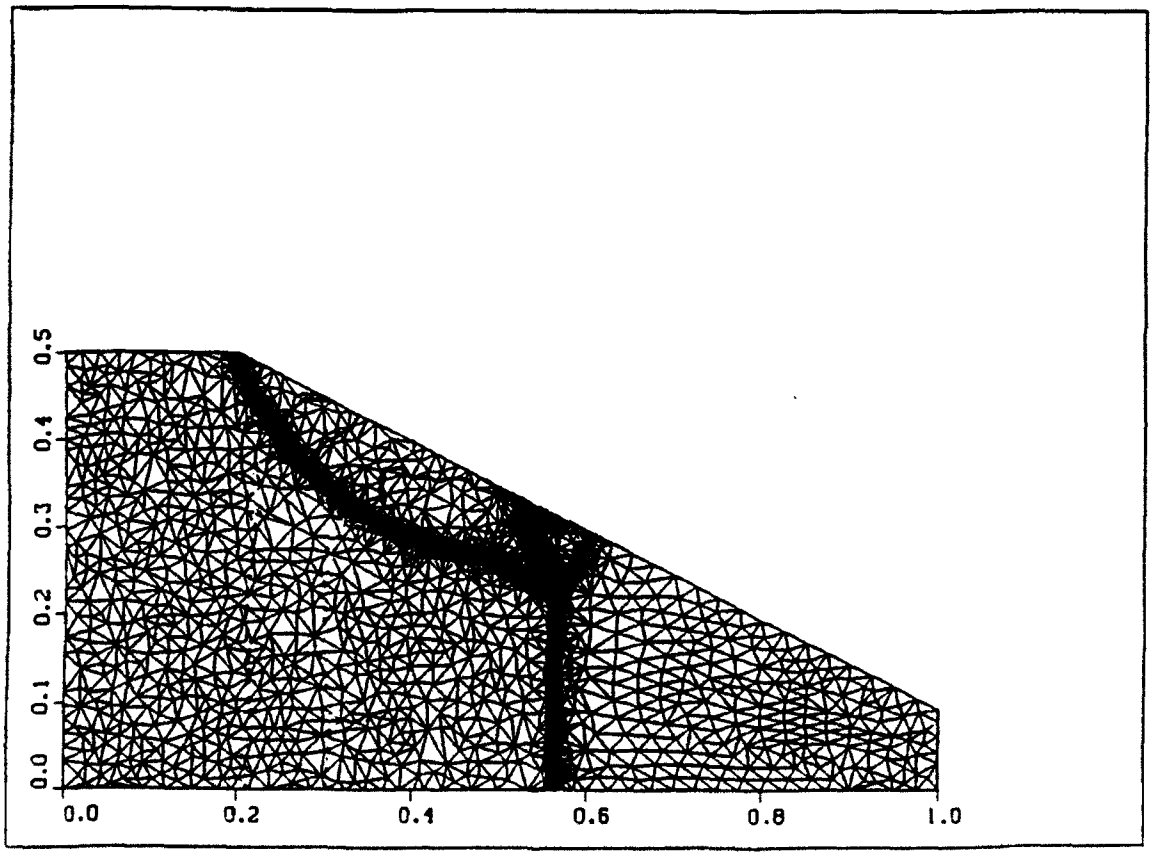


Grid

Figure 8a. Mach Reflection in a planar channel. $M_s = 8.7$; $\alpha = 27°$.

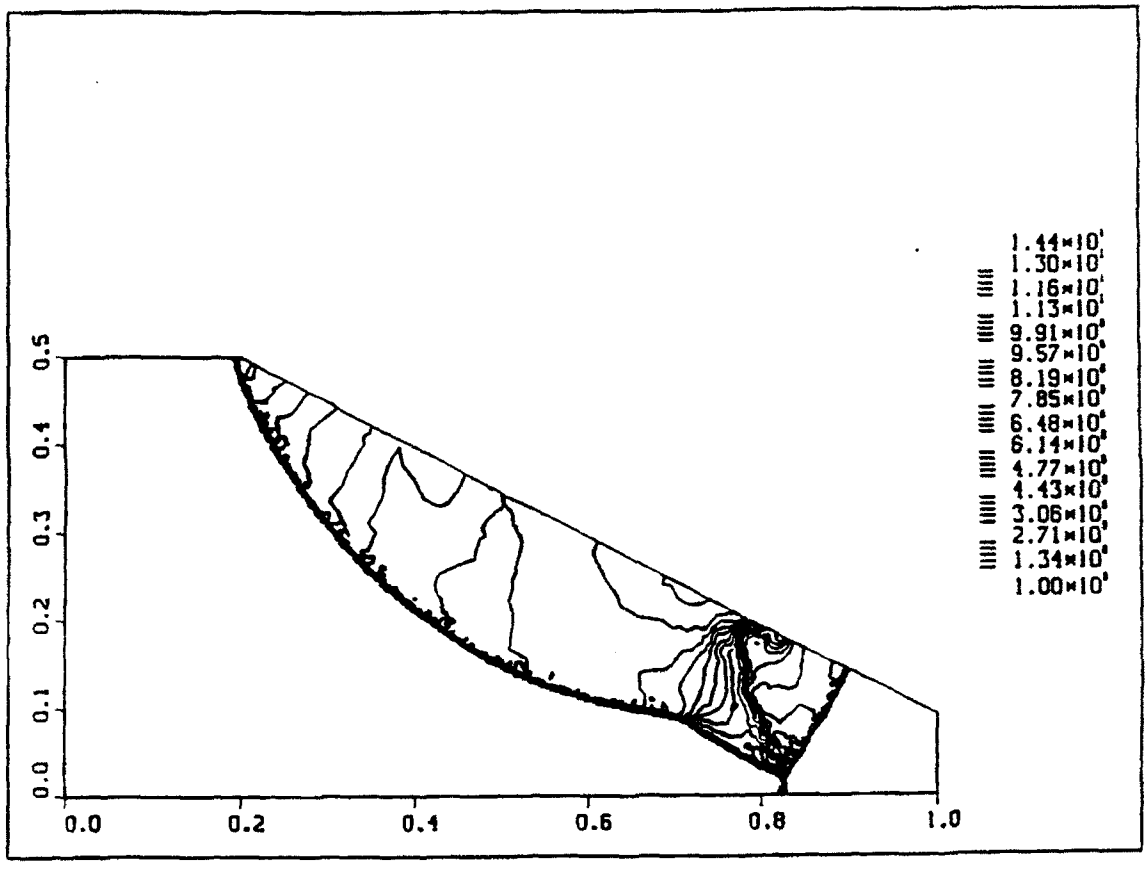


Density contours

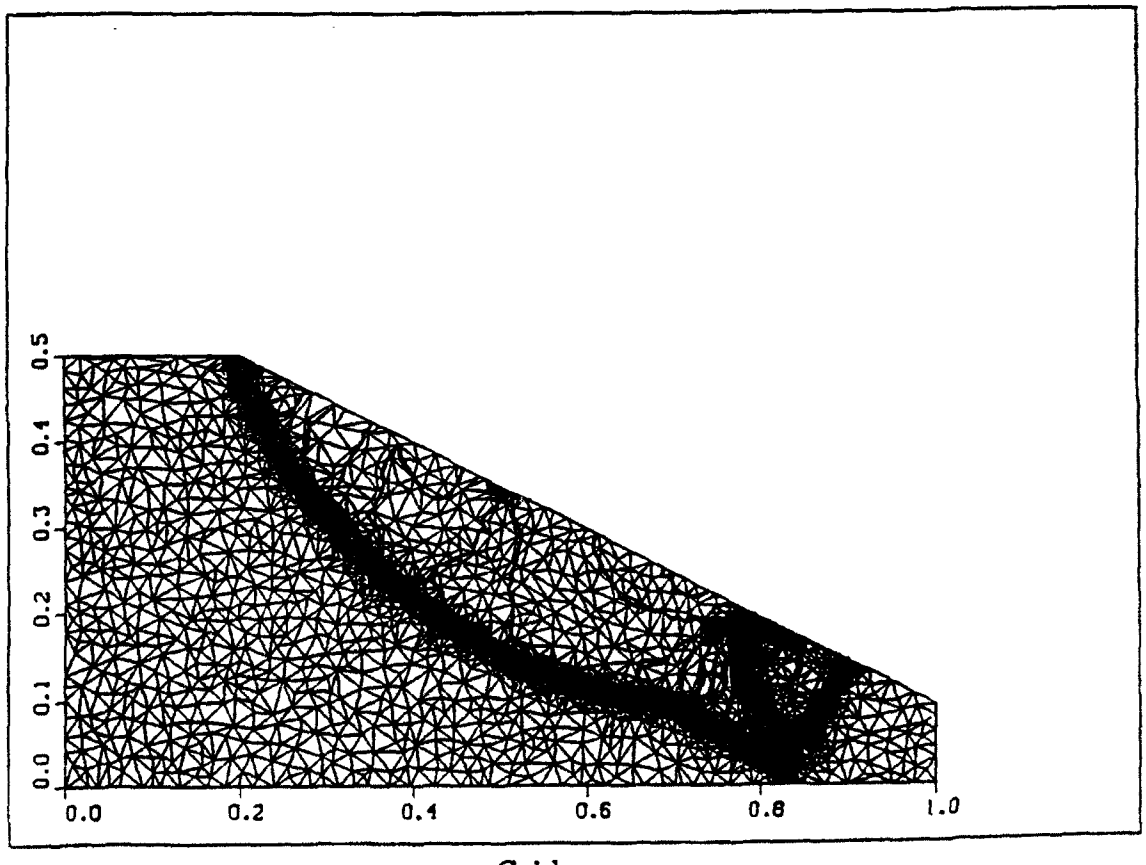


Grid

Figure 8b. Mach Reflection in a planar channel. $M_s = 8.7$; $\alpha = 27°$.



Density contours



Grid

Figure 8c. Mach Reflection in a planar channel. $M_s = 8.7$; $\alpha = 27°$.

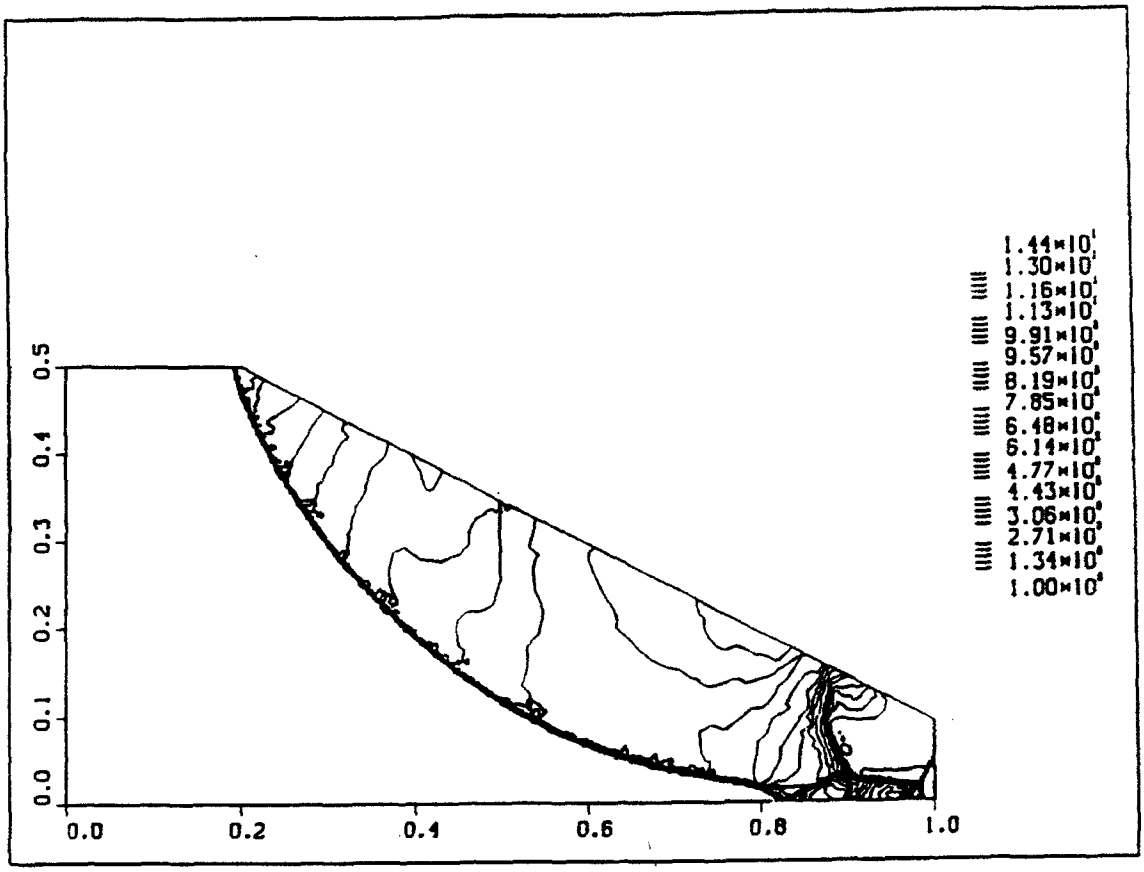
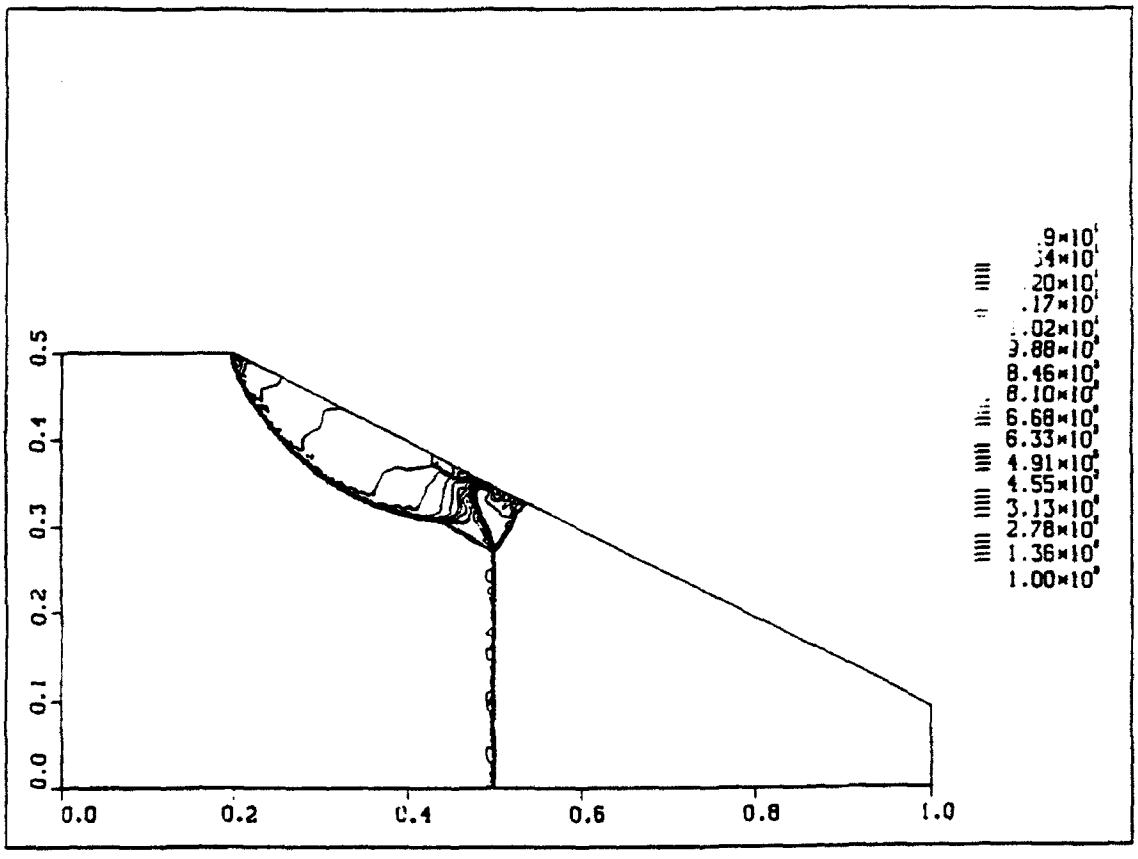
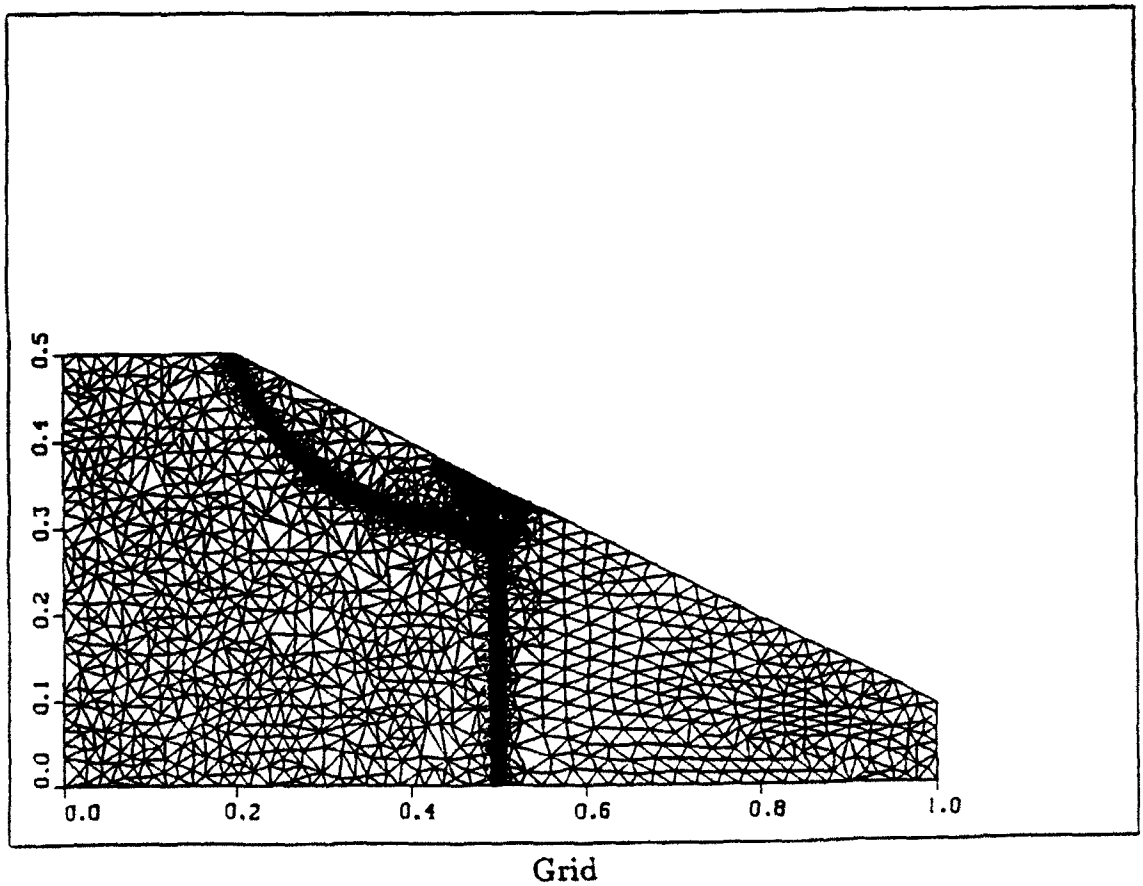


Figure 9a. Secondary Mach Reflection in a planar channel. Density contours.

Figure 9b. A blown up view of the secondary Mach Reflection shown in Figure 9a.

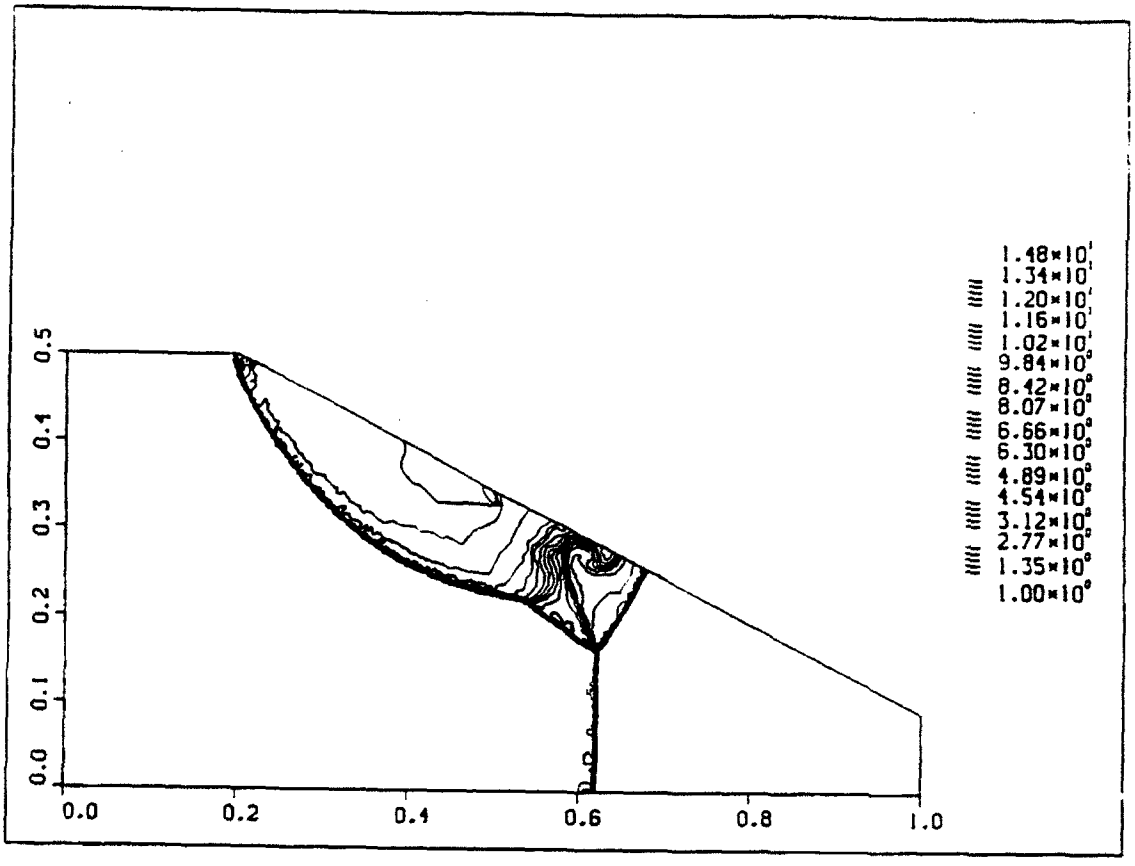


Density contours

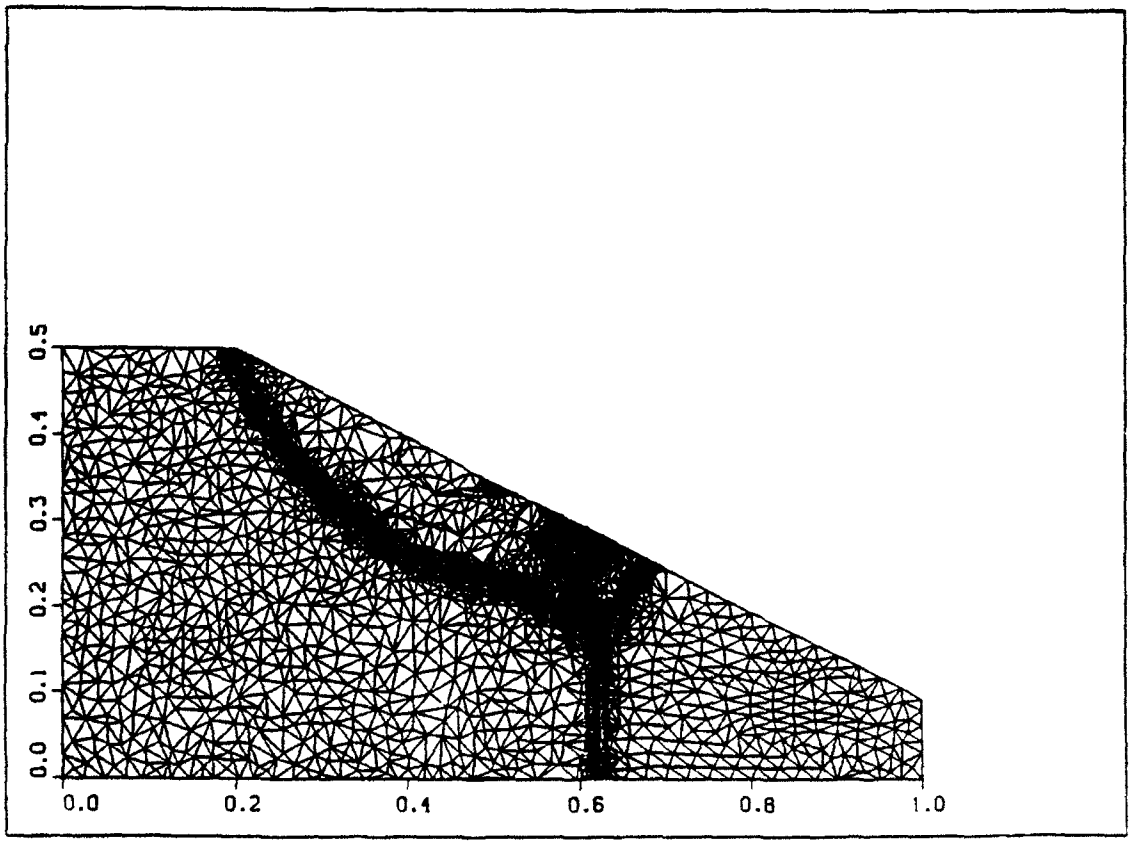


Grid

Figure 10a. Mach Reflection in an axisymmetric channel. $M_s = 8.7$; $\alpha = 27°$.

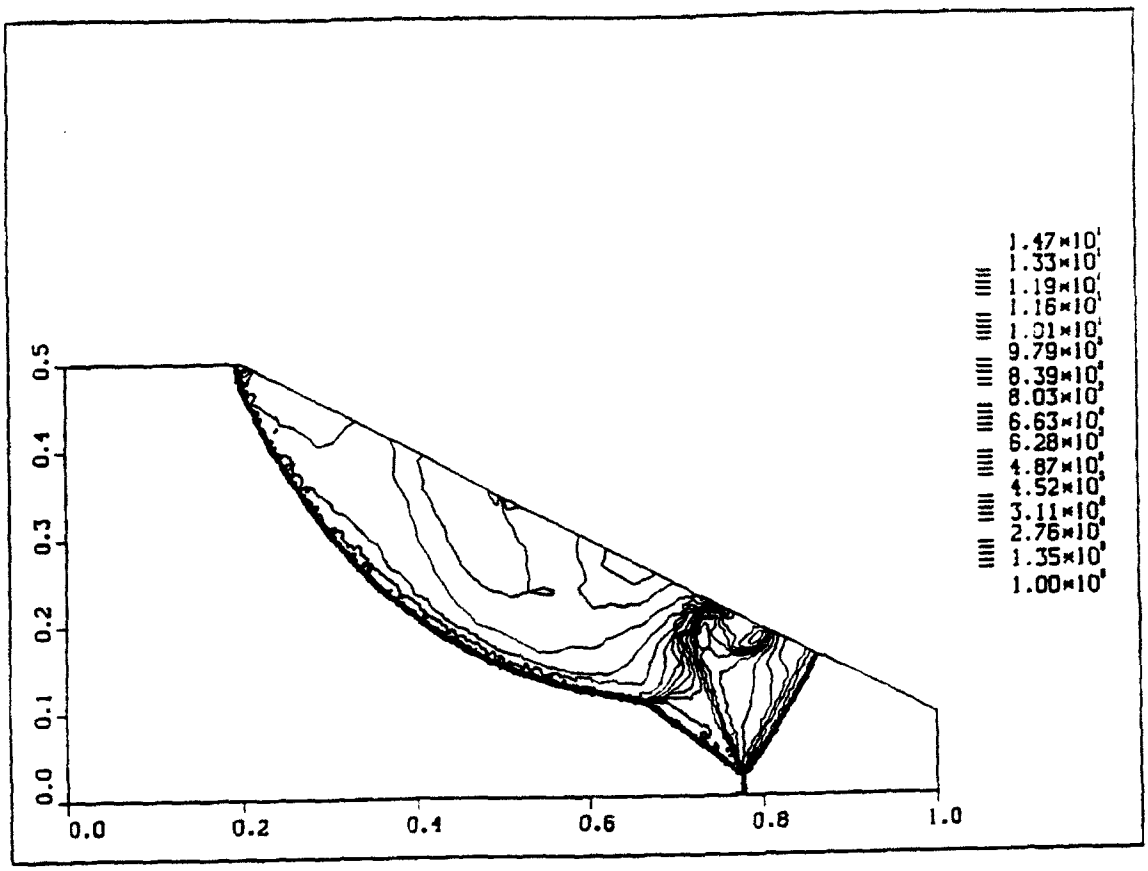


Density contours

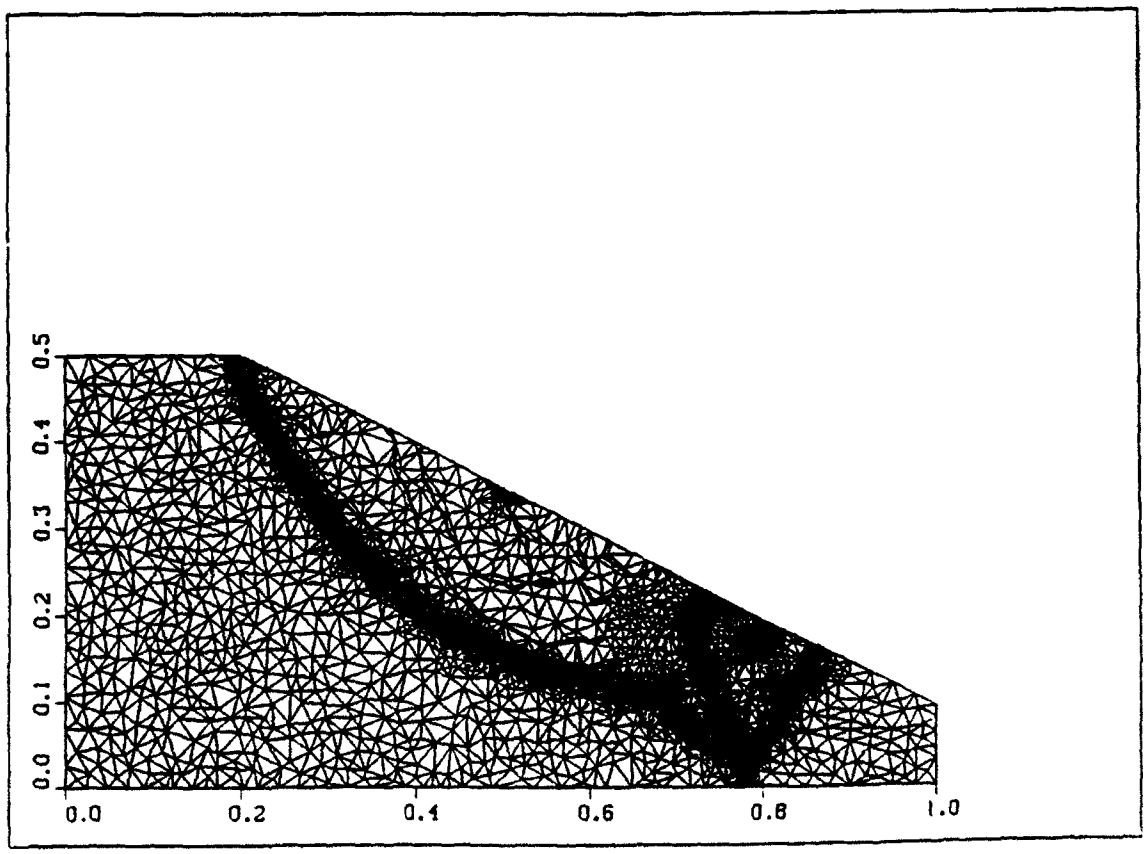


Grid

Figure 10b. Mach Reflection in an axisymmetric channel. $M_s = 8.7$; $\alpha = 27°$.



Density contours



Grid

Figure 10c. Mach Reflection in an axisymmetric channel. $M_s = 8.7$; $\alpha = 27°$.

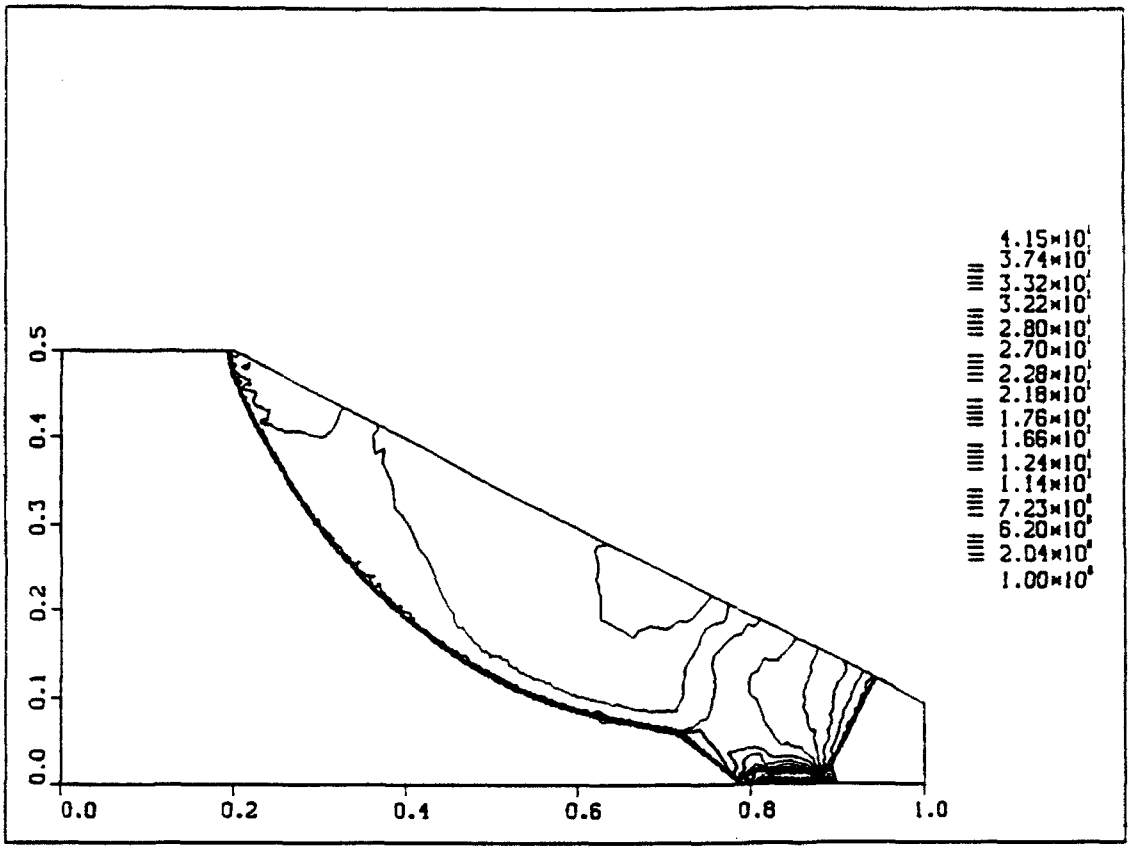


Figure 11a. Start of the secondary Mach Reflection. Axisymmetric channel. Density contours.

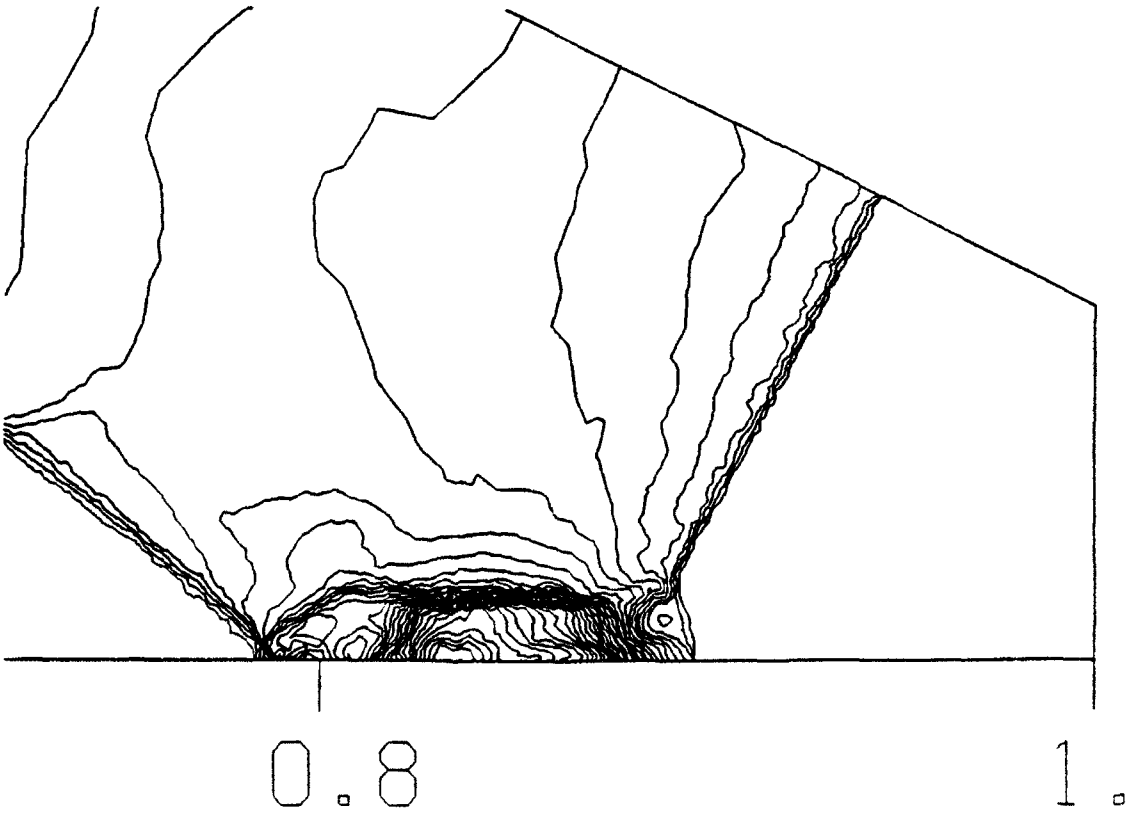


Figure 11b. Blow up of the secondary Mach Reflection area shown in Figure 11a.

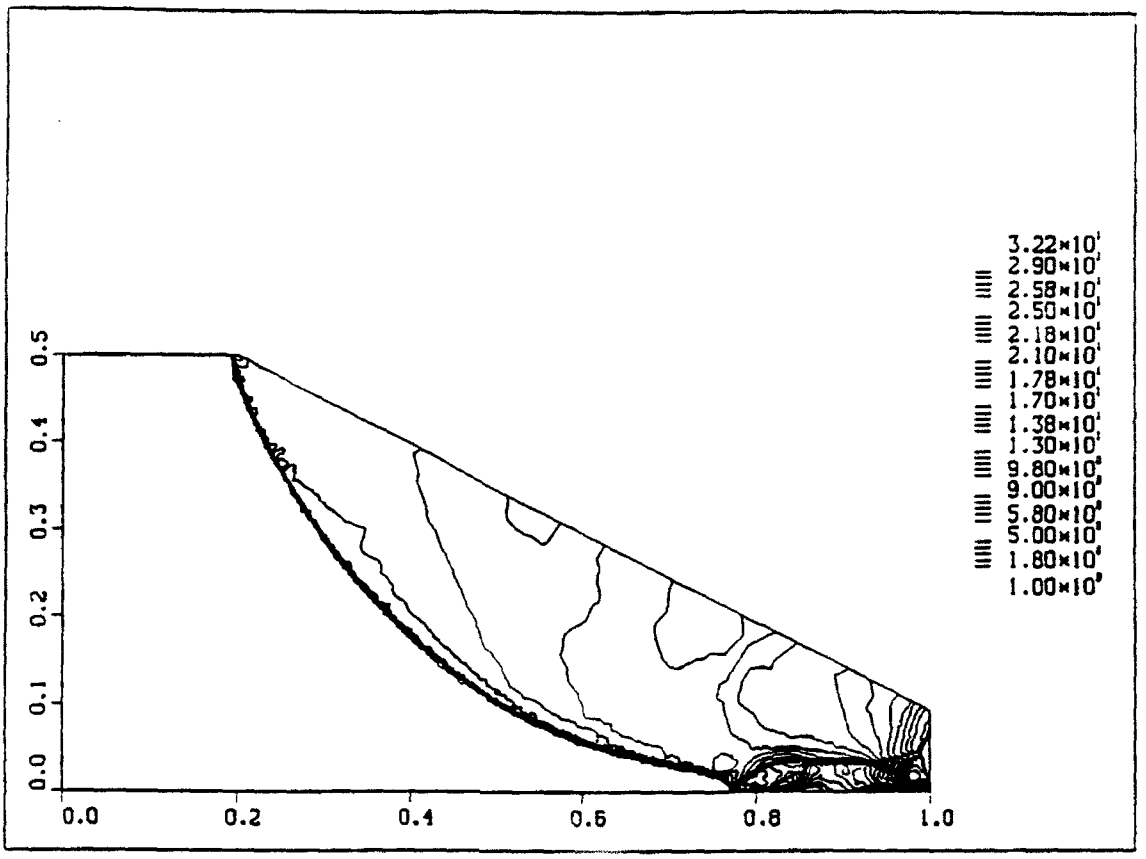


Figure 11c. Secondary Mach Reflection axisymmetric channel. Density contours.

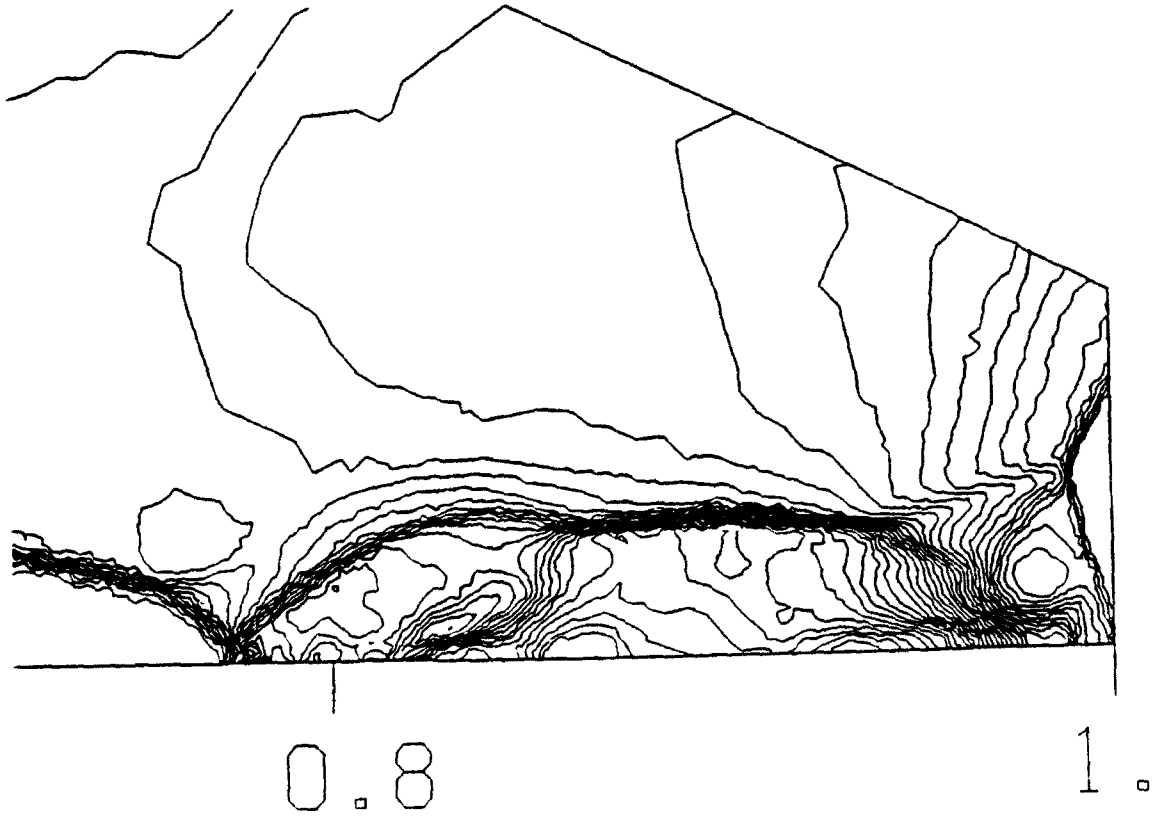


Figure 11d. Blow up of the secondary Mach Reflection area shown in Figure 11c.

Solution of Euler's Equations on Adaptive Grids Using A Fast Unstructured Grid Second Order Godunov Solver (FUGGS)

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Science Applications International Corporation
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Abstract. We describe a new technique for solving Euler's gasdynamic equations on unstructured triangular grids with arbitrary connectivity. The formulation is based on the second order Godunov method. The use of data structure with only one level of indirectness leads to an easily vectorized and parallelized code with a low level of overhead in memory requirement and high computational efficiency. The performance and accuracy of the algorithm has been tested for a very wide range of Mach numbers starting from very low subsonic to high hypersonic flows, without the need to adjust any code parameters. The algorithm was implemented in a vertex based and triangle based scheme. The computational results produced by the triangle based version showed an extremely low level of artificial viscosity.

A new method of direct dynamic refinement of unstructured grids, as described in this paper, allows an automatic adaptation of the grid to regions of pressure or density discontinuity, steep pressure or density gradient, and high vortical activity. Results using the algorithm with dynamic grid refinement are presented.

Flow Solver on an Unstructured Grid

The specific use of triangular meshes provides a very flexible means for simulating flows in extremely complex geometries. The data that identifies a triangular mesh (unstructured grid) provides the flexibility needed to properly discretize the complex geometry of the computational domain, especially on the boundary where the geometry and the implementation of boundary conditions, are extremely crucial for the accuracy of the simulation. The flexibility of unstructured grids enables adaptation to physical features in the flow. The price of resolution results in a local rather than a global penalty. Consequently, it is possible to simulate problems on computers with limited memory and still achieve highly resolved solutions. A typical example, which is illustrated in this paper, is a travelling shock passing over an obstacle. The challenge is to simulate such problems with fine resolution across the shock while limiting the total number of mesh points in the calculation.

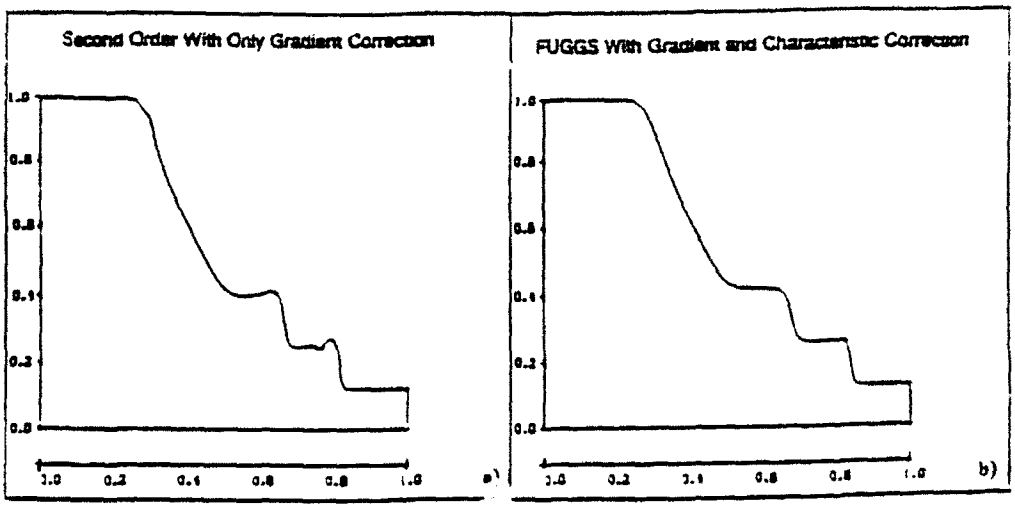


Figure 2: Sod problem, effect of the characteristics correction on the density.

Performance and Validation of FUGGS

FUGGS has proven to be a very robust algorithm capable of high quality solutions while using triangles with large variations of aspect ratios. The code was tested on a variety of unstructured grids and consistently provided results, despite the apparent poor quality of the underlying mesh. We were able to simulate efficiently and accurately a wide spectrum of flow regimes starting from low subsonic to high hypersonic. The code has no free parameters to choose and thus does not require any "tuning" to specific problems. The user has only to specify the boundary conditions (around the grid) and initial flow conditions. The algorithm is fully vectorized and can be easily parallelized in the future. We describe the detailed algorithm below and then present typical results.

Direct Dynamic Refinement Method for Unstructured Triangular Grids

As stated, an unstructured grid is very suitable to implement boundary conditions on complex geometrical shapes and refinement of the grid if necessary. This feature of the unstructured triangular grid is compatible with efficient usage of memory resources. The adaptive grid enables the code to capture moving shocks and high gradient flow features with high resolution. The memory resources available can be very efficiently distributed in the computational domain to accommodate the resolution needed to capture the main features of the physical property of the solution. Dynamic refinement controls the resolution

of the grid according to available memory resources and subject to prescribed priorities. These priorities can be set according to the physical features which the user wishes to emphasize in the simulation. The user has control over the resolution of the physical features resolved in the simulation, without being restricted to the initial grid. The alternative to Direct Dynamic Refinement is the hierarchical dynamic refinement (H refinement) that keeps a history of the initial grid (mother grid) and the subdivision of each level (daughters grid). The H refinement subdivides the initial grid into two or four triangles in each level, and keeps track of the number of subdivision levels each triangle has undertaken. In the H refinement method, one has to keep overhead information on the level of each triangle subdivision, and needs double indirect indexing to keep track of the H refinmenet process. This slows down the computation by partially disabling the vectorization of the code. As mentioned, the H refinement does rely heavily on the initial grid as it subdivides the mother grid and returns back to it after the passage of the shock.

Direct Dynamic Refinement for capturing the shocks basically requires the refinement to be in the region ahead of the shock. This requirement minimizes the dissipation in the interpolation process when assigning values to the new triangles created in the refined region. Additionally, it requires that the coarsening of the grid should be done after the passage of the shock. In principle, the interpolation and extrapolation in the refinement and coarsening of the grid is done in the region where the flow features are smooth.

The physics of the problem should be involved in the process that identifies the region of refinement and coarsening. One can derive error criteria that will allow grid adaptation to stationary or moving pressure or density discontinuities, region of high voritical activity, etc. For each of the physics features to be resolved, there should be an error indicator that is suited best to capture and identify the region of importance corresponding to this feature.

Criteria for Refinement (Error Indicator)

We have implemented an algorithm with multiple criteria for capturing a variety of features in the physics of the problem to be solved. That means that we were able to derive a number of error indicators that enable identification of moving shock waves or stationary shocks in the computational domain.

To identify the location of a moving shock, we use the flux of energy or momentum into triangles. The fluxes entering and leaving triangles are the most accurate physical variables computed by the Godunov algorithm for solving the Euler's equations, and are used to update the physical variables for each time step in each triangle. A shock wave means that there is a "step function" change in the cell that is caused by an influx of energy, momentum or density.

Stationary shock can be identified by density gradients computed as required in the second order Godunov algorithm.

The refinement process is done in two ways: i) adding a vertex in the center of a triangle and ii) adding a vertex on an edge of a triangle. Figure 3 illustrates the two alternative ways used to refine the grid. Figure 4 shows an example of the refinement procedure. In the coarsening stage we identify a vertex to be removed. With the point removal, we delete the connecting edges and triangles surrounding the point. The next step is to triangulate the void polygon by creating new triangles using only the vertices of the polygon. Figure 5 shows an example of how the coarsening proceeds.

In the process of refinement and coarsening, we often create triangles with large aspect ratios (the base-to-height maximum ratio for the three edges). We use reconnection to flip the diagonal between two adjacent triangles to obtain triangles with a "better" aspect ratio. This procedure is referred to as the reconnection step in Figs.4 and 5.

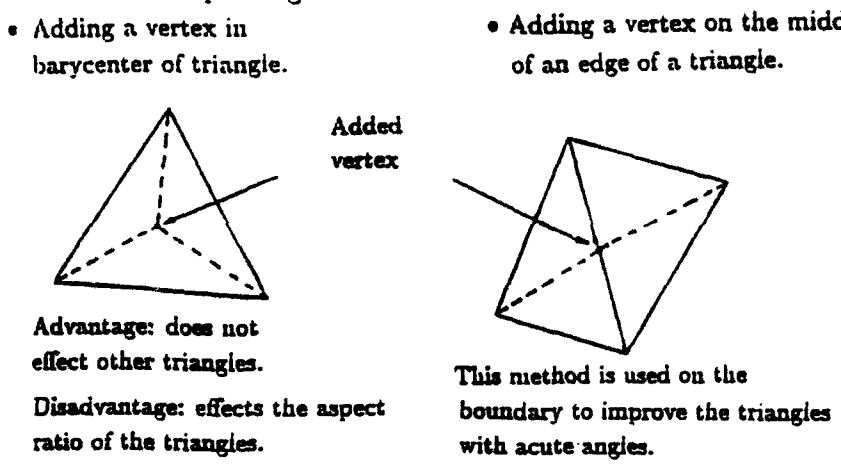
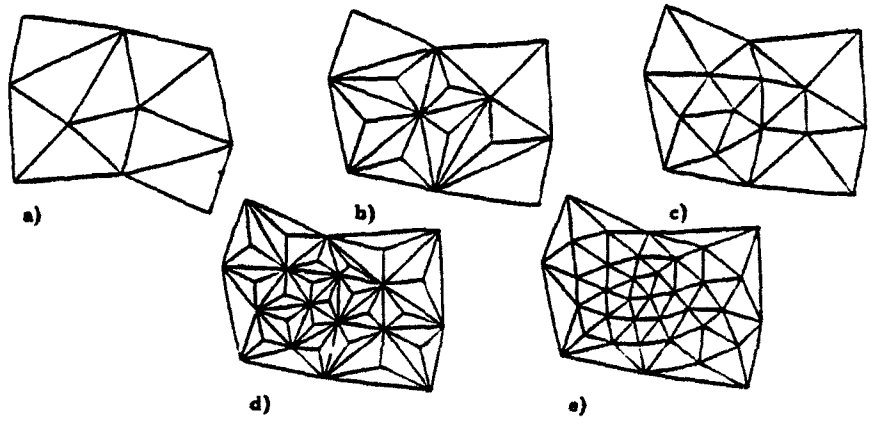
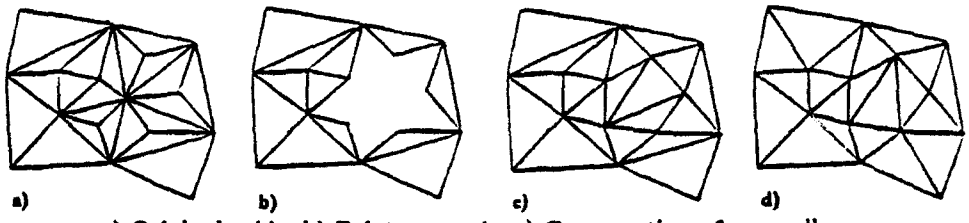


Figure 3: Two Ways of Refinement.



a) Original grid. b) One refinement. c) First reconnection. d) Second refinement. e) Second reconnection.

Figure 4: Illustration of the grid refinement process.



a) Original grid. b) Point removal. c) Constructing of new cells. d) Coarse grid after reconnection.

Figure 5: Illustration of the grid coarsenning process.

Results

Direct dynamic refinement was used to solve the transient behavior of the flow entering a channel with a double wedge having an inclination of 20°. The flow Mach number entering the channel is 2.5. The flow is from left to right. A sequence of snapshots illustrates the density contours, and the grid for each timestep is given in Figs. 6 (countour plots) and 7 (grid). These figures clearly demonstrate the automatic adaptation of the grid to the moving shocks and the ability to capture the detailed physics of the simulation with very high resolution and minimal memory requirements. The initial grid can clearly be seen to the right of the shock ("ahead") in the early stage of the shock propagation from left to right. The coarsening algorithm is able to produce a reasonable mesh in the region trailing the shock as shown in Fig. 7.

The ability to capture stationary shocks is illustrated in Fig. 8 in which a supersonic free flow (M = 2.5) has been run over a diamond shape bump (20° wedge) driven to a steady state. The shock emerges from the first corner (left), the fan of rarefaction waves appears from the apex of the diamond shape bump, and the secondary shock from the second corner (right) is clearly illustrated by the ability of the algorithm to adapt the grid to the physics of the flow. Figure 9 illustrates the sharpness of the reflected shock obtained for an axisymmetric converged channel with an angle of 27° and M = 8.7.

The few examples shown here represent a small subset of results obtained with FUGGS. The examples are indicative of the excellent performance that can be achieved for physically complicated situations. We would like to emphasize that these calculations involved no free parameters.

Acknowledgment

We would like to thank Dr. Aharon Friedman and Dr. Marty Fritts for their valuable contributions. This work was partially supported by the Wright Research and Development Center under contract No. F33615-88-C-3002 and by DARPA through contract F49620-89-C-0087 administered by AFOSR.

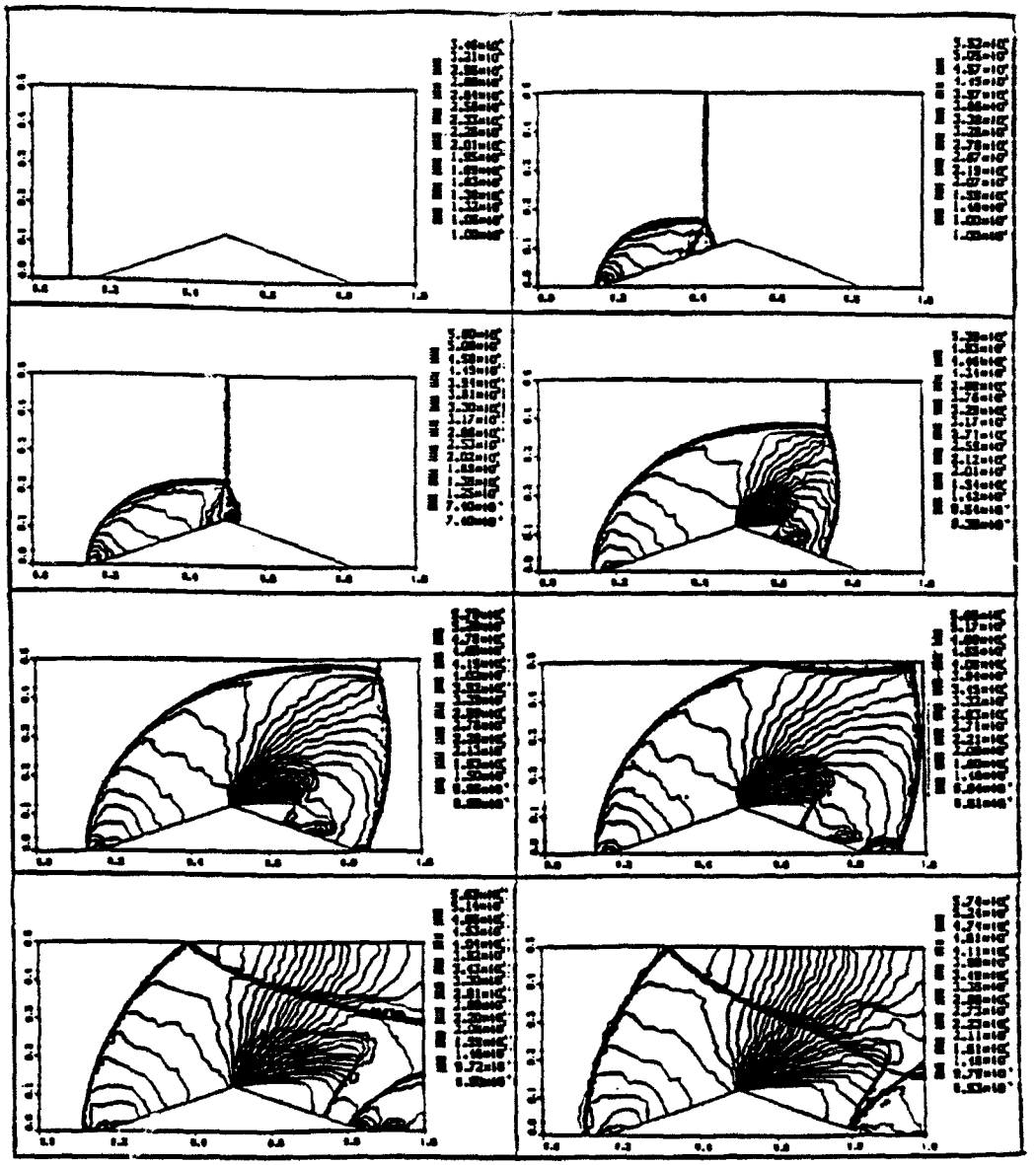


Figure 6. A sequence of density snapshots of countour plots for a propagating shock (M = 2.5, wedge angle = 20°).

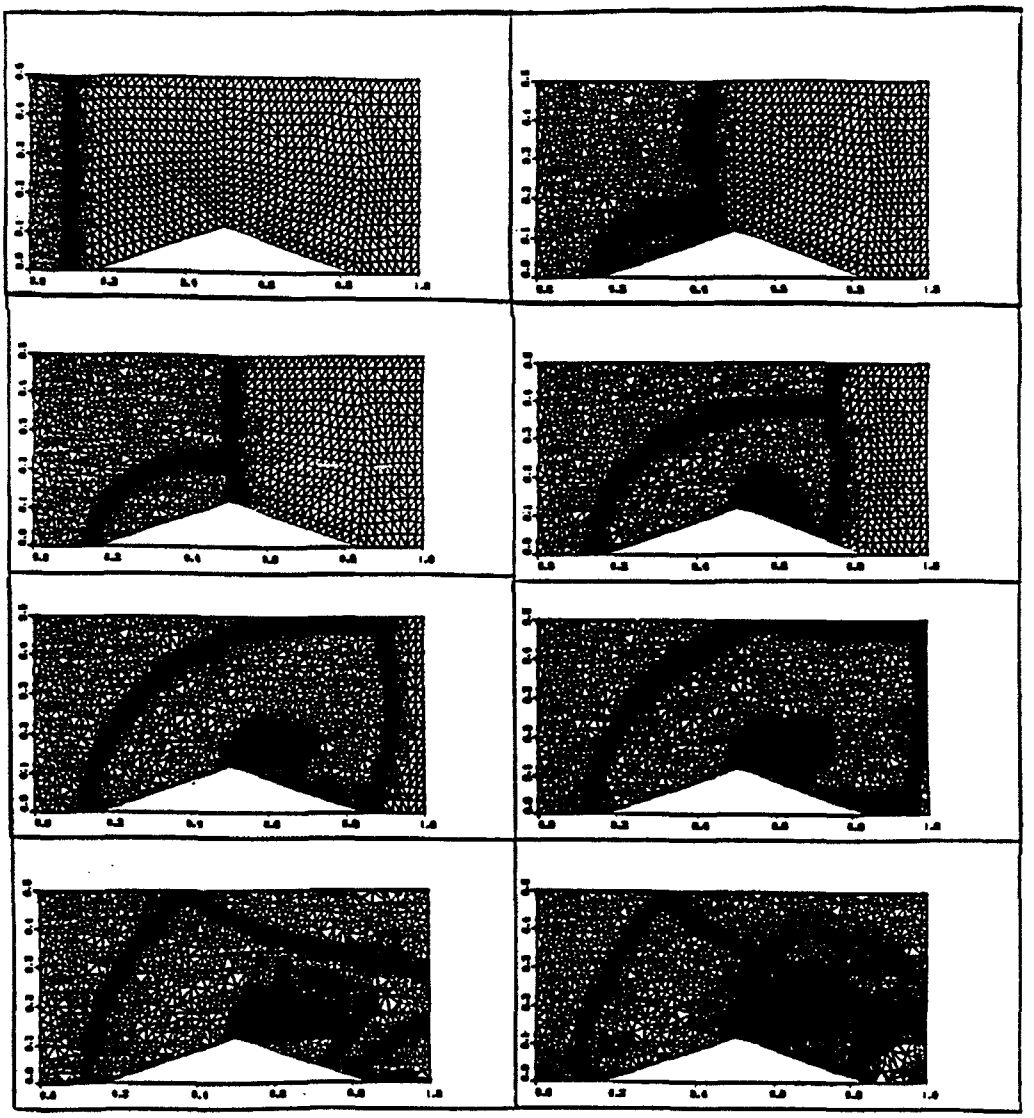


Figure 7. A sequence of grids corresponding to countour plots in figure 6.

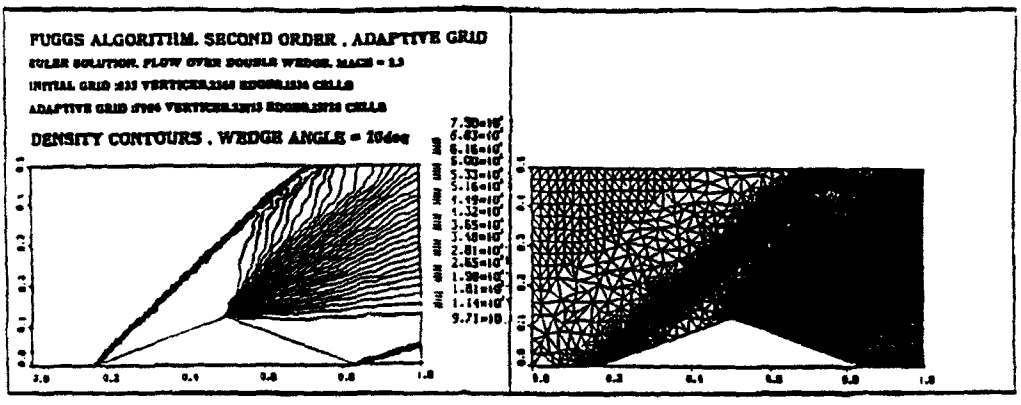


Figure 8. Density contour plot and grid for flow driven to steady state over a double wedge obstacle.

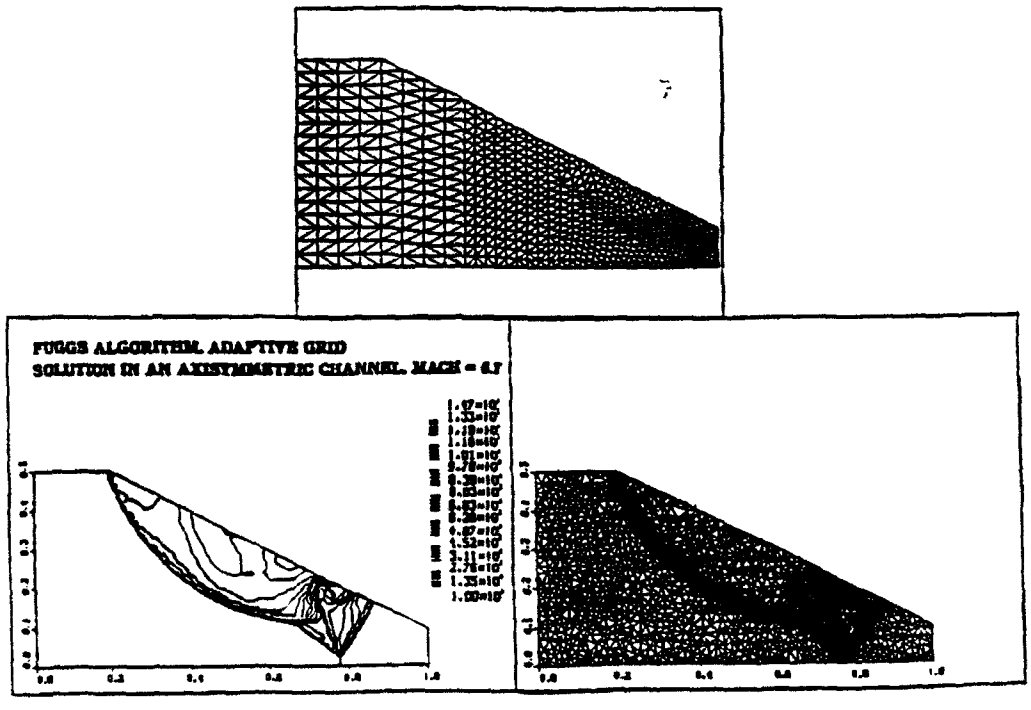


Figure 9. Initial grid, countour plot and the adaptive grid for flow in axisymmetric channel (M = 8.7, wedge angle = 27°).

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Air-Breathing Pulsed Detonation Engine Concept; A Numerical Study

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AIR-BREATHING PULSED DETONATION ENGINE CONCEPT: A NUMERICAL STUDY

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1. Introduction

The airbreathing Pulsed Detonation Engine (PDE) concept was introduced by us and reported on in the past[1,2,3]. As described in the previous reports, we have carried out a systematic series of parametric studies of the PDE via Computational Fluid Dynamics (CFD) and have analyzed engine performance over a wide range of flight regimes including subsonic and supersonic flows and physical geometries including various nozzle and air inlets. In addition, we have performed static table top experiments[1] to demonstrate that the principle of pulsed or repetitive detonation can be achieved in a generic PDE configuration. To date, our results indicate that practical engines for certain vehicles and missions can be conceptualized and designed with the information that has already been generated from the studies. Specifically, our studies have shown that the PDE is an excellent candidate for the primary propulsion source for small aerodynamic vehicles that operate over the flight envelope, $0.2<M<3$ and altitude between sea level and 30,000 ft. Further, our analysis of the simulation results indicate that the PDE is a high thrust to weight ratio device with a specific fuel consumption on the order of one pound per hour per pound fuel. The predicted performance places the PDE propulsion concept in a strongly competitive position compared with present day small turbojets. The PDE concept has the added attractiveness of rapid variable thrust control, no moving parts and the potential for low cost manufacturing. Finally, the PDE concept is scalable over a wide range of engine sizes and thrust levels. For example, it is theoretically possible to produce PDE engines on the order of one to several inches in diameter and thrusts on the order of pounds, as well as devices which provide thousands of pounds thrust.

The parametric studies that we have carried out to date were possible due to the development of a new generation of CFD tools that have allowed us to accurately simulate the details of the complex nonlinear time dependent processes. A brief description of the CFD methods employed in our studies is given in section 3.

The purpose of the present paper is: (1) to report the most recent studies of a full simulation of the operation of the PDE with a generic missile configuration cruising at supersonic speeds, (2) to report the results of a parametric-scaling study of the thrust produced as a function of the variation of a given engine configuration with respect to engine size.

The present paper is organized as follows: Section 2 gives, for completeness, a brief description of the PDE concept, Section 3 describes briefly the CFD methods used in our most recent studies, Section 4 gives the results of the parametric-scaling study and, Section 5 describes the simulations of the complete flow around a generic missile configuration powered by a PDE, Section 6 gives our summary and conclusions.

2. The Pulsed Detonation Engine Concept

A detonation process, due to the very high rate of reaction, leads to a propulsion concept in which the constant volume process can be fully realized. In detonative combustion, the strong shock wave, which is part of the detonation wave, acts like a valve between the detonation products and fresh charge. The speed of the detonation wave is about two orders of magnitude higher than the speed of a typical deflagration. This allows the design of propulsion engines with a very high power density. Each detonation has to be initiated separately by a fully controlled ignition device, with a wide range of variable cycle frequencies. There is no theoretical restriction on the range of operating frequencies; they are uncoupled from acoustical chamber resonance. This is very important feature of the constant volume detonation process that differentiates it from the process occurring in a pulse-jet;[4,5] the pulse jet cycle is tuned to the acoustical resonances of the combustion chamber. This leads to a lack of scalability for the pulse jet concept.

A physical restriction dictating the range of detonation frequency arises from the rate at which the fuel/air mixture can be introduced into the detonation chamber. This also means that a device based on a detonative combustion cycle can be scaled and its operating parameters can be modified for a range of required output conditions. There have been numerous attempts to take

advantage of detonative combustion for engine applications. The most recent and successful of these attempts was carried out at the Naval Postgraduate School (NPS) by Helman et al.[1] During this study, several fundamentally new elements were introduced to the concept distinguishing the NPS research device from previous studies. First, it is important to note that the NPS experimental apparatus was the first successful self aspirating air breathing detonation device. Intermittent detonation frequencies of 25 Hz were obtained. This frequency was in phase with the fuel mixture injection through timed fuel valve opening and spark ignition. The feasibility of intermittent injection was established. Pressure measurements showed conclusively that a detonation process occurred at the frequency chosen for fuel injection. Further, self aspiration was shown to be effective. Finally, the effectiveness of a primary detonation as a driver for the main detonation was clearly demonstrated. Although the NPS studies were abbreviated, many of the technical issues considered to be essential for efficient intermittent detonation propulsion were addressed with positive results.

The generic device we consider here is a small engine shown in Figure 1. Figure 1 shows a schematic of the basic detonation chamber attached to the aft end of a generic aerodynamic vehicle. The combustible gas mixture is injected at the closed end of the detonation chamber and a detonation wave propagates through the mixture. The size of the engine suggests a small payload or aerodynamic vehicle, but the concept can be extended to larger payloads simply by scaling up the size of the detonation chamber and possibly combining a number of chambers into one larger engine.

A key issue in the pulsed detonation engine concept is the design of the main detonation chamber. The detonation chamber geometry determines the propulsion efficiency and the duration of the cycle (frequency of detonations). Since the fresh charge for the generic engine is supplied from the external flow field, the efficiency of the engine depends on the interaction of the surrounding flow with the internal flow dynamics. The range of the physical process requiring simulation in order to model the complex flow phenomena associated with the detonation engine performance is very broad. A partial list is:

1. Initiation and propagation of the detonation wave inside the chamber,
2. Expansion of the detonation products from the chamber into the air stream around the chamber at flight Mach numbers,
3. Fresh air intake from the surrounding air into the chamber.
4. The flow pattern inside the chamber during post-exhaust pressure buildup which determines the strategy for mixing the next detonation charge,
5. Strong mutual interaction between the flow inside the chamber and surrounding the engine.

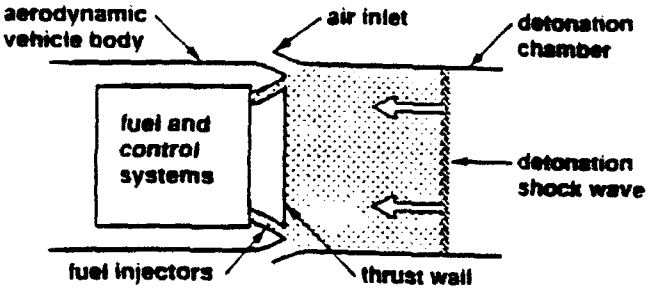

Figure 1. Schematic of the generic PDE showing detonation chamber, inlet, detonation wave, fuel injectors and position relative to an aerodynamic vehicle.

All of these processes are interdependent, and interaction and timing are crucial to engine efficiency. Thus, unlike simulations of steady state engines, the phenomena described above can not be evaluated independently. The need to resolve the flow regime inside the chamber accounting for nozzles, air inlets etc., and at the same time resolve the flow outside and surrounding the engine, where the flow regime varies from high subsonic, locally transonic and supersonic, makes it a challenging computational problem.

The single most important issue is to determine the timing of the air intake for the fresh charge leading to repetitive detonations. It is sufficient to assume inviscid flow for the purpose of simulating the expansion of the detonation products and fresh air intake. The assumption of inviscid flow makes the task of numerically simulating the PDE flow phenomena somewhat easier than if a fully viscous flow model were employed. For the size of the generic device studied in this work the effects of viscous boundary layers are negligible with the exception of possible boundary layer effects on the valve and inlet geometries discussed subsequently..

3. Computational Methods used in the Studies

The basic computational tool that was used for our studies is the FUGGS (Fast Unstructured Grid Second Order Godunov Solver) code, described in detail in Refs. 6,7. This code provides a method for solving the Euler equations of gasdynamics on unstructured grids with arbitrary connectivity. The formulation is based on a second order Godunov method[8]. The use of a data structure with only one level of indirectness leads to an easily

vectorized and parallelized code with a low level of overhead in memory requirement and high computational efficiency. The performance and accuracy of the algorithm has been tested for a very wide range of Mach numbers and geometrical situations, and has demonstrated robustness without the need for any adjustable parameters. The algorithm can either be triangle or vertex based; experience with the method has shown that extremely low levels of artificial viscosity can be achieved using the triangle based version of the method.

A new method of direct dynamic refinement of unstructured grids has been developed, (Ref. 6), and allows an automatic adaptation of the grid to the region of the moving detonation wave inside the PDE geometry. This refinement guarantees that the associated highly inhomogeneous pressure and density contours of the detonation wave are accurately tracked in the simulation. This is an important ingredient in our simulations. since the main component of the detonation process contributing to the thrust generated by the PDE is the total kinetic energy of the wave. Use of the new refinement scheme has more accurately describe the moving detonation wave behavior. These new results concern nonplanar wave evolution and, as pointed out in Section 4, may be a factor in controlling the magnitude of the generated thrust.

4. Scaling Study of the PDE

We have shown in our previous study that in the Pulsed Detonation Engines, thrust is primarily produced by the unsteady interaction of shock wave generated by the propagating detonation wave and the thrust wall of the detonation chamber. This interaction will be nonlinear and scalability of the engine will greatly depend on the extent of nonlinearity. For example, for the engine geometry shown in Figure 1, the engine volume can be increased just by elongating the wall of the detonation chamber. If the area of the thrust wall in Figure 1 remains the same and the composition of the detonation mixture does not change, the increase in the detonation chamber length will result in longer duration of the interaction between the shock wave and the thrust wall. This simple situation poses a question concerning the relationship between the increase in PDE thrust and increase in its volume. This is very practical issue in scaling up the size of the engine, since increase in the detonation chamber diameter will eventually result in difficulty generating a planar detonation front, leading to loss of engine efficiency.

To study this aspect of the detonation engine scalability we have conducted a set of numerical simulations for the engine geometry very similar to these shown in Figure 1. The detonation chamber diameter was kept constant at 8cm and its length varied from 8cm to 16cm. The main objective of our study is to determine how the thrust produced by the detonation engine increases when the engine length doubles and the rest of the engine parameters will remain the same. This section describes the results of two simulations for the detonation chamber geometry described above, using a detonation chamber length of 8 cm and 16 cm. The simulation begins at $t = 0$ when the detonation chamber is placed in an external freestream with the Mach number of 0.8. The detonation wave is initiated at the aft end of the detonation chamber. The detonation chamber for these cases includes a simple annular inlet which remains open during operation. The specific fuel chosen for the present simulations is ethylene. The chemical reaction occurring in the ethylene/air detonation process is given by:

$$C_2H_4 + 3O_2 + 11.24N_2 \longrightarrow 2H_2O + 2CO_2 + 11.24N_2.$$

The detonability limits of ethylene in air range from 4% to 12% by volume and depend somewhat on temperature and pressure. We assume for the sake of simplicity that the fuel/air ratio is 6% by volume. In contrast with our previous presentations here, as well as in case of supersonic PDE simulation presented in this paper, we have simulated a propagating detonation wave by releasing the energy of detonative combustion in our mixture immediately behind the detonation front. In our simulations we have used the Dynamically Adaptive FUGGS code which we have developed recently. Figures 2a, 2b, and 2c, present three frames of the results for simulation in a 16 cm long detonation chamber. In these figures, results are presented in the form of pressure contour plots. For illustration of the dynamic grid adaptation to the evolving flow pattern, we have plotted the unstructured triangular grid corresponding to the stage at which contour plots are shown. In Figure 2a, pressure contour plots are shown shortly after the detonation wave has been initiated at the aft end of the detonation chamber. We can observe that the shock wave front is planar. The detonation wave velocity is 1800 m/sec and the pressure at the front of the detonation wave is $\approx$ 20 atm., corresponding to the CJ condition for the ethylene/air mixture. Figure 2b shows the results of the detonation wave reflecting from the thrust wall and the detonation products starting to expand into the flow stream surrounding the detonation chamber. The detonation products expand through the inlet and into the detonation chamber. This simultaneous expansion results in a complicated wave structure which can be observed in Figure 2b. Here we also note that the dynamically adjustable grid closely follows developing wave structures. In Figure 2c, results are shown at the stage when the two main shock waves generated by the PDE cycle have interacted and are about to leave the computational domain. The maximum pressure here dropped to 1.7 atm.

The computational grid follows the shocks and vortices propagating through the computational domain and we can observe the substantially reduced grid density in the regions of relatively monotonic flow. Figure 2 illustrates the level of detail of this complicated flow regime which can be studied with modern CFD methods and algorithms.

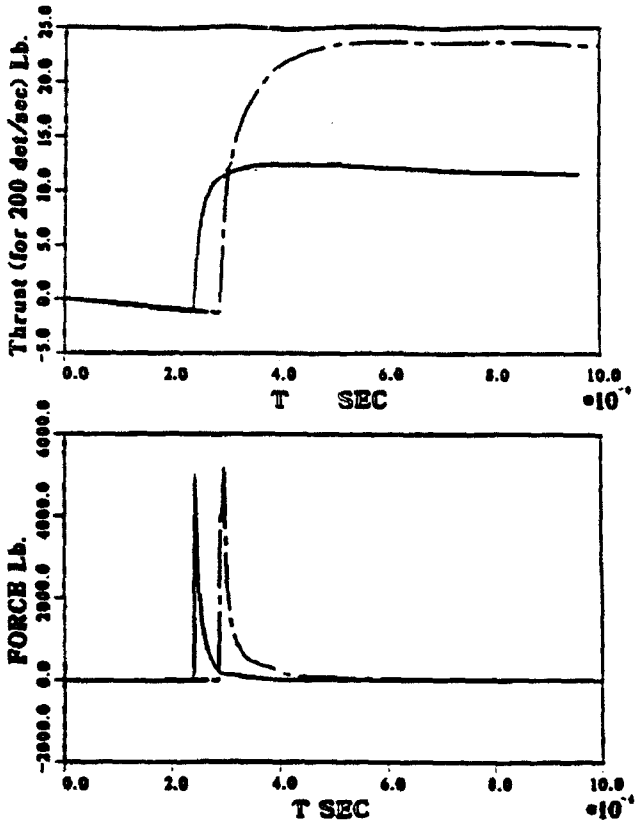

Figure 3. Time averaged thrust and force data from simulation of 8cm (solid lines) and 16cm (dashed lines) detonation chambers, 200 Hz detonation frequency.

In Figure 3 the total force and time averaged thrust generated by the device in the simulations just discussed for 8cm and 16cm long detonation chambers, are shown as a function of time. The time averaged thrust is based on the total time for one cycle defined as 5.0×10^{-3} sec. This time is equivalent to a detonation frequency of 200 Hz. As seen in the figure, initially the force acting on the thrust wall is close to zero. The simulation was run for 2.0×10^{4} sec physical time to establish a flow pattern characteristic of the steady nonreactive flow of ambient air around the detonation chamber. At the time 2.0×10^{4} sec the detonation wave started to propagate from the aft of the chamber. We can see in Figure 3 that the detonation wave reaches the thrust wall at the time 2.45×10^{4} sec (for 8cm case) and 2.9×10^{4} sec (for 16cm case), when a very large force of $\approx 5.0 \times 10^{3}$lb is felt on the end wall of the detonation chamber. This force is a result of the high pressure behind the detonation wave. It rapidly decays to virtually zero level in $\approx 0.5 \times 10^{-4}$ sec in the 8cm case and $\approx 1.0 \times 10^{-4}$ sec in the 16cm case. The maximum force produced on the thrust wall is the same in both cases. The increase of the detonation chamber volume is most noticeable in thrust data. As we can see in Figure 3 the average thrust increases from 12 Lbs in the 8cm chamber case to 24 Lbs in 16cm chamber case. This result shows that the thrust of the detonation chamber will scale linearly with an increase in detonation chamber length when the other parameters are kept constant.

5. Supersonic Missile Simulation

In this section we present the results of a full simulation of a generic supersonic missile powered by a PDE. The purpose of this simulation was to study the requirements placed on the PDE air inlets and internal structures that may be needed to produce a well mixed, uniform flow inside the detonation chamber. In addition, the simulations were carried out on the full vehicle in order to account for all wave drag that a real missile produces; the resulting thrust predictions for the simulations are therefore true net thrust values. We show here the results of a successful geometry that satisfies the requirements of choking flow in the inlet throat and uniform predetonation flow in the chamber produced by means of a grill. The missile geometry and computational grid are shown in figures 4a, 4b, and 4c.

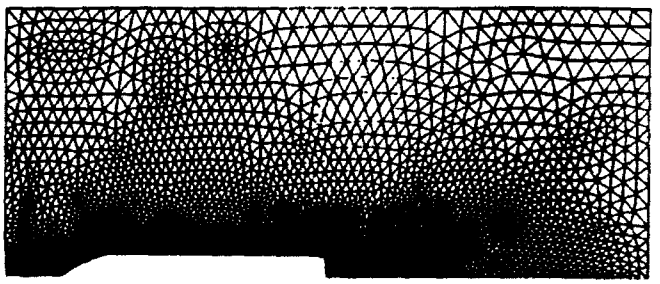

Figure 4a. Unstructured Grid for Missile and Engine Simulation.

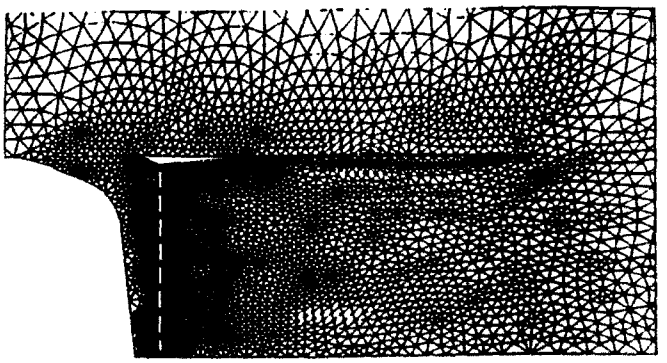

Figure 4b. Grid Detail for Inlet and Manifold.

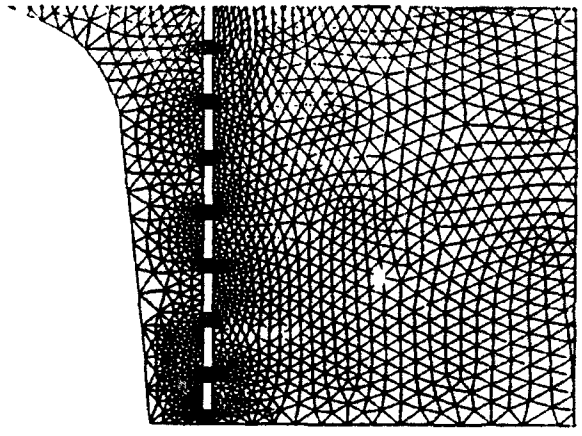

Figure 4c. Grid Detail for Manifold.

Figure 4a shows the main missile body with the PDE covered by the high density of grid points necessary to resolve the details of the PDE chamber, inlets and, grill as shown in the enlarged views of the chamber, figures 4b and 4c.

The simulations were performed by allowing steady subsonic flow conditions to be established in the detonation chamber holding a steady supersonic flow, Mach 2, about the missile. The degree to which this steady and uniform flow can be established in the chamber using the inlet and grill of figure 4 is shown in figure 5. Here the complete flow including the bow shock is shown, figure 5a, as well as an enlarged view of the flow in the vicinity of the inlets showing smaller shocks, figure 5b, and a particle trace showing the streamlines of the uniform chamber flow, figure 5c. When steady flow conditions are reached in the detonation chamber, plane detonation is started at the rear end of the chamber. The detonation then travels towards the inner thrust wall at approximately Mach 4. Figure 6 shows the same sequence of views as figure 5, but with the detonation approximately having travelled halfway to the thrust wall. Notice that the detonation remains more-or-less planar indicating that the flow properties are uniform in the chamber. Figure 7 shows the phenomena associated with the detonation impacting the thrust wall, the high pressure of the detonation wave exhausting from the inlet and particles leaving the chamber through the inlets. The principle results from the simulations of the supersonic missile case are that the use of such a grill structure and inlet shape allow uniform flow to be established before and after detonation in sufficient time that detonation frequencies of 200 cycles per second are obtainable. It is not clear at this time whether such internal grill structures are desirable from the standpoint of structural integritry. This question will be addressed later in planned experimental studies of the PDE.

6. Conclusions

The simulation of the PDE presented in this paper are partial results from an ongoing SAIC research program aimed at development of a practical PDE engine for a wide spectrum of applications including small UAV's and PENAID missiles among others. The primary focus of the results presented here is the scaling of PDE performance with respect to size variation and the establishment of uniform subsonic flow conditions in the detonation chamber before and after detonation.

The results of the scaling studies described in the text lead to scaling laws that can be used to predict the performance of PDE's over some range of parameters assuming that other parameters are held fixed. For example, holding the external Mach number and basic chamber and inlet geometry fixed suggests that the thrust at constant specific fuel consumption produced by the PDE scales as:

$$Thrust = T_1 * \left(\frac{\nu}{\nu_1}\right) * \left(\frac{f}{f_1}\right),$$

where T_1, (v/v_1) and (f/f_1) are the thrust computed for a chamber of volume v_1 operating at frequency f_1, the ratio of a new volume to v_1 and the ratio of the new frequency to f_1 respectively. Thus, thrust should scale linearly with the parameter (v/v_1) * (f/f_1) over some range of this parameter. Departure from this linear variation may occur due to the following reasons: First, since volume is proportional to the product of cross- sectional area and length, $v \sim r^2 l$, ($r \sim$ detonation chamber radius, $l \sim$ chamber length) physical limits will be placed on r and l; if r is too small (less than 1 cm) a detonation will not be sustainable and if l is too small (less than 10 cm) it may be difficult to mix fuel and air effectively. Using the thrust relation established above, we make the following observations. For a PDE device producing 100 pounds thrust at 100 Hz, doubling the frequency and increasing the volume by a factor of 5 yields a thrust level of 1000 pounds. Assuming that the aspect ratio of the chamber (chamber length to radius) is fixed, this would required an engine only 25.5 cm in diameter and 25.5 cm in length. Similarly, scaling the engine down in size to a 5 cm diameter, 5 cm length detonation chamber operatin at 100 Hz yields thrust levels of the order of 3.7 pounds. Of course, the derive relation between thrust and (v/v_1) * (f/f_1) cannot be believed over too wide a range of parameters; but, it does serve to point out the

flexibility in scaleup or scaledown permitted by the PDE concept.

We further conclude that the performance computed for PDEs is encouraging from the point of view of thrust, thrust control, simplicity of the device (no moving parts) and specific fuel consumption (SFC). The specific fuel consumption computed from our simulations ($\sim$ 1Lb/*hr./lb*) is competitive with present day small turbojets (SFCs for small turbojets are in the range of 1.8-2.0 lb./(lb.*hr.)). Thus, for a given mission and vehicle, a PDE propulsion unit could be more fuel efficient resulting in increased range. Moreover, if the expected thrust control in PDEs is realizable, it may be possible to produce propulsion units that can slow down, loiter and maneuver and finally regain full thrust within the time it takes to increase the detonation frequency.

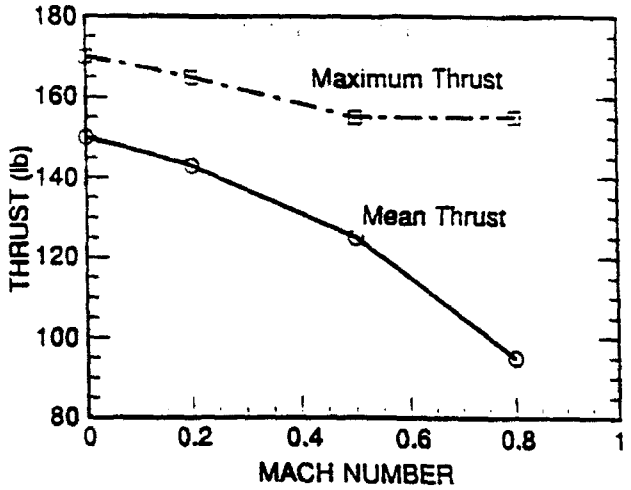

Figure 8. Thrust versus Mach number variation obtained from simulation data.

Another result from the scaling sltudies is that the thrust data show a dependence on the external flight conditions, e.g. Mach number. The Mach number plays a role in the wave drag that the geometry of the PDE will incur; the details of the valve and inlet configurations figure prominentiy in the total wave drag.

On the other hand, the simulations showed that the timing of the fresh air refilling required to recharge the chamber for subsequent detonations is a strong function of the details of the valve and inlet geometry, the expansion of the combustion products, the resulting over-expansion of the chamber flow and the external flow regime and interaction of the external flow with the internal flow. For subsonic flight, Mach 0.2-0.9, the fresh air entering the chamber comes from two separate principle flow processes: one comes from the flow through any valve or inlet and the other comes from the self- aspiration or reverse flow from the aft end of the chamber due to strong over-expansion. All these processes are interdependent and, in order to search for a given performance in a given device, requires variation of many parameters. The simulation results obtained to date provide an understanding of the effects caused by variation of the above-mentioned parameters and, with the information available, we are able to conclude that a PDE propulsion unit can be optimized (although no optimization studies were carried out) for a given flight regime. For example, if we consider the simulations obtained for constant (number and inlet) geometry but at Mach numbers 0.8, 0.5, 0.2, and 0.0 respectively, the variation of maximum time averaged thrust and mean thrust as a function of Mach number can be characterized as shown in Figure 8.

The decrease in thrust with Mach number has been described earlier[3] to be a result of the increased wave drag produced by the inlet geometry. Optimization of the inlet geometry could help in eliminating a large part of the wave drag. The data contained in Figure 8 could be used to determine the detonation frequency at a given Mach number yielding constant thrust. For a constant thrust level of 90 pounds, the required detonation frequency varies from 84 Hz at M = 0.0 to 140 Hz to M = 0.8. In a similar fashion, parametric variations of other important aspects of PDE performance, such as minimum time for refill at given Mach number as a function of air inlet opening, can be obtained. In order to find an optimum configuration satisfying given performance over a wide flight regime, a more extensive simulation study will be required. It was mentioned earlier that the simulations presented here were carried out under the assumption of inviscid flow; boundary layer effects were not included. The addition of boundary layers to the PDE engine inlets and valves, the only components where boundary layers will be significant, will lead to increased performance. Roughly the same amount of fresh air will flow into the over-expanded detonation chamber but at a somewhat slower rate and in a pattern that will promote enhanced circulation and hence fuel/air mixing.

A final conclusion can be made concerning the application of PDE's to supersonic vehicles. As shown in the simulations the ability to refill the detonation chamber with fresh air charge is a very strong function of valve and inlet geometry. Refilling may also be somewhat enhanced by the self-aspiration effect, but; to a much less extent than in the subsonic case. The example of supersonic operation discussed in Section 5 shows that care must be taken in design of the inlet or valve configuration. The flow in the chamber must allow for refill and fuel/air mixing. More than likely choked flow conditions will be required at the inlet entrance to the chamber. This could lead to complications in the design of a PDE with simple geometry; choked flow conditions are a function of the external Mach number and a fixed

inlet will be optimal only for a small range of the operating envelope. On the other hand, if a given vehicle is to fly at supersonic speeds and is launched at supersonic speeds, this problem may not appear. Further, if the given vehicle is launched at subsonic speeds and a booster is used to bring it up to the required supersonic operating speed, the problem may again not appear. We conclude that the PDE has potential for the supersonic flight regime and it is not excluded that a configuration can be found which will operate over the flight regimes 0.2 < Mach number < 3 in a fuel efficient manner.

Acknowledgements

The authors would like to express appreciation to Dr. Adam Drobot of SAIC for helpful suggestions and advice during the course of this work. The work reported on here was partially supported by DARPA under AFOSR contract FY9620-89-(-0087). The authors would like to thank Dr. L. Auslander for his encouragement and interest in this project.

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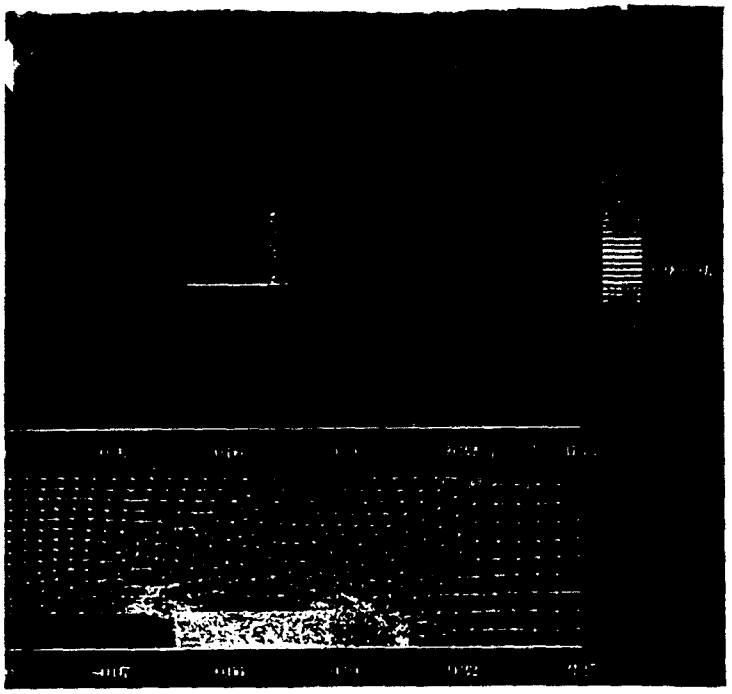

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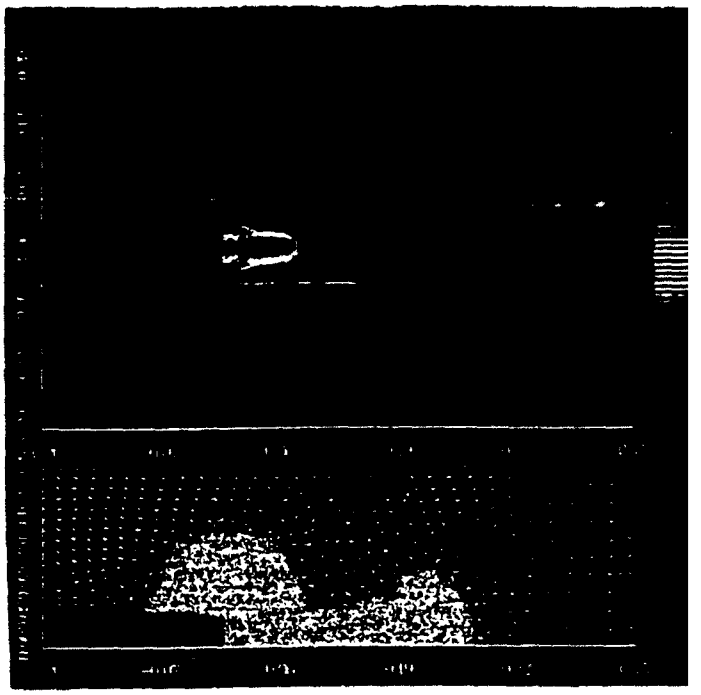

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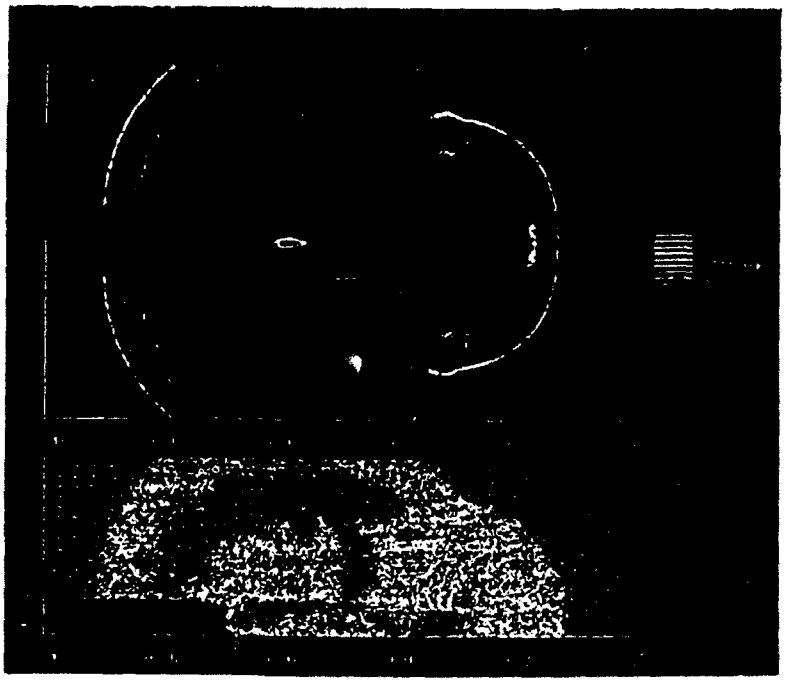
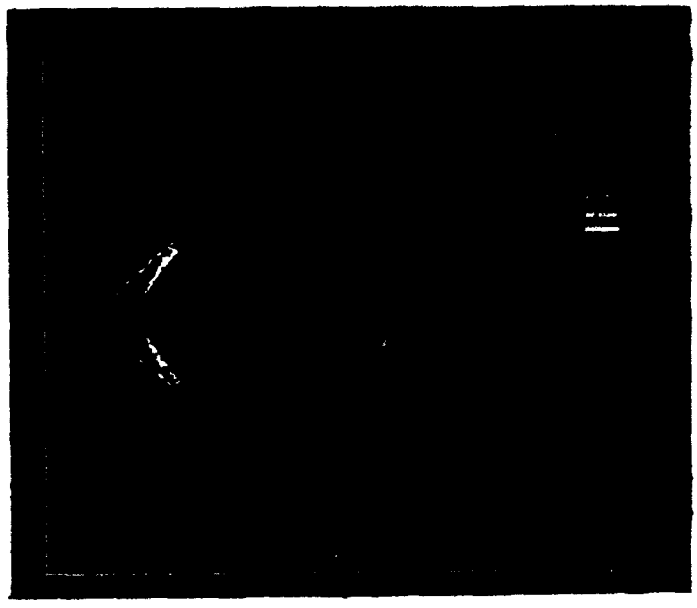
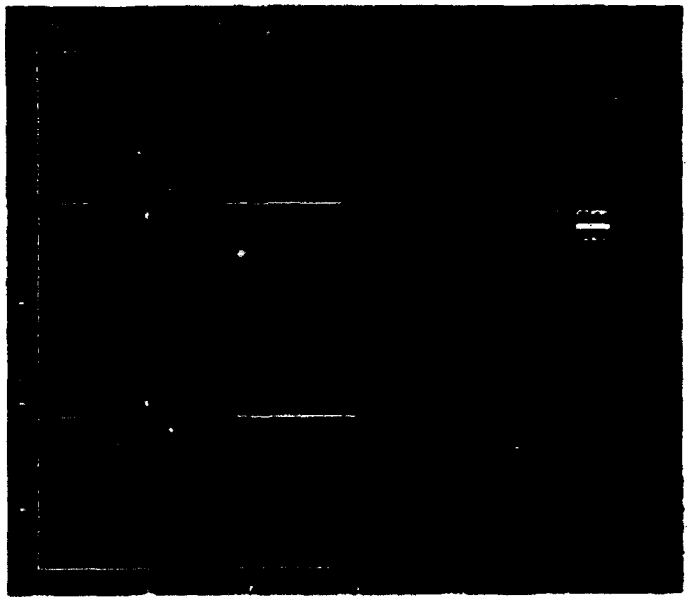


c)

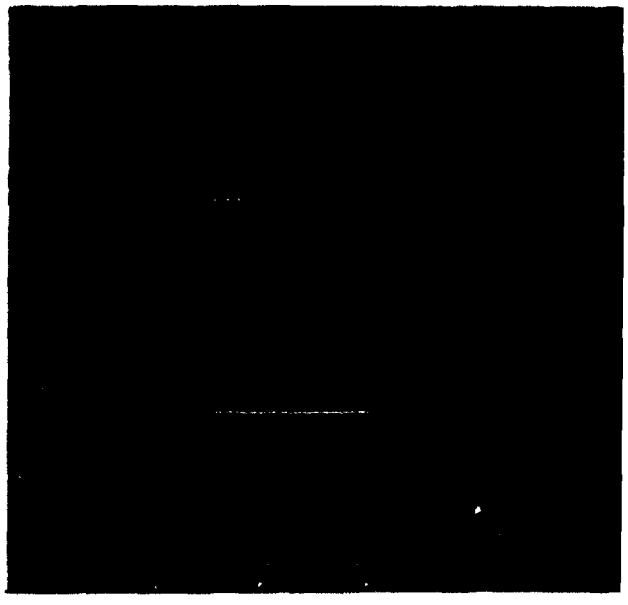
Figure 2. Pressure contours and computational grid for 16 cm long PDE. External flow M = 0.8.



a. Pressure Contours. Missile and Engine.

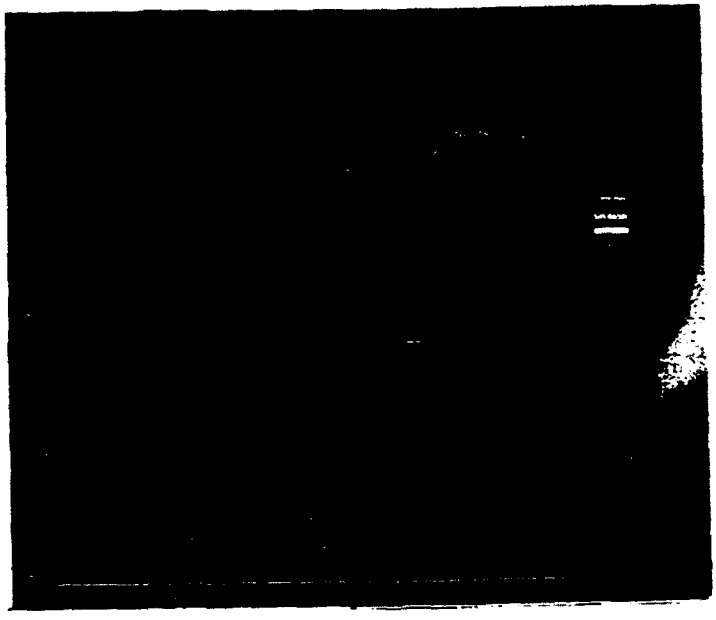


b. Pressure Contours. Detonation Engine.

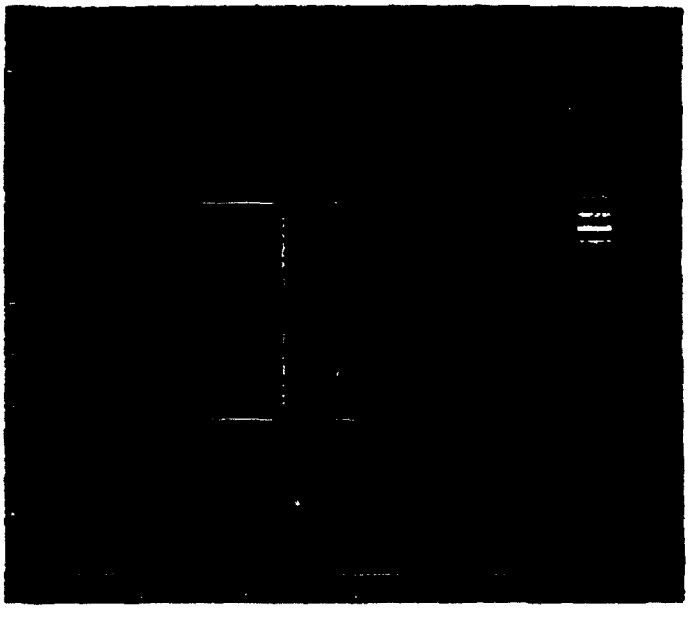


c. Traced Particles. Detonation Engine.

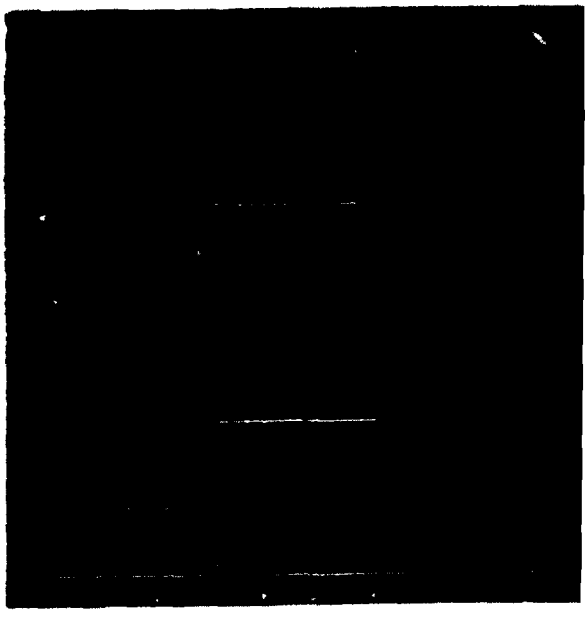
Figure 5. Supersonic missile simulation. Missile speed M = 2.0. Time t = 0.0.



a. Pressure Contours. Missile and Engine.

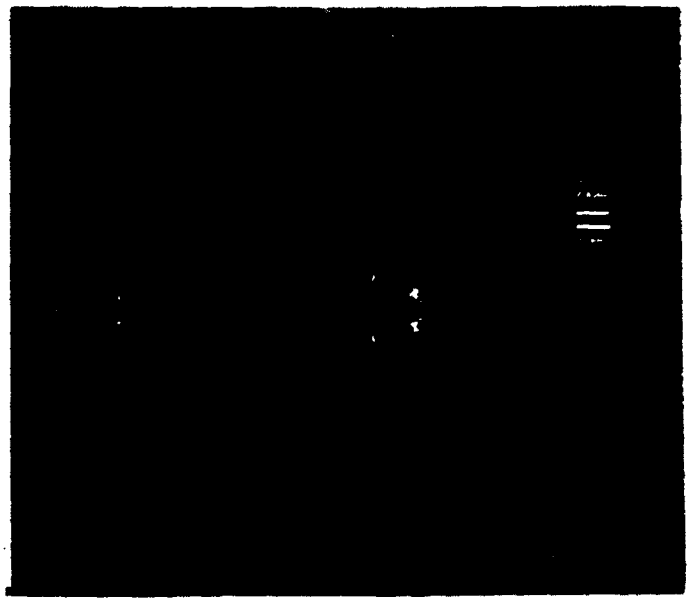


b. Pressure Contours. Detonation Engine.



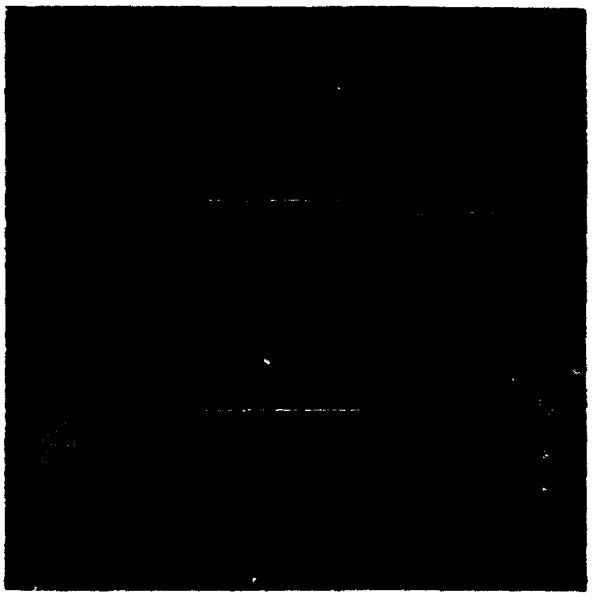
c. Traced Particles. Detonation Engin

Figure 6. Supersonic missile simulation. Missile speed M = 2.0. Time t = $2.0 \cdot 10^{-5}$ sec.



a. Pressure Contours. Missile and Engine.

b. Pressure Contours. Detonation Engine.



c. Traced Particles. Detonation Engine.

Figure 7. Supersonic missile simulation. Missile speed M = 2.0. Time t = $2.0 \cdot 10^{-4}$ sec.

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Plasma enhanced chemical vapor deposition modeling

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Abstract

We are developing a model to simulate the plasma enhanced chemical vapor deposition (PECVD) of thin diamond films. The emphasis to date has been on the development of stand-alone modules to simulate the microwave-induced time-dependent electric and magnetic fields, the generation and energization of plasma electrons in the discharge, the non-equilibrium hydrocarbon chemistry, and the development of a two-dimensional unstructured mesh hydrodynamics solver capable of simulating flow through geometrically realistic reactors. The coupling of the various modules, and the incorporation of a surface chemistry module for the substrate deposition, into a self consistent reactor model is underway. We present some preliminary results from components of a model 2.45 GHz microwave reactor employing H_2 with 1% CH_4 and operating at a gas pressure of 5.3×10^3 Pa (40 Torr). We have completed an electromagnetic model of the microwave energy deposition in the plasma and calculated the field patterns in the reactor. We have also performed point calculations of the time-dependent electron distribution and of the build-up of atomic hydrogen, the gas temperature, and the resulting generation of CH_3, C_2H_2, and other hydrocarbon radicals. We have also completed a fluid simulation of the flow through the reactor using unstructured mesh techniques. The results we discuss in this paper indicate that careful treatment of non-equilibrium processes in PECVD reactors as well as accurate representation of reactor geometry are essential to a useful simulation capability.

1. Introduction

The ability to deposit thin diamond films rapidly onto substrates with a high degree of uniformity using the plasma enhanced chemical vapor deposition (PECVD) technique is a high priority technology goal. It is generally recognized that an improved understanding of the microscopic mechanisms in PECVD reactors and of the sensitivity of the various reactor parameters is needed. The important design issues for PECVD reactors are as follows: efficient coupling of microwave energy to the plasma and to the process gas; efficient transport of activated process gas to the wafer or substrate deposition area; efficient use of the injected gas; uniformity of chemically active species flux across the deposition area. It is desirable to avoid reactor designs that have the following: high microwave electric fields in regions away from the desired plasma formation location, leading to plasma discharge near chamber walls or breakdown of dielectric materials; flow patterns which carry activated species to the reactor walls or out through pumping ports rather than to the wafer; stagnant or circulating flow patterns above the wafer, buffering the wafer from the desired chemically active species.

To understand these issues and to provide input to improved reactor designs we are developing a self-consistent numerical model which simulates each of the essential mechanisms in the PECVD reactor. A physically realistic model requires careful simulation of the electromagnetics, the plasma physics, the neutral gas flow, and the homogeneous and heterogeneous chemistry. Furthermore, the different elementary processes in the reactor are highly interactive; for this reason it is difficult to foresee intuitively the impact of varying one or another reactor parameter. For example, the microwave source induces a complex, geometrically dependent and time varying electric field which ionizes the gas; the resultant build-up of electrons alters the developing electric field distribution. The microwave energy input heats the electrons, and the energetic part of the non-Maxwellian electron energy distribution dissociates the gas, inducing a rise in the gas temperature. The amount of dissociation and heating depends sensitively on the high energy tail of the electron distribution which consequently must be accurately determined. The interaction of the neutral gas with the plasma alters the molecular input stream of H_2 to include a substantial

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component of atomic hydrogen, and this, in turn, affects the ionization rate and the electron distribution. The hydrocarbon chemistry is non-equilibrium and both the flux and the spatial distribution of appropriate radicals reaching the wafer are very sensitive to the geometrical configuration of the reactor and to the details of the flow configuration through the reactor.

We have focused to date on the development of modules to simulate the microwave-induced time-dependent electric and magnetic fields, the generation and energization of plasma electrons in the discharge, the evolution of the molecular and atomic hydrogen gas, the non-equilibrium hydrocarbon chemistry, and the development of a two-dimensional unstructured mesh hydrodynamics solver capable of simulating flow through geometrically realistic reactors. The coupling of these modules, and the incorporation of a surface chemistry module for the substrate deposition, into a self consistent reactor model is underway. In the next section we describe in some detail the generation of the microwave field and the transfer of the field energy to the electrons. This is followed by preliminary model results and our conclusions.

2. Microwave field and plasma generation

The absorption of microwaves and the creation of the plasma which transfers energy to the neutral species in the reactor involves the solution of two closely coupled problems. They are (1) the determination of the electromagnetic field patterns in the complex geometry of the reactor and (2) the formation of the electron distribution function. At a pressure of 5.3×10^3 Pa (40 Torr) and a gas temperature in the plasma region greater than 2000 K, the mean free path of an electron with neutrals is approximately 5×10^{-5} m. During the time an electron gains the average electron energy (approximately 2 eV) typical of the reactors we are modeling, it undergoes around 150 collisions and has a mean displacement of approximately 7×10^{-4} m. Thus, to an excellent approximation, the heating of the electrons results from the microwave electric fields which are local to the electron's spatial location.

The electron distribution function satisfies the Boltzmann equation. Because an electron undergoes many collisions as it is heated, the distribution function is nearly isotropic and can be well approximated by the zero and first order terms of a spherical expansion, the latter representing a distortion of the distribution function in the direction of the applied field, oscillating at the microwave frequency ω. The equation for the electron distribution function is

$$\frac{1}{3}\left[\left(\frac{eE_0}{m_e}\right)^2 \frac{1}{v^2}\frac{\partial}{\partial v}\left(v^2 \frac{\nu_m}{\nu_m^2+\omega^2}\frac{\partial F_0}{\partial v}\right) + v^2\nabla\cdot\left(\frac{1}{\nu_m}\nabla F_0\right) + v\nabla\cdot\left(V\frac{\partial F_0}{\partial v}\right)\right] = L_i + L_x - \frac{2m_e}{M}\frac{1}{v^2}\frac{\partial}{\partial v}(v^3\nu_m F_0)$$

where E_0 is the amplitude of the electric field, e, m_e, and v are the electron charge, mass, and velocity respectively, ν_m is the electron momentum transfer frequency, F_0 is the zero order approximation to the distribution function, V is the bulk fluid velocity, M is the neutral mass, and L_i and L_x are the inelastic loss terms that affect the distribution function respectively via ionization and excitation of rotational, vibrational, and electronic levels. The first term on the left represents the electron velocity diffusion due to the cumulative affect of many small angle scatterings of the electron induced by the oscillating electric field. The next two terms give the affect of the divergence of the diffusive and convective fluxes respectively. The last term on the right gives the energy loss due to elastic collisions.

Below a critical electric field the ionization rate is exceedingly small and hence the electron density and power deposited per unit volume are also small. Above the critical field the ionization rate and power deposition increase rapidly. If the power deposition is kept approximately constant and equal to the power injected into the reactor the electric field will rapidly adjust to a level close to the breakdown value. The power deposited per unit volume scales as $E_0^2 n_e$, where n_e is the electron density; as the electron density rises the electric field drops. The above considerations provide the necessary prescription for determining the time-dependent evolution of the electric field, the electron density, and the electron energy distribution. Using a set of elastic and inelastic cross-sections, the last two parameters define the time-dependent evolution of the fluid, including the build-up of atomic hydrogen and the rise in the gas temperature as the gas dissociates. In addition to H_2 and H, the Boltzmann calculation monitors the evolution of H_2^+, H_3^+, H^+, and H^- and separately tracks each of the three lowest vibrational levels of H_2. The hydrocarbon chemistry is initiated by energetic electrons, but being trace constituents the hydrocarbons do not significantly affect the electron development. It is useful to take advantage of the separation of time scales inherent in this problem. The electron distribution function is established on a time scale of around 10^{-8} s, the electron density growth occurs over approximately 1 μs, and the hydrogen dissociation and hydrocarbon chemistry as well as fluid convection and diffusion occur on a millisecond time scale.

3. Results

We present calculations from the modules of the PECVD model that have been constructed and tested. The results obtained are designed to identify important physical mechanisms and to determine the regimes where they are critical. The calculation of the electric and magnetic fields was accomplished using SAIC's MASK code, a general two-dimensional electromagnetic code designed for the study of microwave devices of arbitrary geometrical configuration. The code introduces the electric fields at the input port and allows them to propagate into the reactor, which can include arbitrarily shaped regions of dielectric or conducting bodies. It employs a finite difference representation of the full set of time-dependent Maxwell equations and solves the initial value problem. Figure 1 shows the results of a simulation for a generic reactor in which the plasma is modeled as a spherical shell with a finite conductivity and a finite dielectric constant. Ultimately the plasma model will be replaced by results of Boltzmann calculations over the plasma region. The MASK calculation retains both the field strength and the phase dependence and determines the energy deposition in the target plasma. The results shown are contours of constant field amplitude for the axial (a) and radial (b) electric components in an azimuthally symmetric configuration. The bottom horizontal line is the axis of symmetry. The input wave is introduced on the left and propagates into the reactor region through a radially expanding transition region. The substrate is on the right in the figure and immediately above it is the outlet for the reacting gases. The figure indicates regions of high and low field concentration which will provide an important tool for reactor design. This calculation determines the energy deposition in the plasma and, hence, the reactor efficiency. When performed self consistently it also predicts the shape of the plasma region and the subsequent coupling to the hydrodynamic calculation.

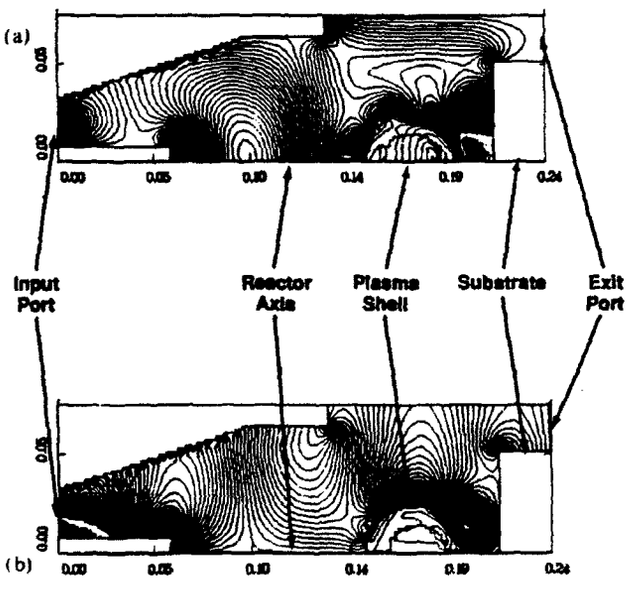


Fig. 1. MASK calculation of (a) the axial and (b) the radial components of the electric field in a model reactor. Shown in the figure are contours of constant amplitude. The reactor axis is the bottom horizontal line. The substrate shelf is at the right and the outlet for the reacting gases is above it. The plasma shell is centered on the axis to the left of the substrate.

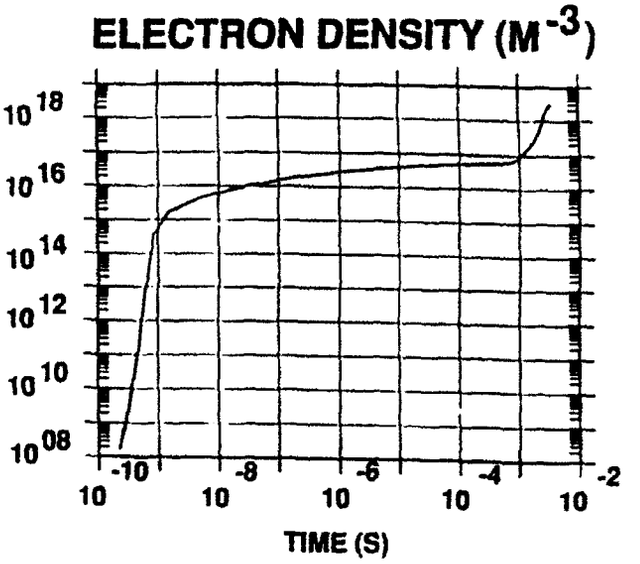
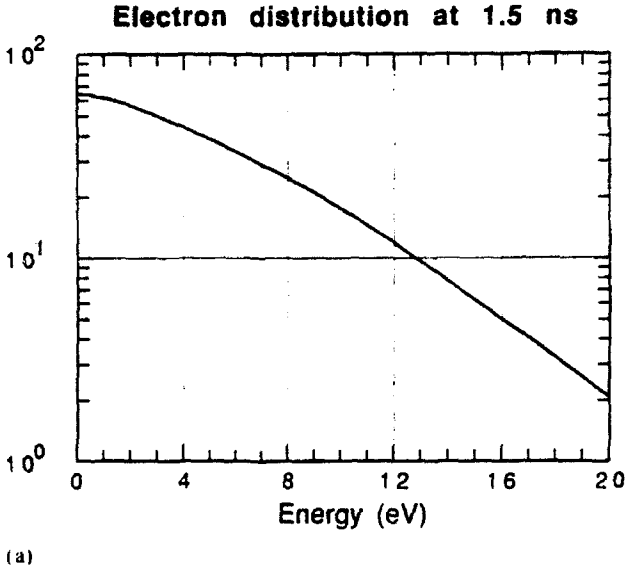
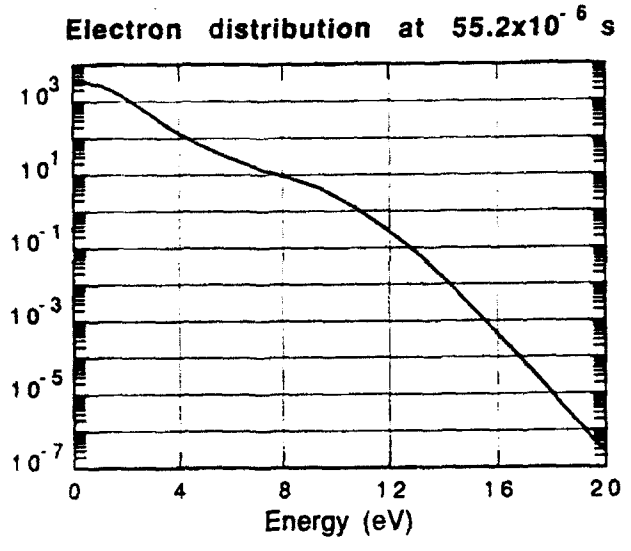


Fig. 2. Time development of the electron density at a point in the reactor of high electric field corresponding to the one-point simulation described in the text.

The Boltzmann module calculation simulates the electron and heavy particle evolution at a location within the reactor where the electric field is sufficiently high to create and sustain a plasma. We maintain a constant deposited microwave power and assume the gas pressure is kept constant at 5.3×10^3 Pa (40 Torr). The simulation runs for several milliseconds, beyond which time advection and diffusion effects, not included in this calculation, would become important. The initial conditions are $[H_2] = 1.28 \times 10^{24}\ m^{-3}$, $[CH_4] = 1.28 \times 10^{22}\ m^{-3}$, gas temperature $T = 300$ K. Figure 2 shows the electron density rising rapidly to approximately $10^{15}\ m^{-3}$ in around 1 ns, a result of the very energetic electron distribution at early times. Thereafter, it increases nearly two more decades over about 10^{-5} s, the slower increase being reflective of the less energetic electron spectrum as the electrons give up energy to the various inelastic processes. The increase on a millisecond time scale is associated with the conversion of the gas from the molecular to the atomic state which leads to an increasing fraction of atomic ions (which recombine much more slowly than molecular ions) and also causes



(a)



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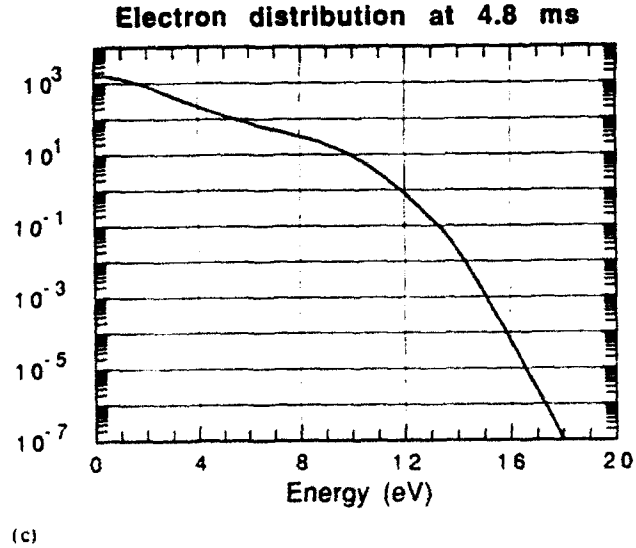


(c)

an adjustment in the electron distribution function. The evolution of the electron distribution function as determined by the Boltzmann equation is illustrated for these three time regimes in Fig. 3 in which the ordinate scale is arbitrary. In Fig. 3(a) at 1.5 ns we see the very energetic electron spectrum: the average electron energy is around 8 eV. In Fig. 3(b) at 55.2 μs the average energy has dropped to 2 eV and in Fig. 3(c) at 4.8 ms when atomic hydrogen predominates, the spectrum has changed again, the average electron energy increasing moderately to about 2.7 eV.

The evolution of the hydrocarbon species is simulated with a chemistry code that uses the output of the Boltzmann code. The reactions used in the hydrocarbon model are listed in Table I along with the constants A, b, and E which determine the rate coefficient k according to $k = AT^b \exp(-E/T)$. The code calculates the rate for each reverse reaction that is not known, using detailed balance. The hydrocarbon chemistry is initiated by the electrons which dissociate H_2 (and also the CH_4), causing the release of chemical energy and heating the gas. Figure 4 shows the gas temperature as a function of time for the simulation described above. In Fig. 5 we show the evolution of 12 hydrocarbon species plus H_2 and H out to 3 ms, at which time the H_2 and H densities are approximately equal. Although the formation of H is initiated by the electron dissociation of H_2, after about 2.5 ms with rise in temperature, thermal dissociation of H_2 becomes predominant. The build-up of CH_3 due to the dissociation of CH_4 occurs very early (approximately 30 μs) but it reacts with itself to form C_2H_6 and drops to a local minimum before 1 ms. As the temperature increases, however, the CH_3 recombination reaction rate decreases and CH_3 increases to a new maximum near 2 ms; thereafter it decreases once more as the CH_4 becomes exhausted. Acetylene (C_2H_2) results from the chain of reactions initiated by the formation of C_2H_6, thence to C_2H_5 and, in turn, to C_2H_4, C_2H_3 and finally to C_2H_2 which persists to the end of the simulation. In general, the hydrocarbon species do not have time to reach the equilibrium values that the gas temperature would dictate. Thus, the time between their formation in the plasma and their reaching the substrate determines the densities of the critical radical species reaching the substrate.

Fig. 3. Electron energy distribution for the simulation as in Fig. 2. (a) at a time before inelastic processes reduce the average electron energy; (b) at an intermediate time when the average electron energy is about 2 eV; (c) at a time when dissociation of the H_2 is nearly complete. The ordinate scale is arbitrary.

TABLE 1. Hydrocarbon reactions and rate coefficients

Reaction	$A(10^{6(n-1)}(\mathrm{m})^{3(n-1)}\mathrm{s}^{-1})^a$	b	E(K)	Range(K)
$H + H + H_2 \rightarrow H_2 + H_2$	2.7×10^{-31}	−0.6	0	100–5000
$H_2 + H_2 \rightarrow H + H + H_2$	1.5×10^{-9}	0	4.84×10^4	2500–8000
$CH_4 + H \rightarrow CH_3 + H_2$	3.6×10^{-20}	3.0	4.40×10^3	300–2500
$CH_3 + H_2 \rightarrow CH_4 + H$	1.1×10^{-21}	3.0	3.90×10^3	300–2500
$CH_4 + {}^{H_2}_{CH_4} \rightarrow CH_3 + H + {}^{H_2}_{CH_4}$	$\frac{(2.9)}{(18.6)} 3.3 \times 10^{-7}$	0	4.45×10^4	1500–3000
$CH_3 + H + {}^{H_2}_{CH_4} \rightarrow CH_4 + {}^{H_2}_{CH_4}$	$\frac{(2.9)}{(18.6)} 2.2 \times 10^{-21}$	−3.0	0	300–2500
$CH_3 + CH_3 \rightarrow C_2H_5 + H$	1.3×10^{-9}	0	1.34×10^4	1500–3000
$C_2H_5 + H \rightarrow CH_3 + CH_3$	5.0×10^{-11}	0	0	300–1500
$CH_3 + CH_3 \rightarrow C_2H_4 + H_2$	1.7×10^{-8}	0	1.61×10^4	1500–2500
$CH_3 + {}^{H_2}_{CH_4} \rightarrow CH_2 + H + {}^{H_2}_{CH_4}$	$\frac{(2.9)}{(18.6)} 1.7 \times 10^{-8}$	0	4.56×10^4	1500–3000
$CH_2 + H \rightarrow CH + H_2$	6.6×10^{-11}	0	0	300–2500
$CH_2 + CH_3 \rightarrow C_2H_4 + H$	6.6×10^{-11}	0	0	300–2500
$C_2H_6 + H \rightarrow C_2H_5 + H_2$	9.0×10^{-22}	3.5	2.62×10^3	300–2000
$C_2H_6 + CH_3 \rightarrow C_2H_5 + CH_4$	9.1×10^{-25}	4.0	4.17×10^3	300–2000
$C_2H_6 + {}^{H_2}_{CH_4} \rightarrow CH_3 + CH_3 + {}^{H_2}_{CH_4}$	$\frac{(2.9)}{(18.6)} 1.7 \times 10^{-5}$	0	3.43×10^4	800–2500
$C_2H_5 + C_2H_5 \rightarrow C_2H_4 + C_2H_6$	2.3×10^{-12}	0	0	300–1200
$C_2H_5 + {}^{H_2}_{CH_4} \rightarrow C_2H_4 + H + {}^{H_2}_{CH_4}$	1.7×10^{-7}	0	1.56×10^4	700–1500
$C_2H_4 + H \rightarrow C_2H_3 + H_2$	2.5×10^{-10}	0	5.14×10^3	700–2000
$C_2H_4 + {}^{H_2}_{CH_4} \rightarrow C_2H_2 + H_2 + {}^{H_2}_{CH_4}$	$\frac{(2.9)}{(18.6)} 4.3 \times 10^{-7}$	0	3.99×10^4	1500–2500
$C_2H_4 + {}^{H_2}_{CH_4} \rightarrow C_2H_3 + H + {}^{H_2}_{CH_4}$	$\frac{(2.9)}{(18.6)} 4.3 \times 10^{-7}$	0	4.86×10^4	1500–2500
$C_2H_4 + CH_3 \rightarrow C_2H_3 + CH_4$	7.0×10^{-13}	0	5.59×10^3	300–1000
$C_2H_3 + H \rightarrow C_2H_2 + H_2$	3.3×10^{-11}	0	0	300–2500
$C_2H_3 + {}^{H_2}_{CH_4} \rightarrow C_2H_2 + H + {}^{H_2}_{CH_4}$	$\frac{(2.9)}{(18.6)} 5.0 \times 10^{-9}$	0	1.61×10^4	500–2500
$C_2H_2 + H + {}^{H_2}_{CH_4} \rightarrow C_2H_3 + {}^{H_2}_{CH_4}$	$\frac{(2.9)}{(18.6)} 1.11 \times 10^{-30}$	0	3.5×10^2	300–500
$C_2H_2 + H \rightarrow C_2H + H_2$	1.0×10^{-10}	0	1.19×10^4	300–3000
$C_2H + H_2 \rightarrow C_2H_2 + H$	2.5×10^{-11}	0	1.56×10^3	300–3000
$C_2H_2 + CH_2 \rightarrow C_3H_3 + H$	3.0×10^{-12}	0	0	>298
$C_2H_2 + C_2H \rightarrow C_4H_2 + H$	5.8×10^{-11}	0	0	300–2500
$C_2H_2 + {}^{H_2}_{CH_4} \rightarrow C_2H + H + {}^{H_2}_{CH_4}$	$\frac{(2.9)}{(18.6)} 6.6 \times 10^{-8}$	0	5.38×10^4	1500–3500

[a] n denotes the number of reactants.

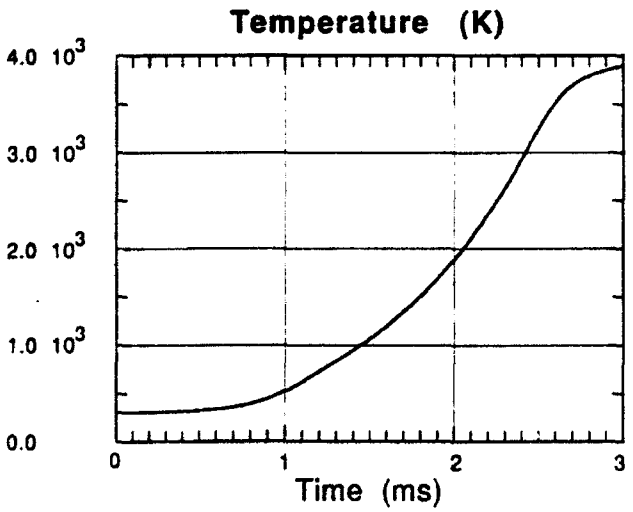
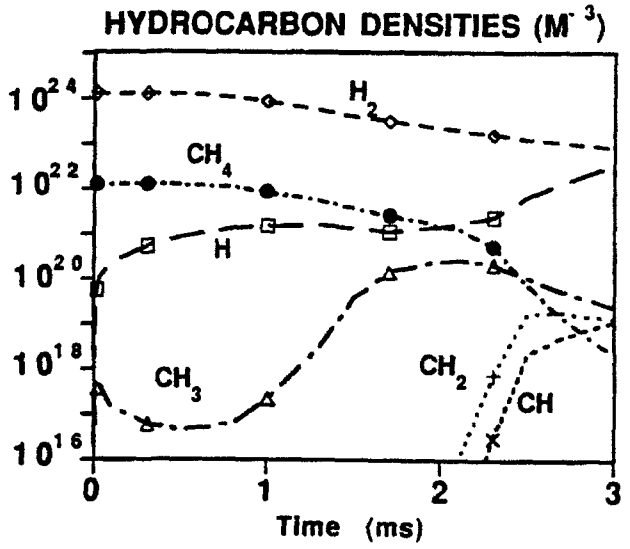
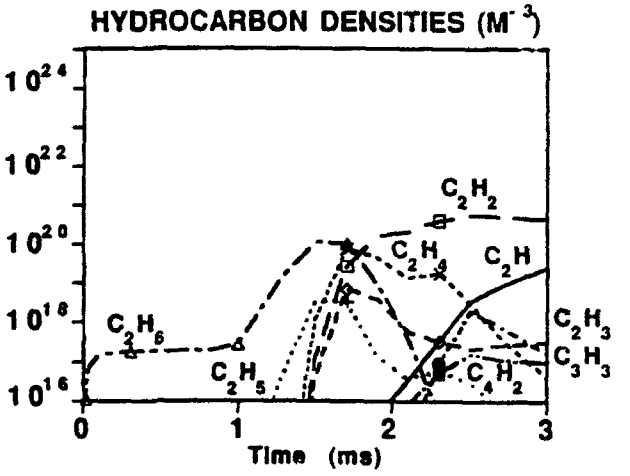


Fig. 4. Evolution of the gas temperature for the simulation as in Fig. 2.

Finally, we present preliminary results of a fluid simulation of a generic PECVD reactor, using SAIC's FUGG code which is capable of performing fluid calculations over arbitrarily complex geometries. The code employs an unstructured grid allowing extremely fine resolution in critical areas while employing coarser gridding in regions where quantities vary slowly. The code was designed for the study of flow problems dominated by convection and is presently being modified to incorporate thermal conduction and viscosity effects. In Fig. 6 we show two examples of the code's triangular gridding capability. In both cases a cross-section of the azimuthally symmetric model reactor is shown, where the left vertical boundary represents the reactor axis. Three gas inlet ports are modeled allowing the gas to enter at the top (in Fig. 6(a) the plenum region above the inlet ports is also modeled). The gas exits through the horizontal boundary at the bottom right. The substrate wafer is represented in Fig. 6(a) by the left half of the lower horizontal boundary and in Fig. 6(b) by the shelf at the lower left. In Fig. 6(a) the variable gridding capability is clearly illustrated and, in particular, the fine gridding needed in the inlet ports is shown. Figure 7 shows results of a fluid calculation for the reactor of Fig. 6(b) in which hydrogen gas enters at 50 m s^{-1} at a pressure of 5.3×10^3 Pa (40 Torr). A heating source of 1.5 kW over a spherical volume of radius 0.035 m, centered on the reactor axis and mid-



(a)



(b)

Fig. 5. Evolution of the hydrocarbon densities for the simulation as in Fig. 2.

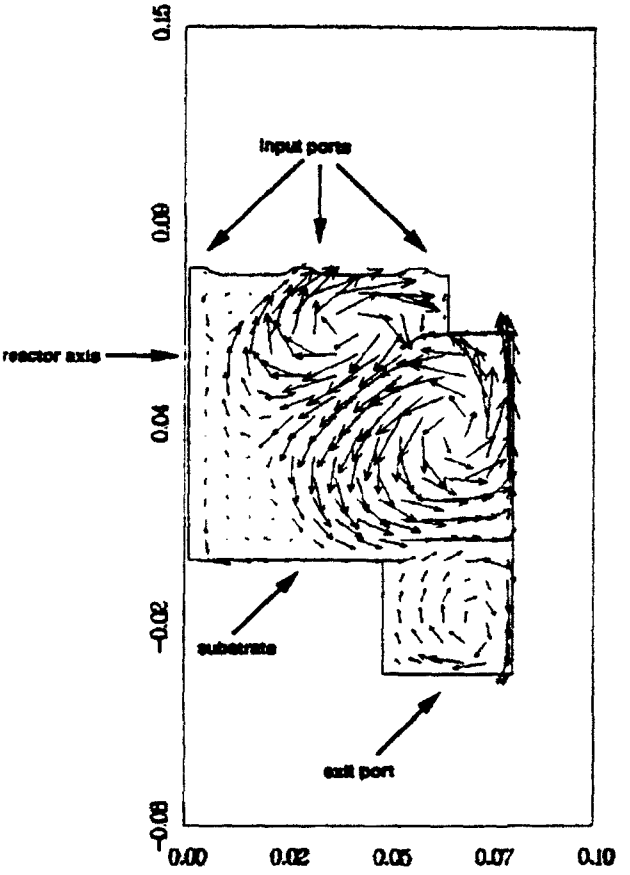


Fig. 7. Velocity field for reactor of Fig. 6(b) in which H_2 enters at a velocity of 50 m s^{-1} at a pressure of 5.3×10^3 Pa (40 Torr). A heating source of 1.5 kW to simulate the effect of the plasma is centered on the axis between the inlet port and the water in a spherical volume of radius 0.035 m. The ordinate and abscissa dimensions are in meters.

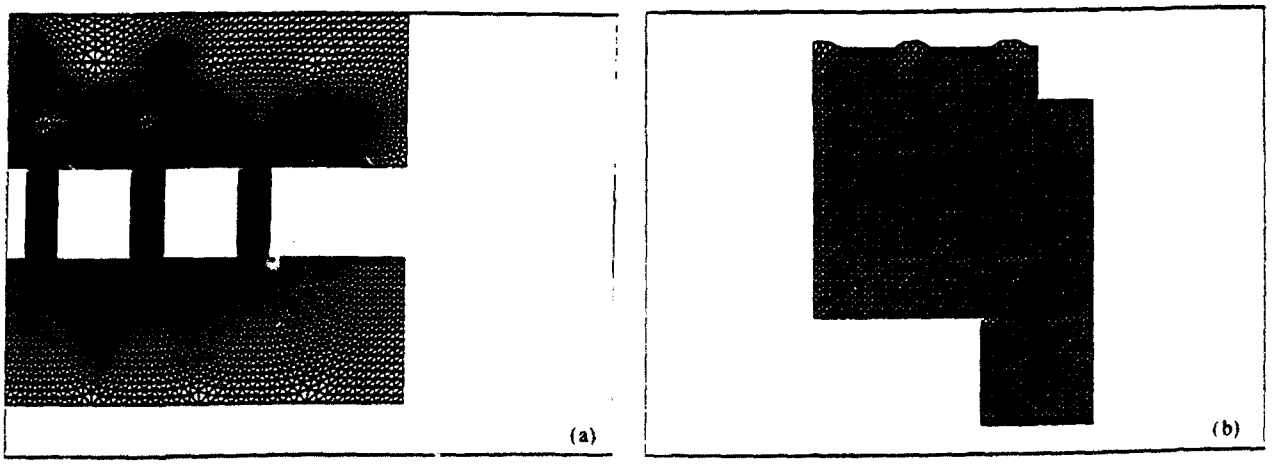


Fig. 6. Examples of the FUGG code's unstructured gridding capability for two model reactors ((a) and (b)).

way between the inlet port and the wafer, is included to simulate approximately the effect of the plasma source. Shown are velocity vectors for the flow 2.6 ms after the plasma is turned on. Also calculated but not shown are the pressure, density, and temperature fields. While conclusions should be tempered because of the current lack of inclusion of thermal effects in the code and because the results represent a transient pre-steady-state stage, the effects of buoyancy are apparent. The complex vortex flows seen suggest this reactor configuration would be very poor for efficient diamond deposition.

4. Discussion and conclusions

We have presented results of a model under development that will permit the simulation of PECVD reactors of arbitrary geometry. The model will be an important tool providing better understanding of the microscopic processes occurring within the reactor, permit parameter studies to identify those parameters which critically affect both the rate of deposition and the uniformity of the deposition over the wafer surface, and ultimately enable the design of improved reactors. We have identified several critical elements in the modeling effort that need to be treated carefully if simulation results are to be meaningful. First, the electromagnetic fields which initiate the plasma formation need to be determined in the realistic reactor geometry, including effects of all metallic, dielectric, and insulator elements actually present, to ensure that the fields are high in the desired plasma formation region but not elsewhere. Second, the coupling of the fields to the plasma electrons, to determine accurately both the time development of the electron density and their energy distribution, is most important for determining the evolution of the rate of hydrogen dissociation and the rise in the gas temperature. This, in turn, critically determines the non-equilibrium hydrocarbon chemistry development, a third area that needs to be carefully modeled. Finally, the flow of hydrocarbon radicals to the wafer is very sensitive to the reactor's geometrical configuration, its thermal properties, and the location of the plasma relative to the wafer. In conclusion, our results emphasize the highly non-equilibrium and coupled nature of PECVD reactor processes and the strong influence of reactor geometry. A numerical simulation that is useful must address all such issues.

Acknowledgment

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Nonlinear signal processing using integration of fluid dynamics equations

by

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1. INTRODUCTION

Very recently, there have been exploratory efforts in image processing based on nonlinear methods.[1] These efforts involve systems of nonlinear hyperbolic partial differential equations in combination with local wave representation, such as wavelets, for signal enhancement.[2,3,4] Techniques based on Kalman filtering for feature extraction from complex time-evolving scenes, as well as neural network approaches to image analysis and feature identification, can also be shown to involve nonlinear PDE analogies. The use of nonlinear methods, however, is largely unexplored and may provide another level of improvement for image processing.

If the purpose of an image enhancement process is to highlight the edges of an image, then the technique used in the frequency domain is usually highpass filtering. An image can be blurred, however, by attenuating the high-frequency component of its Fourier transform. Since edges and other abrupt changes in the gray levels are associated with high-frequency components, image sharpening can be achieved in the frequency domain by a highpass filtering process, which attenuates the low-frequency without disturbing high-frequency information in the Fourier transform. The primary problem with this technique is that an ideal discontinuity will have an infinite spectrum of frequencies associated with it. When filtering is applied, some frequencies are cut off, leading to a loss of some edges in an image.

It is interesting to observe that in the field of Computational Fluid Dynamics (CFD) similar problems exist in simulating flows with discontinuities. The problem of simulating flows with discontinuities is less forgiving, since an incorrect calculation usually leads to a complete distortion of the flow field. This has led CFD scientists to develop sophisticated algorithms that identify and preserve discontinuities while integrating the flow field in the computational domain. In the image domain, sharpening is usually done by differentiation. The most commonly used methods involve the use of either gradients or second derivatives of the pixel information. Central differencing is usually used to calculate the derivatives. CFD research has shown that this strategy will lead in many cases to a smearing of the flow discontinuities (analog of the image edges in image enhancement).

Here, we describe a new and unique image sharpening method based on computational techniques developed for CFD. Our preliminary experience with this method shows its capability for nonlinear enhancement of image edges as well as deconvolution of an image with random noise. This indicates a potential application for image deconvolution from sparse and noisy data resulting from measurements of backscattered laser-speckle intensity.

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2. THE CFD IMAGE ENHANCEMENT TECHNIQUE

Considerable attention has been devoted to the development of numerical methods and algorithms for Computational Fluid Dynamics during the last thirty years. In recent years, however, our understanding of numerical algorithms for a particular class of problems in gas dynamics described by the Euler equations has become more complete. The main numerical difficulty in solving invisid compressible flows described by Euler equations is the occurrence of features that, in the invisid approximation, are discontinuous and even in the presence of viscosity are too small to be resolved on an affordable computational mesh. These flow discontinuities in which the fluid state jumps across shock waves or contact surfaces are extremely important in fluid simulations. Most of the efforts in developing numerical techniques in fluid dynamics over the last twenty years were devoted to accurate simulations of these discontinuities. Initially, naive numerical methods that used a formal finite difference representation of the conservation equations on a computational grid were employed. That led to disastrous results, smearing of the discontinuities, and spurious oscillations. Subsequently, sophisticated nonlinear techniques, which allowed accurate simulations of complex discontinuities without smearing and ringing, were developed. These new methods also satisfy a very demanding criteria for robustness and allow simulation of the wide range of flow problems without adjustment or tuning of the numerical technique.

The numerical methods that allow high accuracy resolution of flow discontinuities are so-called TVD (Total Variation Diminishing) methods. The Second Order Godunov Method is one of the most successful numerical techniques developed for this purpose. In Figure 1, an example is given of a solution using the Second Order Godunov Method for a complicated case of multiple shock waves,[5] illustrating the ability of this method to capture and simulate sharp discontinuities.

The Second Order Godunov Method was developed based on an understanding of the phenomenology of signal propagation in the gasdynamical system. The numerical algorithm implementing this method is not analytic and is based on a set of steps that can be considered as wave filters. These filters are designed to not smear the discontinuity (edge), suppress the spurious oscillations, and propagate the relevant signals through the system. The following algorithmic steps are performed to advance the solution for a single iteration in the Second Order Godunov Method:

1. Local Extrapolation
2. Monotonicity Constraint
3. Characteristics Constraint
4. Riemann Problem Solution
5. Integration

It is interesting to note that most of these steps have an analog in conventional image processing methods. Here, we will give an explanation of the function of each algorithmic step of the Second Order Godunov Method and where applicable, will point to its possible analog in conventional signal processing techniques.

Step 1 consists of extrapolation of the values in the computational grid (pixel) cell to the edges of the cell. Linear or nonlinear extrapolation can be used. This step is analogous to the standard edge sharpening techniques used in image processing, with one important difference: the extrapolation is done not for the value itself but for its flux (change of value across cell boundary).

Step 2 includes a monotonicity constraint for the values at the cells' edges. This is analogous to the nonlinear technique of the locally monotonic regression[6] only recently introduced for signal processing.

Step 3 subjects the values at the edges to the constraints derived from a solution of one dimensional characteristics. This step assures that the values at the edges have not been extrapolated from directions inconsistent with the characteristic solutions. This prevents extrapolation as well as smearing or overshoot of the discontinuities. For the image processing application, this can be regarded as a form of automatic edge detection step where the shock waves are associated with the edges of an image.

Step 4 uses an exact solution of the system of the gas dynamic equations for calculation of the flux values based on the extrapolated values of the parameters at the left and right side of the edges. This step has no analogy in image processing. However, since the analytical solution includes discontinuities, an exact calculation of the flux at the edge location is allowed, even if this flux is calculated through a discontinuity.

Step 5 consists of finite volume integration of the system of conservation laws. Here, the image is effectively treated as a flow field; the flux integration serves as a smoothing filter from the image perspective.

Application of these steps can be considered as the application of a unique filter stack with proven properties of discontinuity preservation and robustness. Below we illustrate uses of this technique for practical problems of image processing that exemplify the feasibility and advantages of this approach.

The use of image analogies for image processing is not new. One widely applied technique treats an image as a potential field where the image potential acts as a force on the edges that are represented as elastic curves with some elastic properties.[3] Our approach, as stated, involves an application of a technique developed for gas dynamic problems for image deconvolution. Although this technique is very new, an analysis of the basic steps presented above and our experience with its application for image deconvolution show that this nonlinear algorithm has considerable potential for edge enhancement and filtering of extremely noisy signals.

3. IMAGE ENHANCEMENT BY THE SECOND ORDER GODUNOV METHOD

The field of gray scale intensity of an image can be translated into a flow field. To every image pixel we add a corresponding cell of the computational domain with values of the gas dynamical parameters proportional to the values of the gray scale. Since there are at least five gasdynamical parameters that can be defined in every cell of the computational domain (pressure, density, two velocity components and γ) and only one parameter in the image domain, cell mapping is not unique. Our understanding of the basic gasdynamical processes plays a major role in completing the analogy. Appropriate mapping of the image gray scale intensity into a flow field creates conditions favorable for the formation or enhancement of field discontinuities. For example, a shock wave reflecting from a wall or a contact surface can increase in strength, or two colliding flow streams will produce a contact surface that will become stronger in time. If we have a numerical technique to resolve these discontinuities accurately, then with successive numerical integration of the flow field, the discontinuities will sharpen as the solution evolves in time. Then by inverse mapping of the flow field to the image gray scale field, we can reconstruct an enhanced image. Below we give some examples of practical application of this technique.

3.1. Edge sharpening for a sinusoidal distribution

In Figure 2 results are given for edge definition of a one dimensional signal. The original sinusoidal signal is shown in Figure 2a. This example was chosen to test the ability of our technique to identify the edges of an image where the signal strength has deteriorated in the vicinity of the

edges, producing a gradual (instead of sharp) increase in the gray scale intensity. We observe that application of our technique results in significant sharpening of the edges, even after 15 or more iterations.

In Figure 3 random noise has been added to the sinusoidal signal shown in Figure 2a. The level of random noise addition corresponds to 10% of the maximum intensity of the original signal. The original signal with the random noise is shown in Figure 3a. In Figures 3b, 3c, 3d we observe successive noise filtering and edge enhancement with application of our algorithm for 15, 30, and 45 interations correspondingly. We see that the edges of the final processed signal are located at exactly the same position as shown in Figure 2d for the uncontaminated signal.

Figure 4 illustrates the application of our algorithm to the signal that has been contaminated with 50% addition of random noise. Significant noise filtering occurs after 15 iterations and edge definition at the exact original locations after 45 iterations.

In Figure 5 the results are shown for a signal with 100% random noise added. Here again the signal is quickly filtered and the edges are picked up exactly at the correct locations.

3.2. Edge sharpening for a two dimensional image

Figure 3 contains a picture of Washington. DC taken from a Russian satellite. Digital representation of this picture had 150 dots per inch resolution. A fragment of the picture shown in Figure 6 is represented on an evenly spaced 400 × 360 grid. We take the gray scale pixel information of this picture and convert the data into initial conditions for a gasdynamic problem by assigning the values of pressure and density in the computational domain directly proportional to the values of the pixels on the gray scale. Now the gasdynamic problem is defined and we can solve it using our high resolution Second Order Godunov Method. In Figures 7a, 7b, and 7c results in the pixel plane are shown after three, six, and nine iterations respectively in the gasdynamic domain. By "iteration," we mean that the flow solver integration algorithm was applied to the given flow field, or in this case, the pressure and density data derived from the initial picture. Even after three iterations, the picture is significantly sharper and continues to improve with more iterations.

A more detailed examination of the sharpening effect can be obtained by looking at the one-dimensional cross section of the picture plane. In Figure 8, an arbitrary cross section of the original picture shown in Figure 6 is given. For clarity we show only the first fourth of the actual pixels in the cross section. We can see here that this particular cross section contains a multitude of sharp edges expressed only by three or four points. Further sharpening of these edges by a standard differentiation technique will lead to significant smearing of a number of the discontinuities. In Figure 9, the same cross section is shown after three iterations with the Second Order Godunov solver. Significant enhancement of all the sharp edges is evident. The process of enhancement can be followed in Figures 6b, 6c and 6d corresponding to six, nine, and twelve iterations. Continuous improvement in the definition of edges can be observed.

In Figures 10, 11a, 11b, 11c, and 11d, we demonstrate the ability of the current nonlinear PDE methodology to enhance simultaneously the high and low frequency features of an image. The amplitudes of both short and long wavelengths are simultaneously enhanced. However, as seen in the circled area, long wavelength features that retain one grid-cell discontinuities exhibit interesting behavior in that the cell-specific discontinuity, which appears in Figure 10, disappears in Figures 11b and 11c, but reappears in Figure 11d. The long wavelength definition continues to be enhanced in Figures 11a-11d. The origin of this behavior is presently unknown.

3.3. Application to Medical Imaging

Images of internal organs obtained with a Gamma Camera are usually of marginal quality and need significant post-processing to be useful for medical diagnostics. This is especially true if multiple pictures are taken of moving parts of the body, such as the heart, with low pixel resolution. In this section, we will demonstrate the application of our CFD technique for deconvolution of Gamma Camera images obtained during medical examinations.

Shown in Figure 12 is an image of the human heart produced by the staff of the Georgetown University Hospital, Department of Nuclear Medicine, using a Siemens Gamma Camera. This image contains a sequence of 64x64 pixel frames showing the heart at a sequence of time intervals. This plane image, originally recorded in 256 shades of gray scale, is presented here in 64 shades of gray. In Figures 12b, 12c and 12d the deconvoluted image is shown after 6, 12 and 18 processing iterations by our nonlinear technique. We observe in these figures a significant improvement in the image quality over the images in Figure 12a. Some of the diffuse edges in Figure 12a are clearly pronounced in Figures 12c and 12d. We have also applied our CFD technique to the Gamma Camera images of the brain and liver and have found a significant image deconvolution and edge enhancement.

4. CONCLUSIONS

The CFD technique described here for nonlinear signal and image processing is based on numerical techniques developed for Computational Fluid Dynamics, namely, the Second Order Godunov Method. We have demonstrated the application of this numerical method to signal processing, resulting in significant signal deconvolution and edge enhancement effects. Our preliminary analysis has shown that the Second Order Godunov Method, when applied to the gray scale intensity field of an image, is equivalent to an application of an unique filter stack. This filter stack has automatic edge detection, noise reduction and edge enhancement properties. We have demonstrated this nonconventional technique for the system of gas dynamic equations, where the Second Order Godunov Method assures high accuracy resolution of the flow discontinuities that are analogous to the edges in the image field. However, the same methodology can be applied to a reduced set of nonlinear hyperbolic partial differential equations, which will result in a significant optimization of the proposed technique.

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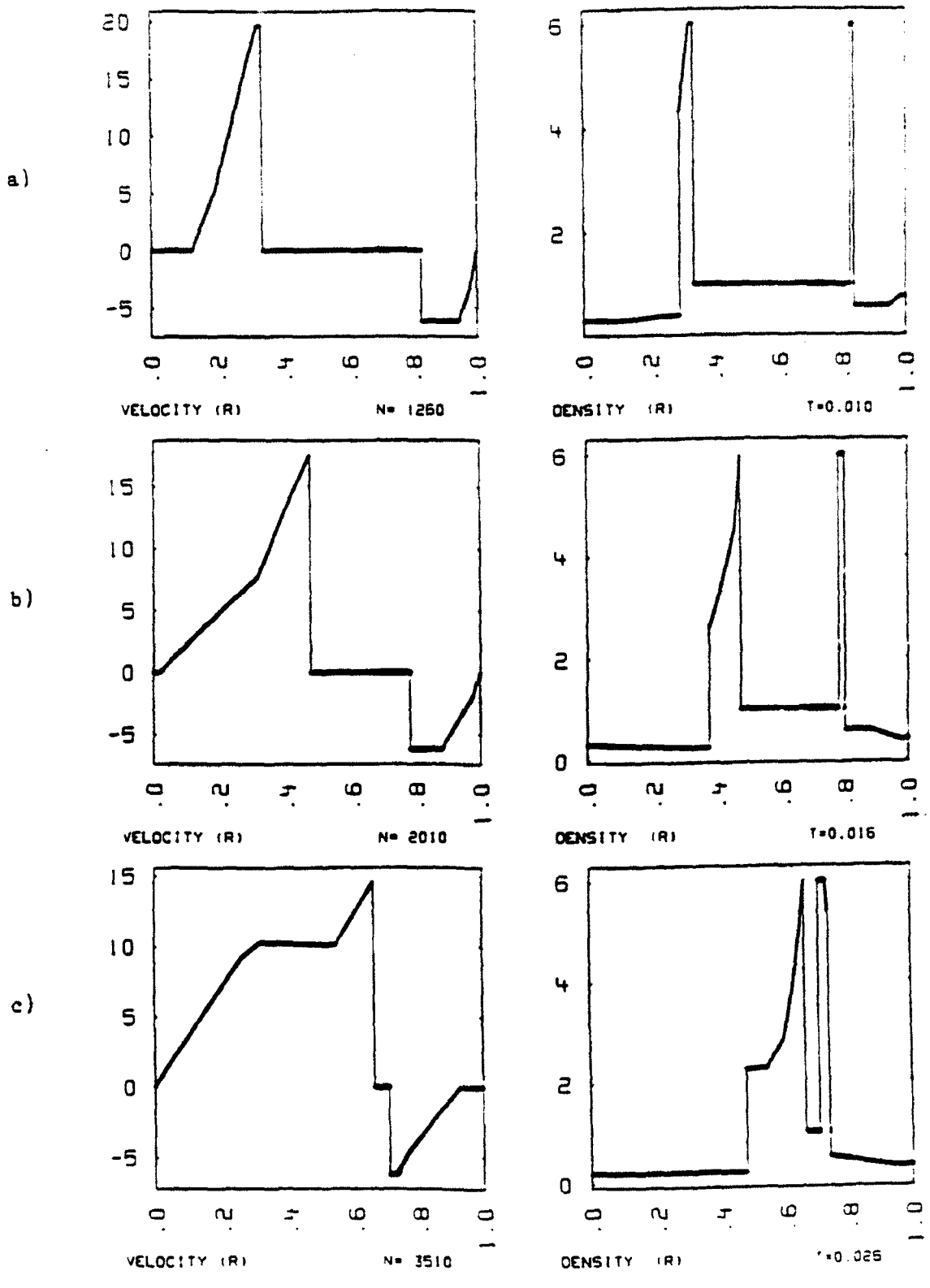


Fig. 1. High resolution of flow discontinuities obtained with the Second Order Godunov Method.

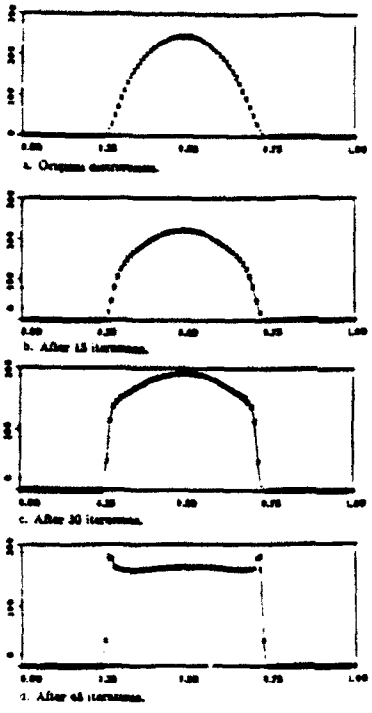


Fig. 2. Edge enhancement for a sinusoidal distribution without noise.

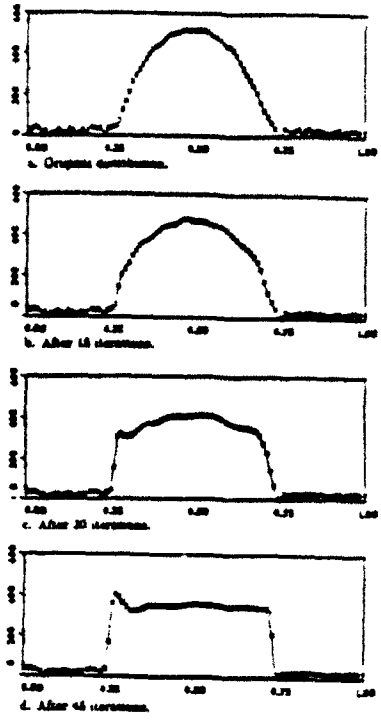


Fig. 3. Edge enhancement for a sinusoidal distribution with 10% intensity random noise.

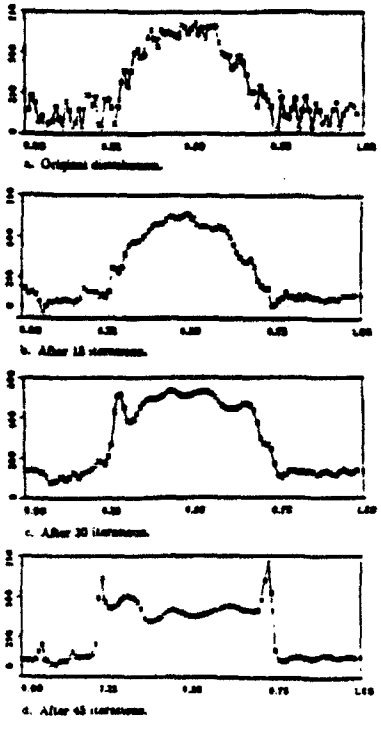


Fig. 4 Edge enhancement for a sinusoidal distribution with 50% intensity random noise.

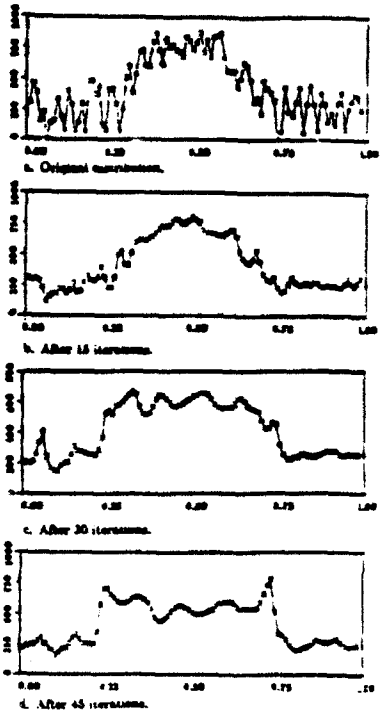


Fig. 5. Edge enhancement for a sinusoidal distribution with 100% intensity random noise.

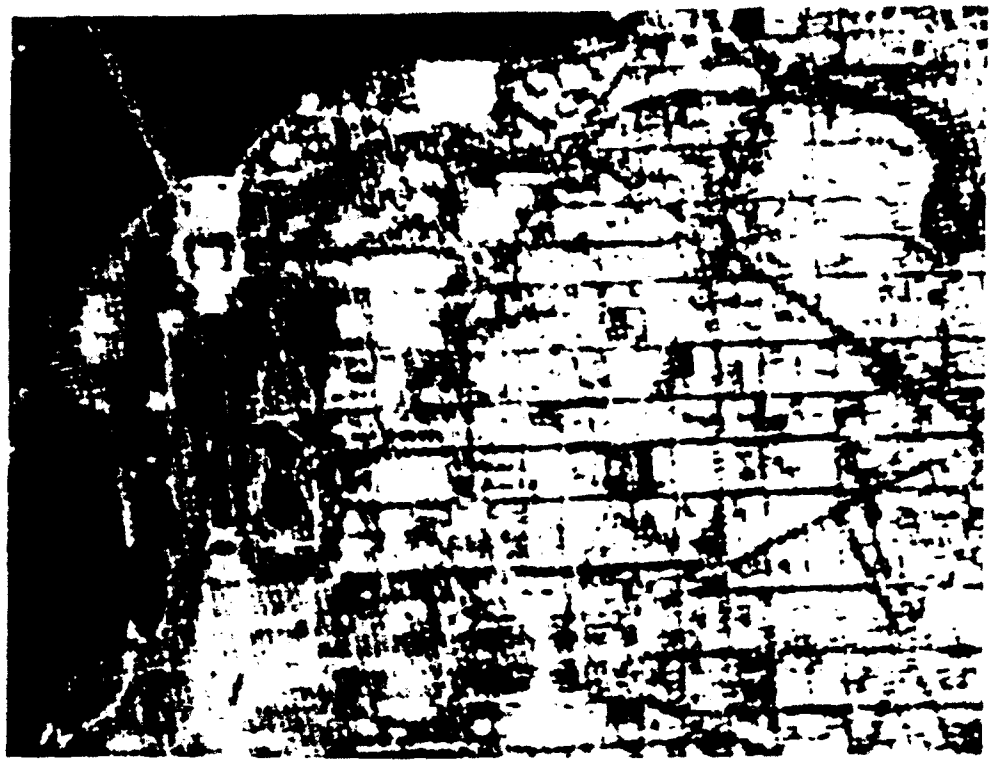


Fig. 6. The original satelite photograph of Washington. DC with resolution reduced to 150 dots/inch.

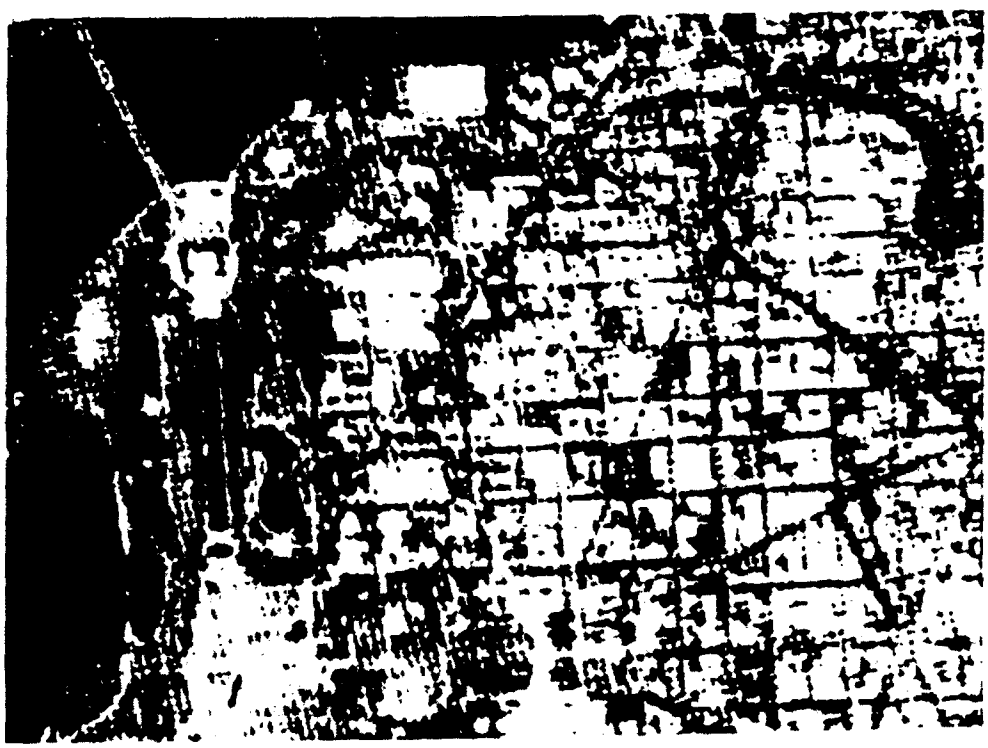


Fig. 7a. The sharpened picture after the Godunov solver has been used. After three iterations. Note the details that appeared on the Potomac. These details are barely visible even on the original high resolution photograph.

Fig. 7b. After six iterations.

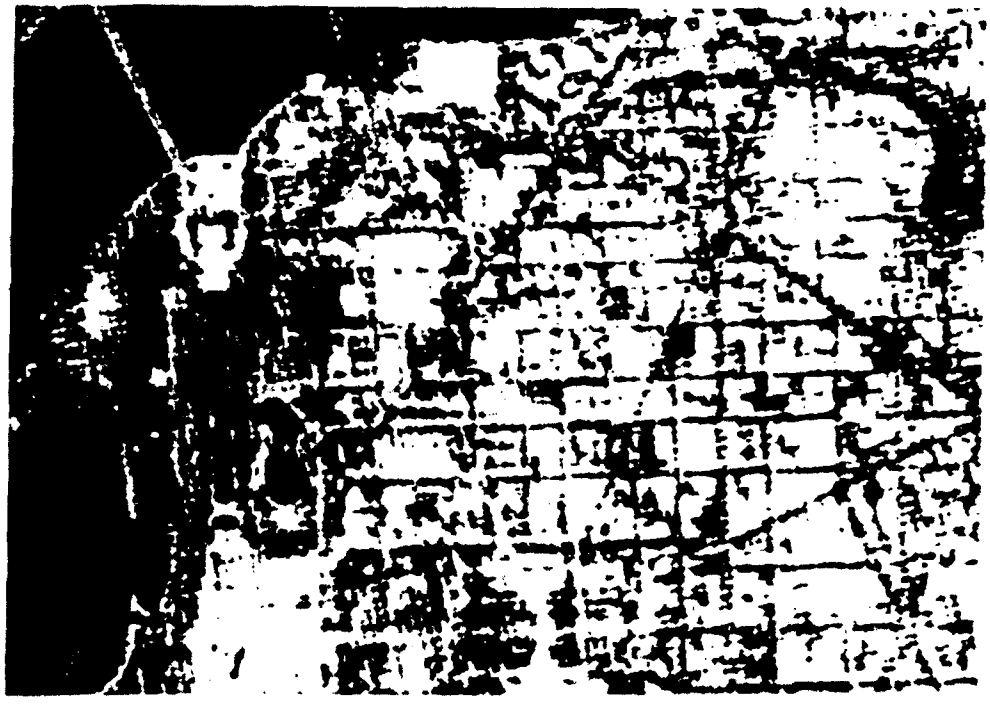


Fig. 7c. After nine iterations.

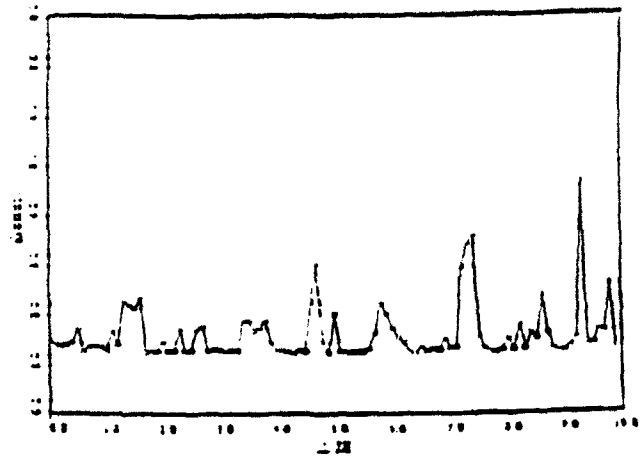


Fig. 8. Gray scale density of a cross section of the original image.

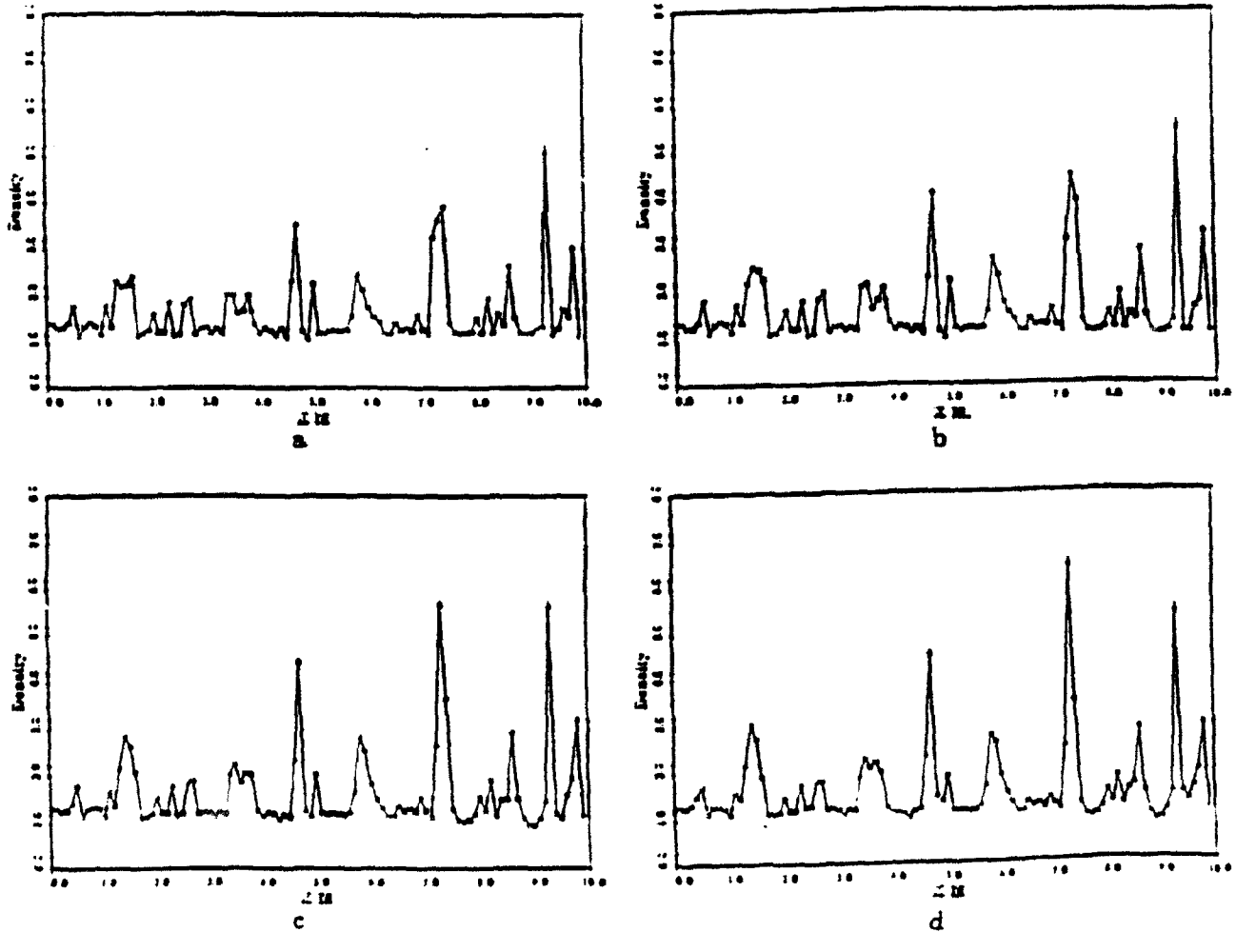


Fig. 9. Gray scale density of the CFD processed image: (a) after 3 iterations; (b) after 6 iterations; (c) after 9 iterations; (d) after 12 iterations.

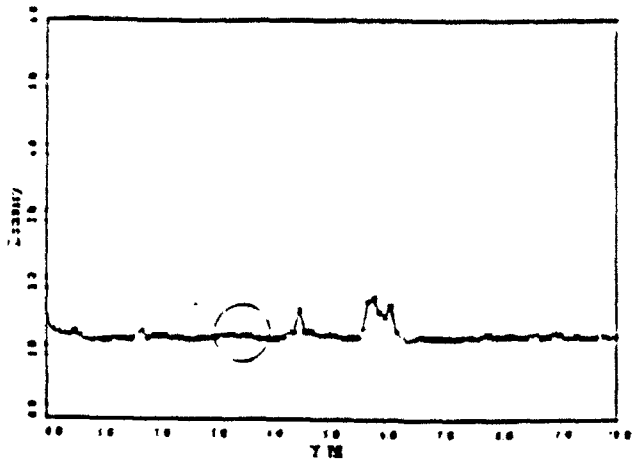


Fig. 10. Gray scale density of a cross section of the original image.

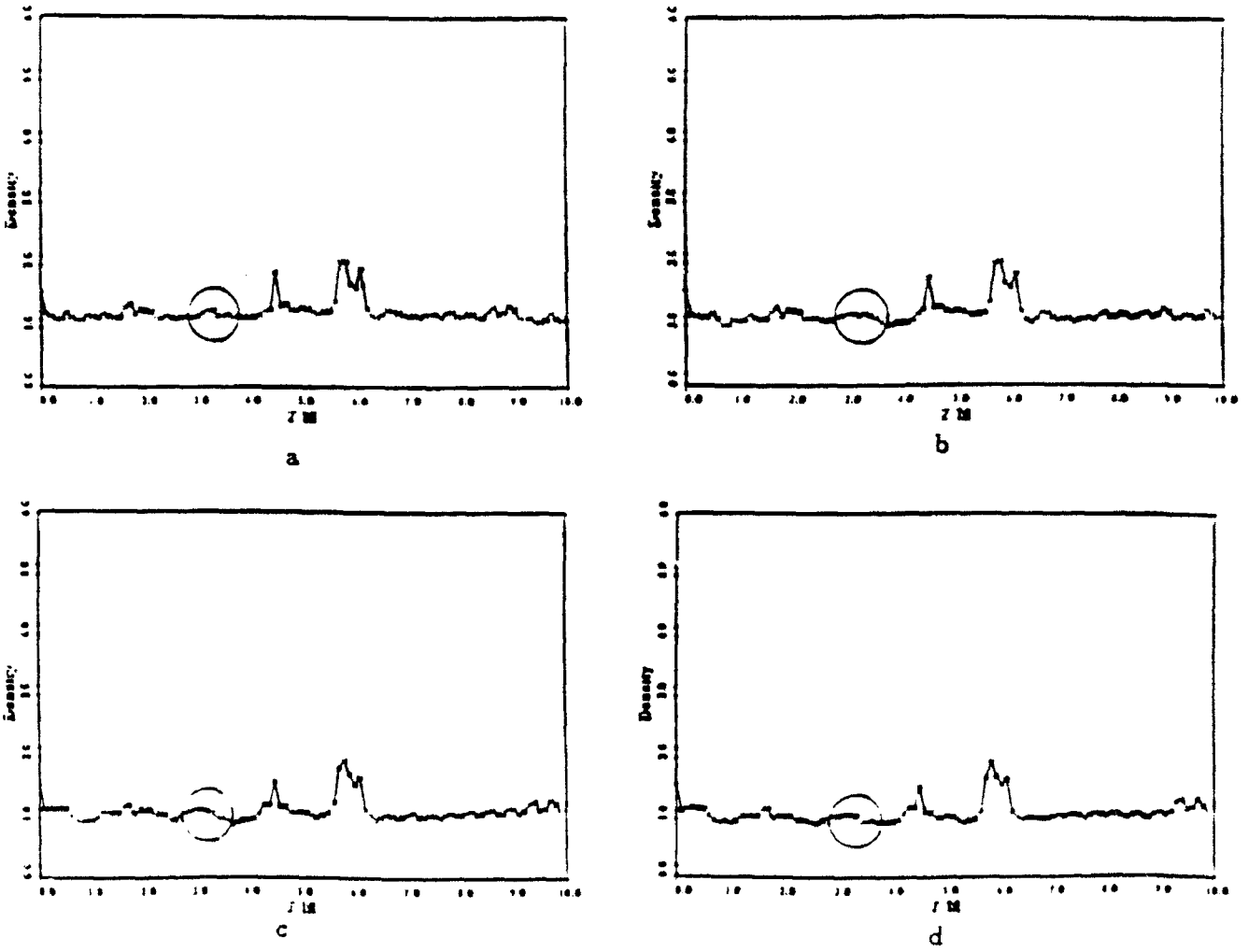
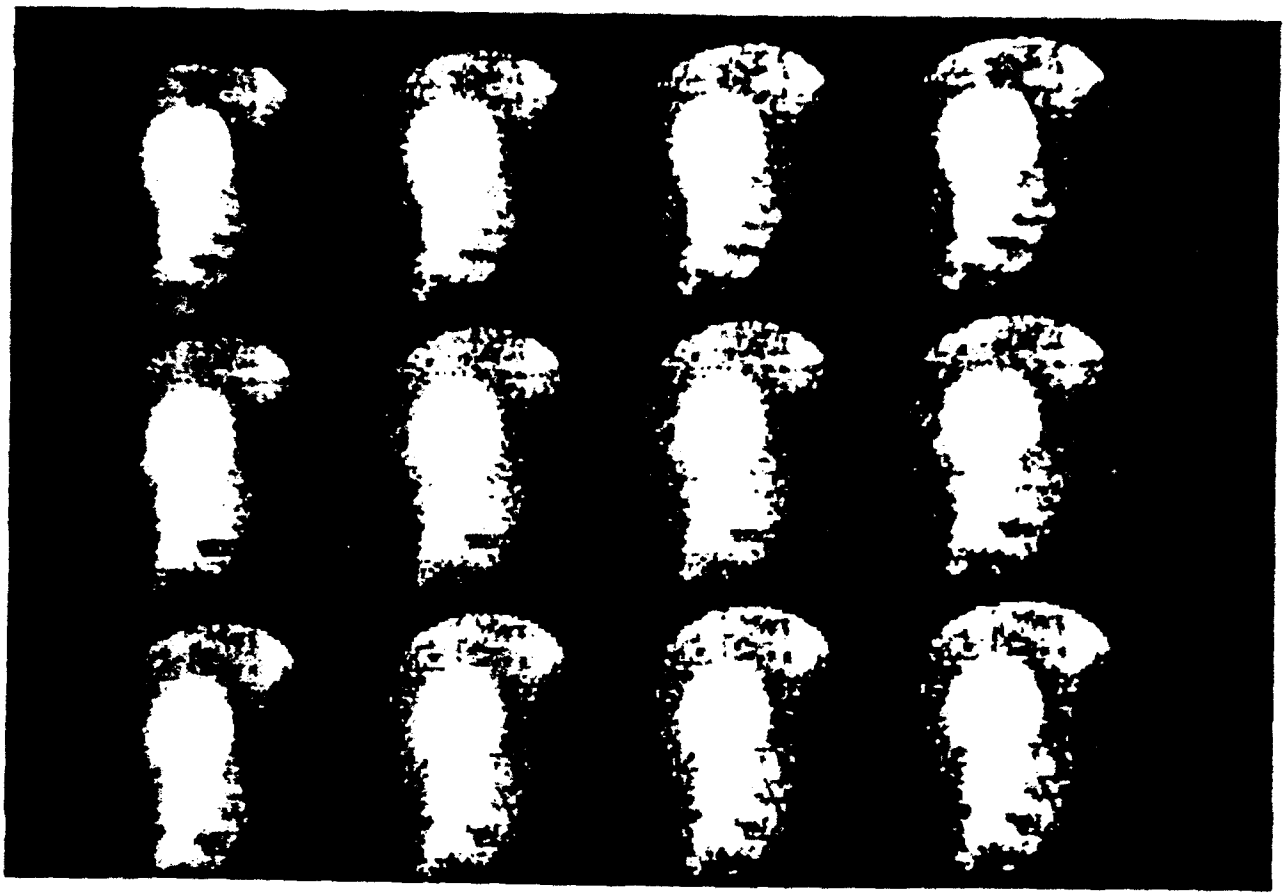


Fig. 11. Gray scale density of the CFD processed image: (a) after 3 iterations; (b) after 6 iterations; (c) after 9 iterations; (d) after 12 iterations.



(a) (b) (c) (d)

Fig.12. Image of human heart taken by a Siemens Gamma Camera. (a) Original image 64x64 pixels per frame; (b) Image after six processing iterations; (c) Image after 12 processing iterations; (d) Image after 18 processing iterations.

Review of Propulsion Applications and Numerical Simulations of the Pulsed Detonation Engine Concept

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Here we review experimental and computational studies of the pulsed detonation engine concept (PDEC) and present results of our recent numerical study of this concept. The PDEC was proposed in the early 1940s for small engine applications; however, its potential was never realized due to a complicated, unsteady operation regime. In this study, we demonstrate the use of current advances in numerical simulation for the analysis of the PDEC. The high-thrust/engine volume ratio obtained in our simulations demonstrates promising potential of the pulsed detonation engine concept.

Introduction

EARLY developments of engine technology leading to practical propulsion engines were almost completely associated with steady-state engine concepts. Unsteady concepts, which initially appeared promising, never evolved from the conceptual state and have remained for the most part unexplored. The early work in unsteady propulsion suffered from a lack of appropriate analytical and design tools, a condition which seriously impeded the advancement of the unsteady concepts to a practical stage.

In this paper, we review the historical development of unsteady propulsion by concentrating on the particular concept of the intermittent detonation engine, and discuss current research activities in this area. A review of the literature[1-24] reveals that a significant body of experimental and theoretical research exists in the area of unsteady propulsion. However, this research has not been extended to the point where a conclusive quantitative comparison can be made between impulsive engine concepts and steady-state concepts. For example, the analysis given in Refs. 8–11 of the performance of a detonation engine concept includes neither frequency dependence nor analysis of losses due to multicycle operation. A new generation of analytical and computational tools exists today and allows us to revisit and analyze such issues with a high degree of confidence. Numerical simulation has developed to the state where it can now provide time-dependent two- and three-dimensional modeling of complex internal flow processes[20,24,25] and will eventually result in tools for systematically analyzing and optimizing engineering design. In addition to a review of applications of the pulsed detonation engine concept (PDEC), we will report results of a numerical study of an air-breathing detonation engine. This study was performed using new unsteady computational fluid dynamics (CFD) tools that we will also describe.

Our paper is structured as follows: 1) historical review of the pulsed detonation development efforts; 2) description of the basic phenomenology of the air-breathing pulsed detonation engine concept; 3) description of the mathematical formulation and new numerical scheme used to simulate the problem; 4) discussion of the simulation results; and 5) conclusions.

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Historical Review

Constant-Volume Combustion

From the very early development of jet-propulsion engines, it was known that an engine based on a constant-volume combustion process achieves higher thermodynamics efficiency than a constant pressure engine. This follows from a thermodynamic analysis of the engine cycle.[1]

Constant-volume combustion was used in gas turbine engines at the beginning of this century, and the first gas turbine engines in commercial use were based on the constant-volume cycle. Jet-propulsion engines were one of the applications of the constant volume cycle (or explosion cycle) which was explored in the late 1940s.[2] Although the explosion cycle operates at a larger pressure variation in the combustion chamber than in a pulse jet,[3,4] the cycle actually realized in these engines was not a fully constant-volume one since the combustion chamber was open-ended.[2] In Ref. 2, the maximum pressure ratio measured in an explosion cycle engine was 3:1, whereas the pressure ratio for the same mixture under the assumption of a constant-volume cycle would be 8:1. Also, this engine was limited by the available frequency of cycles, which in turn was limited by the reaction rate. A simple calculation[2] showed that if the combustion time could be reduced in this engine from 0.006–0.003 s, the thrust per pound of mixture would increase 100%. Thus, the explosion-cycle engine has two main disadvantages:

1) Constrained volume combustion (as distinguished from constant-volume combustion) does not take full advantage of the pressure rise characteristic of the constant-volume combustion process.

2) The frequency of the explosion cycle is limited by the reaction rate, which is only slightly higher than the deflagrative combustion rate.

The main advantage of the constant-pressure cycle is that it leads to engine configurations with the steady-state processes of injection of the fuel and oxidizer, combustion of the mixture, and expansion of the combustion products. These stages can be easily identified and the engine designer can optimize them on the basis of relatively simple steady-state considerations.

At the same time, an engine based on constant-volume combustion will have an intermittent mode of operation, which may complicate its design and optimization. We are interested in the question of whether this complication is worth the potential gains in engine efficiency.

Pulsed Detonation Engine as an Ultimate Constant-Volume Combustion Concept

The detonation process, due to the very high rate of reaction, permits construction of a propulsion engine in which the

constant-volume process can be fully realized. In detonative combustion, the strong shock wave, which is part of the detonation wave, acts like a valve between the detonation products and the fresh charge. The speed of the detonation wave is about two orders of magnitude higher than the speed of a typical deflagration. This allows the design of propulsion engines with a very high power density. Usually, each detonation is initiated separately by a fully controlled ignition device, and the cycle frequency can be changed over a wide range of values. There is only an upper limit for the detonation cycle frequency. This limit is determined by the time it takes to refill the detonation chamber with the fresh combustible mixture. This in turn will depend on chamber geometry and the external flow parameters. In our study, we have established that detonation frequencies of 200–250 Hz appear to be feasible. At the same time, the same PDEC engine can operate at very low detonation frequency with thrust almost linearly proportional to the frequency. This also means that a device based on a detonative combustion cycle can be scaled, and its operating parameters can be modified for a range of required output conditions. There have been numerous attempts to take advantage of detonative combustion for engine applications. In the following, we give a description of the most relevant past experimental and analytical studies of the detonation engine concept.

Hoffmann's Report

The first reported work on intermittent detonation is attributed to Hoffmann[5] in 1940. He operated an intermittent detonation test stand with acetylene-oxygen and benzine-oxygen mixtures. The addition of water vapor was used to prevent the highly sensitive acetylene-oxygen mixture from premature detonation. Hoffmann[5] indicated the importance of the spark plug location in reference to tube length and diffuser length. It was found that a continuous injection of the combustible mixture leads to only a narrow range of ignition frequencies that will produce an intermittent detonation cycle. These frequencies are governed by the time required for the mixture to reach the igniter, the time of transition from deflagration to detonation, and the time of expansion of the detonation products. Hoffmann attempted to find the optimum cycle frequency experimentally. It was discovered that detonation-tube firing occurred at lower frequencies than the spark-plug energizing frequencies, indicating that the injection flow rate and ignition were out of phase. World War II prevented further work by Hoffmann and co-workers.

Nicholls' Experiments

A substantial effort in intermittent detonation engine research was done by a group headed by Nicholls[6-10] of the University of Michigan beginning in the early 1950s. The most relevant work concerns a set of experiments carried out in a 6-ft-long detonation tube.[6] The schematics of the detonation-tube experiments test rig used by Nicholls and co-workers are shown in Fig. 1. The detonation tube was contructed from a 1-in.-i.d. stainless-steel tube. The fuel and oxidizer were injected under pressure from the left end of the tube and ignited at the 10-in. distance downstream. The tube was mounted on a pendulum platform that was suspended by support wires. Thrust for single detonations was measured by detecting tube (platform) movement relative to a stationary pointer. For multicycle detonations, thrust measurement was achieved by mounting the thrust end of the tube to the free end of the cantilever beam. In addition to direct thrust measurements, the temperature on the inner wall of the detonation tube was measured.

Fuel mixtures of hydrogen/oxygen, hydrogen/air, acetylene-oxygen, and acetylene-air were used. The gaseous oxidizer and fuel were continuously injected at the closed end wall of the detonation tube and three fixed flow rates were used. Under these conditions, the only parameters that could be varied were the fuel/oxidizer ratio and frequency of ignition. A maximum gross thrust of ≈ 3.2 lb was measured in hydrogen/air mixture at the frequency of ≈ 30 detonations/s. The most promising results were demonstrated for the hydrogen/air mixture, where a fuel specific impulse of $I_{sp} = 2100$ s was reached. The maximum frequency of detonations obtained in all experiments was 35 Hz. The temperature measurements on the inner wall showed that for the highest frequency of detonations the temperature did not exceed 800°F.

In their later work,[8-10] the University of Michigan group concentrated on development of the rotating detonation wave rocket motor. No further work on the pulsed detonation cycle was pursued.

Krzycki's Experiments

In a setup somewhat similar to Nicholls', Krzycki[11] performed an experimental investigation of intermittent detonations with frequencies up to 60 cps. An attempt was also made to analyze the basic phenomena using unsteady gas dynamic theory. Krzycki's attempt to analyze the basic phenomena relied on wave diagrams to trace characteristics, assumptions of isentropic flow for detonation and expansion, and incompressible flow for mixture injection processes. The most convincing data from the experiments are the measurement of thrust for a range of initiation frequencies and mixture flow rates. Unfortunately, no direct pressure measurement in the device are reported so that only indirect evidence exists of the nature of the process observed.

The basic test stand used by Krzycki is very similar to that used by Nicholls et al.[6] The length of the detonation tube and internal diameter were exactly the same as those in Nicholls' experiments. A propane/air mixture was continuously injected through reversed-flow diffuser for better mixing and

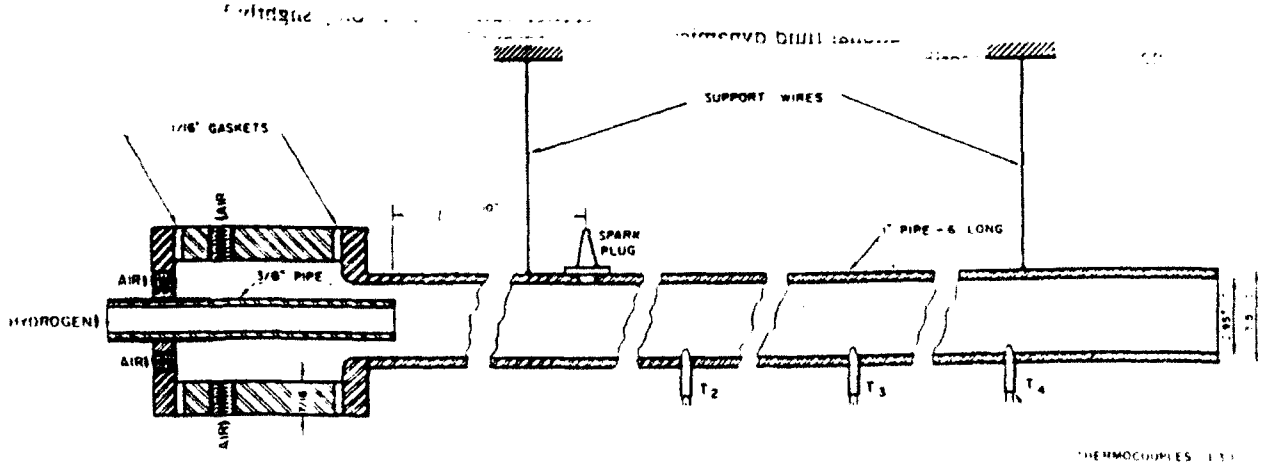


Fig. 1 Detonation tube used in experiments by Nicholls et al.

ignited at the 25-cm distance from the injection point by an automobile spark plug. The spark frequency was varied from 1–60 Hz. The spark plug power output was varied inversely with the initiation frequency and at the frequency of 60 Hz was only 0.65 J. This fact alone eliminated the possibility of direct initiation of the detonation wave by the spark and consequently all of the experiments were performed in the region dominated by transition from deflagration to detonation. According to experimental data and theory,[12] for direct initiation of a mixture of propane/air at the detonability limits, an energy release on the order of 10^6 J is required. Thus, the required deflagration-detonation transition region length would have been prohibitively large for the propane/air mixture. It follows that in all of the experiments a substantial part of the process was deflagrative. This resulted in low efficiency and negligible thrust. Krzycki repeated the experiments of Nicholls using exactly the same size detonation tube and basically the same rates of injection of the detonatable mixture. Krzycki's experimental results are very well-documented, giving enough information to deduce a clear picture of the physical processes occurring in the tube. A conclusion, arrived at by the author, was that thrust was possible from such a device but practical applications did not appear promising. It is unfortunate that, possibly based on Krzycki's extensive but misleading results, all experimental work related to the pulsed detonation engine concept stopped at this time.

Work Reported in Russian Sources on Pulse Detonation Devices

A review of the Russian literature has not uncovered work concerning applications of pulsed detonation devices to propulsion. However, there are numerous reports of applications of such devices for producing nitrogen oxide[13] (an idea proposed in the 1940s by Zeldovich to use detonation for binding nitrogen directly from air to produce fertilizers) and as rock crushing devices.[14]

Korovin et al.[13] provide a most interesting account of the operation of a commercial detonation reactor. The main objective of this study was to examine the efficiency of thermal oxidation of nitrogen in an intermittent detonative process as well as an assessment of such technological issues as the fatigue of the reactor parts exposed to the intermittent detonation waves over a prolonged time. The reactor consisted of a tube with an inner diameter of 16 mm and length 1.3 m joined by a conical diffuser to a second tube with an inner diameter of 70 mm and length 3 m. The entire detonation reactor was submerged in running water. The detonation mixture was introduced at the end wall of the small tube. Methane, oxygen, and nitrogen comprised the mixture composition and the mixture ratios were varied during the continuous operation of the reactor. The detonation wave velocity was measured directly by piezoelectric sensors placed in the small and large tubes. The detonation initiation frequency in the reactor was 2–16 Hz. It is reported that the apparatus operated without significant changes for 2000 h.

Smirnov and Boichenko[14] studied intermittent detonations of a gasoline/air mixtures in a 3-m-long and 22-mm-i.d. tube operating in the 6–8 Hz ignition frequency range. The main motivation of this work was to improve the efficiency of a commercial rock-crushing apparatus based on intermittent detonations of the gasoline/air mixtures.[15] The authors investigated the dependence of the length of the transitional region from deflagration to detonation on the initial temperature of the mixture.

As a result of the information contained in the Soviet reports, it can be concluded that reliable commercial devices based on intermittent detonations can be constructed and operated.

Development of the Blast Propulsion System at JPL

Back,[16] Varsi et al.,[17] Kim et al.,[18] and Back et al.[19] at the Jet Propulsion Laboratory (JPL) studied the feasibility of a rocket thruster powered by intermittent detonations of solid explosive. The main application foreseen by the authors is propulsion in dense or high-pressure atmospheres of certain solar system planets. The JPL work was directed at very specific applications; however, the studies[17-19] addressed some key issues of devices using unsteady processes such as propulsion efficiency. The JPL studies have important implications to pulsed detonation propulsion systems.

Reference 19 gives the basic description of the test stand used. In this work, a data sheet type C explosive was detonated inside a small detonation chamber attached to nozzles of various length and geometry. The nozzles, complete with firing plug, were mounted in a containment vessel that could be pressurized with the mixture of various inert gases from vacuum to 70 atm. The apparatus measured directly the thrust generated by single detonations of a small amount of solid explosive charge expanding into conical or straight nozzles. Thrust and specific impulse were measured by a pendulum balance system.

Results obtained from an extensive experimental study of the explosively driven rocket have led to the following conclusions. First, rockets with long nozzles show increasing specific impulse with increasing ambient pressure in carbon dioxide and nitrogen. Short nozzles, on the other hand, show that specific impulse is independent of ambient pressure. Most importantly, most of the experiments obtained a relatively high specific impulse of 250 s and larger. This result is all the more striking since the detonation of a solid explosive yields a relatively low energy release of approximately 1000 cal/g compared with 3000 cal/g obtained in hydrogen/oxygen combustion. Thus, it can be concluded that the total losses in a thruster based on unsteady expansion are not prohibitive and, in principle, very efficient propulsion systems operating on intermittent detonations are possible.

Detonation Engine Studies at Naval Postgraduate School

A modest exploratory study of a propulsion device utilizing detonation phenomena was conducted at the Naval Postgraduate School (NPS).[20-23] During this study, several fundamentally new elements were introduced to the concept distinguishing the new device from previous ones.

First, it is important to note that the experimental apparatus constructed by Helman et al.[22] showed the first successful self-aspirating, air-breathing detonation device. Intermittent detonation frequencies of 25 Hz were obtained. This frequency was in phase with the fuel-mixture injection through timed fuel-valve opening and spark discharge. The feasibility of intermittent injection was established. Pressure measurements showed conclusively that a detonation process occurred at the frequency chosen for fuel injection. Furthermore, self-aspiration was shown to be effective. Finally, the effectiveness of a primary detonation as a driver for the main detonation was clearly demonstrated. Although the NPS studies were abbreviated, many of the technical issues considered to be essential for efficient intermittent detonation propulsion were addressed with positive results.

Simulations of Pulsed Detonation Engine Cycle at NASA Ames Research Center

Recently Camblier and Adelman[24] carried out numerical simulations of a pulsed detonation engine cycle taking into account finite-rate chemistry. Unfortunately, the simulations were restricted to a quasi-one-dimensional model. The configuration considered had a 6-cm-i.d., 50-cm-long main chamber that was attached to a 43-cm-long diverging nozzle. It was assumed that a stoichiometric mixture of hydrogen/air at 3.0 atm is injected from an inlet on the closed end wall of the detonation chamber. Under these conditions, Camblier and Adelman estimated a large range of possible detonation frequencies of engine operation up to 667 Hz. The origin of this estimate is not clear from their work since, according to their simulations, the detonation, expansion, and fresh charge fill requires 2.5 ms. This value leads to a maximum frequency of

400 Hz. The simulated engine performance yielded a large average thrust of ≈4000 N and an unusually high specific impulse of 6507 s. These simulations were the first to demonstrate the use of modern CFD methods to address the technical issues associated with unsteady pulsed detonation concepts.

In the remaining sections, we discuss a particular propulsion concept based on the results of the experiments of Helman et al.[22] and describe a computational study of its performance characteristics. The unsteady numerical scheme used for the study made use of unique simulation techniques; the key ingredients of these techniques are also described.

Generic Pulsed Detonation Engine

The generic device we consider here is a small cylindrical engine, 15 cm long and 15 cm in diameter. The combustible gas mixture is injected at the closed end of the detonation chamber and a detonation wave propagates through the mixture. The size of the engine suggests a small payload, but the concept can be extended to larger payloads simply by scaling up the size of the detonation chamber and possibly combining a number of engines into one large propulsion engine. A key issue in the pulsed detonation engine concept is the design of the main detonation chamber. The detonation chamber geometry determines the propulsion efficiency and the duration of the cycle (frequency of detonations). Since the fresh charge for the generic engine is supplied from the external flowfield, the efficiency of the engine depends on the interaction of the surrounding flow with the internal flow dynamics. The range of the physical processes requiring simulation in order to model the complex flow phenomena associated with the detonation engine performance is very broad. A partial list is as follows:

1) Initiation and propagation of the detonation wave inside the chamber.

2) Expansion of the detonation products from the chamber into the airstream around the chamber at flight Mach numbers.

3) Reverse flow from the surrounding air into chamber resulting from overexpansion of the detonation products.

4) Pressure buildup in the chamber due to reverse flow. The flow pattern inside the chamber during postexhaust pressure buildup determines the strategy for mixing the next detonation charge.

5) Strong mutual interaction between the flow processes inside the chamber and flow around the engine.

All of these processes are interdependent and their timing is crucial to the engine efficiency. Thus, unlike simulations of steady-state engines, the phenomena described above cannot be evaluated independently.

The need to resolve the flow inside the chamber accounting for nozzles, air inlets, etc., and at the same time resolve the flow around the engine, where the flow regime varies from high subsonic, locally transonic, and supersonic, makes it a challenging computational problem.

The main issue is to determine the timing of the air intake for the fresh gas charge. It is sufficient to assume inviscid flow for the purpose of simulating the expansion of the detonation products and fresh gas intake. In the following, we present the first results of an inviscid simulation of the detonation cycle in a cylindrical chamber. First, we describe our computational method for solving the time-dependent Euler equations used in the study.

Unsteady Euler Solver

A new second-order algorithm for solving the Euler equations on an unstructured grid was used in our study of the detonation concept. The approach is based on first- and second-order Godunov methods. The method leads to an extremely efficient and fast flow solver that is fully vectorized and easily lends itself to parallelization. The low memory requirements and speed of the method are due to the use of a unique data structure.

Until recently most CFD simulations were carried out with logically structured grids. Vectorization and/or parallelization did not present a problem. The increased need for simulation of flow phenomena in the vicinity of complex geometrical bodies and surfaces has led to the development of CFD codes for logically unstructured grids. The most successful of these unstructured grid codes are based on finite elements or finite volume methods. For an unstructured grid in two dimensions, the computational domain is usually covered by triangles, and the indices of the arrays containing the values of the hydrodynamic flow quantities are not related directly to the actual geometric location of a node. The calculations performed on unstructured grids evolve around the elemental grid shape (e.g., the triangle for two-dimensional problems), and there is no obvious pattern to the order in which the local integrations should be performed. Explicit integration of hydrodynamic problems on an unstructured grid requires that a logical substructure should be created which identifies the locations in the global arrays of all of the local quantities necessary for the integration of one element. This usually results in a large price in computational efficiency, in memory requirements, and in code complexity. As a consequence, vectorization for the conventional unstructured grid methods has concentrated on rearrangement of the data structure in a manner such that these locally centered data structures appear as global arrays. This can be done to some extent using machine dependent gather-scatter operations.[25,26] Additional opumization can be achieved using localization and search algorithms. However, these methods are complex and result in marginal improvement. Most optimized unstructured codes to date run considerably slower and require an order of magnitude more memory per grid cell than their structured counterparts. Parallelization of the conventional unstructured codes is even more difficult, and there is very little experience with unstructured codes on massively parallel computers.

The method we have developed overcomes these difficulties and results in codes with speed and memory requirements comparable to those found in structured grid codes. Moreover, the ability to construct grids with arbitrary resolution leads to a flexibility in dealing with complex geometries not attainable with structured grids. The essence of the method is based on an independent flux calculation across the edges of a dual baricentric grid, followed by node integration. This approach is order independent. Below we give the essential details of our algorithm; a complete description follows later.

Basic Integration Algorithm

We begin by describing the first-order Godunov method for the system of two-dimensional (axisymmetric) Euler equations written in conservation law form as

$$\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial r} = -\frac{1}{r} C \tag{1}$$

where

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{bmatrix}, \quad F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (e + p)u \end{bmatrix}$$

$$G = \begin{bmatrix} \rho v \\ \rho vu \\ \rho v^2 + p \\ (e + p)v \end{bmatrix}, \quad C = \begin{bmatrix} \rho v \\ \rho vu \\ \rho v^2 \\ (e + p)v \end{bmatrix}$$

Here u and v are the x and r velocity vector components, p the pressure, ρ the density, and e the total energy of the fluid per unit volume. It is assumed that a mixed (initial conditions, boundary conditions) problem is properly posed for the set,

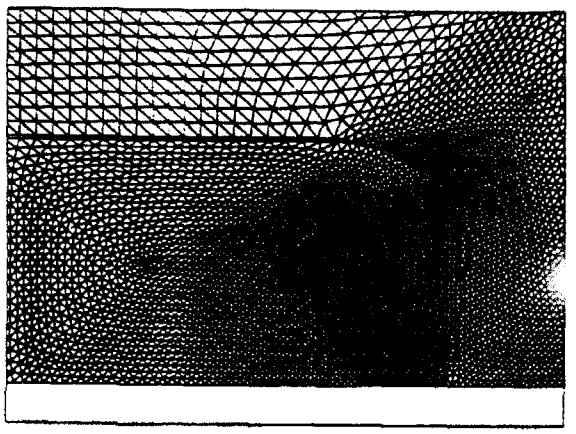


Fig. 2a Computational domain and grid used in simulation of PDEC operation.

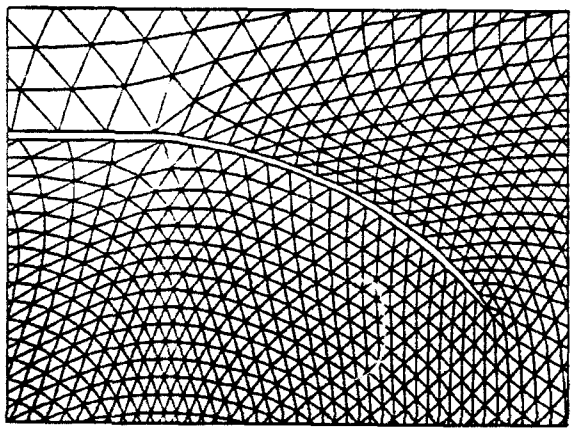


Fig. 2b Enlargement of computational grid in the vicinity of the PDEC nozzle.

Eq. (1), and that an initial distribution of the fluid parameters is given at $t = 0$ and some boundary conditions defining a unique solution are specified on the boundary of the computational domain.

We look for a solution of the system of equations represented by Eq. (2) in the computational domain covered by an unstructured grid. As an example, Fig. 2a shows the unstructured triangular grid used in the pulsed detonation engine simulation. Here most of the computational effort is committed to the resolution of the flow inside the engine detonation chamber and in the immediate vicinity of the nozzle. In Fig. 2b, an enlargement of the nozzle region is shown, illustrating the ability to represent geometry of arbitrary complexity and with localized resolution.

Figure 3 displays a fragment of the computational domain with the corresponding dual grid. The secondary or dual grid is formed by connecting the baricenters of the primary mesh, thus forming finite polygons around the primary vertices.

We have found, as have others,[27] that the best practical representation of the integration volume is obtained when the dual grid is formed by connecting baricenters of the triangles. Integration by the Godunov method[28] can be divided into two basic steps: 1) calculation of the fluxes at the edges of the secondary grid using solutions of a set of one-dimensional Riemann problems; and 2) integration of the system of partial differential equations, which amounts to addition of all of the fluxes for every polygon at a particular time step.

To define the fluxes for the grid shown in Fig. 3 at every edge of the main grid, it is necessary to solve the corresponding Riemann problem. For example, to define the flux at the edge *ab*, we solve the Riemann problem between points *A* and *B*. The solution of this problem is in coordinates local to the

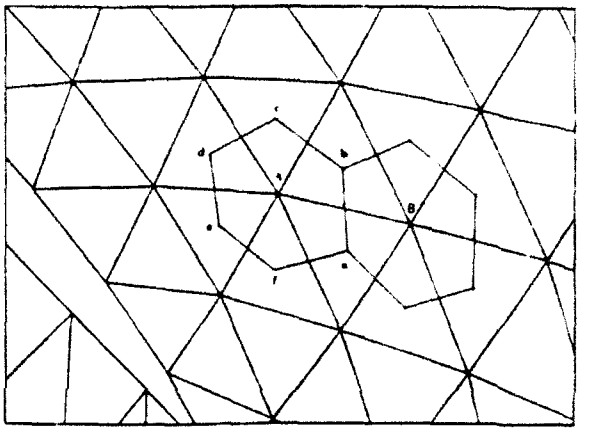


Fig. 3 The primary (triangles) and secondary (polygons) unstructured grids.

edge of the dual grid *ab* so that the tangential component of velocity will be directed along this edge (*ab*). Implementation of our approach requires maintaining strict consistency when defining the "left" and "right" states for the Riemann problems at the edges *ab*, *bc*, *cd*, *de*, *ef*, and *fa*. For this reason, we define not only the location of the vertices and lengths of the edges but also the direction of the edges with respect to the primary grid. For the clockwise integration pattern in the same polygon, point *A* will be the "right" state for all of the Riemann problems related to this point, and the neighbor will represent the "left" side of the diaphragm.

It is easy to see that the flux calculation is based on information at only two nodes and requires single geometrical parameters defining the edge of the secondary grid that dissects the line connecting the two points. Thus, we can calculate all of the values needed for flux calculation in one loop over all edges of the primary grid without any details related to the geometrical structures that these edges form. This in turn assures parallelization or vectorization of the algorithm for the bulk of the calculations involving the Riemann solver that provides the first-order flux. The only procedure not readily parallelizable is the integration of the fluxes for the flow variables at the vertices of the grid. Here we use the "edge coloring" technique that allows us to split the flux addition loop into seven or eight loops for edges of different color. Each of these loops is usually large enough not to impair vectorization. At this stage, all of the fluxes are added with their correct sign corresponding to the chosen direction of integration within the cell. The amount of calculation required here is minimal since the fluxes are known and need only to be multiplied at each time step by a simple factor and added to the vertex quantity.

Second-Order Integration Algorithm

The second-order solver is constructed along lines similar to that of the first-order method. At each cell edge, the Riemann problem is solved for some specified pair of left and right conditions. The solution to this Riemann problem is then used in the calculation of fluxes that are added later to advance to the next integration step. The extension to second-order is achieved by using extrapolation in space and time to obtain time-centered left and right-limiting values as inputs for the Riemann problem. The basic implementation of the method of calculation of second-order accurate fluxes is fundamentally the same as for one-dimensional cases. The only difference is in the method of obtaining linear extrapolation of the flow variables as a first guess of their value at the edges of the dual grid. To obtain the first guess, we need to know the gradient of some gasdynamical parameter U at the vertices of the primary mesh. The value of ∇U can be evaluated by using

a linear path integral along the edges, which delineates the finite volume associated with the vertex. For vertex A in Fig. 3,

$$\int_A \nabla U \mathrm{d}A = \oint_l U n \, \mathrm{d}l \tag{2}$$

where integration along the path l in this case is equivalent to integration along the edges *ab, bc, cd, de, ef,* and *fa*. Knowing the gradient of the gasdynamic parameter in the volume related to vertex A will allow us to extrapolate the values of this parameter at any location within the volume. This permits us to evaluate the first guess for U at the edges of the dual grid. The final implementation of the second-order algorithm has been described previously.

A schematic flowchart of the basic steps of the second-order algorithm implementation is shown in Fig. 4.

Simulations of the Generic Pulsed Detonation Engine

In this section, we present sample results of simulations of the generic PDE device using the numerical code described in the preceding section. In Fig. 2a, the computational domain containing the PDE main detonation chamber is shown covered with the unstructured grid. In our sample simulation, we have chosen a small ≈ 15-cm-long and ≈ 15-cm-i.d. cylindrical chamber with a small converging nozzle. This geometry is one of a number of the geometries we have analyzed in a parametric study whose goal was to evaluate and optimize a typical PDEC device. The device shown in Fig. 1a does not represent the optimum and is given here to illustrate our methodology. We consider a situation when the PDEC serves as a main thruster for a vehicle traveling in air with the velocity of $M = 0.9$ and located at the aft end of the vehicle. The main objectives of the simulations presented here are as follows:

1) To find the maximum cycle frequency. This is determined by the time required from detonation, exhaust of combustion products, and intake of fresh charge for the next detonation.

2) To calculate the thrust produced during each cycle and the integrated thrust as a function of time.

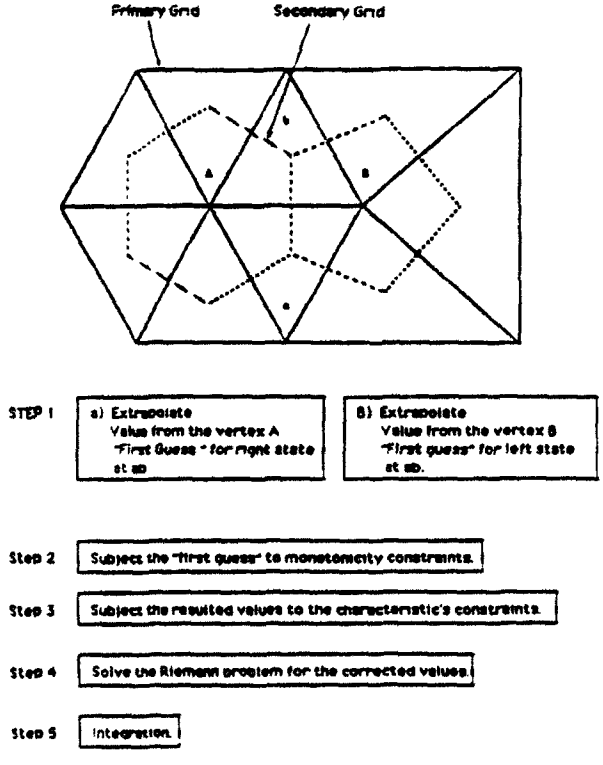


Fig. 4 Grid schematic and outline of steps for second-order Godunov method.

The simulation begins at $t = 0$ when we assume an ideal detonation process has taken place in a stochiometric propane/air mixture. Initially the detonation wave has traveled from the open aft end of the chamber toward the interior with a maximum velocity of 1800 m/s and maximum pressure of 20×10^5 Pa. The distribution of pressure, velocity, and density of the detonation wave is defined through the self-similar solution for a planar detonation wave. These distributions are shown schematically in Fig. 5. The wave was directed toward the interior of the chamber to capture the kinetic energy of the wave and to prolong exposure of the inner chamber walls to the high pressure. In Fig. 6, simulation results are shown at time $t = 0.19$ ms in the form of pressure contours and particle paths from different locations inside and outside the detonation chamber. From the pressure contour plots, we observe that the shock reflection from the inner wall has taken place and detonation products are expanding into the ambient airstream. The flow inside the chamber is choked due to the converging nozzle and the maximum pressure behind the shock is ≈ 8 atm. The pressure inside the chamber is less than 3 atm. The strong expansion of the detonation products into the ambient airstream produces a shock wave with a spherical-like front rapidly decaying in strength. As a result of the interaction of the expanding detonation products with the external flow, a large toroidal vortex is created. The vortex is carried away quickly from the chamber by the external flow and by its own flow momentum.

In Fig. 6a, we also show trajectories of the particles introduced inside the chamber and just above the nozzle. Examination of these trajectories allows us to follow the dynamics of the chamber evacuation and refill. In order to track the detonation products, we initially place marker particles inside the chamber at three cross sections in clusters of four distributed normally to the detonation chamber axis. Each particle has a *different* color; however, particles in the same cluster have the same shade of color. At the three chosen cross sections, we have designated shades of red, yellow, and green for the particles located correspondingly at the left end, center, and beginning of the nozzle cross sections of the chamber. The movement of these particles is shown by connecting them with a continuous line beginning with particle location at $t = 0$ to the present time. In Fig. 6a, we observe that at time $t = 0.19$ ms all particles originally in the nozzle cross section and three of the particles originally in the midsection have left the detonation chamber. However, particles originally introduced on the inner wall of the chamber have only advanced to the nozzle region.

We use a different technique for observing the motion of the ambient gas outside the chamber. Here a cluster of seven

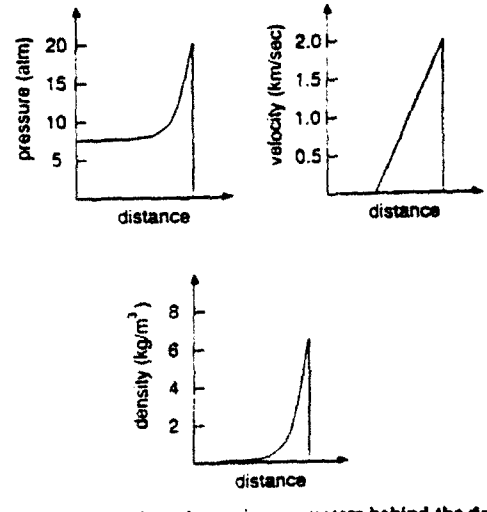
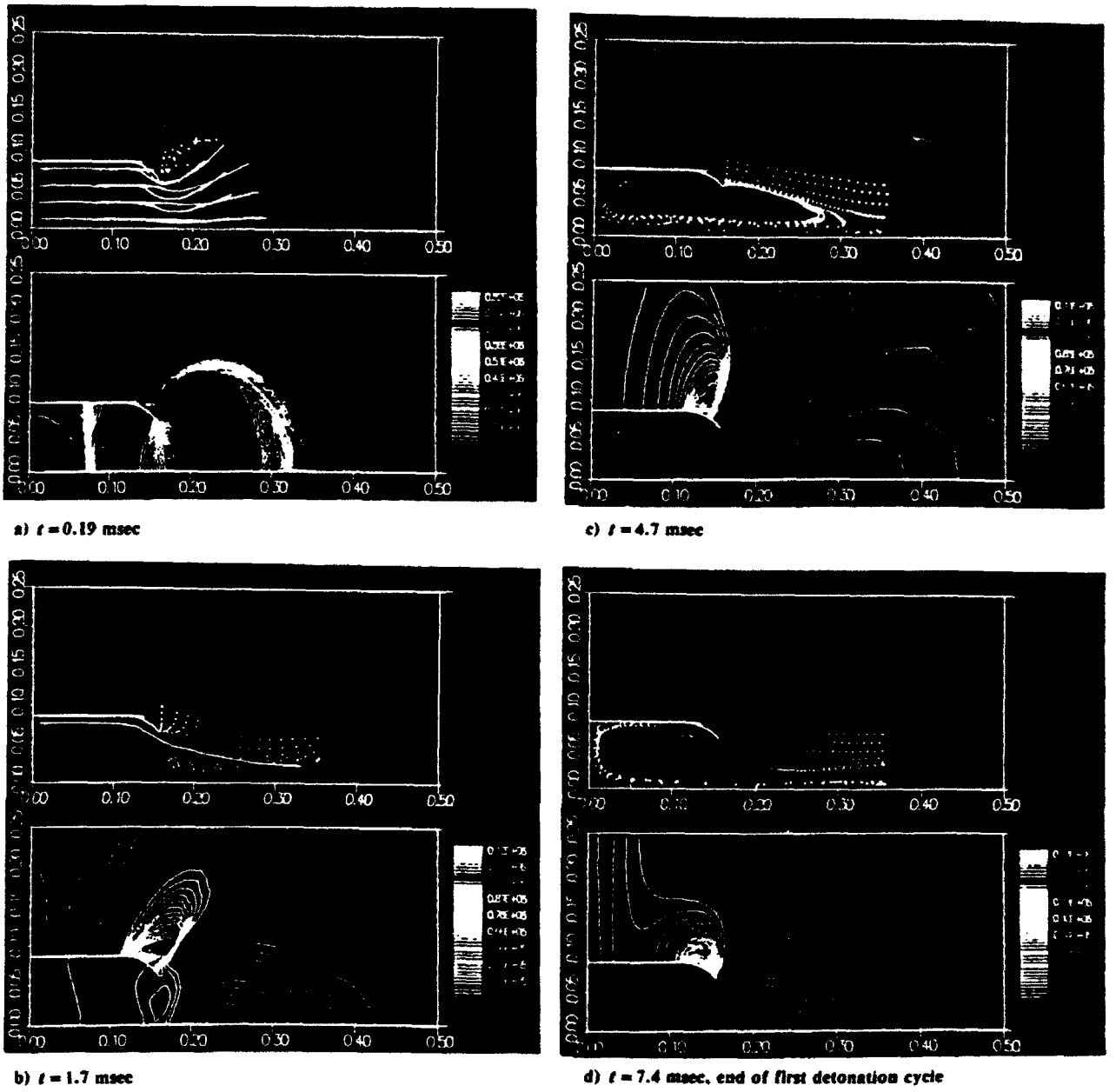


Fig. 5 Distribution of gasdynamic parameters behind the detonation wave according to a one-dimensional self-similar solution.



a) $t = 0.19$ msec

c) $t = 4.7$ msec

b) $t = 1.7$ msec

d) $t = 7.4$ msec, end of first detonation cycle

Fig. 6 Pressure contours and particle paths for various times during the PDEC simulation.

particles is introduced every 0.05 μs in the external flow above the nozzle. All such particles are traced as they move with the flow until they leave the computational domain. At any given time only the current location of the particle is displayed, and since the particles are introduced periodically with time there are a large number of particles to trace. We assign a color to every cluster of external particles to keep track of the time when they were introduced in the calculation. The colors vary from magenta, for those particles introduced early in calculation, to blue, for those introduced shortly before the end of a detonation cycle. In Fig. 6a, corresponding to very early times, only one cluster of external particles is visible. This cluster was introduced at $t = 0$ and is tracking the expanding flow of the detonation products.

In Fig. 6b, the simulation results are shown for $t = 1.7$ ms. The pressure contours show that a shock wave develops at the external edge of the nozzle as a result of a strong expansion of the Mach 0.9 external flow. As a result of overexpansion of the detonation products, the pressure inside the detonation chamber is lower than the ambient pressure, causing the shock to be located lower on the external surface of the nozzle. The external flow about the chamber has a stagnation point on the axis of symmetry downstream at ≈ 25 cm. At this time, it is evident from the particles' trajectories that most of the detonation products have left the chamber. Figure 6b shows one continuous trace of the particles originating at the back wall of the detonation chamber having advanced well ahead of the stagnation point in the external flow.

The marker particles released outside and just above the nozzle's exit show two distinct flow paths. One path takes the flow past the stagnation point to the right of the detonation chamber; this flow path is marked by the four upper particle traces. Another flow path is marked by three lower particle paths released close to the nozzle surface and is deflected toward the detonation chamber exit. Figure 5b shows particles marking this deflected stream approaching the detonation chamber nozzle. The magenta color of these particles indicates they were released at ≈ 0.5 ms.

Figure 6c corresponds to the simulation time $t = 4.7$ ms. The pressure inside the chamber has risen ≈ 1 atm. Higher

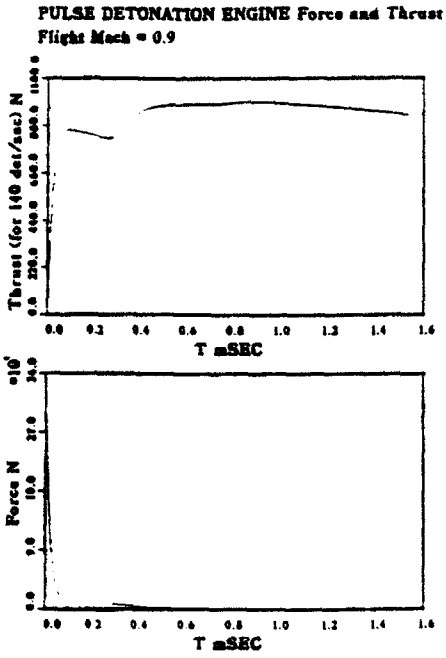


Fig. 7 Thrust and force generated by PDEC as a function of time.

pressure at the chamber exit has resulted in the shock standing on the external surface of the nozzle to move upward. The particles marking the movement of fresh air into the chamber show these to be well inside with some reflecting from the end wall giving a second stagnation point for the reversed fresh airflow.

Figure 6d corresponds to the end of the first cycle when the detonation chamber is filled with fresh charge and ready for the next detonation. In this figure, the particles' paths indicate that the chamber refills in a pattern suitable for fast mixing of the fuel-air mixture. We conjecture then that fuel injection along the chamber axis will promote fast fuel-air mixing. We can see in Fig. 6d that further injection of external air inside the chamber stopped, and from that point on the mixture composition in the chamber will be fixed.

In Fig. 7, the total force and time-averaged thrust generated by the device in the simulations discussed previously are shown as a function of time. The time-averaged thrust is based on the total time for one cycle. As seen in Fig. 7, initially a very large force of $\approx 1.5 \times 10^5$ kg is felt on the end wall of the detonation chamber. This is a result of the inwardly moving detonation wave used in our simulation. Very early during the sequence, this wave reflects from the left wall of the detonation chamber briefly generating a large force. This force rapidly decays and at $t \approx 0.1$ ms changes sign due to interaction of the strong shock wave with the converging nozzle. This effect is noticeable in the thrust data; the average thrust decreases somewhat after reaching levels of ≈ 1980 N. The shock partially reflects from the converging nozzle walls and generates a wave moving to the left wall. The reflected wave thereafter generates positive thrust from $t \approx 0.3$ ms. Finally, thrust levels reach the maximum of ≈ 2200 N and then decay slowly as a result of the cross-sectional drag force. The simulations predict that to sustain this level of thrust will require a detonation frequency of about 150 Hz. All simulations were performed on a Stellar workstation.

Conclusions

The main intent of the present study was to carry out a review of the relevant literature in the area of detonation propulsion, to assess the state of the art, and to recommend future research based on our findings. We have reviewed the literature and presented our summary in the first section of this paper. Our initial conclusion from the review is that there is a substantial body of evidence leading toward the possibility of producing propulsion engines with significant thrust levels based on an intermittent detonation.

Most of the historical attempts at producing thrust based on the intermittent detonation cycle were carried out with the same basic experimental setup; namely, a long straight detonation tube employing forced fuel injection at the closed tube end. We have discussed the many reasons why such a device cannot take proper advantage of the physical processes associated with detonation.

The experiments performed at the Naval Postgraduate School using a self-aspirating mode of operation for a pulsed detonation thruster produced very useful results which, upon further examination, provide us with a route toward practical propulsion engines of variable thrust levels that are both controllable and scalable.

We have explored some of the implications of the possible applications of the self-aspirating detonation engine concept and have developed a suitable numerical simulation code to be used as a design, analysis, and evaluation tool. In fact, the preliminary analysis of a candidate detonation chamber flow was shown to be dominated completely by unsteady gasdynamics. An attempt to understand the flow properties based on any steady-state model or one-dimensional unsteady analytical model will miss such important aspects as fuel-air mixing and shock reflection from internal geometrical obstacle such as the converging nozzle. The unsteady simulation code developed during the course of our study is a necessary tool that we plan to use in a study leading to a feasible prototype engine design realizing the full potential of the intermittent detonation process.

Acknowledgments

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Numerical and analytical study of transverse supersonic flow over a flat cone

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Abstract. Quasisteady supersonic flow over a flat cone on a plane surface is studied. A formula is derived for the angle through which the flow lines turn at the cone. The results are used to justify the use of two-dimensional simulations of the flow. Peak pressures and total impulses are obtained numerically for various cone angles.

Key words: Cone, Euler equation, Mach reflection, CFD, Supersonic flow

1. Introduction

The purpose of this study is to determine the maximum pressure on the surface of a flat cone (one for which the height is much less than the diameter) in the quasi-uniform flow behind a strong blast wave propagating at right angles to the axis of the cone. If the cone is small compared with the radius of the blast wave, the undisturbed flow is approximately rectilinear. First, the blast wave passes over the cone and an unsteady load builds up on the surface. In general the shock will undergo Mach reflection over at least part of the surface of the cone, the extent depending on the cone angle α, the adiabatic index γ, and the Mach number M. After a short transitional stage the cone will then be subject to the quasisteady supersonic flow field behind the blast front. (For a strong blast wave in air, the pressure drops to one-half the peak value about one-tenth of the way back from the front toward the origin of the blast (Sedov 1959). Thus, if the blast center is located $\sim$ 100 radii from the cone, the pressure arriving at the cone is reduced to half its initial value $\sim$ 10 radii behind the front.) The post-shock flow velocity varies on the same scale. We would like to find whether the pressure on the cone reaches its maximum during the quasisteady or the unsteady regime of the flow and determine its magnitude.

The cone, shown schematically in Fig. 1, is located on a plane surface. We take its axis to be normal to the surface, and we model the front of the spherical blast wave as a planar shock wave propagating normally to this axis. This is a reasonable approximation when the distance to the blast center is much larger than the radius, i.e., in the same limit for which we can assume that the state behind the front is uniform. The flow over the cone is substantially three-dimensional. The only symmetry is with respect to inversion about the midplane (the plane through the cone axis and parallel to the flow). In the general case in which the cone axis is not normal to the plane, the problem is totally asymmetrical.

Previous studies of the effect of supersonic flows on conical bodies have focused primarily on situations in which the flow is parallel or nearly parallel to the axis of the cone. Those results are applicable to, e.g., the aerodynamical effects associated with the nose cones of re-entry vehicles. In contrast, the problem we are considering may be regarded as an idealized model of the interaction between a blast wave and a ground or shipboard structure. It can also model the flow over a bump or a housing on the skin of a supersonic aircraft or missile. The results may thus be relevant to both damage studies and flight characteristics.

A number of experimental studies related to the problem of oblique supersonic flow over a cone have been carried out, beginning at least three decades ago (Tracy 1963; Damkevala and Zumwalt 1968). Most of this work has dealt with small deviations from axisymmetry, although angles of attack as large as 30° have been studied (Yahalom 1971). Less experimental effort seems to have been devoted to transverse flows (angle of attack equal to 90°). Likewise, theoretical studies by Goman and Davydov (1975) and Gusarov et al. (1979) have concentrated on small deviations from conical shapes in axisymmetric flow. Numerical simulations have been car-

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ried out at large angles of attack (30°–50°) by Fletcher and Holt (1976). These results are useful, and the same techniques can be applied to transverse flows, but they have definite limitations. At the Mach numbers investigated ($M \lesssim 6$–8) the flow is strongly conditioned by the presence of a viscous boundary layer. This necessitates solution of the Navier-Stokes equations instead of the Euler equations, and it may be necessary to incorporate a turbulence model as well. In three dimensions it is difficult to obtain good resolution even for inviscid flow; the presence of a thin boundary layer makes the problem even more formidable.

In the next section we determine the streamlines associated with transverse flow over a cone in the Newtonian approximation, i.e., assuming that the streamlines follow the contours of the body surface. We show that for a flat cone the streamlines deviate very little from the vertical plane in which they were propagating before reaching the cone. We use this result to argue that the flow over the cone can be accurately modeled by treating each cross section made by a vertical plane separately, i.e., by solving a series of two-dimensional problems. In the section following that, we describe the results of such calculations. For this purpose we use an Euler code, which is only valid at low flow Mach numbers ($M \lesssim 5$). In our calculations the shock Mach number equals 25, but the Mach number of the flow in the heated region behind the shock is ~ 3, so we are justified in ignoring viscous effects. At higher values of M our results are at least indicative and can be expected to yield accurate values of the peak pressures on the cone. (Of course the reduction of the problem to two dimensions is a consequence of the cone geometry and would be equally useful for Navier-Stokes applications.) We show that these results can be combined to draw a picture of most of the flow field. In the final section we summarize our conclusions.

2. Streamline trajectories

If the flow deflected by a solid object remains supersonic after deflection, the angle between the flow direction and the surface determines the flow parameters behind the shock for given inlet flow parameters. For shock Mach numbers $M \gtrsim 10$, the shock angle is small and the deflected flow on the upwind side closely follows the form of the deflecting object. The streamlines are determined by the condition that the angle through which they are deflected be as small as possible. We would like to analyze how this deflection angle varies on the surface of the cone shown in Fig. 1. Based on this analysis we can estimate most of the characteristics of steady supersonic flow directed transversely toward the cone.

The equation for the frustrum of a cone with the geometrical center of its base located at the center of coordinates (see Fig. 1) is

$$(x^2 + y^2)\tan^2\alpha = (z - h)^2, \tag{1}$$

where h is the height of the cone and α is the angle between the side of the cone and the base. The angle

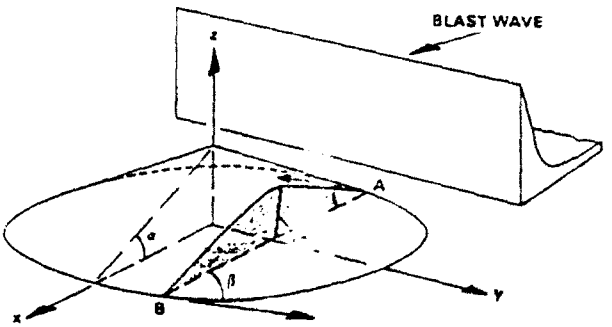

Fig. 1. Schematic of the model. The z axis coincides with the axis of the cone and the flow is taken in the direction of the positive x axis. The angles α, β, γ, and ω are defined in the text

δ between the propagation direction n (taken to be the positive x-direction) and the deflected streamline at the leading edge of the cone, which determines the shock strength, is bounded above by the angles between n and the conic sections in the x–y and x–z planes.

The cross sections of the cone parallel to the x–y plane are circles given by

$$x^2 + y^2 = (z_0 - h)^2/\tan^2\alpha \equiv r^2, \tag{2}$$

where z_0 is constant for each particular cross section and r is the radius of the circle. The angle β between n and the tangent to this circle at the point with ordinate y is given by

$$\tan\beta = \frac{\partial y}{\partial x} = -\frac{x}{(r^2 - x^2)^{1/2}} = -\frac{(r^2 - y^2)^{1/2}}{y}. \tag{3}$$

The sign is chosen so that positive values of β correspond to negative values of x (i.e., the upwind side).

The cross sections parallel to the x–z plane form hyperbolas on the surface of the cone. The equation for this family of curves is

$$\frac{(z - h)^2}{\tan^2\alpha} - x^2 = {y_0}^2, \tag{4}$$

where y_0 is constant for each particular cross section. The angle γ between n and the tangent to this hyperbola is given by

$$\begin{aligned}\tan\gamma = \frac{\partial z}{\partial x} &= \tan\alpha/\left(1 + {y_0}^2/x^2\right)^{1/2} \\ &= \left(1 - {y_0}^2/r^2\right)^{1/2}\tan\alpha\end{aligned} \tag{5}$$

Let us examine now how $\tan\beta$ and $\tan\gamma$ vary on the intersection of the cone with the x–y plane when y changes from 0 to $\pm R$, where $r = R = h/\tan\alpha$. From (3), $\tan\beta$ approaches ∞ and 0, i.e., $\beta = 90°$ and $\beta = 0°$, in the limits $y \to 0$ and $y \to \pm R$, respectively. From (5), $\tan\gamma$ approaches $\tan\alpha$ and 0 in the same limits, corresponding to $\gamma = \alpha$ and $\gamma = 0°$.

Comparing (3) and (5), we readily conclude that for $\tan\alpha < 1$

$$\begin{aligned} &\tan\gamma < \tan\beta, \quad 0 < y < R; \\ &\tan\gamma = \tan\beta = 0, \quad y = R, \end{aligned} \tag{6}$$

and for $\tan\alpha > 1$

$$\begin{aligned} &\tan\gamma < \tan\beta, \quad 0 < y < R/\tan\alpha; \\ &\tan\gamma = \tan\beta, \quad y = R/\tan\alpha; \\ &\tan\gamma > \tan\beta, \quad R/\tan\alpha < y < R; \\ &\tan\gamma = \tan\beta = 0, \quad y = R. \end{aligned} \tag{7}$$

Thus, at any point with $x \leq 0$ on the cone specified by (1) for $\tan\alpha < 1$, the propagation vector **n** makes a smaller angle with the cone in the cross section parallel to the x–z plane than in the one parallel to the x–y plane. For supersonic flow over the cone shown in Fig. 1, condition (6) implies that the velocity vectors behind the shock front in the region of compression of the flow will always be directed over the cone and not around it.

Now we consider intermediate cross sections of the cone, obtainable by rotating through an angle ω about the line AB defined by the intersection of the x–y plane and a plane parallel to the x–z plane. We would like to find the minimum angle between **n** and the tangent in these cross sections when ω varies from 0° (cross section parallel to the x–y plane) to 90° (cross section parallel to the x–z plane).

This family of cross sections is defined by (1) together with the equation of the cross-section plane,

$$z - Z = (y - Y)\tan\omega. \tag{8}$$

where ω is the angle between the cross-section plane. We restrict ourselves to points lying in the x–y plane as shown in Fig. 1, since the bow shock produced by the interaction between the flow and the cone will either be attached at this point or will stand off slightly ahead of the cone. The coordinates of the point where the flow encounters the cone are $X = (R^2 - Y^2)^{1/2}$, Y, and $Z = 0$. The tangent line is the intersection of this plane and the plane tangent to the cone at (X, Y, Z). The equation of the latter is obtained from (1):

$$(xX + yY)\tan^2\alpha + h(z - h) = 0. \tag{9}$$

Solving (8) and (9) simultaneously yields the equations describing the tangent line:

$$z = (y - Y)\tan\omega = \frac{-(x - X)X\tan^2\alpha\tan\omega}{h\tan\omega + Y\tan^2\alpha}. \tag{10}$$

The angle δ between this line and **n** is given by

$$\begin{aligned} \tan\delta &= \frac{\left[(y - Y)^2 + z^2\right]^{1/2}}{x - X} \\ &= \frac{(h^2 - Y^2\tan^2\alpha)^{1/2}\tan\alpha}{h\sin\omega + Y\tan^2\alpha\cos\omega} \equiv f(\omega). \end{aligned} \tag{11}$$

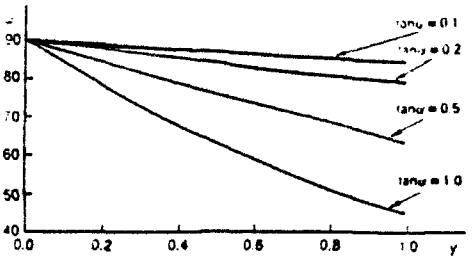

Fig. 2. Value of angle ω which minimizes deflection angle as a function of Y/R

Now we look for the extrema of $f(\omega)$ when ω varies from 0° to 90°:

$$\frac{df}{d\omega} = \frac{\tan\delta\,(Y\tan^2\alpha\sin\omega - h\cos\omega)}{h\sin\omega + Y\tan^2\alpha\cos\omega}, \tag{12}$$

which vanishes only for

$$\tan\omega = \frac{h}{Y\tan^2\alpha} \equiv \tan\omega_{\min}. \tag{13}$$

It is easy to show that (13) defines the minimum of f. Substituting (13) into (11), we find

$$\tan\delta_{\min} = \frac{(h^2 - Y^2\tan^2\alpha)^{1/2}\tan\alpha}{(h^2 + Y^2\tan^4\alpha)^{1/2}}, \tag{14}$$

which determines the angle $\delta_{\min}$ through which the streamline of the supersonic flow behind the shock wave turns as a function of Y.

From (13) we see that $\tan\omega > 1$ holds for $\tan\alpha < 1$, since $Y \leq h/\tan\alpha$. Figure 2 shows how $\omega_{\min}$ changes when Y varies from 0 to R for various values of $\tan\alpha$. This figure implies that for flat cones the supersonic flow will be almost parallel to the x–z plane.

Another way to reach the same conclusion is by finding the maximum y-displacement of a streamline from its original trajectory. This occurs for $x = 0$, when the trajectory reaches its highest point on the surface of the cone. The tangent to the cone at $x = 0$, i.e., the section of the cone in the y–z plane, is described by

$$y\tan\alpha + z = h. \tag{15}$$

Solving this equation together with

$$z = (y - Y)\tan\omega_{\min} = \frac{h(y - Y)}{Y\tan^2\alpha}, \tag{16}$$

we obtain

$$y = \frac{hY\sec^2\alpha}{h + Y\tan^3\alpha} \equiv y_0. \tag{17}$$

Maximizing $\Delta y = y_0 - Y$ with respect to Y, we find that the largest value of Δy occurs for

$$Y = \frac{h\cos^2\alpha}{\sin\alpha(1 + \cos\alpha)} = \frac{R\cos\alpha}{1 + \cos\alpha} \tag{18}$$

and equals

$$(\Delta y)_{\max} = \frac{h \sin\alpha \cos\alpha}{(1+\cos\alpha)^2} = \frac{h \tan^2 \alpha/2}{\tan\alpha}. \qquad (19)$$

For $\alpha \ll 1$ we have $Y_{\max} \approx R/2$ and $(\Delta y)_{\max} \approx h\alpha/4$.

In summary, the vertical deflection of the streamlines over a cone of small edge angle α is of order α, while the horizontal deflection is of order α^2. For $\alpha \lesssim 0.1$ we see that the flow over the cone deviates from the vertical plane in which it starts out by an amount 0.01. Thus the compression region of supersonic flow over flat cones can be calculated accurately by modeling the flow over separate cross sections of the cone made by planes parallel to the x–z plane. A wedge, being two-dimensional, is easier to model than a cone. For this reason we carried out several calculations of the interaction between blast waves and wedges, described in the next section.

We can also conclude that the maximum change in the direction of a streamline for such cones will be α. If the shock undergoes regular reflection, uniform supersonic flow over a wedge with base angle α gives an upper bound for the pressure on the cone. Where Mach reflection occurs it is necessary to model the transient regime, as the pressure peaks associated with the Mach stem and the contact surface could conceivably be larger.

3. Numerical modeling

Let us consider a cone with $\alpha = 10°$ ($\tan\alpha = 0.176$) at the base. According to the analysis in the preceding section of a transversely directed supersonic flow over a cone, an upper limit can be obtained by modeling the same supersonic flow over a wedge with opening angle α.

Here we present the result obtained by numerically solving the equations for the flow over the wedge when it is loaded by a passing blast wave. For the simulation we used the Fast Unstructured-Grid Second-Order Godunov Solver, described by Eidelman and Lottati (1990). This code, which is based on a second-order Godunov method (Eidelman et al. 1984), provides a method for solving the Euler equations of gasdynamics on unstructured grids with arbitrary connectivity. The use of a data structure with only one level of indirectness leads to an easily vectorized and parallelized code with low memory requirements and high computational efficiency. The algorithm has been tested for performance and accuracy over a wide range of Mach numbers and geometrical situations, and has demonstrated robustness without the need for any adjustable parameters. It can be implemented in either a triangle- or vertex-based form; experience with the method has shown that extremely low levels of artificial viscosity can be achieved using the triangle-based version of the method. Direct dynamic refinement of the grid (Eidelman and Lottati 1990) allows automatic adaptation to the front of the moving blast wave. This refinement guarantees that the associated highly inhomogeneous pressure and density features are accurately tracked.

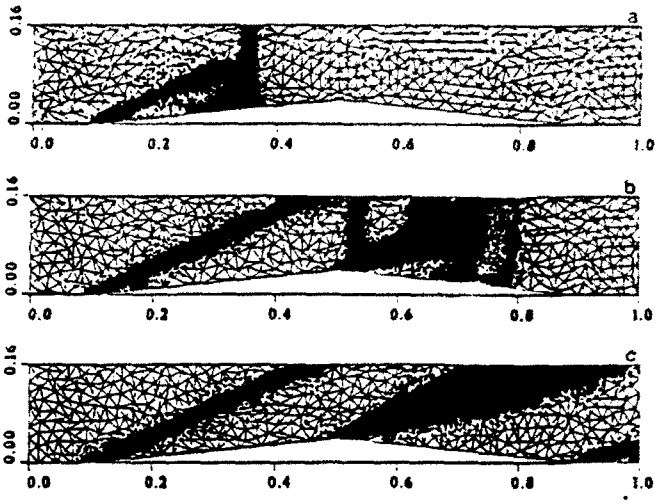

Fig. 3. Unstructured grid for $\alpha = 10°$ at times (a) 35 μs, (b) 55 μs, and (c) 130 μs, associated with the density and pressure contour plots of Figs. 4 and 5.Distances are in meters. These reproductions are unable to resolve the smallest triangles, which show up as dark regions roughly coincident with the locations of gasdynamic discontinuities

For the initial conditions in the computational domain we assume air at standard temperature and pressure. At $t = 0$, a strong (M = 25) blast wave, propagating to the right, is located at the left boundary. We assume that the blast wave is "square" and that conditions at the left boundary of the computational domain remain constant for the whole time of the simulation. A constant value of $\gamma = 1.2$ was used (appropriate to flow behind shocks with this value of M on account of real-gas effects). For these values of α, γ, and M, shock tube measurements described by Glass (1987) of diffraction over a wedge indicate that double Mach reflection should occur.

Figure 3 shows the computational grid at various times t: (a) at $t = 35\,\mu$s, shortly before the blast front reaches the apex of the wedge, located at a horizontal distance $l = 1$ m from the corner; (b) at $t = 55\,\mu$s, just after it passes the apex; and (c) at $t = 130\,\mu$s, after the leading shock has exited from the computational domain and a quasisteady state has developed. The highly refined portions of the grid follow shock fronts, contact discontinuities, etc. The numbers of vertices shown are 4166, 11785, and 10959, respectively, reflecting the complexity of the corresponding states, i.e., the amount of structure in the gasdynamic processes present.

Figure 4 shows contours of density scaled by the ambient density $\rho_0 = 1.29\,\mathrm{kg\,m^{-3}}$ at the same times as in Fig. 3. In the first frame the flow is still identical with that for a shock reflecting from a single wedge with opening angle α, and therefore is evolving self-similarly (Glass 1987). The first Mach stem and incident shock are clearly defined. The associated contact surface is barely discernible, both because the contour levels are bunched near the much larger jumps at the shocks and because at very high Mach numbers the slip line is found quite close

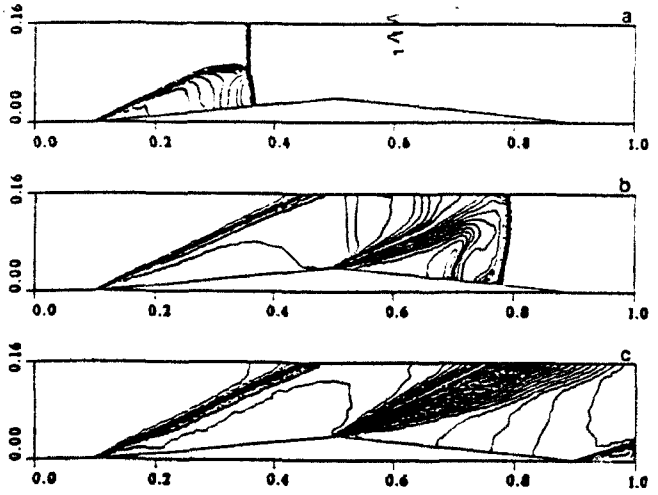

Fig. 4. Scaled density contours for $\alpha = 10°$ at times (a) 35 μs, (b) 55 μs, and (c) 130 μs. Thirty-five contour levels are plotted, with ρ/ρ_0 varying from 1.0 to 13.5. They are concentrated at the large density jumps in the strong shocks. This causes the shocks to be emphasized more than the contact discontinuity, where the density change is relatively small. The structure of the Mach reflection is discernible only in the earliest frame. In the final frame the flow has become essentially steady

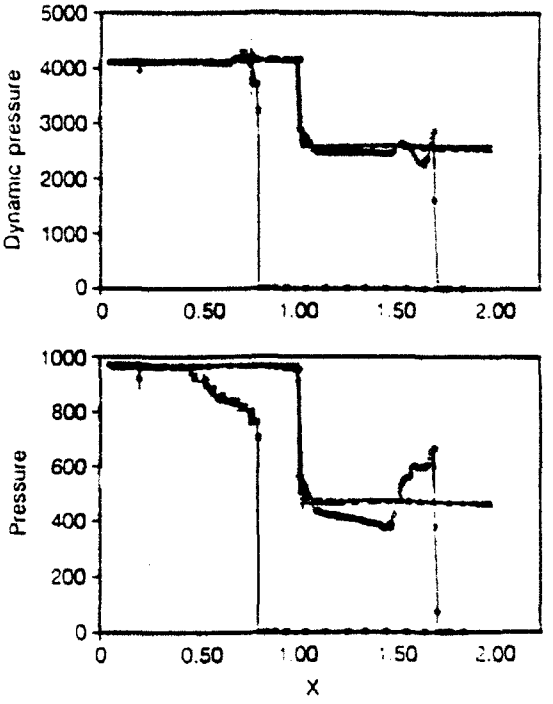

Fig. 5. Scaled dynamic and static pressure on the wedge surface in the case $\alpha = 10°$ as functions of the distance for times 35 μs (□), 55 μs (○), and 130 μs (△). Ahead of the shock these quantities have their ambient values; far behind the shock they become essentially steady

to the Mach stem (Glaz et al. 1985). In Fig. 4b the front has passed the apex and the evolution is no longer self-similar. The flow behind the front expands through an expansion fan attached to the corner. Also clearly visible is the recompression shock two-thirds of the way from the corner to the front. This shock, which serves to reconcile the high pressures in the region following the Mach stem with the lower values appropriate to the expanded flow downstream from the corner, is propagating backward but is being swept to the right by the strong flow behind the leading shock. The triple points have moved far above the cone and no longer appear on the grid. Note that the supersonic outflow boundary condition imposed at the top of the mesh allows material and waves to pass out of the system without reflecting and without causing other signals to propagate back inside. Figure 4c depicts the flow at late times, when transients have essentially disappeared. The only gasdynamic features visible are shocks at the leading and trailing edges and the expansion fan.

Figure 5 shows traces of the static and dynamic pressure scaled by the ambient pressure $p_0 = 101.3\,\mathrm{kPa}$ along the top surface of the wedge as functions of the horizontal distance x in meters at the three specified times. Ahead of the blast these quantities are at ambient levels, they rise sharply when the shock sweeps past, fluctuate, and finally reach their asymptotic values. Note that, as is seen experimentally in shock-tube studies (Glass 1987), the pressure on the surface of the wedge is highest at the leading edge. It is also important to notice that, although these traces exhibit considerable structure (especially the static pressure), the maximum values of the pressure and density for the transient stages are always smaller than those in the quasisteady flow regime. At the same time, values of the Mach number in the transitional stage can be higher than in the quasisteady state. For our case, however, the maximum Mach number is at most 10% higher than the steady-state value. This shows that the maximum force is applied to any point on the surface of the wedge in the quasisteady state.

Figure 6 shows as functions of time the drag and lift coefficients, defined by

$$C_D = \frac{\int p_{\parallel} dx}{\rho_\infty u_\infty^2 l} \tag{20}$$

and

$$C_L = \frac{\int p_{\perp} dx}{\rho_\infty u_\infty^2 l}. \tag{21}$$

Here $p_{\parallel} = p\cos\theta$ and $p_{\perp} = p\sin\theta$ are the horizontal and vertical components of the pressure in terms of the angle θ between the normal to the surface and the x axis, the integrals are carried out over the surface of the wedge, and ρ_∞ and u_∞ are the density behind the undisturbed shock front. The lift grows monotonically, but the drag first rises, then drops to its quasisteady value. The decrease results from the increase in pressure on the trailing side of the wedge when the shocked air reaches that side.

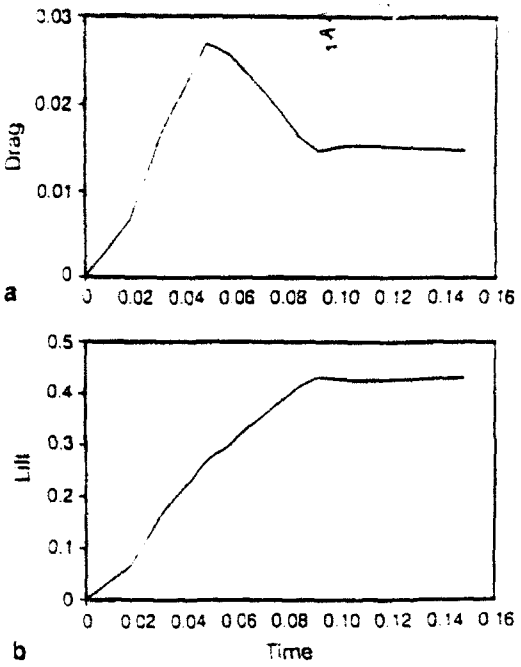

Fig. 6. Lift and drag coefficients for $\alpha = 10°$ as functions of time

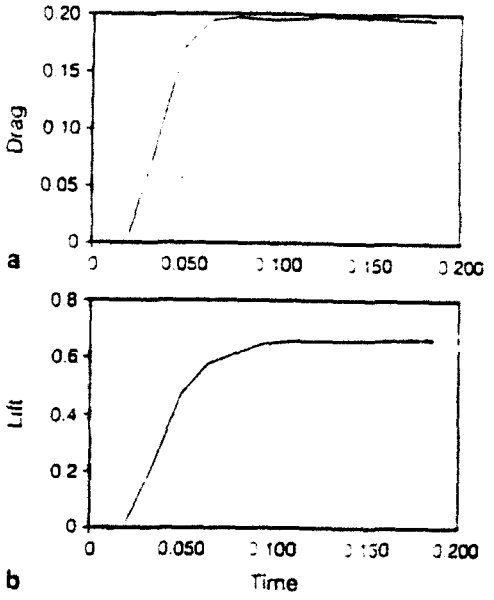

Fig. 8. Lift and drag coefficients for $\alpha = 20°$ as functions of time (in milliseconds)

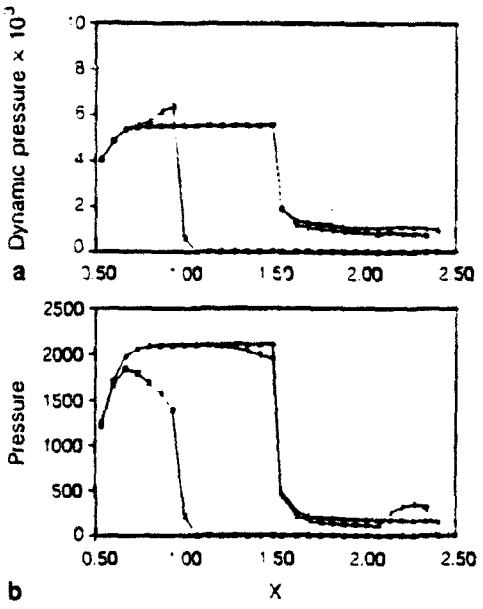

Fig. 7. Scaled dynamic and static pressure on the wedge surface in the case $\alpha = 20°$ as functions of the distance for times 34 μs (□), 94 μs (○), and 168 μs (△)

To learn how sensitive the flow is to the wedge angle, we carried out a second calculation with $\alpha = 20°$ ($\tan\alpha = 0.364$) and the other parameters unchanged. This calculation was done with a coarser grid than the previous one, with triangles about a factor of three larger. Most of the features resembled those of the first case. For example, the traces of the static and dynamic pressure along the top surface, shown in Fig. 7, are qualitatively similar to those for $\alpha = 10°$. One difference is that the drag rises monotonically as a function of time (Fig. 8), rather than decreasing after the shock has passed. This is because the expansion fan attached to the top of the cone is stronger and a low-pressure "bubble" forms on the lee side.

We carried out additional calculations with other values of the parameters. As long as α was small and M was large the results resembled those discussed above. They are not described here, since in no case did the transient pressures exceed those in the quasisteady state, nor were the features in the flow qualitatively different.

4. Conclusions

From the foregoing treatment it is clear that the same modeling technique can be used to determine the pressure distribution in cross sections other than the midplane. So long as $|y|$ does not approach R, the deflection is mostly vertical. The corresponding profile is now a hyperbola, but it differs noticeably from a wedge only near the top. The principal difference is in the expansion wave at the top, which becomes broader than the centered rarefaction wave seen above. For larger values of y the cross section of minimum deflection, found by solving (1) and (8) together, is more rounded at the top but the leading edge of this hyperbolic "wedge" has a smaller angle. By combining pressure distributions at several representative values of y we can find the pressure loading over the entire cone. The picture breaks down only at the lateral extremities of the cone ($|y| \sim R$).

On the basis of qualitative arguments and numerical simulation, our study of the flow resulting from a blast wave propagating transversely over a cone leads to the following conclusions:

1. Flow over a cone with small base angle can be accurately simulated by individually modeling the two-dimensional flows over cross sections of the cone made by vertical planes perpendicular to the shock front.
2. The maximum load on the cone can be calculated from the solution of the flow over the cross section determined by the plane through the cone axis (Fig. 1).
3. In this solution the pressure attains its maximum as a function of time in the quasisteady supersonic regime established after the front has passed.

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Detonation Wave Propagation in Variable Density Multi-Phase Layers

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Detonation Wave Propagation in Variable Density Multi-Phase Layers

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ABSTRACT

A mathematical model is presented describing a physical system of detonation waves propagating in a solid particle/air mixture with a wide range of solid phase concentrations. The mathematical model was solved numerically using the Second Order Godunov method, and numerical solutions were validated for detonation waves propagating in mixtures with concentrations of solid phase from 0.75 kg/m^3 to 1000 kg/m^3. Numerical solution was obtained for detonation waves propagating in a system consisting of layers of explosive powder with substantial variation in particle density between the layers. The study revealed a specific detonation front structure that is dependent on the thickness of the layers and their energetic content. The dynamics of lateral initiation of the adjacent layers and the structure of detonation waves in this system were investigated. Results are given for detonation of clouds having a small concentration of particles and a ground layer in which solid particle densities are three orders of magnitude larger than in the cloud.

1. INTRODUCTION

It is of considerable practical interest to study diffraction and transmission of the detonation waves into bounding layers of explosives. When combustible particles are intentionally or unintentionally dispersed into the air, the resulting mixture can be detonable. Formation of this potentially explosive dust environment and the properties of its detonation are of significant practical interest in view of its destructive or creative effects. The experimental and theoretical study of these phenomena until now has addressed only homogeneous particle/oxidizer mixtures. However, intentional or accidental processes of the explosive dust dispersion will always lead to inhomogeneous particle density distribution. Some industrial methods of explosive forming rely on detonation of explosive powder. This powder can be deposited as a thin layer over the surface area of the forming metal, with some remaining concentration in the vicinity of the layer. Also a multi-layer system can be formed from several layers of condensed explosives of different density. The structure of the detonation waves, phenomenology of its initiation, and propagation in these environments, are the main subjects of this paper.

When the detonation wave is generated in a homogeneous mixture by a"direct initiation," it starts with a strong blast wave from the initiating charge. As the blast wave decays, combustion of the reactive mixture behind its shock front starts to have a larger role in support of the shock wave motion. When the initial explosion energy exceeds some critical value, transition to steady state detonation occurs.[1-4] In explosive dust mixtures with a nonuniform distribution of particle density, the initiation dynamics is significantly more complicated. The critical initiation energy sufficient for one of the explosive particle density regions is not necessarily adequate for other regions. Also, when there is a significant variation in density between the different layers (regions) of the mixture, steady detonation in one layer can result in an overdriven detonation in an adjacent layer. Liu et al.[5] has studied experimentally a system of gaseous layers and lateral interactions for gaseous detonations. Our paper demonstrates that the phenomenoiogy of these interactions is somewhat different from these experimental studies of multi-layer detonations in gases. This is primarily because the energy content of adjacent layers in a typical multi-gas layer experiment[5] varies by a factor of less then two, whereas the energy content in explosive dust/air mixtures can vary by several orders of magnitude.

In this paper we use detailed numerical simulation to study the initiation dynamics and propagation phenomenology for a general case of explosive dust dispersion. We will consider particle density variation from 1000 kg/m^3 in the ground layer to 0.75 kg/m^3 for the upper edges of the cloud. The effects of variation of the cloud density on detonation wave parameters will be examined for different cases of cloud particle density distribution. When possible, the results of computer simulations are validated in comparison with experimental and theoretical studies.

Section 2 of this paper describes a mathematical model that includes governing conservation equations for two phases and the constitutive laws, as well as the model for a particle gas interaction, combustion and equation-of-state for gas phase. The numerical integration technique for solving the mathematical model will is also outlined. In Section 3, we present our numerical simulation results. We first validate our model by comparing one-dimensional detonation wave simulation with available experimental results. We then give the two-dimensional simulation for detonation wave propagation in combustible particle/air mixtures with variable parti-

cle density distribution. Concluding remarks are given in Section 4.

2. THE MATHEMATICAL MODEL AND THE NUMERICAL SOLUTION

The mathematical model consists of conservation governing equations and constitutive laws that provide closure for the model. The basic formulation adopted here follows the two-phase fluid dynamics model presented in the text by Kuo[7]. The approach assumes that there are two distinct continua, one for gas and one for solid particles, each moving at its own velocity through its own control volume. The sum of these two volumes represents an average mixture volume. With these assumptions, distinct equations for continuity, momentum and energy are written for each phase. The interaction effects between the two phases are accounted as the source terms on the right hand side of the governing equation. The following is a short description of the two phase flow model used in our study, with conservation equations written in Eulerian form for two-dimensional flow in Cartesian coordinates.

Conservation Equations

Continuity of gaseous phase

$$\frac{\partial \rho_1}{\partial t} + \frac{\partial(\rho_1 u_g)}{\partial x} + \frac{\partial(\rho_1 v_g)}{\partial y} = \Gamma \; ; \qquad (2.1)$$

Continuity of solid particle phase

$$\frac{\partial \rho_2}{\partial t} + \frac{\partial(\rho_2 u_p)}{\partial x} + \frac{\partial(\rho_2 v_p)}{\partial y} = -\Gamma \; ; \qquad (2.2)$$

Conservation of momentum of gaseous phase in x-direction

$$\frac{\partial(\rho_1 u_g)}{\partial t} + \frac{\partial(\rho_1 u_g^2 + \phi p_g)}{\partial x} + \frac{\partial(\rho_1 u_g v_g)}{\partial y} = -F_x + \Gamma u_p \; ; \qquad (2.3)$$

Conservation of momentum of solid particle phase in y-direction

$$\frac{\partial(\rho_1 v_g)}{\partial t} + \frac{\partial(\rho_1 u_g v_g)}{\partial x} + \frac{\partial(\rho_1 v_g^2 + \phi p_g)}{\partial y} = -F_y + \Gamma v_p \; ; \qquad (2.4)$$

Conservation of momentum of solid particle phase in x-direction

$$\frac{\partial(\rho_2 u_p)}{\partial t} + \frac{\partial(\rho_2 u_p^2)}{\partial x} + \frac{\partial(\rho_2 v_p u_p)}{\partial y} = F_x - \Gamma u_p \; ; \qquad (2.5)$$

Conservation of momentum of solid particle phase in y-direction

$$\frac{\partial(\rho_2 v_p)}{\partial t} + \frac{\partial(\rho_2 u_p v_p)}{\partial x} + \frac{\partial(\rho_2 v_p^2)}{\partial y} = F_y - \Gamma v_p \; ; \qquad (2.6)$$

Conservation of energy of gas phase

$$\frac{\partial(\rho_1 E_{gT})}{\partial t} + \frac{\partial(\rho_1 u_g E_{gT} + u_g \phi p_g)}{\partial x} + \frac{\partial(\rho_1 v_g E_{gT} + v_g \phi p_g)}{\partial y}$$

$$\Gamma\left(\frac{u_p^2 + v_p^2}{2} + Echem + C_s \bar{T}_p\right) - \left(F_x u_p + F_y v_p\right) - \dot{Q} \; ; \qquad (2.7)$$

Conservation of energy of solid particle phase

$$\frac{\partial(\rho_2 E_{pT})}{\partial t} + \frac{\partial(\rho_2 E_{pt} u_p)}{\partial x} + \frac{\partial}{\partial y}(\rho_2 E_{pt} v_p) = \dot{Q} + (F_x u_p + F_y v$$

$$-\Gamma\left(\frac{u_p^2 + v_p^2}{2} + Echem + C_s \bar{T}_p\right) \; ; \qquad (2.8)$$

Conservation of number density of solid particle

$$\frac{\partial N_p}{\partial t} + \frac{\partial(N_p u_p)}{\partial x} + \frac{\partial(N_p v_p)}{\partial y} = 0 \; . \qquad (2.9)$$

In the above equations, $\phi = 1 - \frac{N_p M_p}{\rho_g}$, $\rho_1 = \phi\rho_g, \rho_2 = (1-\phi)\rho_p$, where N_p and M_p are the number density and mass of each particle, respectively, and ρ_g and ρ_p are the material density of gas and particle densities, respectively. u_g, v_g, p_g are gas phase x-velocity, y-velocity and pressure, respectively; $u_p, v_p, \bar{T}_p$, are x-velocity, y-velocity and average temperature of particle, respectively. C_s is specific heat of solid particle and *Echem* is chemical energy of solid phase, Γ is the rate of phase change from solid to gas and Q is heat transfer between the two phases; F_x, F_y are the drag force between the two phases in x and y directions, respectively.

Equations (2.2) and (2.7) are linked through the relation $\rho_2 = nM_p$. In the case of a reactive solid phase, M_p decreases due to combustion. The mass of a single particle at any point can be obtained from $M_p = \rho_2(x,y)/n(x,y)$, and the diameter of a particle at any spatial location is $D(x,y) = [6M_p(x,y)/\pi\rho_p]^{1/3}$. The total internal energy of gaseous phase

$$E_{gT} = E_g + \frac{1}{2}(u_g^2 + v_g^2) \quad and \quad E_g = E_g(p_g, \rho_g) \qquad (2.10)$$

where $E_g(P_g, \rho_g)$ is the equation-of-state for the gas phase, which will be discussed later.

The total internal energy of solid particle phase is

$$E_{pt} = E_p + \frac{1}{2}(v_p^2 + v_p^2) \quad and \quad E_p = Echem + C_s \bar{T}_p \ . \tag{2.11}$$

In order to close the above system of conservation equations, it is necessary to define certain criteria and interaction laws between the two phases, which include mass generation rate, Γ, drag force between particles and gas, F_x, F_y and the interphase heat transfer rate $\dot{Q}$. The model for particle and gas interaction and particle combustion that results in the constitutive relation for the conservation equations, is explained in detail in the next subsection.

Model for a Particle Gas Interaction and Combustion

Presently, the physics of the energy release mechanisms in solid particles/air mixtures is not clearly understood. This can be attributed to the obvious difficulties of making a direct non-obtrusive measurement in the optically thick environment typical for this system. In the experimental and theoretical work done for the grain dust detonation conditions,[7] it was demonstrated that the volatile components released by the particle heated behind the shock front play a major role in determining the detonability limits of the mixture. Eidelman and Burcat[8] successfully applied a combination of fast evaporation and aerodynamic shattering mechanisms to simulate a two-phase detonation process.

The chemical processes of a single particle combustion, which mainly occur in the gaseous phase, are significantly faster than the physical processes of particle gasification or disintegration. Thus, in the multi-phase mixtures, the rate of energy release will be mostly determined by physics of particle disintegration. It is very difficult to describe the details of particle disintegration in the complex environment prevalent behind the shock or detonation wave. For example, Reinecke and Waldman[9] defined five different disintegration regimes for a relatively simple environment of water droplets passing through a weak shock. Fortunately, in most cases of multi-phase detonation, only the main features of the particle disintegration dynamics need to be captured to describe the phenomena. For example, Eidelman and Burcat,[10] using simple models for particle evaporation and shattering, obtained simulation results that compared very favorably with experimental data. Because of our inability to resolve the particle disintegration problem in all its complexity, the validation of the model against known experimental data is essential.

In this paper we consider solid particles consisting of explosive material. Explosive material contains fuel and oxidizer in a passive state at low temperature; however, when the temperature rises the fuel and oxidizer react, leading to detonation or combustion. The initiation of reaction for explosives will occur at relatively low temperature. For example, TNT will detonate when heated to the temperature[11] of 570°C. Only particles larger than a critical detonation size can detonate directly when initiated by a shock wave. We consider here particles smaller than 4mm in diameter that will not detonate when heated, but will burn when the temperature on the particle surface reaches a critical value. Since the heat conduction inside the explosive material is relatively slow, the process of particle heating needs to be resolved in detail. Our simulations numerically solve the temperature field in the particles at every step of numerical integration of the global conservation equations. The explosive particle combustion model examined in this paper assumes that the fraction of the particle that reaches the critical temperature will burn instantaneously.

Energy transfer by convection and conduction is simulated by solving the unsteady heat conduction equation in each computational cell at each time step. Assuming a particle's temperature T_p to be a function of time and radial position only, the unsteady heat conduction equation may be transformed to:

$$\frac{d^2 w}{dr^2} = \frac{1}{\alpha}\frac{dw}{dt} \ , \tag{2.12}$$

subject to the boundary conditions:

$$w = 0 \quad at \quad r = 0, \quad t > 0$$

$$k_s \frac{dw}{dr} = (h - \frac{1}{R})w = hRT_g \quad at \quad r = R, \quad t > 0 \tag{2.13}$$

where:

$w(r,t) = rT_p(r,t)$
r = radial position
T(r,t) = temperature
R = particle radius
T_g = temperature of surrounding gas
k_s = thermal conductivity of particle
h = convective heat transfer coefficient.

The Nusselt number, used to find h, is given by an empirical relation provided by Drake.[12] The gas viscosity is found from Sutherland's Law. The gas thermal conductivity is calculated by assuming a constant Prandtl number. Lastly, the boiling temperature at a given pressure is found from the Clapeyron-Clausius equation, assuming: 1) constant latent enthalpy of phase change, 2) the vapor obeys the ideal equation of state, and 3) the specific volume of the solid/liquid is negligible compared to that of the vapor. A critical temperature is also employed to serve as an upper limit to the boiling point, regardless of pressure.

Equation (2.13) with boundary condition (2.14) can be numerically integrated using either implicit or explicit schemes.

Since the particle radius, R, will become very small due to evaporation, the implicit Crank-Nicolson algorithm is used because of its stability properties and its second order temporal and spatial accuracy. Using the Crank-Nicolson scheme to predict the particle temperature profiles at times t_1 and t_2 permits easy calculation of the total energy exchange, Q between t_1 and t_2 due to convection and conduction.

Knowledge of the particle temperature profile also allows us to determine Γ, the rate of phase change from solid particle to gas. Once any point at a radial location $0 \leq r \leq R$ has a temperature exceeding the boiling temperature, the entire mass between r and R is transferred to the gas phase in one time step. In so doing, an energy equal to the product of the mass lost and the particle intrinsic energy is transferred by the particle to the gas.

The interphase drag force (Fx, Fy) is determined from the experimental drag for a sphere, as presented by Schlichting[13].

$$F_x = \left(\frac{\pi}{8}\right) N_{pg} C_D |\mathbf{V}_g - \mathbf{V}_p| (u_g - u_p) R^2 \qquad (2.14)$$

where

$$C_D = \begin{cases} \frac{24}{Re}\left(1 + \frac{Re^{2/3}}{6}\right) & \text{for Re} < 1000; \\ 0.44 & \text{for Re} > 1000, \end{cases} \qquad (2.15)$$

and $Re = \frac{2R|\mathbf{V}-\mathbf{V}_g|}{\mu_g}$, R is radius of partricle and μg is gas viscosity at temperature of $T_{film} = \frac{1}{2}(T_g + \bar{T}_p)$. Similarly, the formulae for Fy is

$$Fy = \frac{\pi}{8} N_p \rho_g C_D |\mathbf{v}_g - \mathbf{v}_p| (v_g - v_p) R^2. \qquad (2.16)$$

Equation of State for Detonation Products

To close the system of governing equations, one needs a constitutive relation between density, pressure, temperature and energy for gas phase, which is an equation-of-state. This study uses the Becker-Kistiakowsky-Wilson (BKW) equation-of-state[14,15] that is,

$$p_g V_g / \bar{R} T_g = 1 + x e^{bx}, \qquad (2.17)$$

where V_g = volume of gas phase
p_g = pressure of gas phase
T_g = temperature of gas phase
$\bar{R}$ =- universal gas constant
$x = k/F_g(T + \Theta)^a$ $k = K\Sigma_i X_i k_i$
with empirical constants a, b, K, Θ and k_i. The constants k_i, one for each molecular species, are co-volumes. The co-volumes are multiplied by their mole fraction of species, X_i, and are added to find an effective volume for a mixture. For a particular explosive, if we know the composition of detonation products and a, b, Θ, K, and all k_i's can be found in Ref. 15.
The internal energy is determined by thermodynamics relation

$$\left(\frac{\partial E_g}{\partial V_g}\right)_T = T_g \left(\frac{\partial_{pg}}{\partial T_g}\right)_V - p_g . \qquad (2.18)$$

Integration of this equation for a fixed composition of the detonation products will allow us to calculate the energy of the detonation products as a function of temperature and volume. For each component, its thermodynamic properties as functions of temperature were calculated from the NASA tables compiled by Gordon and McBride[16].

The BKW equation-of-state is the most common and well calibrated of those equations-of-state used to calculate the properties of detonation products. The detailed discussion and review of the BKW equation-of-state can be found in Ref. 15.

Numerical Method of Solutions

The system of partial differential equations described in the previous paragraph is integrated numerically. The Second Order Godunov method is used for the integration of the subsystem of equations describing flow of gaseous phase material. This method is described in Ref. 17. In the following, we will elaborate only on some specifics of its application to simulations of detonation products. The subsystem of equations describing the flow of particles is integrated using a simple upwind integration. This is done because our mathematical model neglects pressure of interparticle interaction and that prevents formulation of a Second Order Godunov scheme for particles.

The physical system under study will have concentrations of solid explosive powder ranging from 1000 kg/m^3 near the ground to 0.75 kg/m^3 or less in the cloud. Detonation of this mixture will create detonation products with effective γ ranging from 3 to 1.1. To describe the flow of detonation products, we use the BKW equation-of-state described above. Since the Second Order Godunov method uses primitive variables to calculate Riemann problems at the edges of the cells, its implementation for non-ideal EOS is difficult. In our simulations, we have resolved this problem by using direct and inverse equations-of-state. After integrating a system of gas conservation laws, we use the direct BKW

equation-of-state to calculate pressure, gamma and temperature as functions of thermal energy, density, and mixture composition. After this step, we have a complete set of parameters allowing calculation of the fluxes in the Second Order Godunov method as well as interaction of the multi-phase processes. The "inverse" EOS calculates internal energy as a function of density, pressure and mixture composition. In our code we use the "inverse" EOS to calculate the fluxes of conserved variables after calculation of the flux of primitive variables.

For the multi-phase system under study, dx=dy=1mm was used to allow explicit integration of the gasdynamic and physical processes of evaporation and heat release. When a mismatch occurred between the physical and gasdynamical characteristic times, the time step was adjusted by some fraction to assure stability. However, this did not result in a significantly smaller time step as compared with that calculated by CFL criteria. For larger cell sizes, this approach is impractical. Recently we implemented a scheme in which multi-phase processes are calculated implicitly; however, this will be reported elsewhere.

The numerical method is implemented in a code named MPHASE, which is fully vectorized and supported by number of graphics and diagnostics codes.

3. RESULTS

Model Validation for One-Dimensional Detonation Wave Problem

The main advantage of our particle combustion model is its description of the phenomenology of detonation for a wide range of explosive particle sizes and densities. We will demonstrate this capability on a set of one-dimensional test problems. For these test problems, we simulated the initiation and propagation of the detonation waves in a shock tube-like setting, where the explosive particles are distributed uniformly through the shock tube volume.

Results of these simulations are summarized in Table 1, which shows detonation wave velocity, peak pressure, and peak density given as a function of the average density of the solid explosive. Here the explosive two-phase mixture is composed from RDX particles and air, where RDX particle concentration varies from 0.75 kg/m^3 to 1000 kg/m^3. This concentration variation covers the whole range of solid explosive concentrations of interest to our problem. The simulations performed with the MPHASE code were compared with the experimental results,[15,18] and the calculations presented in Ref. 19 were done with the TIGER code.

From Table I, it is clear that our simulation results compare favorably with other simulation results and experimental data. The maximum deviation between our results and referenced results is no greater than 15% for the entire range of explosives densities. Considering that our results were obtained with a single model for particle combustion applied to the extreme range of densities, our model gives an excellent prediction of the detonation wave parameters.

Two-Dimensional Simulation Results

In our two-dimensional simulations, we first study the dynamic of the lateral initiation in a simple system formed by two layers of explosive with different concentrations of the explosive powder in the layers. These layers of explosive will be considered confined in a rectangular shock tube with rigid walls. The schematics of the set up for a typical simulation of this type are shown in Figure 1. The detonation wave is initiated in the lower layer, and its propagation though the shock tube causes lateral initiation of the adjacent layer. In one of the test cases, both layers are initiated simultaneously with a planar front.

First we simulated initiation and propagation of the detonation in a system of two layers of detonable RDX powder/air mixture contained in a rectangular channel 4 cm wide and 35 cm long. The lower layer has an RDX powder concentration of 800 $\frac{kg}{M^3}$ and occupies half of the channel width, and the upper layer of the channel has a mixture concentration of 200 $\frac{kg}{M^3}$. Detonation is initiated in the lower layer by a planar front that is propagating from left to right. In Figures 2a:2f, results of this simulation are shown in the form of pressure contours on a logarithmic scale in MPa for a sequence of time frames. In these figures, we can follow the evolution of the lateral initiation and formation of the detonation wave structure in this system.

In Figure 2a, contour plots are shown at time t=0, which corresponds to the beginning of the simulation and depicts initial conditions of the planar wave in the lower layer. This initial wave causes lateral initiation of the upper layer through an oblique detonation front shown in Figure 2b at $t=9 \times 10^{-6}$ sec. The oblique front reflects from the upper wall of the channel, and in Figure 2c we observe that the wave pattern indicates it is a single Mach reflection. The Mach stem is very short at this point. In Figure 2d, the pressure contours are shown at the time $t=31 \times 10^{-6}$ sec. Here the Mach stem is clearly visible and the reflected shock has reached the lower wall of the channel. The Mach stem will continue to grow and the triple point will propagate towards the high density layer. In Figure 2e, the simulation results are shown at $t=52 \times 10^{-6}$ sec when detonation wave complex has reached steady state propagation regime. The triple point has reached the interface between the two layer and is unable to continue propagation downwards due to the high level of pressure and density in the lower layer. Also at this stage of the detonation wave propagation, the reflected shock has reached the upper wall

of the channel. In Figure 2f, the simulation results are shown at t=64 × 10^{-6} sec. Here the structure of the detonation front is basically unchanged from the previous picture, except for an additional reflection from the upper wall of the channel. The detonation wave parameters are also unchanged from the previous time frame, indicating that the detonation wave in this two layer system has reached steady state.

To validate that the detonation waves complex observed in above reported simulation is not a function of the initial conditions, we simulated a test case in which all problem parameters, except the initiation wave, are the same as in the previous case. The initiation is done by a single planar wave that starts propagating simultaneously in both layers of the explosive. In Figures 3a:3e, results for this simulation are shown in the form of pressure contours for a sequence of time frames. The initial conditions are shown in Figure 3a. Here we can observe a planar front impinging simultaneously on both layers of explosive in the channel. At first, this front propagates some distance planarly, as observed in Figure 3b. However, a significant difference in the explosive powder density quickly leads to formation of the oblique front in the upper layer, as shown in Figure 3c. As in the previous case, the oblique front reflects from the upper wall in the single Mach reflection shown in Figure 3d. And as in the previous case, the triple point of the Mach stem propagates downward to the interfaces between the layers to form the stable wave pattern shown in Figure 3e. The parameters of the detonation waves and the structure of the detonation wave complex are identical to those observed in the previous case, which proves that it is not a function of the initial conditions, but physical conditions of the layers.

We studied the effects of the channel walls using a system that included a 2cm thick lower layer of high density (800 $\frac{kg}{M^3}$) RDX powder and a 10cm thick upper layer of low density (200 $\frac{kg}{M^3}$) RDX powder. The results of this simulation are shown as pressure contours on a logarithmic scale in Figures 4a:4d. Figure 4a shows the initial conditions. In Figure 4b, we can see at the time t = 25 × 10^{-6} a planar detonation wave is propagating through the lower layer and an oblique wave is propagating through the upper layer. In Figure 4c, the detonation wave is shown at the time t=41 × 10^{-6} from the initiation. Here the oblique wave is reflecting from the upper wall; however, it is distinct from the previous cases because only a regular reflection pattern is formed. This is due to the shallow angle of incidence of the detonation wave, that corresponds to the large wedge angles in classical reflection problems. Figure 4d shows the results of the simulation at t = 52 × 10^{-6}. Here we can observe the same regular reflection pattern as in the previous stage; however, the incidence angle of the oblique wave in the upper layer is increasing. Thus, if this trend continues, later in the detonation wave evolution we will see the formation of the Mach reflection pattern, as we have in previous cases.

We have also examined propagation of the detonation wave in the system shown in Figure 5 that corresponds to the situation where the upper layer is not confined by the channel wall. Here the computational domain is 25cm × 25cm in size. The explosive powder density is distributed according to the 4th power law of vertical distance, starting from the ground where the density is 860 kg/m^3, to 1.2cm, where the density is 0.75 kg/m^3. From this point to 25cm height, the density is constant and equal to 0.75 kg/m^3. The density distribution in the direction of the"x" axis is uniform. The boundary conditions for the computational domain shown in Figure 5 are specified as follows: solid wall along the "x" axis; symmetry conditions along the "y" axis; supersonic outflow for upper boundary and at the right of the computational domain. The mixture consists of RDX powder and air at ambient conditions and it is assumed to be quiescent at the time of initiation.

The simulation starts at t=0 when the mixture is initiated at the lower left corner of the computational domain, as shown in Figure 5. The energy released by the initiating explosion leads to formation of the detonation wave propagating through the multi-phase media. Figure 6a shows pressure contours for the propagating detonation wave at the time of t=12 × 10^{-6} msec after initiation. Here the pressure contour levels are shown on logarithmic scale in MPa. The maximum pressure value of 7940 MPa is observed in the layer of condensed explosive located near the ground. The pressure in this layer is two to three orders of magnitude higher than pressure behind the detonation wave in the 0.75 kg/m RDX cloud and air, which is located above the distance of 1.2cm from the ground. Figure 6a demonstrates that the detonation wave in the cloud is overdriven, since the pressure behind the shock continuously rises and reaches its maximum in the layer. From this figure, we also observe that the overdriven wave propagates faster in the cloud than in the layer. This is explained by the fact that it is easier to compress air that is very lightly loaded with particles and located above the ground layer, than it is to compress air heavily loaded with a particle mixture near the ground. It is interesting to note a discontinuous pressure change between the yellow contours and the light blue and green contours behind the detonation front. This discontinuity is over-emphasized by our presentation of contour lines on the logarithmic scale however, further examination of our simulation results indicates this feature is real and is similar in nature to barrel shocks observed for strong jets. It is different in nature from the triple shock structures described above

In Figure 6b, gas phase density contours are shown for the time $t = 12 \times 10^{-6}$ sec. Here the contour lines are distributed on logarithmic scale. The main features of the shock wave structure are very similar to those observed in the pressure contours figure. Here we see that a jet of high density gases reflects from the center of symmetry axis, creating a contact discontinuity that we will observe at a later time. The barrel shock is clearly visible in this figure. In Figure 6c, the particle density contour plots are shown for $t=12 \times 10^{-6}$ sec. The contour levels in this figure are given on the logarithmic scale and the initial deposition of the explosive material in the ground layer of the computational domain can be clearly observed. The black contour lines delineate the beginning and the end of the reaction zone in the cloud. To the left of these contours lies an area with combustion products and to the right unburned particles in the cloud. Here we can see that the reaction zone length is of the order of 1cm.

Figure 6d shows pressure contours for the same simulation for the time $t = 55 \times 10^{-6}$ sec, just before the detonation wave leaves the computational domain. In this figure, we see that the global structure of the wave did change slightly from Figure 6a. We observe that the barrel shock wave is fully developed and has a half ellipse shape. The detonation wave in the cloud is still overdriven; however, part of the shock wave front that propagates vertically weakened as it got further away from the detonation front in the layer. In Figure 6e, gas temperature contours are shown at $t = 55 \times 10^{-6}$ sec. In this case, it is interesting to note that the highest temperatures are observed behind the front of the overdriven detonation wave in the cloud, in the immediate vicinity of the upper strata of the layer. Very high temperatures in this region can be explained by the high pressure generated by the detonation of the explosive material in the layer and by relatively low density of strata of the cloud in the immediate vicinity to the layer. Here, as in the pressure contours graph, the area of barrel shock can be clearly identified.

We also observe in Figure 6 a clear development of two detonation fronts, one moving vertically in the cloud and another moving horizontally in the layer. Because the energy density of the explosive powder in the layer is about three orders of magnitude larger than that in the cloud, the vertical parts of the front represent overdriven detonation waves in the cloud. Even though the vertical front has slowed down compared with the horizontal front, its speed and parameters far exceed those typical for detonation waves in a cloud. In fact, the self-sustained detonation regime in the cloud will develop at the distance of about three meters from the layer. The area of the front close to the detonation wave in the layer will remain hot and overdriven, since it is located very close to detonation front in the layer. In Figure 6f, particle density contours are shown on a logarithmic scale. We can clearly observe the reaction zone delineated by black contour lines. In this case, the reaction zone length in the cloud is about 1cm. Consistent with the gradual transition from overdriven to self-sustained detonation, the reaction zone length is larger for the vertical part of the detonation front. The detonation wave velocity observed in our simulation is approximately 4048 m/sec, which is significantly lower than the detonation wave velocity observed in RDX with a density of 860 kg/m^3 (see Table 1), which is the highest density in the ground layer. This can be explained by the high gradient of particle density distribution in the layer, where the density drops rapidly from 860 kg/m^3 at the bottom of the layer to 0.75 kg/m^3 at the top strata of the layer at 12 mm above the ground.

4. CONCLUSIONS

We have presented a mathematical model and numerical solution for the simulation of initiation and propagation of the detonation waves in multi-phase mixtures consisting of solid combustible particles and gas. Using this model, we studied detonations in mixtures of solid RDX particles and air for the purpose of examining the effects of wide variation in particle density distribution on the dynamics and structure of detonation waves. We considered a physical system of layers of explosive RDX powder confined in a channel and studied initiation and propagation of the detonation waves in this system. This study revealed a specific structure of the detonation front that is dependent on the thickness of the layers and their energetic content. We showed that for the system consisting of two layers of the same thickness but of vastly different powder density, a Mach stem reflection occurs that propagates to the interface between the layers and helps create a stable detonation front. However, formation of the Mach stem reflection will be a strong function of the relative thickness of the layer; in one of the simulated examples, only a regular reflection would form in the simulation time frame.

For the system consisting of a solid particle cloud in air and a layer of high particle density near the ground, our simulations have revealed a specific detonation front shape with a characteristic precursor of the blast front in the strata immediately above the layer. This feature of the detonation front can be explained by the fact that the energy released in the detonation wave in the ground layer produces a faster shock wave in the dilute cloud than in these heavily loaded with solid particles stratums of the ground layer. However, these structures were not observed experimentally, and more studies are needed to examine their parameters.

The maximum pressure affecting the ground was di-

rectly related to the maximum particle density in the lower strata of the layer. However, the detonation front velocity for the fourth power distribution case was considerably lower than calculated for a one-dimensional case with 860 kg/m^3 particle density, reflecting the significant effect of two-dimensional expansion. Existence of the high density strata at the bottom of the ground layer in the fourth power case significantly increased the maximum pressure at the ground, and produced higher detonation wave velocity.

Using a variable density layer, one can reach a combination of pressure and velocity conditions outside of Chapmen-Jougett limitations. The range of conditions that can be obtained in the variable density system and its parametrics of that system needs a more systematic study. In this article, we introduced only the mathematical formulation and numerical simulation method validated for the range of conditions of interest. In addition, we have given some examples of its application for two-dimensional simulations. However, this methodology should be linked to an experimental study for a more in-depth analysis of the phenomenology discussed here.

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D[m/sec] - Detonation wave velocity,
P_{CJ}[Pa] - Pressure at Chapman-Jouguet Point
P_p[Pa] - Peak pressure; ρ_p[kg/m^3] - Peak density

RDX Density (kg/m^3)	Parameters	Present Calculation	Expt'l Ref. 1	Tiger Calculation Ref. 2	BKW Calculation Ref. 1	Soviet Experiments Ref. 3
1000 kg/m^3	D	6155	5981		6128	
	P_{CJ}	1.220×10^{10}			1.08×10^{10}	1.00×10^{10}
	P_p	2.57×10^{10}				
	ρ_p	1936				
860 kg/m^3	D	6031		5900		
	P_{CJ}	0.986×10^{10}		0.88×10^{10}		0.82×10^{10}
	P_p	1.95×10^{10}				
	ρ_p	1722				
466 kg/m^3	D	4800		4500		
	P_{CJ}	0.379×10^{10}		0.30×10^{10}	0.3×10^{10}	
	P_p	0.625×10^{10}				
	ρ_p	924				
250 kg/m^3	D	4049		3600		
	P_{CJ}	0.2478×10^{10}		0.13×10^{10}		
	P_p	0.4538×10^{10}				
	ρ_p	552				
100 kg/m^3	D	3495				
	P_{CJ}	0.5013×10^9				
	P_p	0.7658×10^9				
	ρ_p	220				
0.75 kg/m^3	D	1622	1410*	1870*		
	P_{CJ}	0.25×10^7	0.284×10^{7}*	0.26×10^{7}*		
	P_p	0.484×10^7				
	ρ_p	8				

Ref. 1 - Mader, C., "Numerical Modeling of Detonation," (University of California Press, Ltd., 1979), p. 47.
Ref. 2 - Wiedermann, A., "An Evaluation of Bimodal Layer Loading Effects," IITRI Report, Feb., 1990.
Ref. 3 - Stanukovitch, K.P., "Physics of Explosion" (in Russian), Nauka, 1975.

Table 1. One Dimensional Validation Result.

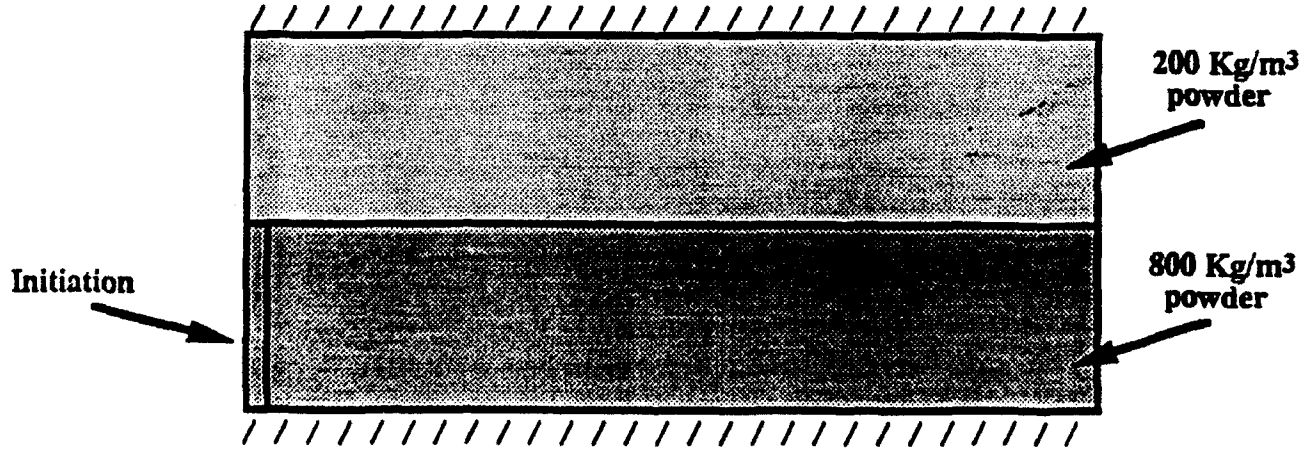

Figure 1. Setup for the two-layer detonation simulation problem.

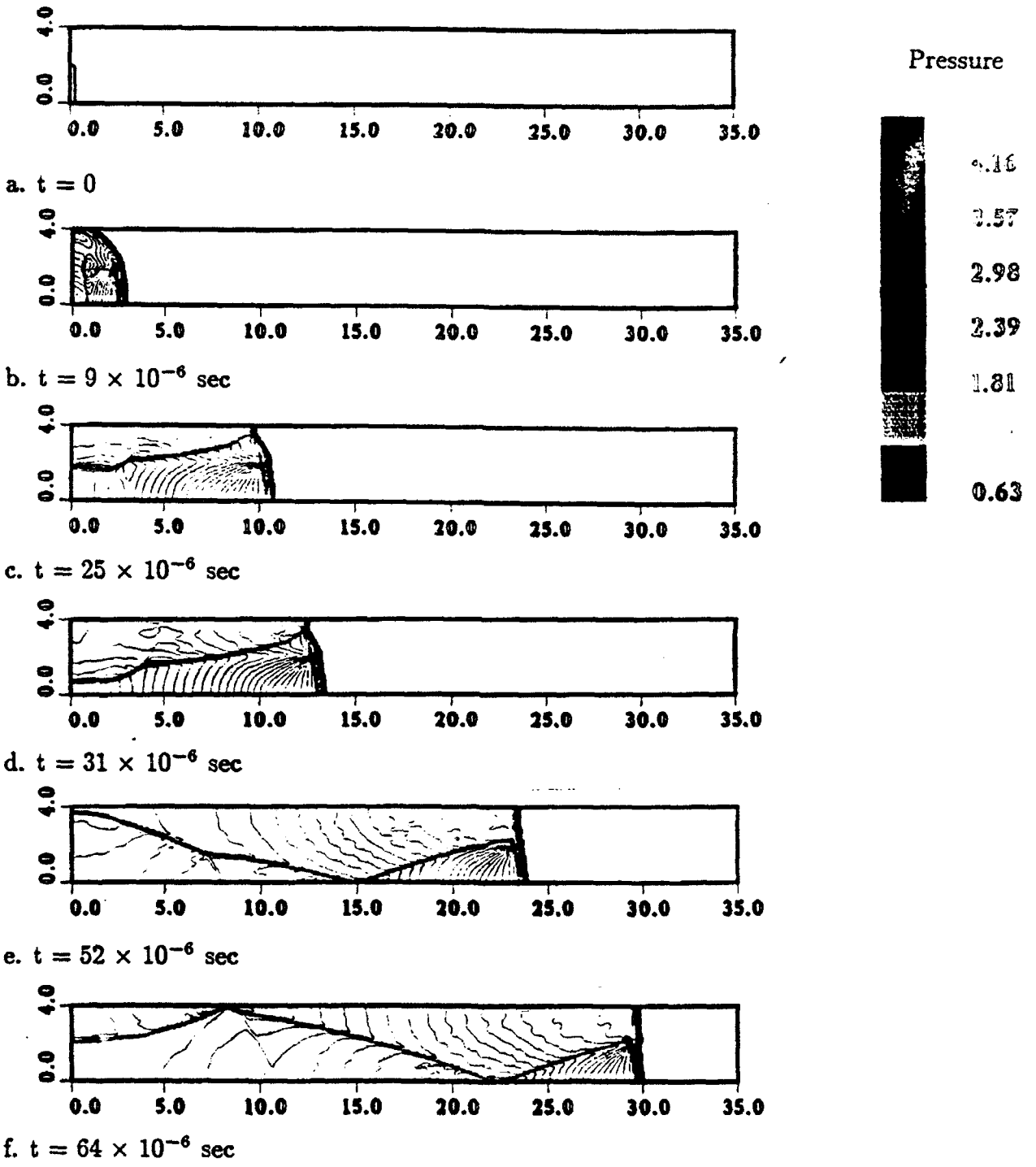

Figure 2. Initiation and propagation of the detonation wave in a two layers system. Only lower layer is initiated. Pressure contours.

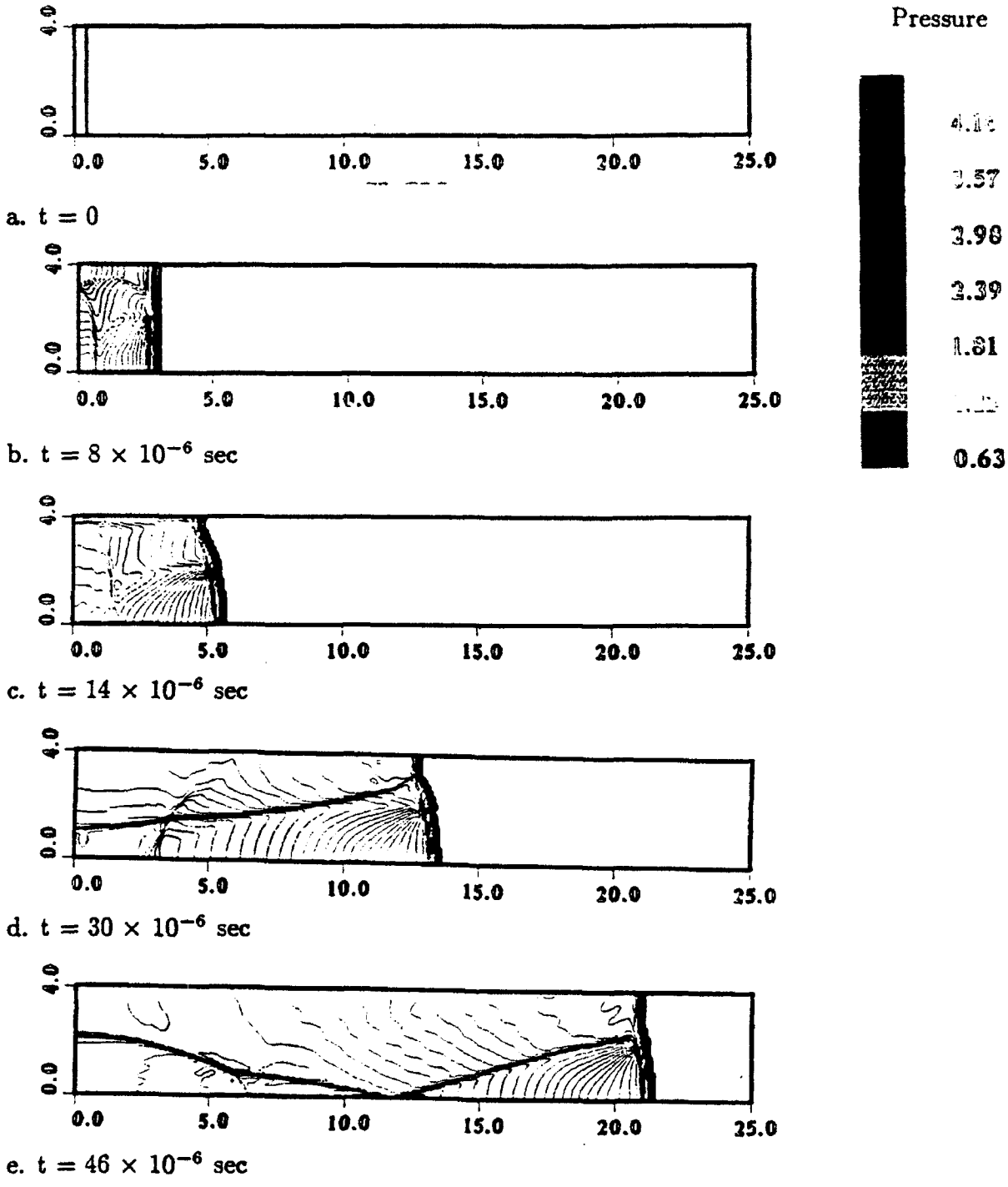

Figure 3. Initiation and propagation of the detonation wave in a two layers system. Both layers are initiated. Pressure contours.

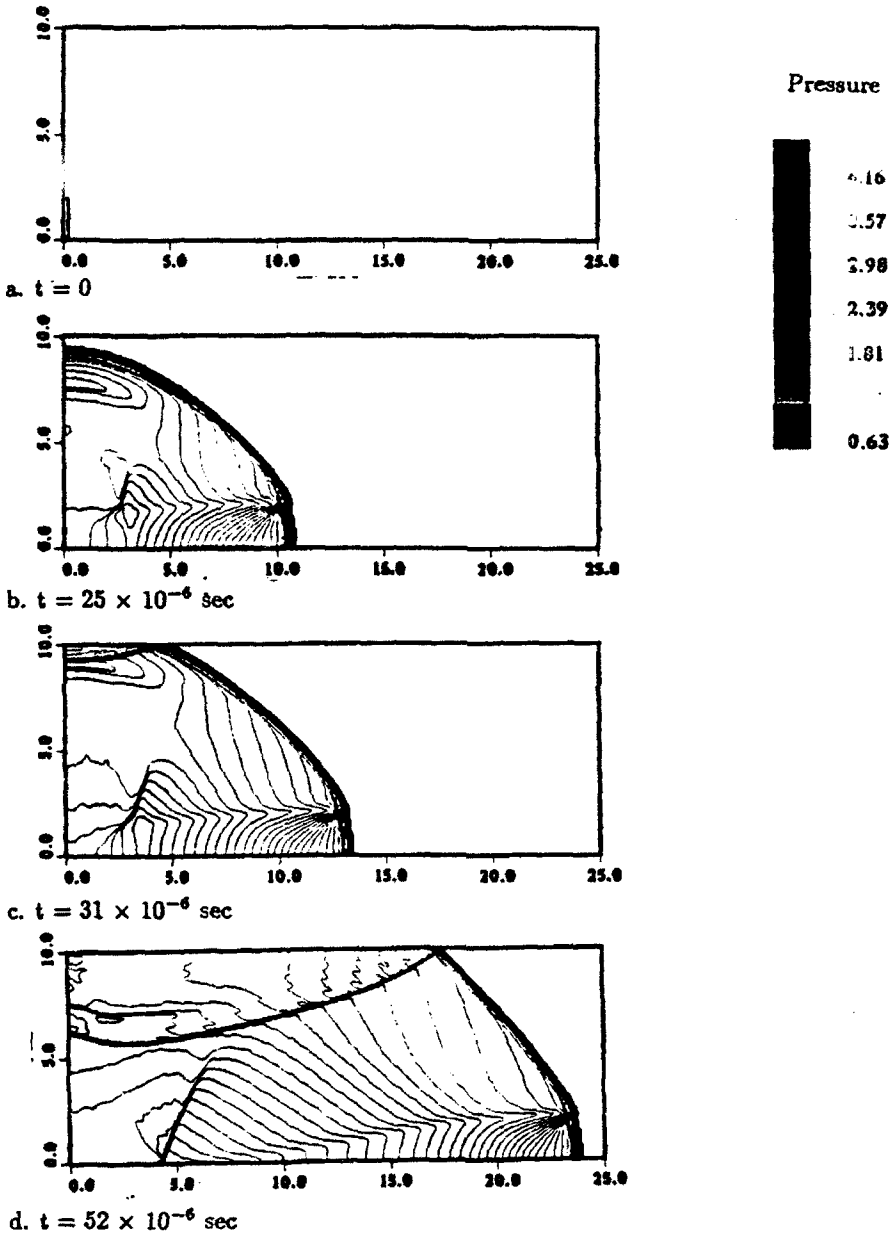

Figure 4. Propagation of the detonation wave in a system with different thickness of explosive layers. Pressure contours.

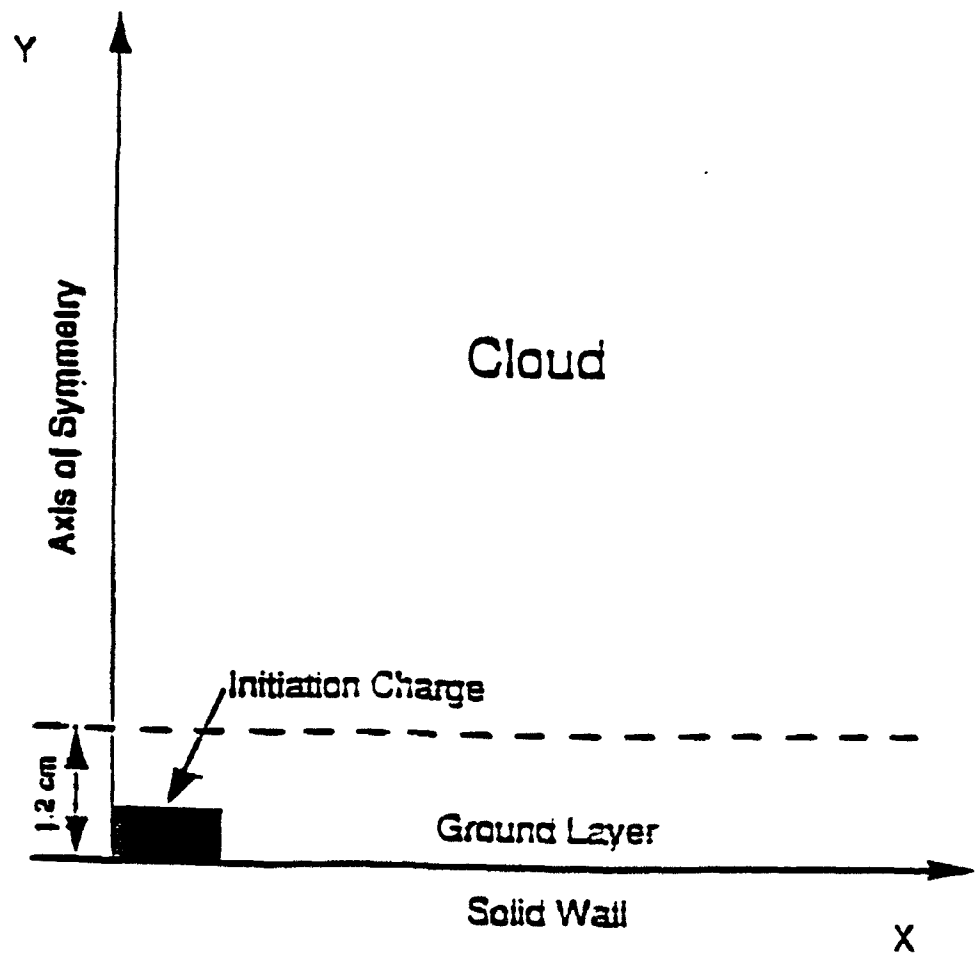

Figure 5. Computational domain and boundary conditions.

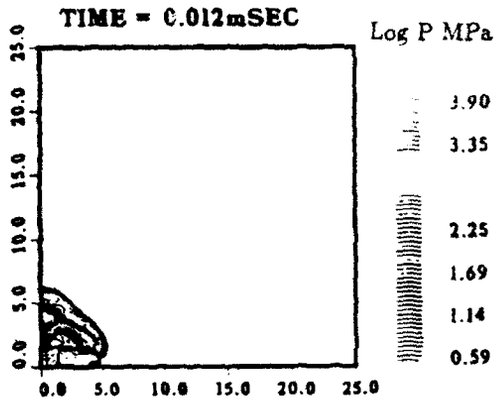

Fig. 6a. Pressure.

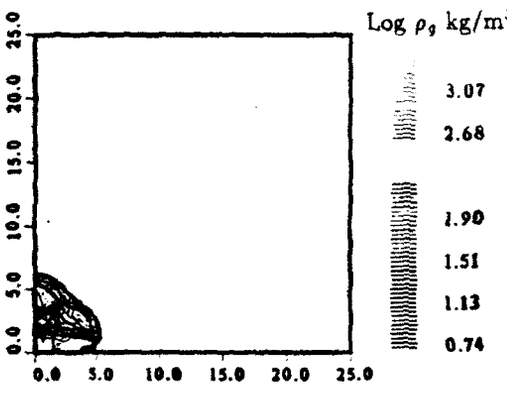

Fig. 6b. Gas Density.

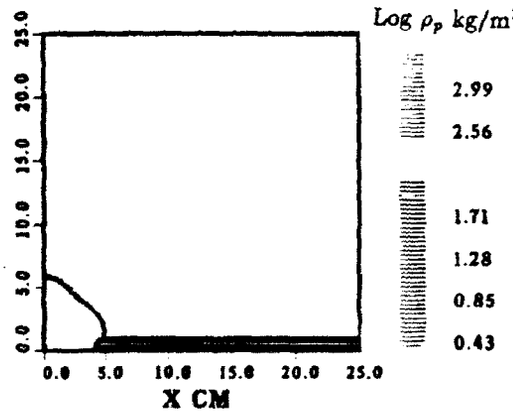

Fig. 6c. Particle Density.

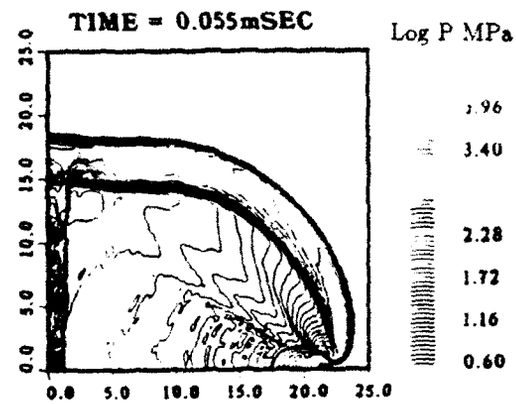

Fig. 6d. Pressure.

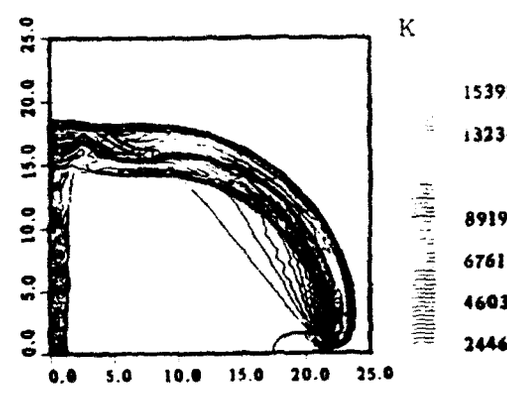

Fig. 6e. Temperature.

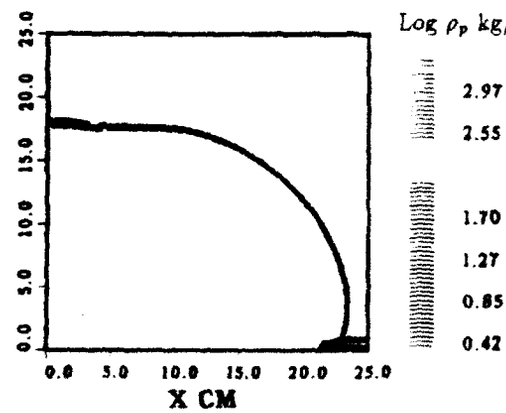

Fig. 6f. Particle Density.

Figure 6. Fourth power layer distribution. Maximum density in the layer 800 kg/m^3. Density in the cloud 0.75 kg/m^3. Time 0.012 msec and 0.055 msec after initiation.

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A Parametric Study of the Air-Breathing Pulsed Detonation Engine

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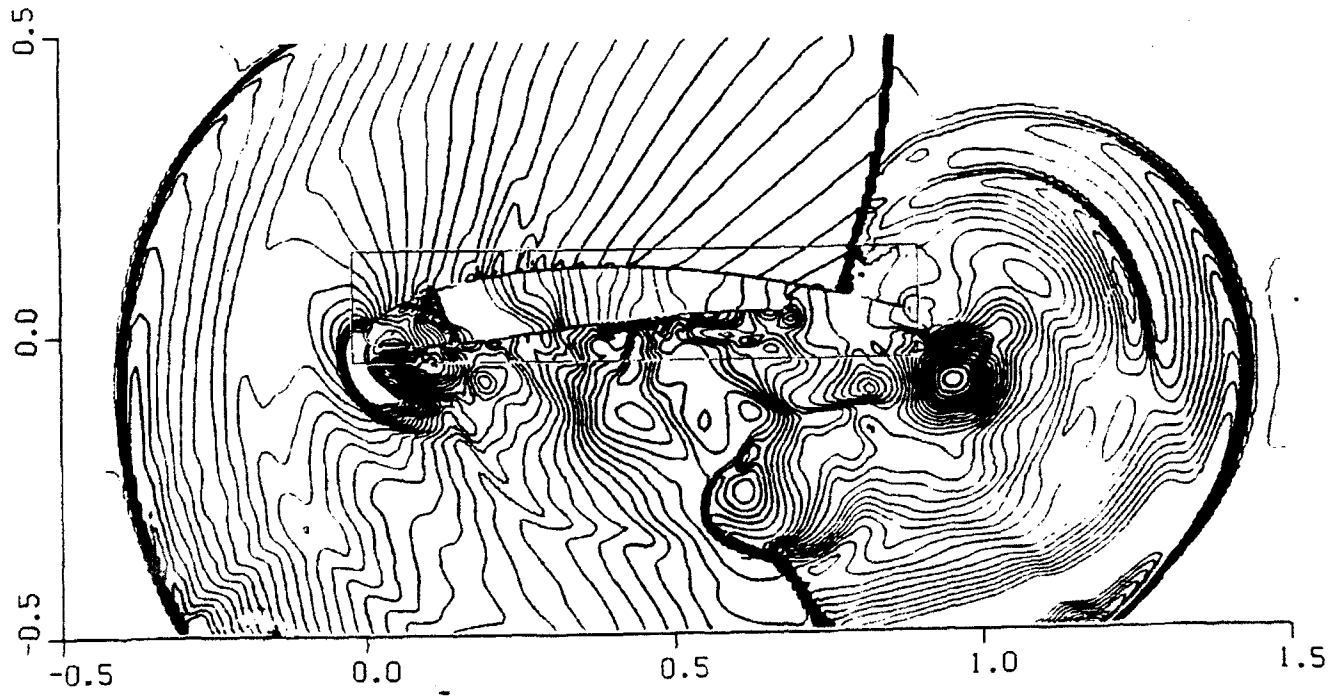

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A PARAMETRIC STUDY OF AIRBREATHING PULSED DETONATION ENGINE

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Abstract

The airbreathing Pulsed Detonation Engine (PDE) is analyzed by direct simulations of its cycle using Computational Fluid Dynamics. We describe a new CFD methodology of composite structured/unstructured grids, which is used for detailed analysis of the PDE performance. This performance is analyzed for a unique engine geometry in which the PDE is located in a wing section. Examination of the key processes in the PDE device shows that the largest portion of its thrust is produced during the very short time interval when the detonation wave reflects from the thrust wall, and that detonation cycle frequency up to 200Hz is feasible. We conclude that the PDE type devices can compete with small diameter turbojet engines in performance characteristics while surpassing them in simplicity of design, flexibility of geometrical configuration, and price.

1. Introduction

Our first reports on the airbreathing Pulsed Detonation Engine (PDE) concept[1-5] described a systematic series of parametric studies of the PDE via computational fluid dynamics (CFD). They also detailed an analysis of engine performance over a wide range of flight regimes, including subsonic and supersonic flows and physical geometries with various nozzle and air inlets. Additionally, static table top experiments[1] demonstrated that the principle of pulsed or repetitive detonation can be successfully applied. To date, our results indicate that practical engines for certain vehicles can be conceptualized and designed with the information that has already been generated from the studies. Specifically, our studies have shown that the PDE is an excellent candidate for the primary propulsion source for small aerodynamic vehicles that operate over the flight envelope, $0.2<M<2.0$. Further, our analysis of the simulation results indicates that the PDE is a high thrust-to-weight ratio device. The predicted performance places the PDE propulsion concept in a strongly competitive position compared with present day small turbojets. The PDE concept has the added attractiveness of rapid variable thrust control, no moving parts and the potential for low cost manufacturing. The PDE concept is scalable over a wide range of engine sizes and thrust levels.[4] For example, it is theoretically possible to produce PDE engines on the order of one to several inches in diameter and thrusts on the order of pounds, as well as devices that provide thousands of pounds thrust. One of the unique features of the PDE that will be explored in this paper is its geometric flexibility. All the configurations of the engine that we have examined in previous papers had an axisymmetric geometry. However, the PDE concept allows a tremendous flexibility in engine geometry. In this paper we will investigate the possibility of fitting a PDE det onation chamber into a section of a conventional wing One of the obvious advantages of this design is reductior of the drag and weight penalty; other advantages can b associated with stealth quality of the Wing-PDE design

The parametric studies to date were made possible by the development of a new generation of CFD tools. These tools have allowed us to accurately simulate the details of the complex nonlinear time dependent processes. In this article, we used a new algorithm implemented on a composite structured/unstructurec grid. This algorithm combines the flexibility of describing complicated geometries characteristic of the unstructured triangular grids with the computational efficiency of the structured grids. A brief description of the CFD methods employed in our studies is given in Section 3.

2. The Pulsed Detonation Engine Concept

A detonation process, due to the very high rate of reaction, leads to a propulsion concept in which the constant volume process can be fully realized. In detonative combustion, the strong shock wave, which is part of the detonation wave, acts like a valve between the detonation products and fresh charge. The speed of the detonation wave is about two orders of magnitude higher than the speed of a typical deflagration. This allows the design of propulsion engines with a very high power density. Each detonation has to be initiated separately by a fully controlled ignition device with a wide range of variable cycle frequencies. A physical restriction dictating the range of detonation frequency arises from the rate at which the fuel/air mixture can be introduced into the detonation chamber. This also means that a device based on a detonative combustion cycle can be scaled and its operating

parameters can be modified for a range of required output conditions.

There have been numerous attempts to take advantage of detonative combustion for engine applications,[6,7,8] the most recent and successful which was carried out at the Naval Postgraduate School[1] (NPS) by Helman et al. During this study, several fundamentally new elements were introduced to the concept that distinguished the NPS research device from previous studies. First, it is important to note that the NPS experimental apparatus was the first successful self- aspirating air breathing detonation device. Intermittent detonation frequencies of 25 Hz were obtained, which was in phase with the fuel mixture injection through the timed fuel valve opening and spark ignition. The feasibility of intermittent injection was established. Pressure measurements showed conclusively that a detonation process occurred at the frequency chosen for fuel injection. Further, self- aspiration was shown to be effective. Finally, the effectiveness of a primary detonation as a driver for the main detonation was clearly demonstrated. Although the NPS studies were abbreviated, many of the technical issues considered to be essential for efficient intermittent detonation propulsion were addressed with positive results.

The generic device we considered in our previous studies[2-5] is a small engine shown in Figure 1, which is a schematic of the basic detonation chamber attached to the aft end of a generic aerodynamic vehicle. In the current study, we considered a Wing-PDE configuration that will be described below; however, for the sake of simplicity we will describe the basics of the PDE concept using the illustration in Figure 1. For the engine configuration shown in this figure, the combustible gas mixture is injected at the closed end of the detonation chamber and a detonation wave, initiated at the aft end of the detonation chamber, propagates through the mixture. The main portion of the thrust is produced by the detonation wave in a very short period of time as it impinges on the thrust wall. After the detonation wave has reflected from the thrust wall, the detonation products will vent from the volume of the detonation chamber through the open aft end of the chamber and air inlets shown in Figure 1. Then the chamber volume will be filled with the fresh combustible gas mixture and the process will be repeated with the frequency of 100 to 200Hz. A key issue in the pulsed detonation engine concept is the design of the main detonation chamber. The detonation chamber geometry determines the propulsion efficiency and the duration of the cycle (frequency of detonations). Since the fresh charge for the generic engine is supplied from the external flow field, the efficiency of the engine depends on the interaction of the surrounding flow with the internal flow dynamics. The range of the physical processes requiring simulation in order to model the complex flow phenomena associated with the detonation engine performance is very broad. These processes include 1) initiation and propagation of the detonation wave inside the chamber; 2) expansion of the detonation products from the chamber into the air stream around the chamber at flight Mach numbers; 3) fresh air intake from the surrounding air into the chamber; 4) the flow pattern inside the chamber during post-exhaust pressure buildup which determines the strategy for mixing the next detonation charge; and 5) strong mutual interaction between the flow inside the chamber and surrounding the engine.

All of these processes are interdependent, and interaction and timing are crucial to engine efficiency. Thus unlike simulations of steady state engines, the phenomena described above cannot be evaluated independently. The need to resolve the flow regime inside the chamber and account for nozzles, air inlets, etc., and at the same time resolve the flow outside and surrounding the engine where the flow regime varies from high subsonic locally transonic and supersonic, makes it a challenging computational problem.

The single most important issue is to determine the timing of the air intake and mixing of the fresh charge leading to repetitive detonations. It is sufficient to assume inviscid flow for the purpose of simulating the expansion of the detonation products and fresh air intake. This assumption makes the numerical simulation of the PDE flow phenomena somewhat easier than using a fully viscous flow model. For the size of the generic device studied in this work, the effects of viscous boundary layers are negligible, with the exception of possible boundary layer effects on the valve and inlet geometries discussed subsequently.

3. Computational Method Used in the Study

The basic computational tool used for our studies is the AUGUST (Adaptive Unstructured Godunov Upwind Second Order on Triangular Grids) code, described in detail by Lottati et al.[9,10] This code provides a method for solving the Euler equations of gasdynamics on unstructured grids with arbitrary connectivity. The formulation is based on a second order Godunov method.[11] For the current study, the AUGUST code has been implemented on a composite structured/unstructured grid. The combined structured/unstructured method is a much more efficient approach to domain decomposition than the separate application of each method. In the following discussion, we show that the results of applying this technique to the complex problem of the external/internal reactive flow typical for the PDE engine show complex wave patterns propagating seamlessly through interfaces between structured/unstructured grids without reflections or distortions. This new approach provides ultimate flexibility

in domain decomposition with maximum code efficiency.

Introduction

Structured rectangular grids allow the construction of numerical algorithms that perform an efficient and accurate integration of fluid conservation equations. The efficiency of these schemes results from the extremely low storage overhead needed for domain decomposition and the efficient and compact indexing that also defines domain connectivity. These two factors allow code construction based on a structured domain decomposition that can be highly vectorized and parallelized. Integration in physical space on orthogonal and uniform grids produces the highest possible accuracy of the numerical algorithms. The disadvantage of structured rectangular grids is that they cannot be used for decomposition of computational domains with complex geometries.

The early developers of computational methods realized that, for many important applications of Computational Fluid Dynamics (CFD), it is unacceptable to describe curved boundaries of the computational domain using the stair-step approximation available with the rectangular domain decomposition technique. The techniques of boundary-fitted coordinates were developed to overcome this difficulty. With these techniques, the computational domain is decomposed on quadrilaterals that can be fitted to the curved domain. The solution is then obtained in the physical space using the geometrical information defining the quadrilaterals, or in the computational coordinate system that is obtained by transformation of the original domain into a rectangular domain. The advantage of this technique is that it employs the same indexing method as the rectangular structured domain decomposition methods that also serve to define domain connectivity. The boundary fitted coordinated approach leads to efficient codes, with approximately a 4:1 penalty in terms of memory requirement per cell as compared with rectangular domain decomposition. However, this approach is somewhat restricted in its domain decomposition capability, since distortion or large size variations of the quadrilaterals in one region of the domain lead to unwanted distortions or increased resolution in other parts of the domain. An example of this is the case of structured body fitted coordinates that are used for simulations of flows over a profile with sharp trailing edges. In this case, increased resolution in the vicinity of the trailing edge leads to increased resolution in the whole row of elements connected to the trailing edge elements.

The most effective methods of domain decomposition developed to overcome this disadvantage are those using unstructured triangular grids. These methods were developed to cope with very complex computational domains. The unstructured grid method, while efficient and powerful in domain decomposition, results in codes that must store large quantities of information defining the grid geometry and connectivity, and have large computational and storage overheads. As a rule, an unstructured grid code requires greater storage by a factor of 10, and will run about 20 times slower when compared on a per cell per iteration basis with a structured rectangular code.

Unstructured grid methods are used to their best advantage when combined with grid adaptivity. This feature usually allows dynamic decomposition of the computational domain subregions, thus leading to an order of magnitude reduction in the number of cells for some problems, as compared to the unstructured grid without this adaptive capability. However, this advantage is highly dependent on the problem solved. Adaptive unstructured grids have an advantage over the unadaptive unstructured domain decomposition if the area of high resolution domain decomposition is less than one tenth of the global area of the computational domain. This explains the fact that while the adaptive unstructured method may be extremely effective for solutions with multiple shock waves in complex geometries, it becomes extremely inefficient when high resolution is needed in a substantial area of the computational domain.

Our approach to domain decomposition combines the structured and unstructured methods for achieving better efficiency and accuracy. Using this method, structured rectangular grids are used to cover most of the computational domain, and unstructured triangular grids are used only to patch between the rectangular grids (Figure 2), or to conform to the curved boundaries of the computational domain (Figure 3). In these figures, an unstructured triangular grid is used to decompose the regions of the computational domain that have a simple geometry.

Our paper will illustrate the performance gains achieved from the use of this composite grid decomposition approach. We apply the Second Order Godunov method[11] to solve the Euler equations on both structured and unstructured sections of the grid.

Mathematical Model and Integration Algorithm

We consider a system of two-dimensional Euler equations written in conservation law form as:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0 \qquad (1)$$

where

$$U = \begin{vmatrix} \rho \\ \rho u \\ \rho v \\ \rho e \end{vmatrix}, \quad F = \begin{vmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(e+p) \end{vmatrix}, \quad G = \begin{vmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(e+p) \end{vmatrix}.$$

Here u, v are the x, y velocity vector components, p is the pressure, ρ is the density and e is total energy of the fluid. We assume that the fluid is an ideal gas and the pressure is given by the equation-of-state.

$$p = (\gamma - 1)(e - \frac{\rho}{2}(u^2 + v^2)) \tag{2}$$

where γ is the ratio of specific heats and typically taken as 1.4 for air. It is assumed that an initial distribution of the fluid parameters is given at $t = 0$, and the boundary conditions defining a unique solution are specified for the computational domain.

The system of governing equations in Eq. (1) can be written as

$$\frac{\partial U}{\partial t} + \nabla \cdot Q = 0 \tag{3}$$

where Q represents the convective flux vector. By integrating Eq. (3) over space and using Gauss' theorem, the following expression is obtained

$$\frac{\partial}{\partial t}\int_{\Omega} U dA + \oint_{\partial\Omega} Q dl = 0 \tag{4}$$

where $dl = n d\mathcal{L}, n$ is the unit normal vector in the outward direction, and $d\mathcal{L}$ is a unit length on the boundary of the domain. The variable Ω is the domain of computation and $\partial\Omega$ is the circumference boundary of this domain.

Equation (4) can be discretized for each element (cell) in the domain

$$\frac{(U_i^{n+1} - U_i^n)}{\Delta t} A_i = \sum_{j=1}^{M} Q_j^n n_j \Delta L_j \tag{5}$$

where A_i is the area of the cell; Δt is the marching time step; U_i^{n+1} and U_i^n are the primitive variables at the center of the cell at time n and at the update $n = 1$ time step; Q_j is the value of the fluxes across the M boundaries on the circumference of the cell where n_j is the unit normal vector to the boundary edge j, and ΔL_j is the length of the boundary edge j. The fluxes Q_j^n are computed by applying the Second Order Godunov algorithm, and Eq. (5) is used to update the physical primitive variables U_i according to computed fluxes for each marching time step Δt. The marching time step is subjected to the CFL (Courant-Fredrichs-Lewy) constraint.

We seek a solution to the system of Eq. (1) in the computational domain, which is decomposed in part into triangles with arbitrary connectivity and in part into rectangles using a logically structured grid. We use the advantage of the unstructured grid[12-15] to describe the curved boundary of the computational domain and areas that need increased local resolution; this covers 10% of the total computational domain. The structured grid occupies the remaining 90% of the computational domain in our example. The numerical technique for solving Euler's equation on an unstructured grid is described in Refs. 9-10, and the technique for the structured grid is described in Ref. 11. These numerical techniques apply some of the ideas that were introduced in Refs. 17-18. The structured and unstructured codes apply the center-based formulation, i.e., the primitive variables are defined in the center of the cell, which makes the cell the integration volume, while the fluxes are computed across the edges of the cell. The basic algorithmic steps of the Second Order Godunov method can be defined as follows:

1. Find the value of the gradient at the baricenter of the cell for each gas dynamic parameter U_i;
2. Find the interpolated values of U at the edges of the cell using the gradient values;
3. Limit these interpolated values based on the monotonicity condition;
4. Subject the projected values to the characteristic's constraints;
5. Solve the Riemann problem by applying the projected values at the two sides of the edges;
6. Update the gas dynamic parameter U according to the conservation equations (1) applying to the fluxes computed and the current time step.

As was advocated in Ref. 9, we prefer the triangle center-based over the vertex-based version of the code. For the same unstructured grid, a triangle-based algorithm will result in smaller control volumes than a vertex-based. In addition, for the Second Order Godunov solver, implementation of the boundary conditions is more straightforward and accurate for the center-based algorithm than in the vertex-based. These two factors, along with the effects of grid connectivity, strongly affect the algorithm accuracy and performance, and are the main reasons for the superiority of the center-based version over the vertex version.

4. Results for Wing-PDE configuration

All of our previous studies considered axisymmetric configurations of the PDE devices. However, because PDE does not have rotating parts, it allows another degree of flexibility that enables us to configure the PDE devices in other than axisymmetric geometries. To illustrate this, we used the inner volume of a section of the wing as a detonation chamber for a PDE device. The schematic of the Wing-PDE geometry considered in this study is shown in Figure 4. We assume that the wing is located in a subsonic air flow stream with M = 0.8. The particular wing shape used is the Gastelow cusped supercritical airfoil.[12] Two significant modifications of the original Gastelow airfoil geometry, provision for an inlet

at the leading edge and an outlet nozzle at the trailing edge, allow its use as a PDE device.

In Figure 5, the cross section of the Wing-PDE geometry is shown in the computational domain that is decomposed into structured rectangular and unstructured triangular grids. For clarity, we show only every sixth point of the grid used in simulation. In our simulations we have used a structured grid with 255×131 nodes and an unstructured grid with 7229 nodes. The area covered by the unstructured grid is about 10% of the total area of the computational domain. It is obvious from Figure 5 that the unstructured grid is used in the regions of the computational domain having complex geometry, i.e., wing external and internal surfaces, inlet, and nozzle. The structured rectangular grid is used to cover the rest of the computational domain. As mentioned previously, this method of domain decomposition leads to the most efficient use of computer resources. Our results demonstrate that flow propagates through the interfaces between the triangular unstructured and rectangular structured sections seamlessly.

First, we have to examine the flow pattern for the steady state flow regime of the Wing-PDE device shown in Figure 5. This will also establish the reference values of the airdynamic drag and lift for this configuration. In Figure 6a, the results are shown in form of the pressure contours for the converged steady state solution for the Wing-PDE configuration in M=0.8 external flow stream at zero angle of attack. We can observe in Figure 6a a very complex internal/external flow pattern around Wing-PDE geometry. In addition to the shock wave near the trailing edge on the upper surface of the wing, we can observe two additional shock waves. One is created by the flow exiting from the inner volume of the wing through the nozzle at the trailing edge, and another is created at the flow inlet located under the leading edge. The air flow enters the inner volume of the wing through the inlet and creates a complex flow field with an average pressure of ≈ 1.0 atm. It is easy to improve the flow uniformity in the inner volume of the inlet geometry and geometry of the inner surfaces. However, these aspects of the Wing-PDE design will be considered in future studies; for the purposes of this paper, we examine only the main features of the Wing-PDE configuration. The air flow in the inner volume of the wing create considerable drag. By integrating the pressure over the inner and outer surface of the Wing-PDE configuration, we have calculated the basic air dynamic characteristics of this profile at M = 0.8 flow. The following values for the steady state flow:

Lift: $C_l = 0.18$; *Drag:* $C_d = -0.138$; *Pitching Moment:* $C_m = 0.034$.

We have assumed that at $t = 0$, the inner volume of the wing is filled with a detonable gas mixture. The detonation wave is initiated at the aft end of the inner volume of the wing by a planar front. The fuel chosen for these simulations was ethylene. The detonability limits of ethylene in air range from 4% to 12% concentrations by volume, and depend somewhat on temperature and pressure. We assume for the sake of simplicity that the fuel/air ratio is 6% by volume.

In Figure 6b, the pressure contours are shown at $t = 1.18 \times 10^{-4}$ sec. The propagation of the detonation front is planar. However, because of the curved inner walls of the wing, the detonation front reflects from the wall surfaces and the maximum pressure in the reflected waves reach 36.6 atm. However, this level of pressure is observed in a very small area of the detonation front where reflected or colliding transverse waves can cause a local maximum. The detonation wave velocity for this mixture is about 1800 m/sec.

In Figure 6c, the pressure contours are shown at the time $t = 5.24 \times 10^{-4}$ sec, shortly after the detonation front has reflected from the inner surface of the leading edge. Here the maximum pressure was dropped to 12.1 atm, the reflected shock is moving in the direction of the trailing edge, and the expansion of the detonation products through the inlet was created a semicircular shock wave that propagates in the opposite direction to the external flow stream. In Figure 6d at the time $t = 9.5 \times 10^{-4}$ sec, the reflected wave reaches the nozzle at the trailing edge, and expansion of the detonation products through this nozzle creates an additional shock wave that expands in the direction of the flow stream. When the original reflected shock has reached the converging area at the trailing edge, it will partially reflect and send a shock wave towards the inner surface of the leading edge. In Figure 6e, the pressure contours are shown at $t = 1.39 \times 10^{-3}$ sec. Here the shock waves created by the detonation products emitting from the inlet and nozzle of the Wing-PDE device collide, creating a complex flow pattern with two triple point shocks, a vortex at the trailing edge and a complex system of waves propagating through the inner volume of the wing. The maximum pressure observed in Figure 6e at the wave shock wave interaction is 3.2 atm. It is important to note that the numerical method simulates the flow evolution seamlessly through the structured/unstructured grid interfaces.

In Figure 6f, the simulation results are shown at $t = 5.7 \times 10^{-3}$ sec; this corresponds to the end of one cycle for the Wing-PDE configuration. Here we can observe that the flow pattern is very similar to the one in Figure 6a, except for some vortices propagating in the lower right part of the computational domain. The maximum pressure is reached at the leading edges and has the same values as shown in Figure 6a. The inner volume of the wing has a relatively uniform flow pattern

with an average pressure of 0.83 atm. At this time the gaseous mixture in the inner chamber of the wing will be initiated at the trailing edge and the second cycle will get started.

Examination of the details of the flow pattern resulting from a single detonation not only allows evaluation of the timing between the subsequent detonations but also provides important information for optimization of mixing, detonation products expansion, and other gasdynamic processes related to operation of the PDE cycle. Performance characteristics of the PDE device can be analyzed by integrating in time the forces exerted by pressure on the inner and outer surfaces of the Wing-PDE device. In Figure 7, results for such an integration of the force parallel to the ground as a function of time are shown. Calculation of this force, taking into account the drag and the thrust resulting from the detonation cycle, yields the net thrust force. Figure 7 gives this force for a linear meter of the wing in pounds. In this figure, we observe that the net thrust force is negative before the detonation is initiated, reaches the value of 4.6×10^5 Lb/M during the reflection of the main detonation front from the inner walls of the wing, and quickly decays to its negative initial values that correspond to the drag of the Wing-PDE configuration in M=0.8 ambient flow stream. The positive thrust force is produced by the detonation engine in a very short time interval; $\approx 3.0 \times 10^{-4}$ sec.

The time integral of the force shown in Figure 7 is thrust produced by the PDE device. Because of its intermittent operation, we need to assume the cycle frequency to be able to calculate the net thrust. In Figure 8, the results of thrust force integration are shown in the assumption of 200Hz detonation frequency of the Wing-PDE device. Our analysis above of a single cycle shows that this frequency of operation is feasible. In Figure 8, we observe that the maximum thrust of 5000 lb per linear meter of the wing is achieved in the first $\approx 4.0 \times 10^{-4}$ sec after the detonation wave impinges on the thrust wall. This period of time corresponds to the duration of the positive thrust force shown in Figure 7. After this, the thrust will erode because of drag force to the value of 4000 lb at the end of the cycle. The average thrust for the duration of the cycle is 4250 lb per linear meter of the wing.

One of the advantages of the Wing-PDE configuration is that it will generate lift. Our simulations show that the chosen configuration will produce significant lift even at zero angle of attack because of the flow of detonation products. In Figure 9, the net integrated lift is presented as a function of time in the same format as the net thrust shown in Figure 8. The integrated lift shown in Figure 9 is not a linear function of time, as will be the case for the steady state flow regime. Substantial lift is generated shortly after the detonation products start to expand into the surrounding flow stream. The average lift generated is about 2250 lb per meter of wing length: this is comparable to the net thrust of 4250 lb. Our estimates indicate that about half of this lift is generated by the detonation products and the other half by the free stream flow through the chamber.

5. Conclusions

We have presented a powerful numerical technique for analysis of nonsteady flow over a complex geometrical configuration in the computational domain decomposed on unstructured triangular and structured rectangular grids. Simulations of the Wing-PDE cycle have demonstrated flexibility and efficiency of this technique of domain decomposition. Numerical results show seamless propagations through structured/unstructured grid interfaces of the multiple shocks, contact discontinuities. vortices, rarefaction waves and other complex flow features.

Use of this powerful numerical technique allowed us to examine the operation cycle and propulsion characteristics of the Wing-PDE device. We demonstrated in this study that in principle, the Wing-PDE device can operate with the 200 Hz cycle frequency producing 4250 lb per linear meter of the wing of the net thrust. We examined the Wing-PDE configuration to illustrate the geometric flexibility of this engine. This is an additional advantage to efficiency,[3] scalability,[4] thrust control,[3] simplicity, and low cost of this device discussed in our previous publications.

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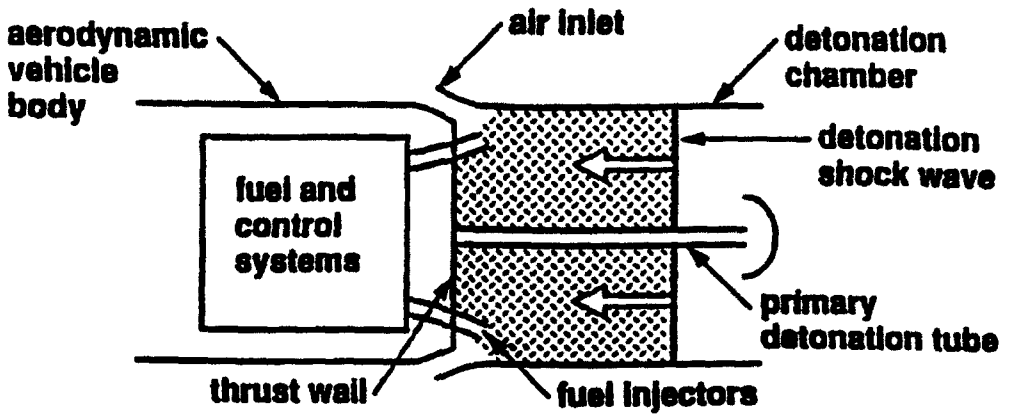


Figure 1. Schematic of the generic PDE showing detonation chamber, inlet, detonation wave, fuel injectors and position relative to an aerodynamic vehicle.

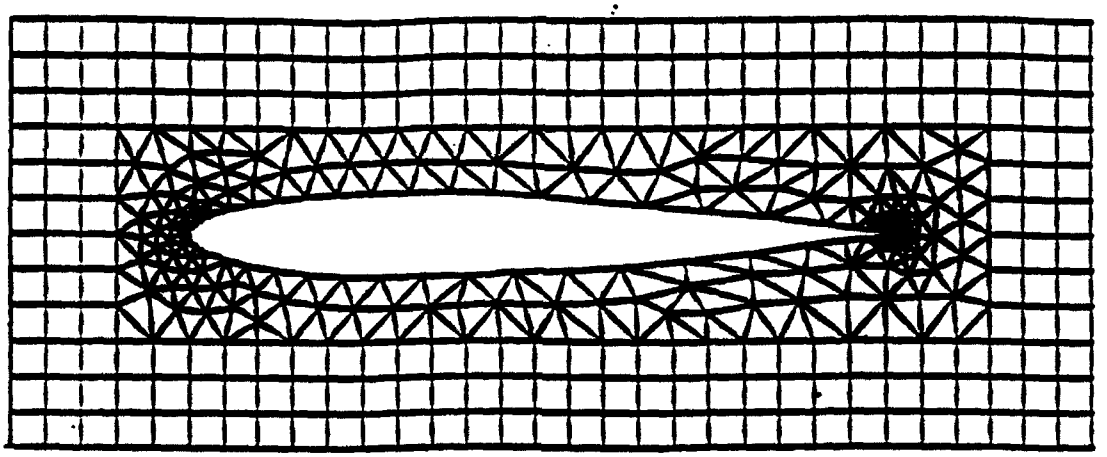


Figure 2. An example of hybrid structured/unstructured domain decomposition.

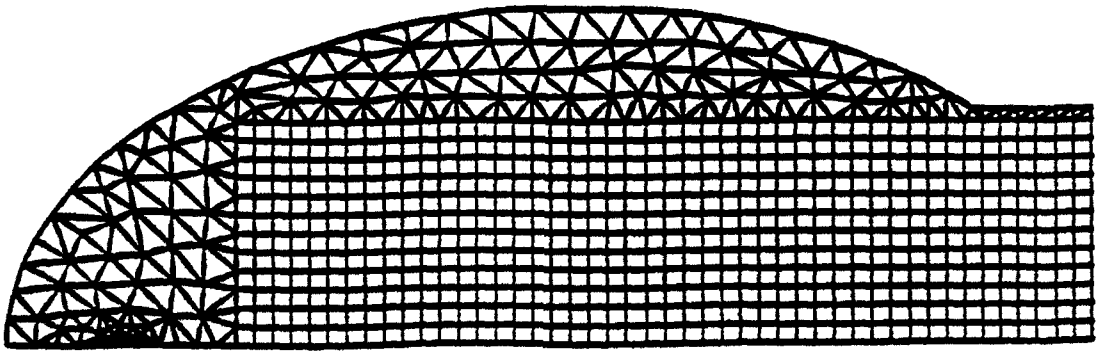


Figure 3. An example of hybrid structured/unstructured domain decomposition.

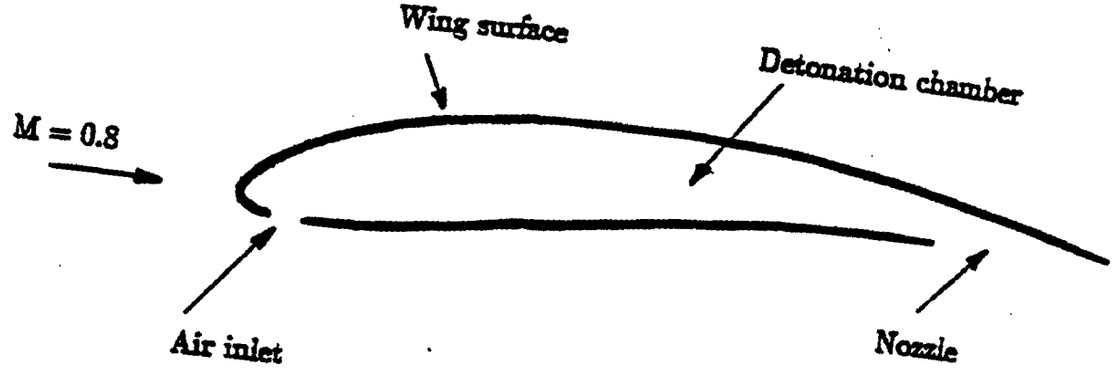


Figure 4. Schematics drawing of the wing-PDE configuration.

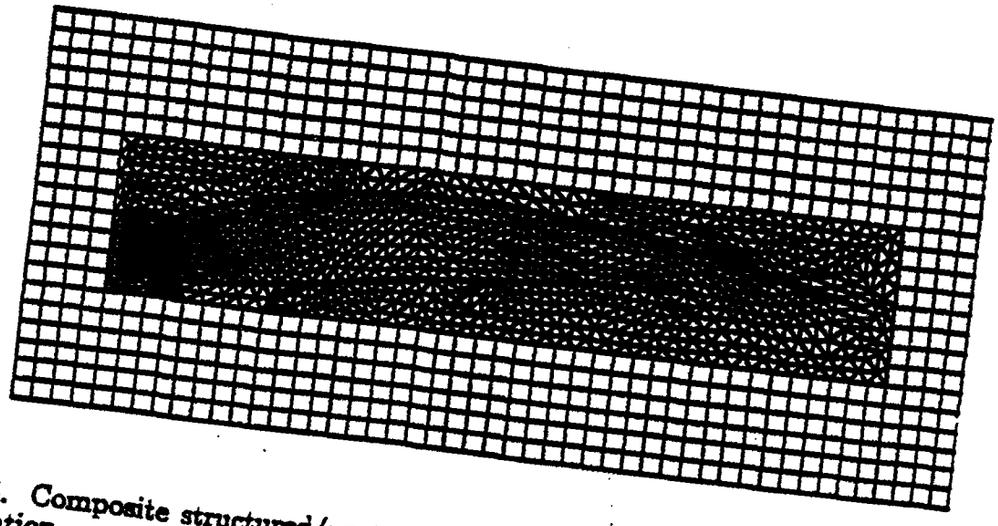
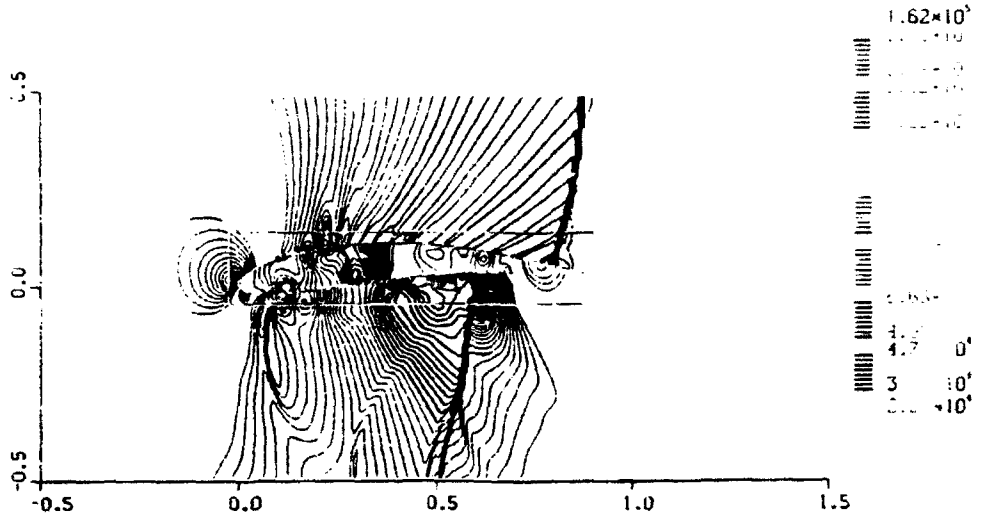
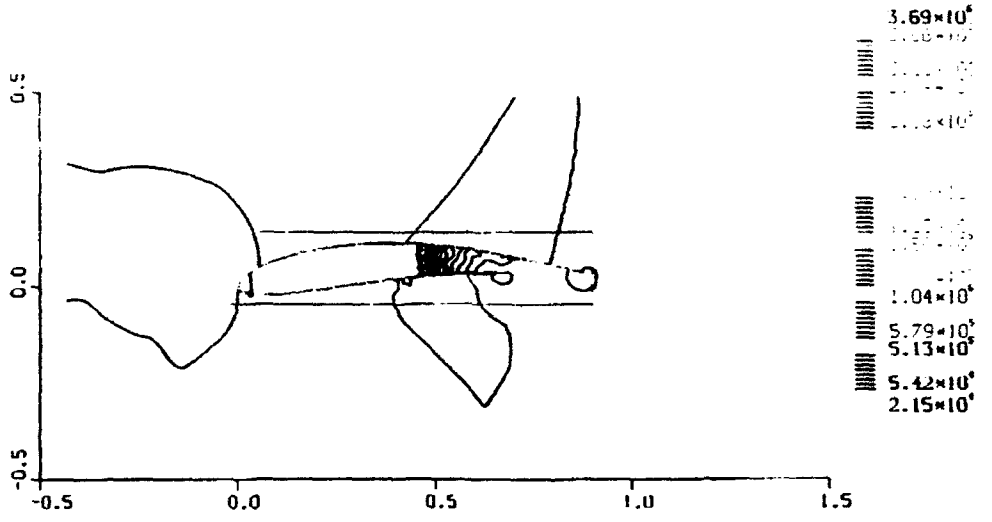


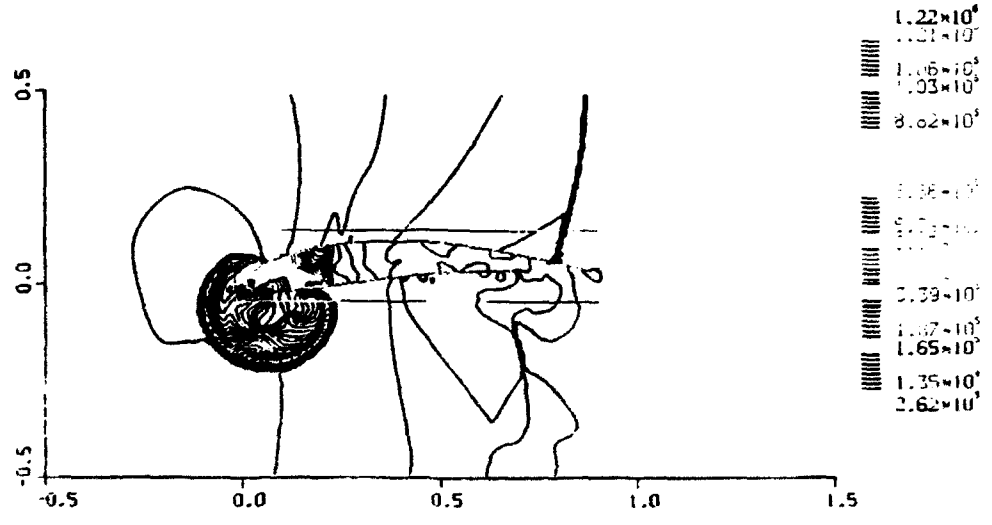
Figure 5. Composite structured/unstructured computational domain for the wing-PDE configuration.



a. Steady state

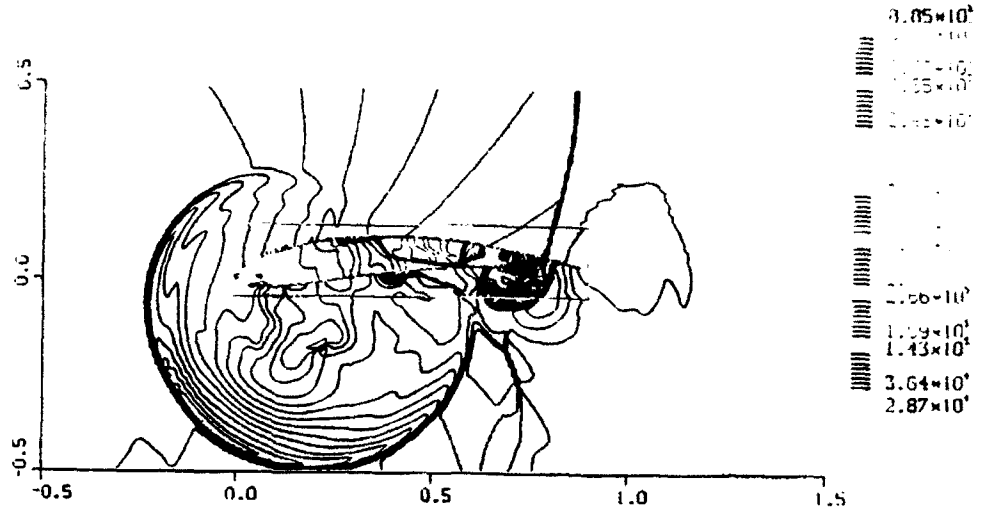


b. $t = 1.18 \times 10^{-4}$ sec

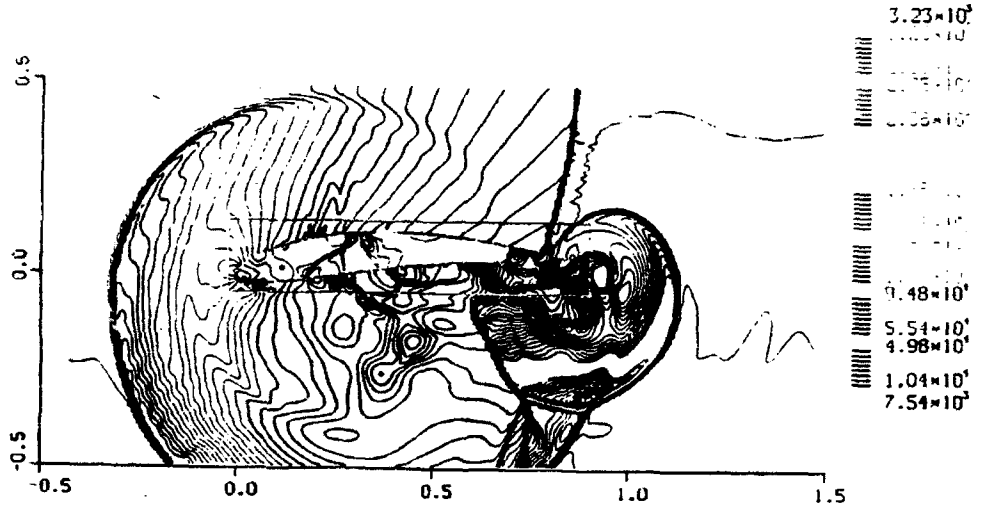


c. $t = 5.24 \times 10^{-4}$ sec

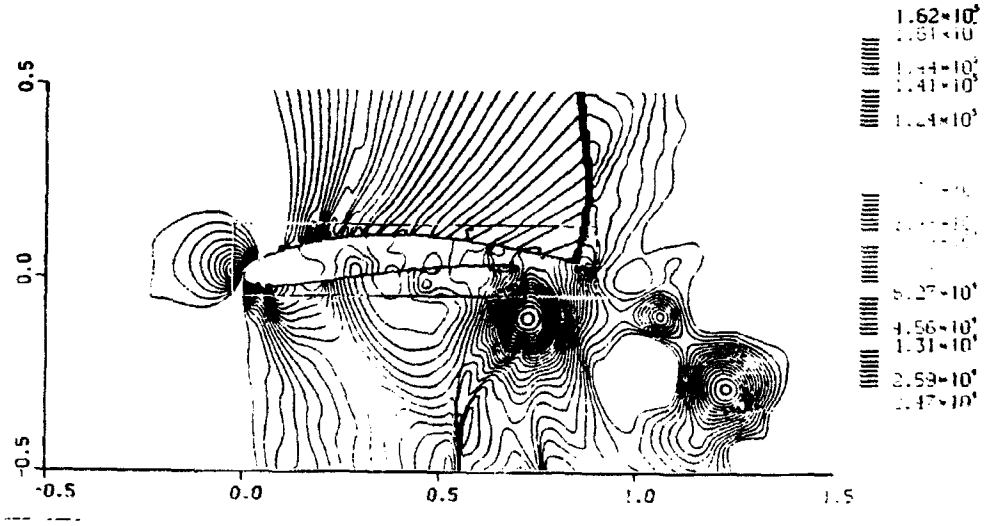
Figure 6. Pressure contours for the various time intervals of the wing-PDE cycle.



d. $t = 9.50 \times 10^{-4}$ sec



e. $t = 1.39 \times 10^{-3}$ sec



f. $t = 5.77 \times 10^{-3}$ sec

Figure 6. Pressure contours for the various time intervals of the wing-PDE cycle (continued).

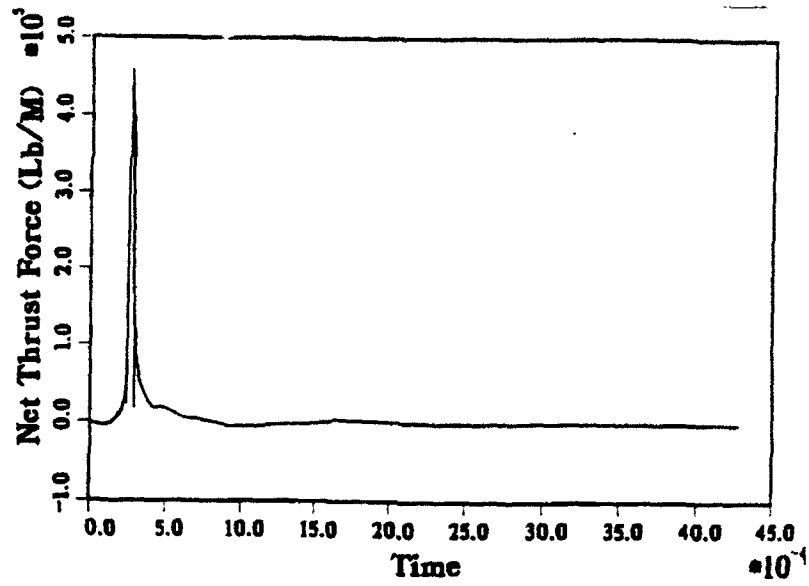


Figure 7. Thrust force as function of time for the wing-PDE device simulation.

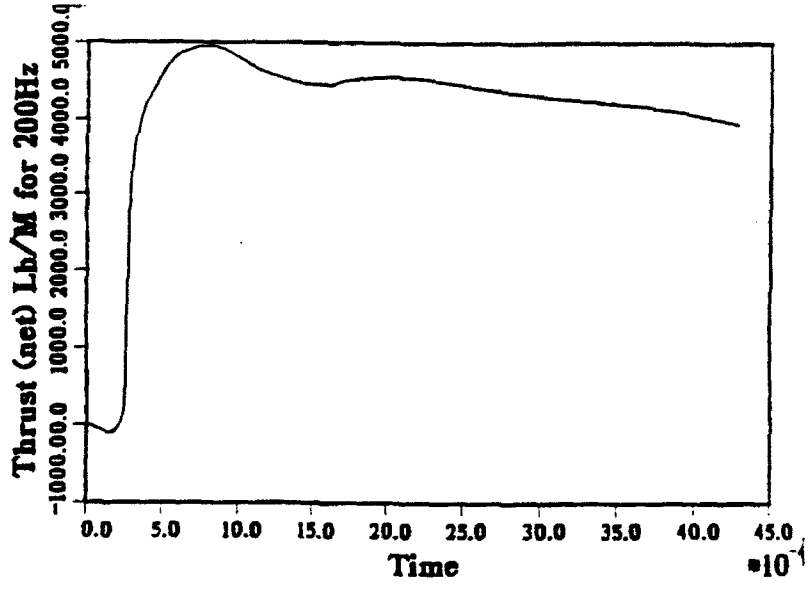


Figure 8. Net integrated thrust for the wing-PDE simulation.

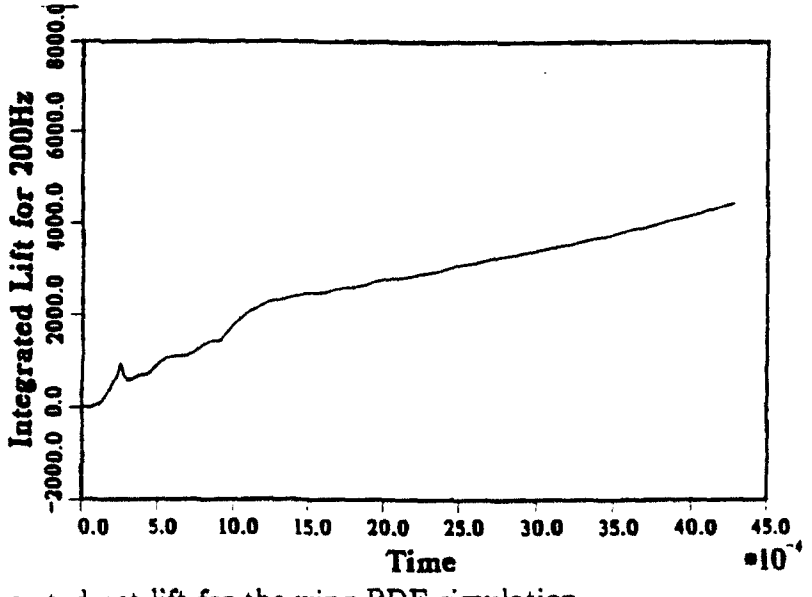


Figure 9. Integrated net lift for the wing PDE simulation.

A Second Order Godunov Scheme on Spatial

Adapted Triangular Grid

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ABSTRACT

Spatial adaptation procedure for the accurate and efficient solution of unsteady inviscid flow simulation is described. The adaptation procedures were developed and implemented applying a second order Godunov scheme. These procedures involve mesh enrichment/coarsening to either add/remove vertices in high/low gradient regions of the flow, respectively. The goal is to achieve solutions of high spatial accuracy at minimal computational cost. The paper describes a very effective error estimator to detect high/low activity regions of the flow to be enriched or coarsened, respectively. The error estimator is based on total energy and density fluxes into the cell combined with gradient of density. Included in the paper is a detailed description of the direct dynamic refinement method that is used for adaptation. A detailed simulation of a reflection and diffraction of multiple shock waves flowing over a diamond shape wedge is presented and compared with experimental results. The simulated results are shown to be in excellent agreement with the experiment primarily in that all the complicated features of the physics are accurately accounted for and the shock waves, slip lines, vortices are sharply captured.

INTRODUCTION

Considerable progress has been made over the past decade in developing methods for spatial adaptation of the computational meshes based on the numerical solution of the simulated physics. These methods are being developed to produce higher spatial accuracy in such simulation more efficiently. The goal of mesh adaptation is to enrich meshes locally, based on the numerical solution, in order to capture physical features of importance; in contrast to globally fine meshes, this process will minimize computer run times and memory costs. The methods of mesh adaptation can be categorized into three general classes: 1) mesh regeneration, 2) mesh movement, and 3) mesh enrichment.

The idea of mesh regeneration is systematically to identify high/low activity region in the flow and accordingly remesh those regions applying mesh generation code. This is done by assigning criteria for spatial accuracy and number of vertices. This procedure requires a mapping of the "old" flow solution into the "new" generated meshes by using one of the interpolated schemes. For the second method, mesh movement, the number of points in the computational domain remains fixed. The adaptation procedure moves vertices from low activity regions to high gradient regions to achieve a high concentration of vertices to resolve high activity regions. The movement of the points is dictated by forcing functions in the Poisson - equation in the grid generator code. The final method of spatial adaptation is mesh

enrichment. In this method. vertices are added or removed according to the spatial resolution of the physical features in the flow. The advantages of mesh enrichment over regeneration and movement are its higher degree of flexibility in being able to add points where they are needed and to remove points where they are not needed. In our mesh enrichment method, we add points ahead of the shock wave, thus preventing the need of interpolation in the high gradient region for achieving higher accuracy of the results. Adding and removing points are done in monotone/very low activity regions to prevent numerical dissipation.

Lohner[1] has developed procedures to enrich the mesh for transient flow problems locally by subdividing elements in the grid according to specific spatial resolution criteria. The method, referred to as H-refinement, keeps a history of the initial grid (mother grid) and the subdivision of each level (daughter grids). The H-refinement relies heavily on the initial grid as it is subdivided for enrichment and recovered in the coarsening stage. A similar adaptive strategy to Lohner is adopted by Rausch[2] et al., but applies a different error estimator and upwind type algorithm for a solver.

In our paper, we describe a Godunov scheme to solve Euler equations on an unstructured adaptive triangle mesh. We discuss the methodology of a cell centered Second Order Godunov scheme applied to a triangular mesh, and the method of Direct Dynamic Refinement that is used for adaptation of the unstructured triangular grid. Simulation and experimental results

are compared for a test case applying the adaptive unstructured grid to a complicated pattern of planar shock wave flow diffraction over a half diamond shape wedge.

SECOND ORDER GODUNOV ALGORITHM ON UNSTRUCTURED GRID

This section describes the implementation of the Second Order Godunov algorithm on a triangular unstructured grid. The algorithm is explicit and is cell-center based.

We consider a system of two-dimensional Euler equations written in conservation law form as:

$$\frac{\partial \bar{U}}{\partial t} + \frac{\partial \bar{F}}{\partial x} + \frac{\partial \bar{G}}{\partial y} = 0 \qquad \text{(i)}$$

where

$$U = \begin{Bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{Bmatrix}, F = \begin{Bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(e+p) \end{Bmatrix}, G = \begin{Bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(e+p) \end{Bmatrix}.$$

Here u, v are the x, y velocity vector components, p is the pressure, ρ is the density and e is total energy of the fluid. We assume that the fluid is an ideal gas. The total energy of gas is given by the following equation:

$$e = \frac{p}{\gamma - 1} + \frac{\rho}{2}(u^2 + v^2) \qquad (2)$$

where γ is the ratio of specific heats. It is assumed that an initial distribution of the fluid parameters is given at $t = 0$, and the boundary conditions defining a unique solution are specified for the computational domain.

The system of governing equation (1) can be written in the following form:

$$\frac{\partial U}{\partial t} + \bar{\nabla} \cdot \bar{Q} = 0 \tag{3}$$

where $\bar{Q}$ represents the convective flux vector. By integrating Eq. (3) over space and using Gauss' theorem, the following expression is obtained

$$\frac{\partial}{\partial t} \int_{\Omega} U dA + \oint_{\partial \Omega} \bar{Q} \cdot d\bar{l} = 0 \tag{4}$$

where $d\bar{l} = \bar{n} d\mathcal{L}$, $\bar{n}$ is the unit normal vector in the outward direction, and $d\mathcal{L}$ is a unit length on the boundary of the domain. The variable Ω is the domain of computation and $\partial\Omega$ is the circumference boundary of this domain.

Equation (4) can be discretized for each element (cell) of the domain

$$\frac{(U_i^{n+1} - U_i^n)}{\Delta t} A_i = \sum_{j=1}^{3} \bar{Q}_j^{n+\frac{1}{2}} \bar{n}_j \Delta L_j \tag{5}$$

where A_i is the area of the cell; Δt is the marching time step; U_i^{n+1} and U_i^n are the primitive variables at the center of the cell at time n and at the update $n + 1$ time step; $\bar{Q}_j$ is the value of the fluxes across the three boundaries edges on the circumference of the cell where $\bar{n}_j$ is the unit normal

vector to the boundary edge j, and ΔL_j is the length of the boundary edge j. Equation (5) is used to update the physical primitive variables U_i according to computed fluxes for each time step Δt. The time step is subjected to the CFL (Courant-Fredrichs-Lewy) constraint.

To obtain a second order spacial accuracy, the gradient of each primitive variable is computed in the baricenter of the cell. This gradient is used to define the projected values of primitive variables at the two sides of the cell's edge, as is shown in Figure 1. The gradient is approximate by a path integral

$$\int_{\Omega} \bar{\nabla} U_i^{cell} dA = \oint_{\partial\Omega} U_j^{edge} d\bar{l} \,. \tag{6}$$

The notation is similar to the one used for Eq. (5) except the domain Ω is a single cell and U_i^{cell} and U_j^{edge} are values at the baricenter and on the edge respectively. The gradient is estimated as

$$\bar{\nabla} U_i^{cell} = \frac{1}{A} \sum_{j=1}^{3} \tilde{U}_j^{edge} \bar{n}_j \Delta L_j \tag{7}$$

where $\tilde{U}_j^{edge}$ is an average value representing the primitive variable value for edge j.

The gradients that are computed at each baricenter are used to project values for the two sides of each edge by piecewise linear interpolation. The interpolated values are subjected to monotonicity constraints.[3] The monotonicity constraint assures that the interpolated values are not creating new

extrema.

The monotonicity limiter algorithm can be written in the following form:

$$U^{edge}_{projected} = U^{cell}_i + \phi \bar{\nabla} U_i \cdot \Delta \bar{r} \tag{8}$$

where $\Delta \bar{r}$ is the vector from the baricenter to the point of intersection of the edge with the line connecting the baricenters of the cells over the two sides of this edge. ϕ is the limiter coefficient that limits the gradient $\bar{\nabla} U_i$.

First, we compute the maximum and minimum values of the primitive variable in the i's cell and its three neighboring cells that share common edges (see Fig. 1):

$$\left.\begin{aligned} U^{\max}_{cell} &= Max\left(U^{cell}_k\right) \\ U^{\min}_{cell} &= Min\left(U^{cell}_k\right) \end{aligned}\right\} k = i, 1, 2, 3 \ . \tag{9}$$

The limiter can be defined as:

$$\phi = Min\left\{1, \phi^{lr}_k\right\} \quad k = 1, 2, 3 \tag{10}$$

where superscript lr stands for left and right of the three edges (6 combinations in total). ϕ^{lr}_k is defined by:

$$\phi^{lr}_k = \frac{\left[1 + Sgn\left(\Delta U^{lr}_k\right)\right] \Delta U^{\max}_{cell} + \left[1 - Sgn\left(\Delta U^{lr}_k\right)\right] \Delta U^{\min}_{cell}}{2(\Delta U^{lr}_k)} \quad k = 1, 2, 3 \tag{11}$$

where $\Delta U_k^{lr} = \bar{\nabla} U_i^{lr} \cdot \Delta \bar{r}_k$. and

$$\left.\begin{aligned} \Delta U_{cell}^{\max} &= U_{cell}^{\max} - U_i^{cell} \\ \Delta U_{cell}^{\min} &= U_{cell}^{\min} - U_i^{cell} \end{aligned}\right\} . \tag{12}$$

To obtain a second order of accuracy in time and space, we subject the projected values of the left and right side of the cell edge to characteristic constraints following Ref. 4. The one dimensional characteristic predictor is applied to the projected values at half time step $t^n + \frac{\Delta t}{2}$. The characteristic predictor is formulated in the local system of coordinates for the one dimensional Euler equation. We illustrate the implementation of the characteristic predictor in the direction of the unit vector $\bar{n}_c$. The Euler equations for this direction can be written in the following form:

$$W_t + A(W) W_{nc} = 0 \tag{13}$$

where

$$W = \begin{Bmatrix} \tau \\ u \\ p \end{Bmatrix} ; \; A(W) = \begin{pmatrix} u & -\tau & 0 \\ 0 & u & \tau \\ 0 & \rho c^2 & u \end{pmatrix} \tag{14}$$

where $\tau = \rho^{-1}$, ρ denotes density while u, p are the velocity and pressure. The matrix $A(W)$ has three eigenvectors $(l^{\#}, r^{\#})$ (l for left and r for right where $\#$ denote +,o,−) associated with the eigenvalues $\lambda^+ = u + c$, $\lambda^\circ = u$, $\lambda^- = u - c$.

An approximation of projected value to an edge accurate to second order in space and time can be written as:

$$\begin{aligned} W_{i+\Delta r}^{n+1/2} &\approx W_i^n + \frac{\Delta t}{2}\frac{\partial W}{\partial t} + \Delta r \frac{\partial W}{\partial r_{nc}} \\ &\approx W_i^n + \left[\Delta r - \frac{\Delta t}{2} A(W_i)\right]\frac{\partial W}{\partial r_{nc}} . \end{aligned} \tag{15}$$

An approximation to $W_{i+\Delta r}^{n+1/2}$ can be written as:

$$W_{i+\Delta r}^{n+1/2} = W_i + (\Delta \bar{r}_i - \frac{\Delta t}{2}(M_x M_n)\cdot \bar{n}_c)\bar{\nabla} W_i \tag{16}$$

where

$$(M_x M_n) = \begin{cases} Max(\lambda_i^+, o) & \text{for cell left to the edge} \\ Min(\lambda_i^-, o) & \text{for cell right to the edge} . \end{cases} \tag{17}$$

The gradients applied in the process of computing the projected values at $t^n + (\Delta t/2)$ are subjected to the monotonicity limiter.

Following the characteristic predictor described above, the full Riemann problem is solved at the edge. The solution of the Riemann problem defines the flux $\bar{Q}^{n+\frac{1}{2}}$ through the edge. The fluxes through the edges of triangles are then integrated (Eq. 5), thus giving an updated value of the variables at t^{n+1}. One of the advantages of the described algorithm is that calculation of the fluxes is done over the largest loop in the system (loop over edges) and can be carried out in the vectorized or parallelized loop. This fact leads to an efficient algorithm.

The algorithm presented is a modification of the algorithm of Ref. 5 which was derived for structured mesh. This algorithm has been applied to simulate a wide range of flow problems and has been found very accurate in predicting the features of the physics. The performance of the algorithm is well documented in Refs. 6-8. The next section, the spatial adaptive procedure, is described in detail. These descriptions include explanations of the error estimator for flow feature detection and the Direct Dynamic Refinement Method used to enrich and coarsen the mesh.

DIRECT DYNAMIC REFINEMENT METHOD FOR ADAPTATION ON AN UNSTRUCTURED TRIANGULAR GRID

The Direct Dynamic Refinement method (DDR) is a new method for adapting unstructured triangular grids during the computational process. As stated, an unstructured grid is very suitable for implementing boundary conditions on complex geometrical shapes as well as the adaptation of the grid, if necessary. The adaptation of the unstructured triangular grid leads to efficient usage of memory resources. The adaptive grid enables the user to capture moving shocks and high gradient flow features with high resolution. The available memory resources can be very efficiently distributed in the computational domain to accommodate the resolution needed to capture features of the physical property of the solution as they are evolved. Dynamic refinement controls the resolution priorities. These priorities can be set according to the physical features that the user wishes to emphasize

in the simulation. The user has control over the accuracy of the physical features resolved in the simulation, without being restricted to the initial grid. The alternative to Direct Dynamic Refinement (DDR) is the hierarchical dynamic refinement (H-refinement) that keeps a history of the initial grid (mother grid) and the subdivision of each level (daughter grids). In the H-refinement method, it is necessary to keep overhead information on the level of each triangle subdivision, and double indirect indexing is needed to keep track of the H-refinement process. As mentioned, the H-refinement relies heavily on the initial grid as it subdivides this grid and returns to it after the passage of the shock.

To minimize the dissipation caused by the interpolation and extrapolation in the refinement and coarsening of the grid, the addition and deletion of point is done in the region where the flow features are smooth. Thus for capturing the shock, the refinement should be applied in the region ahead of the shock. The coarsening of the grid is done in the flow regions where the gradients of the flow parameters are small.

In the present version of AUGUST (Adaptive Unstructured Godunov Upwind Second order Triangular), we implemented an algorithm with multiple criteria for capturing a variety of features that might exist in the physics of the problem to be solved. To identify the location of a moving shock, we use the flux of total energy into triangles. The fluxes entering and leaving triangles are the most accurate physical variables computed by the Godunov

algorithm for solving Euler's equations, and are used to update the physical variables for each time step in each triangle. Supplementary to the flux of energy as an error indicator, we use the flux of total density into triangles and the density gradient. The error indicator is the only sensor that is solely responsible for identifying the area to be refined or coarsened in the computational domain. As such, the error indicator should be sensitive enough to detect physical features that are of interest to the user, such as shock waves, rarefaction waves, slip lines and vortices. The error indicators that are implemented in the code are able to sense very weak slip lines in the presence of strong shock waves. The ability of the error indicators to identify weak physical features in the presence of strong ones, without picking up numerical noises, is essential to the simulation of adaptive grids. As stated, the quality of the results is as good as the error indicators applied. If the error indicators fail to identify the physical feature, this feature probably will be overlooked in the simulated results. It should be noted that the process of applying error indicators for identifying the areas to be adaptively refined or coarsened is an expensive loop that has to check the whole triangles table in the simulation. Thus, the error indicators are applied each 9 to 15 time steps. This process is preceded by application of an algorithm that refines a buffer zone ahead of the features and coarsens the grid after it was moved away. The buffer zone ahead of the feature is identified by using a search pattern of finding the neighbors of the flagged triangles sorted by the error indicators.

We are not applying any physical parameters to identify the ones "ahead."

The refinement algorithm follows several basic steps. The process of adding points to refine the grid locally is done by either adding a new vertex in the baricenter of the triangle or adding a new vertex in the middle of the edge. Adding a new vertex in the baricenter of a triangle is very efficient in the sense that the refinement affects this individual triangle only. We apply this process exclusively for refinement. As a supplement, especially on the boundary, we apply the method of adding a new vertex on an edge. As a complement to adding new vertices, we apply the reconnection/swapping algorithm that flips the diagonal (common edge) of two adjacent triangles to improve the quality of the triangles constructed. Figure 2 displays a chain of those basic steps to illustrate the refinement process. Figure 2a shows the original grid. Figure 2b illustrates a one step scheme refinement in which a new vertex is introduced into a triangular cell forming three cells (two new ones). On the boundary edges, a new vertex is introduced in the middle of those edges to form two cells (one new one). This refinement is followed by reconnection that modifies the grid as demonstrated in Fig. 2c. The process of refinement and reconnection can be continued until the necessary grid resolution is achieved. As an example, another loop of refinement is illustrated in Figs. 2d and 2e. This direct approach to grid refinement provides extreme flexibility in resolving local flow features.

A similar direct approach is applied to grid coarsening. The basic step

in this process is deleting the cells and edges associated with a vertex to be removed, as shown in Fig. 3b. During the second step, this void in the grid is filled with new larger triangles (Fig. 3c) without introducing new vertices. The last step is local reconnection and relaxation as shown in Fig. 3d. The relaxation procedure is a simple relocation of the vertex moved to the center of the polygon surrounding this vertex (only if the polygon is a convex).

The algorithm of direct dynamic refinement proved to be very efficient in refining and coarsening the grid adaptively. The refinement and coarsening followed a short inquiry on the quality and shape of the triangle flagged and its close neighbors. Since we do not keep any history or tree for each triangle, the DDRM algorithm has much less checking to do as compared to the H-refinement algorithm. The vectorization and parallelization of the solver is straightforward.

NUMERICAL RESULTS FOR THE TWO DIMENSIONAL TEST PROBLEM

We have tested the Second Order Godunov algorithm in a variety of flow simulations ranging from the low subsonic to the high hypersonic Mach [6-8] regime. The AUGUST code proved to be very robust and accurate. The results obtained are comparable to or better than those obtained applying leading flow solvers in all of the regimes tested.

To validate our DDRM implemented in the AUGUST code, we simulated the problem of interaction of a Mach 2.85 planar shock wave, propagating

are accurately accounted for and the shock waves, slip lines, vortices are sharply captured.

in a channel with a 45° symmetrical double ramp. Figure 4 shows the experimental interferogram of the problem to be simulated (reproduced). The example that we chose to simulate is most appropriate to test the performance of an adaptive algorithm. The experimental results show a complex flow pattern containing a mix of strong discontinuities, as shock waves, and very weak features such as slip lines, vortices, and rarefaction waves. The error estimator must recognize and flag all these features for refinement. The error estimator should be sensitive enough to identify very weak slip lines without picking up numerical noises present in the simulation. We have simulated the shock wave reflection and diffraction over a 45° corner at the conditions that correspond to the experimental result shown in Fig. 4. Here we present results for several shapes of the flow evolution. The flow in the channel is from left to right. Figure 5 displays density contour plots after the shock passed the apex of the double wedge obstacle. In Fig. 5a, the density contours are overlayed on the grid used at this stage of the evolving flow. For clarity, only the density contours are displayed in Fig. 5b. The grid displayed in Fig. 5a shows how well the adaptation technique follows the high activity region in the flow. The grid is adapting to regions with high pressure gradients and high density gradient. In Fig. 5a, one can observe high quality grid produced by the DDR method. The shock has a relatively thin buffer zone ahead of its front, allowing us to avoid the interpolations related to grid adaptation of the flow variables in the area of high gradient.

The flow features are resolved accurately, and the contact discontinuity and triple point are clearly defined.

Figure 6 shows the density contours at a later time in the same format as in Fig. 5. This figure demonstrates the ability of the DDRM to identify and follow flow features in the computational domain. In this figure we can observe a complicated flow pattern developing as a result of interaction of the rarefraction wave with the complex pattern of shock waves. A recompression shock and a strong vortex that are developed in this time frame are well resolved. We can also observe a slip line originating at the triple point. The adaptation algorithm, as in the previous time frame, follows both shock waves and contact discontinuities.

Figure 7 displays the density contours at the stage comparable to that shown in Fig. 4 for the experimental results. The computed results as displayed in Fig. 7b show a flow pattern similar to the experiment. The slip line and the formation of vertices along it are clearly depicted. The shock and reflected shock as well as the recompression shock are very sharply defined with very low numerical noise. The vortex developed after the compression shock is distinctly displayed. A new reflected shock can be seen developing at the channel wall behind the double wedge.

The results shown in Figs. 5-7 display the ability of the algorithm to simulate a complex transient flow problem on dynamically adapting grid. The error estimates used in our algorithm allow detection of strong and

weak shock waves, conducted discontinuities, vortices or other fronts that need enhanced resolution.

CONCLUSION

The Direct Dynamic Refinement (DDR) method was developed and tested for a challenging problem of reflection and diffraction of a strong shock over a double ramp. For this test problem we have demonstrated that a set of error indicators developed for the DDR allow capturing strong and weak features of the complex wave structure developing in this test case.

The above described algorithms were implemented in the AUGUST code. The AUGUST code was used for a range of subsonic, transonic, and supersonic transient and steady problems. For all these conditions the AUGUST code produced robust results with the error indicators proving to be applicable for all these diverse flow regimes.

ACKNOWLEDGMENT

The work reported here was partially supported by DARPA and AFOSR under Contract #F49620-89-C-0087. The authors would like to thank Col. James Crowley and Dr. A. Nachman for their interest in this project.

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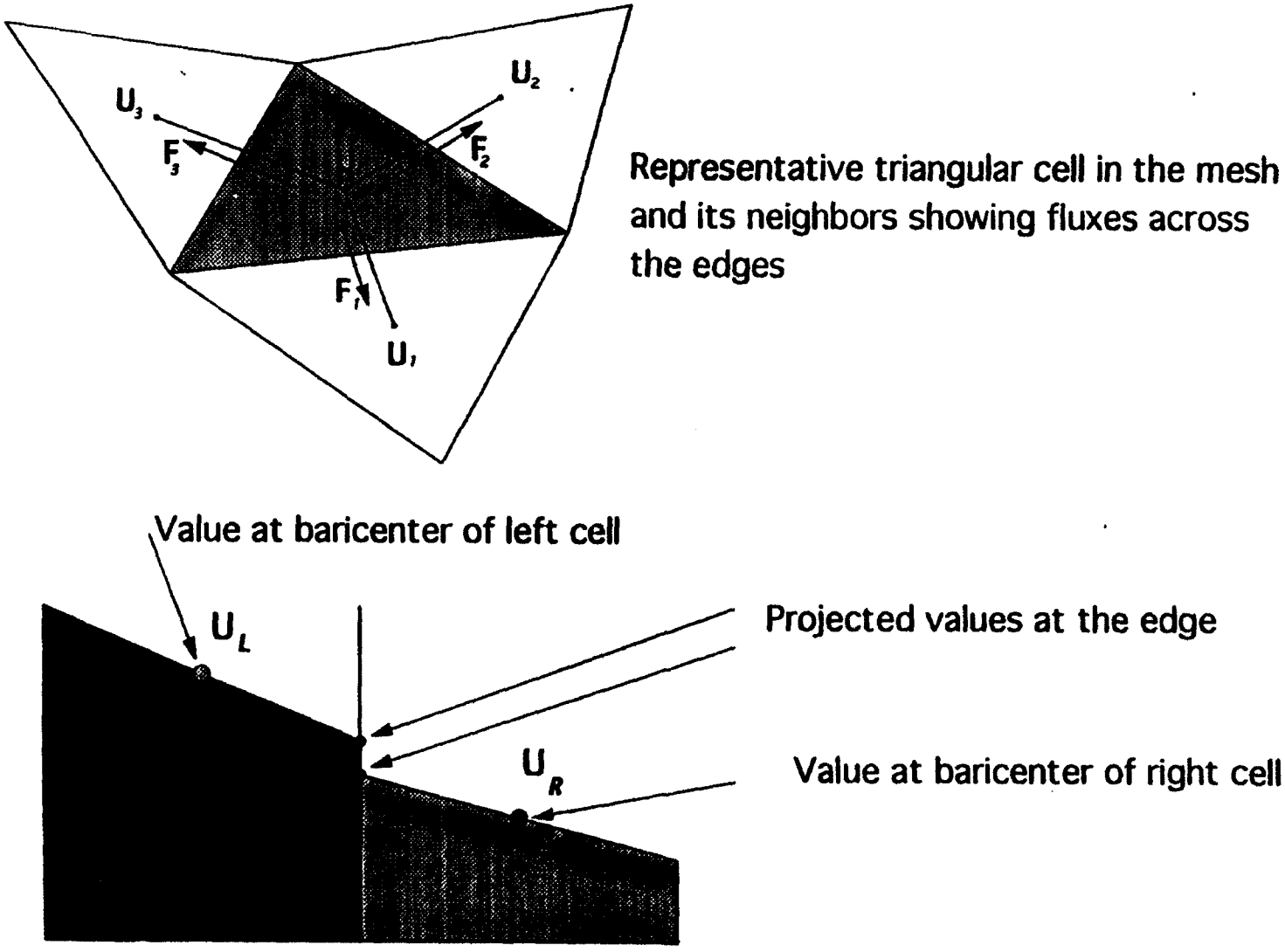
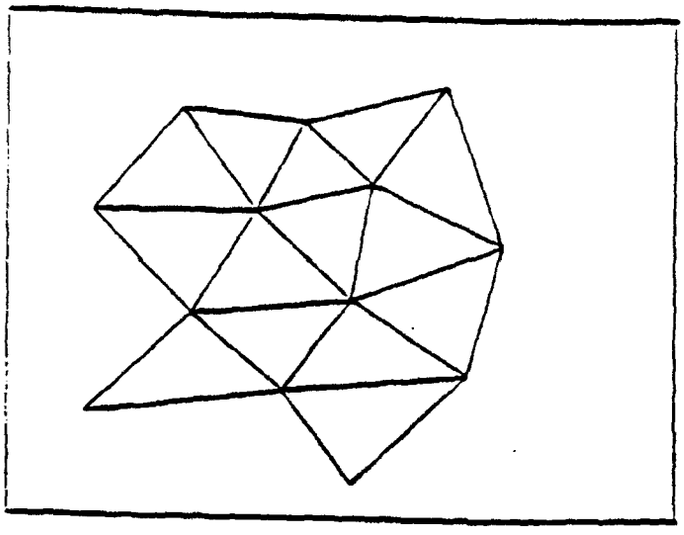
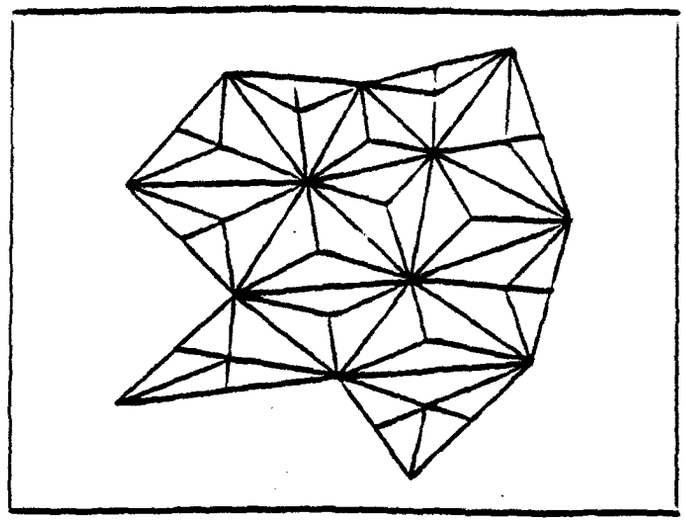


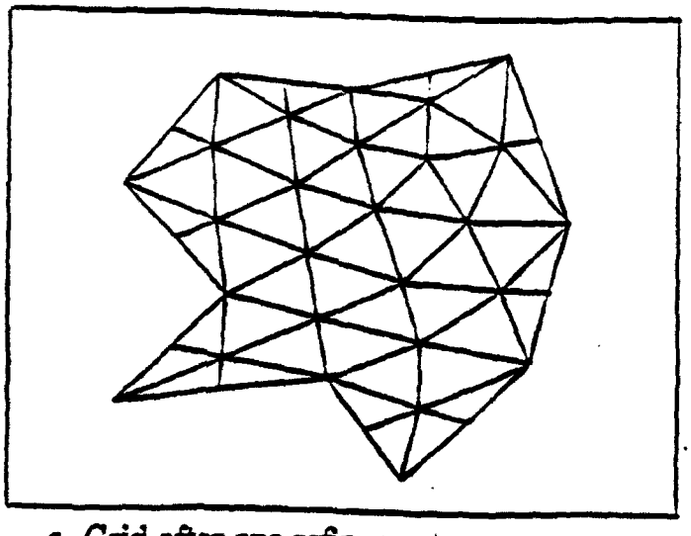
Figure 1. Representative triangular cell in the mesh showing fluxes and projected values.



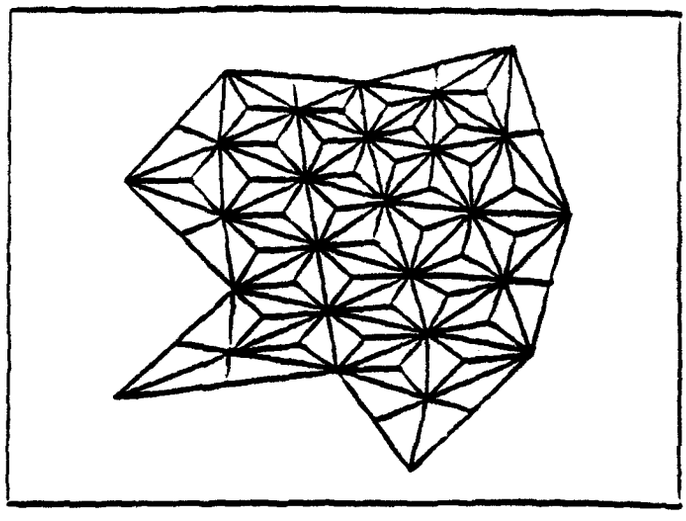
a. Original grid.



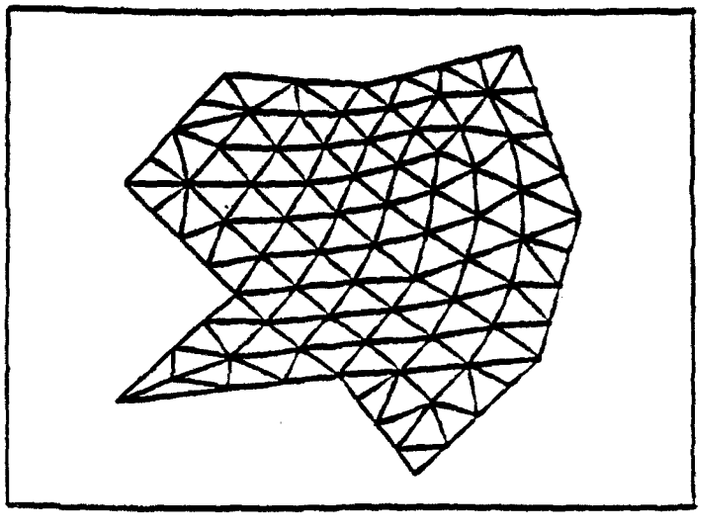
b. Grid after one refinement.



c. Grid after one refinement and one reconnection.

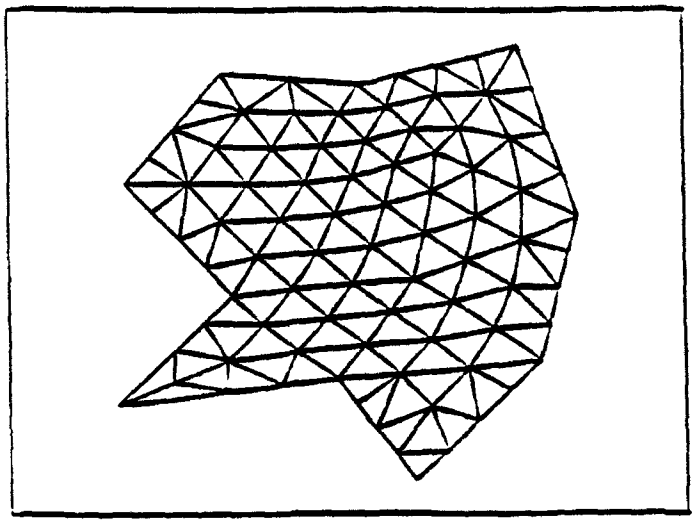


d. Second refinement.

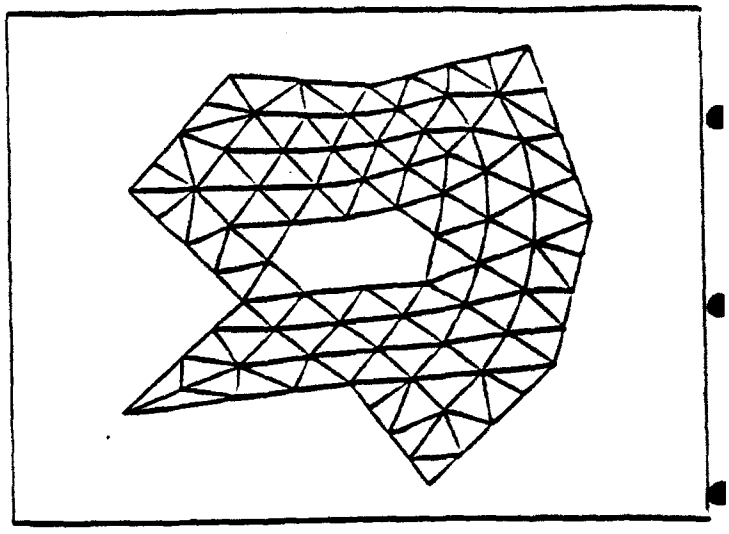


e. Second reconnection.

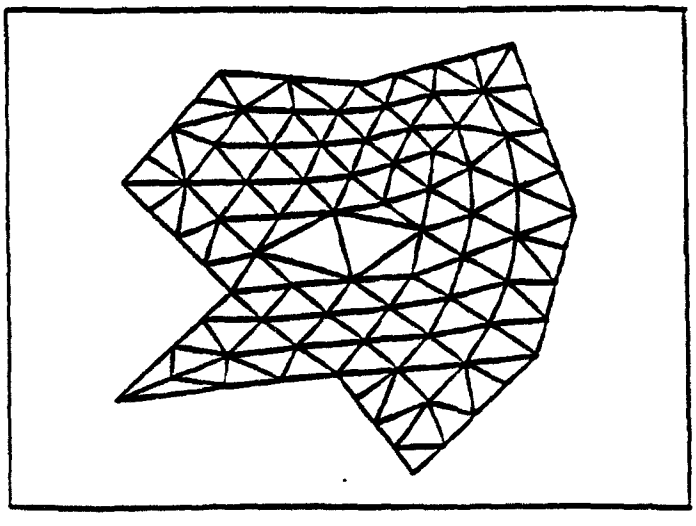
Figure 2. Illustration of the grid refinement process.



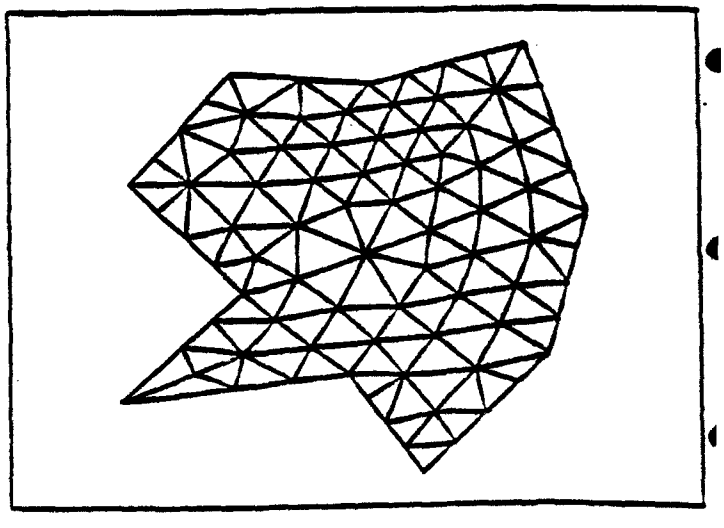
a. Original grid.



b. Point removal.



c. Constructing of new cells.



d. Grid after reconnection and relaxation.

Figure 3. Illustration of the grid coarsenning process.

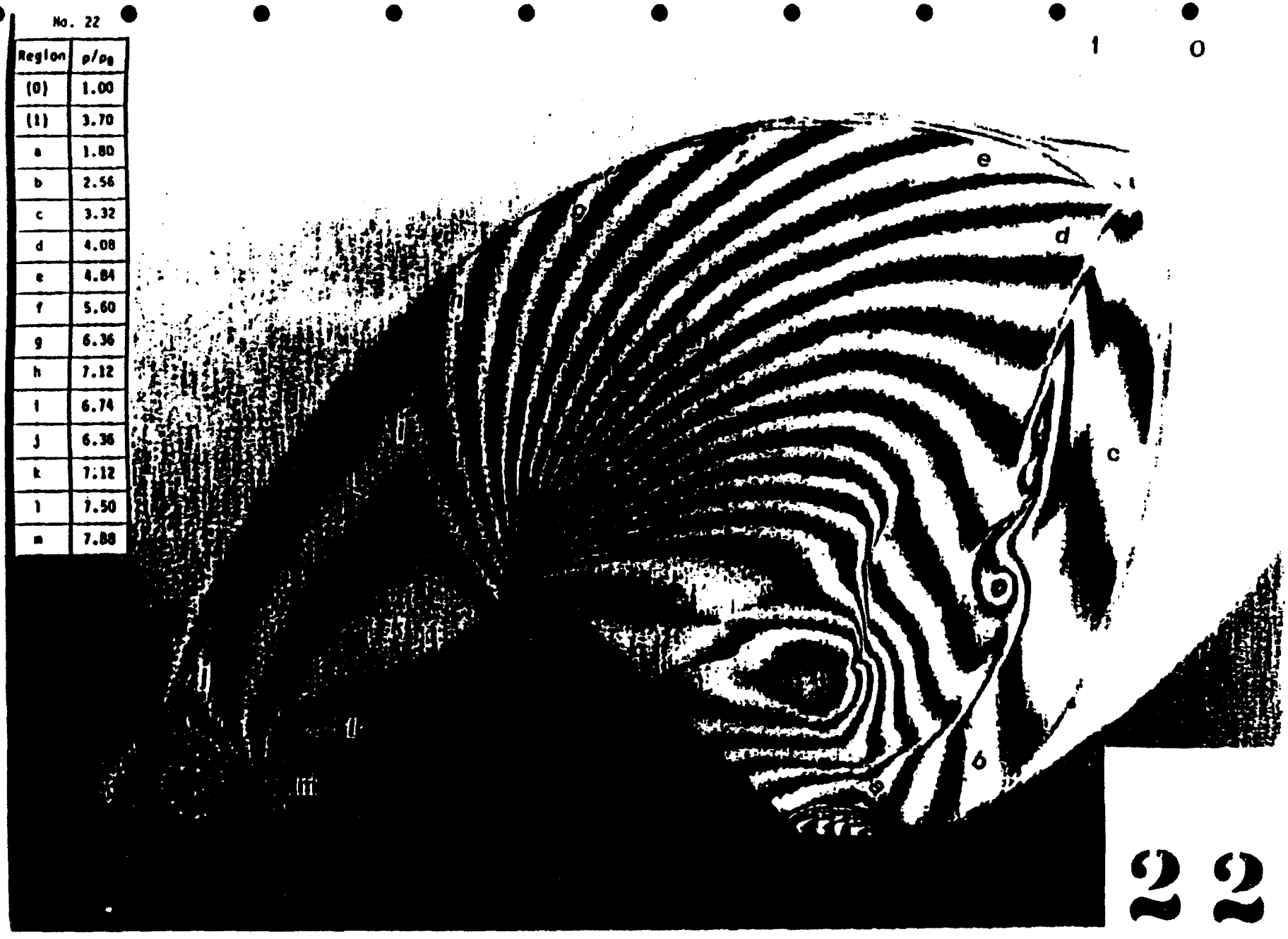


Figure 4. An experimental interferogram taken at 96 μs after shock wave hits a diamond shaped obstacle, Mach $M_s = 2.85$.

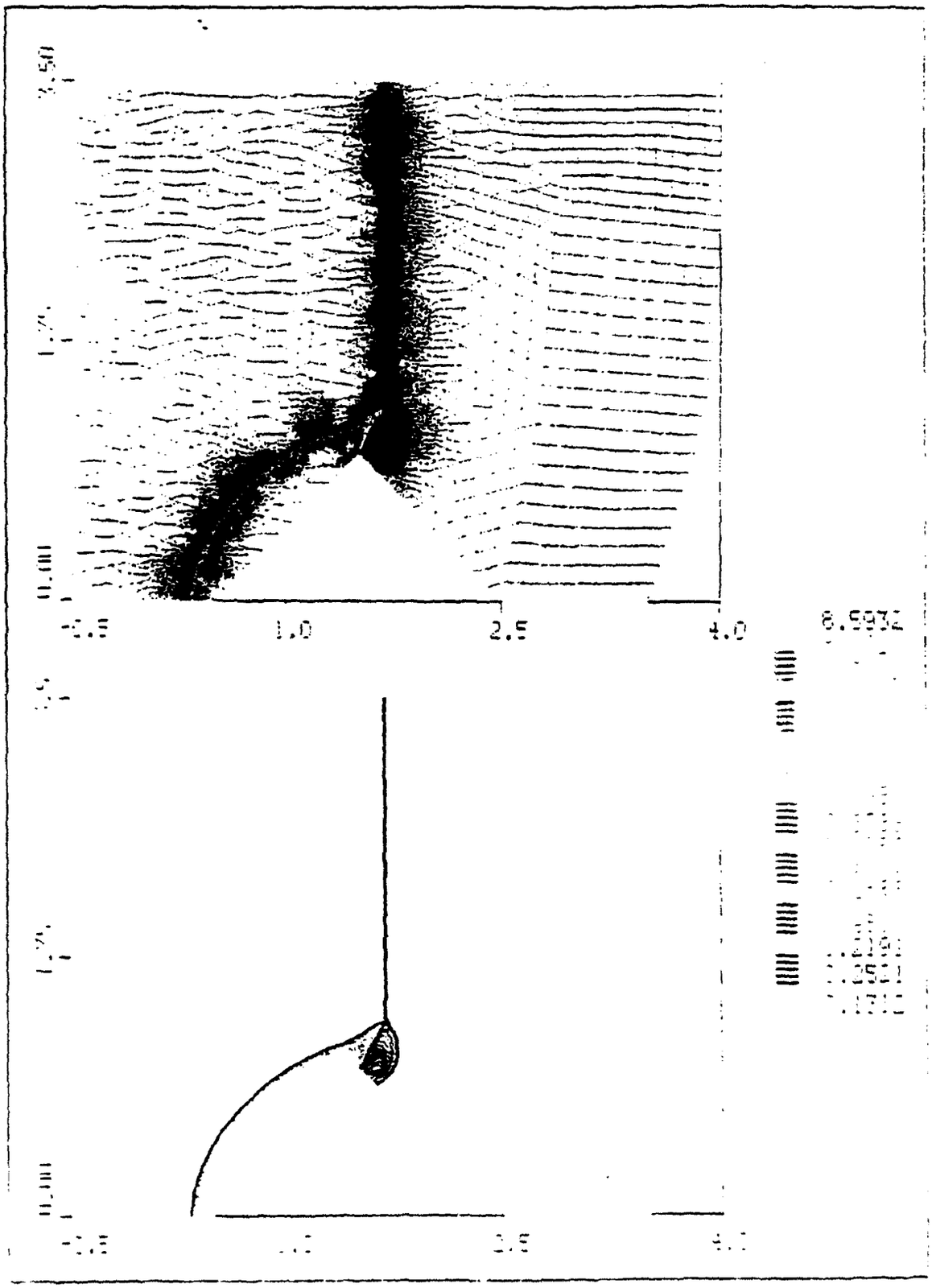


Figure 5. Computed density contours simulating flow identical to the setup of the experiment of Fig. 4. The grid is composed of 21121 vertices.

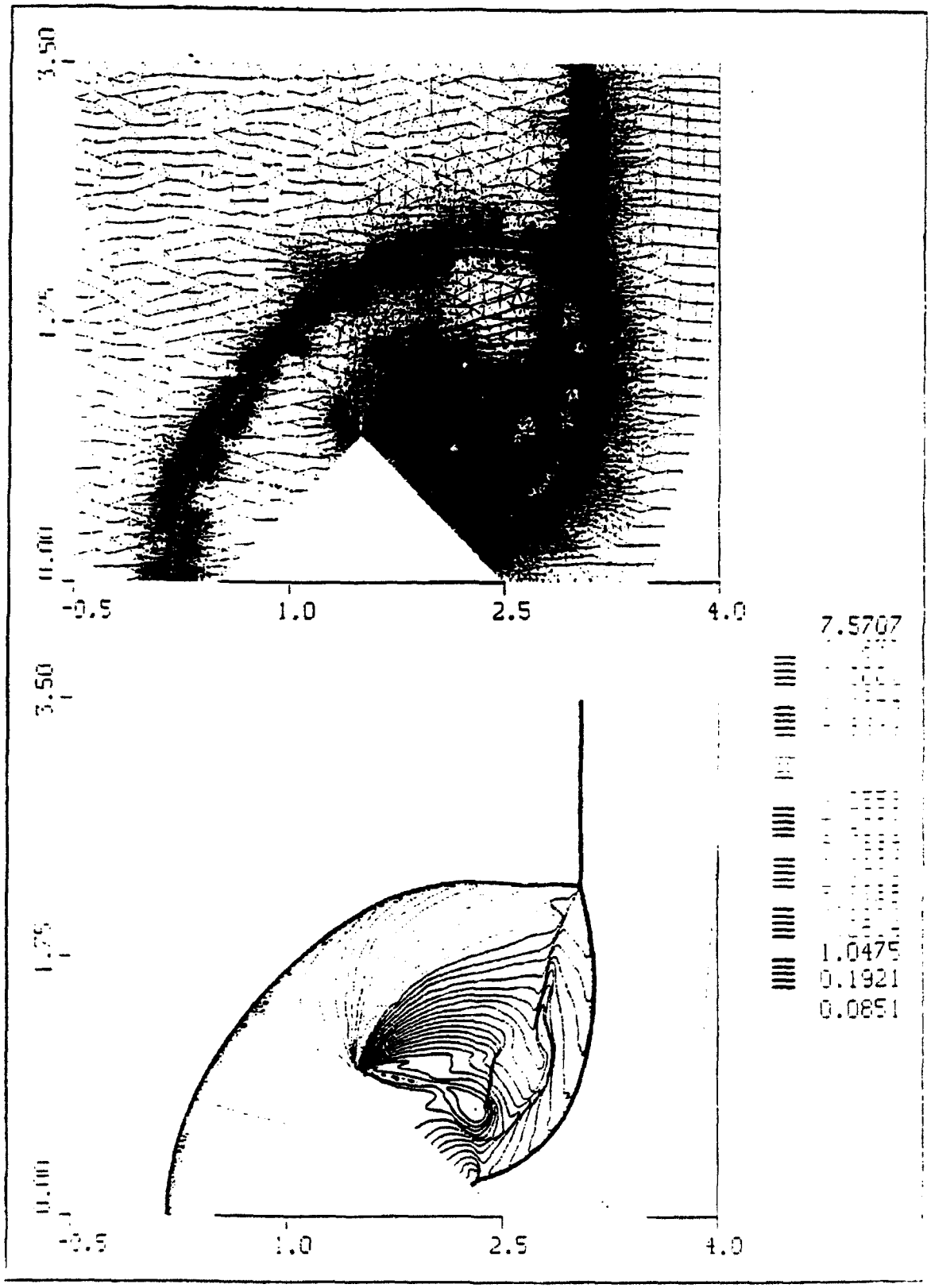


Figure 6. Computed density contours simulating flow identical to the setup of the experiment of Fig. 4. The grid is composed of 65624 vertices.

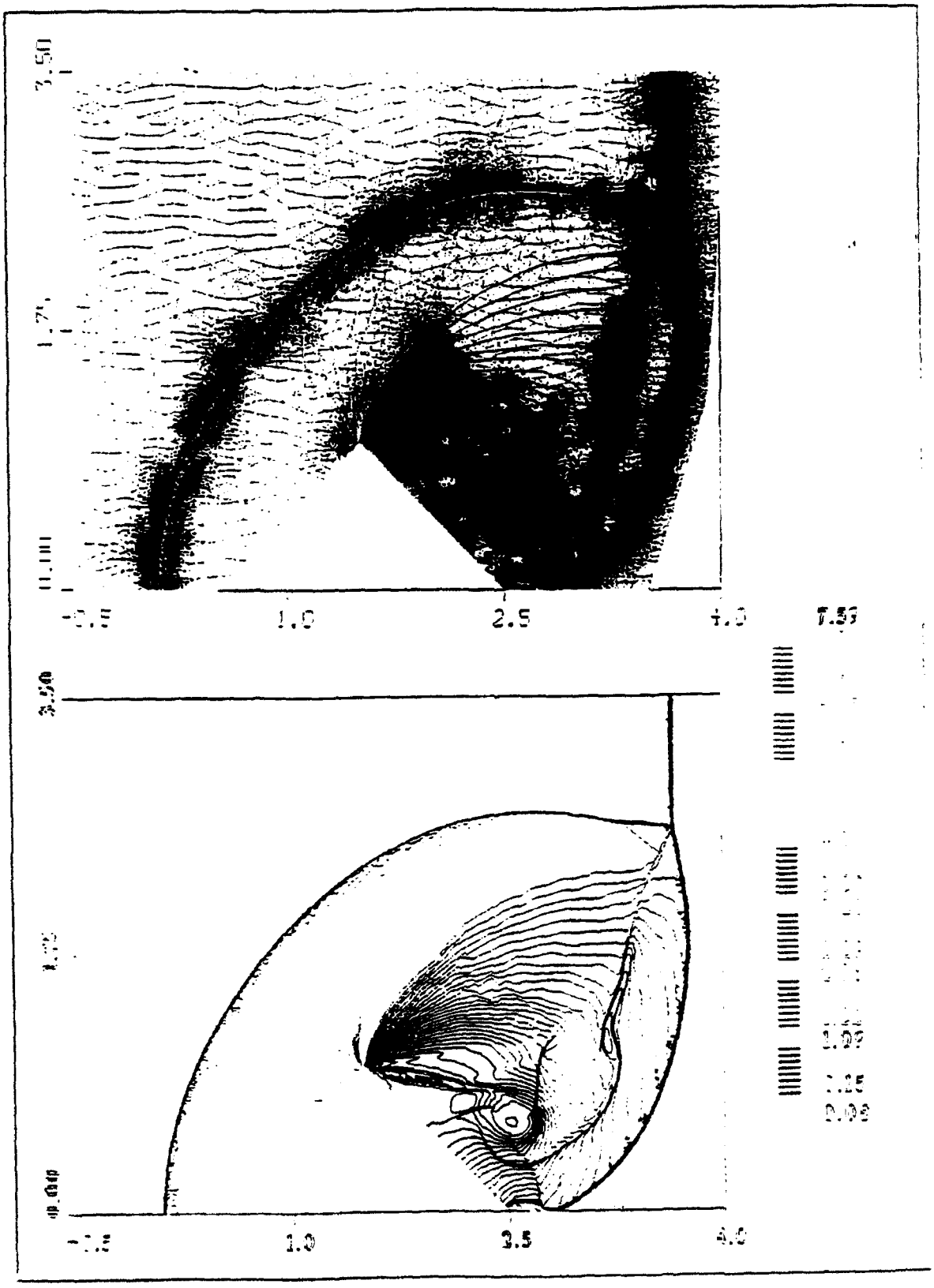


Figure 7. Computed density contours comparable to time of the experimental results shown in Fig. 4. The grid is composed of 79352 vertices.

A Second Order Godunov Scheme on Spatial Adapted Triangular Grid

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ABSTRACT

Spatial adaptation procedure for the accurate and efficient solution of unsteady inviscid flow simulation is described. The adaptation procedures were developed and implemented applying a second order Godunov scheme. These procedures involve mesh enrichment/coarsening to either add/remove vertices in high/low gradient regions of the flow, respectively. The goal is to achieve solutions of high spatial accuracy at minimal computational cost. The paper describes a very effective error estimator to detect high/low activity regions of the flow to be enriched or coarsened, respectively. The error estimator is based on total energy and density fluxes into the cell combined with gradient of density. Included in the paper is a detailed description of the direct dynamic refinement method that is used for adaptation. A detailed simulation of a reflection and diffraction of multiple shock waves flowing over a diamond shape wedge is presented and compared with experimental results. The simulated results are shown to be in excellent agreement with the experiment primarily in that all the complicated features of the physics are accurately accounted for and the shock waves, slip lines, vortices are sharply captured.

INTRODUCTION

Considerable progress has been made over the past decade in developing methods for spatial adaptation of the computational meshes based on the numerical solution of the simulated physics. These methods are being developed to produce higher spatial accuracy in such simulation more efficiently. The goal of mesh adaptation is to enrich meshes locally, based on the numerical solution, in order to capture physical features of importance; in contrast to globally fine meshes, this process will minimize computer run times and memory costs. The methods of mesh adaptation can be categorized into three general classes: 1) mesh regeneration, 2) mesh movement, and 3) mesh enrichment.

The idea of mesh regeneration is systematically to identify high/low activity region in the flow and accordingly remesh those regions applying mesh generation code. This is done by assigning criteria for spatial accuracy and number of vertices. This procedure requires a mapping of the "old" flow solution into the "new" generated meshes by using one of the interpolated schemes. For the second method, mesh movement, the number of points in the computational domain remains fixed. The adaptation procedure moves vertices from low activity regions to high gradient regions to achieve a high concentration of vertices to resolve high activity regions. The movement of the points is dictated by forcing functions in the Poisson - equation in the grid generator code. The final method of spatial adaptation is mesh

related to grid adaptation of the flow variables in the area of high gradient.

enrichment. In this method, vertices are added or removed according to the spatial resolution of the physical features in the flow. The advantages of mesh enrichment over regeneration and movement are its higher degree of flexibility in being able to add points where they are needed and to remove points where they are not needed. In our mesh enrichment method, we add points ahead of the shock wave, thus preventing the need of interpolation in the high gradient region for achieving higher accuracy of the results. Adding and removing points are done in monotone/very low activity regions to prevent numerical dissipation.

Lohner[1] has developed procedures to enrich the mesh for transient flow problems locally by subdividing elements in the grid according to specific spatial resolution criteria. The method, referred to as H-refinement, keeps a history of the initial grid (mother grid) and the subdivision of each level (daughter grids). The H-refinement relies heavily on the initial grid as it is subdivided for enrichment and recovered in the coarsening stage. A similar adaptive strategy to Lohner is adopted by Rausch[2] et al., but applies a different error estimator and upwind type algorithm for a solver.

In our paper, we describe a Godunov scheme to solve Euler equations on an unstructured adaptive triangle mesh. We discuss the methodology of a cell centered Second Order Godunov scheme applied to a triangular mesh, and the method of Direct Dynamic Refinement that is used for adaptation of the unstructured triangular grid. Simulation and experimental results

are compared for a test case applying the adaptive unstructured grid to a complicated pattern of planar shock wave flow diffraction over a half diamond shape wedge.

SECOND ORDER GODUNOV ALGORITHM ON UNSTRUCTURED GRID

This section describes the implementation of the Second Order Godunov algorithm on a triangular unstructured grid. The algorithm is explicit and is cell-center based.

We consider a system of two-dimensional Euler equations written in conservation law form as:

$$\frac{\partial \bar{U}}{\partial t} + \frac{\partial \bar{F}}{\partial x} + \frac{\partial \bar{G}}{\partial y} = 0 \tag{1}$$

where

$$U = \begin{Bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{Bmatrix}, F = \begin{Bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(e+p) \end{Bmatrix}, G = \begin{Bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(e+p) \end{Bmatrix}.$$

Here u, v are the x, y velocity vector components, p is the pressure, ρ is the density and e is total energy of the fluid. We assume that the fluid is an ideal gas. The total energy of gas is given by the following equation:

$$e = \frac{p}{\gamma - 1} + \frac{\rho}{2}(u^2 + v^2) \tag{2}$$

where γ is the ratio of specific heats. It is assumed that an initial distribution of the fluid parameters is given at $t = 0$, and the boundary conditions defining a unique solution are specified for the computational domain.

The system of governing equation (1) can be written in the following form:

$$\frac{\partial U}{\partial t} + \bar{\nabla} \cdot \bar{Q} = 0 \tag{3}$$

where $\bar{Q}$ represents the convective flux vector. By integrating Eq. (3) over space and using Gauss' theorem, the following expression is obtained

$$\frac{\partial}{\partial t} \int_{\Omega} U dA + \oint_{\partial\Omega} \bar{Q} \cdot d\bar{l} = 0 \tag{4}$$

where $d\bar{l} = \bar{n} d\mathcal{L}$, $\bar{n}$ is the unit normal vector in the outward direction, and $d\mathcal{L}$ is a unit length on the boundary of the domain. The variable Ω is the domain of computation and $\partial\Omega$ is the circumference boundary of this domain.

Equation (4) can be discretized for each element (cell) of the domain

$$\frac{(U_i^{n+1} - U_i^n)}{\Delta t} A_i = \sum_{j=1}^{3} \bar{Q}_j^{n+\frac{1}{2}} \bar{n}_j \Delta L_j \tag{5}$$

where A_i is the area of the cell; Δt is the marching time step; U_i^{n+1} and U_i^n are the primitive variables at the center of the cell at time n and at the update $n + 1$ time step; $\bar{Q}_j$ is the value of the fluxes across the three boundaries edges on the circumference of the cell where $\bar{n}_j$ is the unit normal

vector to the boundary edge j, and ΔL_j is the length of the boundary edge j. Equation (5) is used to update the physical primitive variables U_i according to computed fluxes for each time step Δt. The time step is subjected to the CFL (Courant-Fredrichs-Lewy) constraint.

To obtain a second order spacial accuracy, the gradient of each primitive variable is computed in the baricenter of the cell. This gradient is used to define the projected values of primitive variables at the two sides of the cell's edge, as is shown in Figure 1. The gradient is approximate by a path integral

$$\int_{\Omega} \bar{\nabla} U_i^{cell} dA = \oint_{\partial\Omega} U_j^{edge} d\bar{l} \,. \tag{6}$$

The notation is similar to the one used for Eq. (5) except the domain Ω is a single cell and U_i^{cell} and U_j^{edge} are values at the baricenter and on the edge respectively. The gradient is estimated as

$$\bar{\nabla} U_i^{cell} = \frac{1}{A} \sum_{j=1}^{3} \tilde{U}_j^{edge} \bar{n}_j \Delta L_j \tag{7}$$

where $\tilde{U}_j^{edge}$ is an average value representing the primitive variable value for edge j.

The gradients that are computed at each baricenter are used to project values for the two sides of each edge by piecewise linear interpolation. The interpolated values are subjected to monotonicity constraints.[3] The monotonicity constraint assures that the interpolated values are not creating new

extrema.

The monotonicity limiter algorithm can be written in the following form:

$$U^{edge}_{projected} = U^{cell}_i + \phi \bar{\nabla} U_i \cdot \Delta \bar{r} \tag{8}$$

where $\Delta \bar{r}$ is the vector from the baricenter to the point of intersection of the edge with the line connecting the baricenters of the cells over the two sides of this edge. ϕ is the limiter coefficient that limits the gradient $\bar{\nabla} U_i$.

First, we compute the maximum and minimum values of the primitive variable in the i's cell and its three neighboring cells that share common edges (see Fig. 1):

$$\left.\begin{aligned} U^{max}_{cell} &= Max\left(U^{cell}_k\right) \\ U^{min}_{cell} &= Min\left(U^{cell}_k\right) \end{aligned}\right\} k = i, 1, 2, 3 \; . \tag{9}$$

The limiter can be defined as:

$$\phi = Min\left\{1, \phi^{lr}_k\right\} \;\; k = 1, 2, 3 \tag{10}$$

where superscript lr stands for left and right of the three edges (6 combinations in total). ϕ^{lr}_k is defined by:

$$\phi^{lr}_k = \frac{\left[1 + Sgn\left(\Delta U^{lr}_k\right)\right] \Delta U^{max}_{cell} + \left[1 - Sgn\left(\Delta U^{lr}_k\right)\right] \Delta U^{min}_{cell}}{2(\Delta U^{lr}_k)} \quad k = 1, 2, 3 \tag{11}$$

where $\Delta U_k^{lr} = \bar{\nabla} U_i^{lr} \cdot \Delta \bar{r}_k$. and

$$\left.\begin{aligned} \Delta U_{cell}^{\max} &= U_{cell}^{\max} - U_i^{cell} \\ \Delta U_{cell}^{\min} &= U_{cell}^{\min} - U_i^{cell} \end{aligned}\right\} . \tag{12}$$

To obtain a second order of accuracy in time and space, we subject the projected values of the left and right side of the cell edge to characteristic constraints following Ref. 4. The one dimensional characteristic predictor is applied to the projected values at half time step $t^n + \frac{\Delta t}{2}$. The characteristic predictor is formulated in the local system of coordinates for the one dimensional Euler equation. We illustrate the implementation of the characteristic predictor in the direction of the unit vector $\bar{n}_c$. The Euler equations for this direction can be written in the following form:

$$W_t + A(W) W_{nc} = 0 \tag{13}$$

where

$$W = \begin{Bmatrix} \tau \\ u \\ p \end{Bmatrix} ; \; A(W) = \begin{pmatrix} u & -\tau & 0 \\ 0 & u & \tau \\ 0 & \rho c^2 & u \end{pmatrix} \tag{14}$$

where $\tau = \rho^{-1}$, ρ denotes density while u, p are the velocity and pressure. The matrix $A(W)$ has three eigenvectors $(l^{\#}, r^{\#})$ (l for left and r for right where # denote +,o,-) associated with the eigenvalues $\lambda^+ = u + c$, $\lambda^\circ = u$, $\lambda^- = u - c$.

An approximation of projected value to an edge accurate to second order in space and time can be written as:

$$\begin{aligned} W_{i+\Delta r}^{n+1/2} &\approx W_i^n + \frac{\Delta t}{2}\frac{\partial W}{\partial t} + \Delta r \frac{\partial W}{\partial r_{nc}} \\ &\approx W_i^n + \left[\Delta r - \frac{\Delta t}{2} A(W_i)\right]\frac{\partial W}{\partial r_{nc}} . \end{aligned} \tag{15}$$

An approximation to $W_{i+\Delta r}^{n+1/2}$ can be written as:

$$W_{i+\Delta r}^{n+1/2} = W_i + (\Delta \bar{r}_i - \frac{\Delta t}{2}(M_x M_n)\cdot \bar{n}_c)\bar{\nabla} W_i \tag{16}$$

where

$$(M_x M_n) = \begin{cases} Max(\lambda_i^+, o) & \text{for cell left to the edge} \\ Min(\lambda_i^-, o) & \text{for cell right to the edge .} \end{cases} \tag{17}$$

The gradients applied in the process of computing the projected values at $t^n + (\Delta t/2)$ are subjected to the monotonicity limiter.

Following the characteristic predictor described above, the full Riemann problem is solved at the edge. The solution of the Riemann problem defines the flux $\bar{Q}^{n+\frac{1}{2}}$ through the edge. The fluxes through the edges of triangles are then integrated (Eq. 5), thus giving an updated value of the variables at t^{n+1}. One of the advantages of the described algorithm is that calculation of the fluxes is done over the largest loop in the system (loop over edges) and can be carried out in the vectorized or parallelized loop. This fact leads to an efficient algorithm.

The algorithm presented is a modification of the algorithm of Ref. 5 which was derived for structured mesh. This algorithm has been applied to simulate a wide range of flow problems and has been found very accurate in predicting the features of the physics. The performance of the algorithm is well documented in Refs. 6-8. The next section, the spatial adaptive procedure, is described in detail. These descriptions include explanations of the error estimator for flow feature detection and the Direct Dynamic Refinement Method used to enrich and coarsen the mesh.

DIRECT DYNAMIC REFINEMENT METHOD FOR ADAPTATION ON AN UNSTRUCTURED TRIANGULAR GRID

The Direct Dynamic Refinement method (DDR) is a new method for adapting unstructured triangular grids during the computational process. As stated, an unstructured grid is very suitable for implementing boundary conditions on complex geometrical shapes as well as the adaptation of the grid, if necessary. The adaptation of the unstructured triangular grid leads to efficient usage of memory resources. The adaptive grid enables the user to capture moving shocks and high gradient flow features with high resolution. The available memory resources can be very efficiently distributed in the computational domain to accommodate the resolution needed to capture features of the physical property of the solution as they are evolved. Dynamic refinement controls the resolution priorities. These priorities can be set according to the physical features that the user wishes to emphasize

in the simulation. The user has control over the accuracy of the physical features resolved in the simulation, without being restricted to the initial grid. The alternative to Direct Dynamic Refinement (DDR) is the hierarchical dynamic refinement (H-refinement) that keeps a history of the initial grid (mother grid) and the subdivision of each level (daughter grids). In the H-refinement method, it is necessary to keep overhead information on the level of each triangle subdivision, and double indirect indexing is needed to keep track of the H-refinement process. As mentioned, the H-refinement relies heavily on the initial grid as it subdivides this grid and returns to it after the passage of the shock.

To minimize the dissipation caused by the interpolation and extrapolation in the refinement and coarsening of the grid, the addition and deletion of point is done in the region where the flow features are smooth. Thus for capturing the shock, the refinement should be applied in the region ahead of the shock. The coarsening of the grid is done in the flow regions where the gradients of the flow parameters are small.

In the present version of AUGUST (Adaptive Unstructured Godunov Upwind Second order Triangular), we implemented an algorithm with multiple criteria for capturing a variety of features that might exist in the physics of the problem to be solved. To identify the location of a moving shock, we use the flux of total energy into triangles. The fluxes entering and leaving triangles are the most accurate physical variables computed by the Godunov

algorithm for solving Euler's equations, and are used to update the physical variables for each time step in each triangle. Supplementary to the flux of energy as an error indicator, we use the flux of total density into triangles and the density gradient. The error indicator is the only sensor that is solely responsible for identifying the area to be refined or coarsened in the computational domain. As such, the error indicator should be sensitive enough to detect physical features that are of interest to the user, such as shock waves, rarefaction waves, slip lines and vortices. The error indicators that are implemented in the code are able to sense very weak slip lines in the presence of strong shock waves. The ability of the error indicators to identify weak physical features in the presence of strong ones, without picking up numerical noises, is essential to the simulation of adaptive grids. As stated, the quality of the results is as good as the error indicators applied. If the error indicators fail to identify the physical feature, this feature probably will be overlooked in the simulated results. It should be noted that the process of applying error indicators for identifying the areas to be adaptively refined or coarsened is an expensive loop that has to check the whole triangles table in the simulation. Thus, the error indicators are applied each 9 to 15 time steps. This process is preceded by application of an algorithm that refines a buffer zone ahead of the features and coarsens the grid after it was moved away. The buffer zone ahead of the feature is identified by using a search pattern of finding the neighbors of the flagged triangles sorted by the error indicators.

We are not applying any physical parameters to identify the zones "ahead."

The refinement algorithm follows several basic steps. The process of adding points to refine the grid locally is done by either adding a new vertex in the baricenter of the triangle or adding a new vertex in the middle of the edge. Adding a new vertex in the baricenter of a triangle is very efficient in the sense that the refinement affects this individual triangle only. We apply this process exclusively for refinement. As a supplement, especially on the boundary, we apply the method of adding a new vertex on an edge. As a complement to adding new vertices, we apply the reconnection/swapping algorithm that flips the diagonal (common edge) of two adjacent triangles to improve the quality of the triangles constructed. Figure 2 displays a chain of those basic steps to illustrate the refinement process. Figure 2a shows the original grid. Figure 2b illustrates a one step scheme refinement in which a new vertex is introduced into a triangular cell forming three cells (two new ones). On the boundary edges, a new vertex is introduced in the middle of those edges to form two cells (one new one). This refinement is followed by reconnection that modifies the grid as demonstrated in Fig. 2c. The process of refinement and reconnection can be continued until the necessary grid resolution is achieved. As an example, another loop of refinement is illustrated in Figs. 2d and 2e. This direct approach to grid refinement provides extreme flexibility in resolving local flow features.

A similar direct approach is applied to grid coarsening. The basic step

in this process is deleting the cells and edges associated with a vertex to be removed, as shown in Fig. 3b. During the second step, this void in the grid is filled with new larger triangles (Fig. 3c) without introducing new vertices. The last step is local reconnection and relaxation as shown in Fig. 3d. The relaxation procedure is a simple relocation of the vertex moved to the center of the polygon surrounding this vertex (only if the polygon is a convex).

The algorithm of direct dynamic refinement proved to be very efficient in refining and coarsening the grid adaptively. The refinement and coarsening followed a short inquiry on the quality and shape of the triangle flagged and its close neighbors. Since we do not keep any history or tree for each triangle, the DDRM algorithm has much less checking to do as compared to the H-refinement algorithm. The vectorization and parallelization of the solver is straightforward.

NUMERICAL RESULTS FOR THE TWO DIMENSIONAL TEST PROBLEM

We have tested the Second Order Godunov algorithm in a variety of flow simulations ranging from the low subsonic to the high hypersonic Mach [6-8] regime. The AUGUST code proved to be very robust and accurate. The results obtained are comparable to or better than those obtained applying leading flow solvers in all of the regimes tested.

To validate our DDRM implemented in the AUGUST code, we simulated the problem of interaction of a Mach 2.85 planar shock wave, propagating

in a channel with a 45° symmetrical double ramp. Figure 4 shows the experimental interferogram of the problem to be simulated (reproduced). The example that we chose to simulate is most appropriate to test the performance of an adaptive algorithm. The experimental results show a complex flow pattern containing a mix of strong discontinuities, as shock waves, and very weak features such as slip lines, vortices, and rarefaction waves. The error estimator must recognize and flag all these features for refinement. The error estimator should be sensitive enough to identify very weak slip lines without picking up numerical noises present in the simulation. We have simulated the shock wave reflection and diffraction over a 45° corner at the conditions that correspond to the experimental result shown in Fig. 4. Here we present results for several shapes of the flow evolution. The flow in the channel is from left to right. Figure 5 displays density contour plots after the shock passed the apex of the double wedge obstacle. In Fig. 5a, the density contours are overlayed on the grid used at this stage of the evolving flow. For clarity, only the density contours are displayed in Fig. 5b. The grid displayed in Fig. 5a shows how well the adaptation technique follows the high activity region in the flow. The grid is adapting to regions with high pressure gradients and high density gradient. In Fig. 5a, one can observe high quality grid produced by the DDR method. The shock has a relatively thin buffer zone ahead of its front, allowing us to avoid the interpolations related to grid adaptation of the flow variables in the area of high gradient.

The flow features are resolved accurately, and the contact discontinuity and triple point are clearly defined.

Figure 6 shows the density contours at a later time in the same format as in Fig. 5. This figure demonstrates the ability of the DDRM to identify and follow flow features in the computational domain. In this figure we can observe a complicated flow pattern developing as a result of interaction of the rarefraction wave with the complex pattern of shock waves. A recompression shock and a strong vortex that are developed in this time frame are well resolved. We can also observe a slip line originating at the triple point. The adaptation algorithm, as in the previous time frame, follows both shock waves and contact discontinuities.

Figure 7 displays the density contours at the stage comparable to that shown in Fig. 4 for the experimental results. The computed results as displayed in Fig. 7b show a flow pattern similar to the experiment. The slip line and the formation of vertices along it are clearly depicted. The shock and reflected shock as well as the recompression shock are very sharply defined with very low numerical noise. The vortex developed after the compression shock is distinctly displayed. A new reflected shock can be seen developing at the channel wall behind the double wedge.

The results shown in Figs. 5-7 display the ability of the algorithm to simulate a complex transient flow problem on dynamically adapting grid. The error estimates used in our algorithm allow detection of strong and

weak shock waves, conducted discontinuities, vortices or other fronts that need enhanced resolution.

CONCLUSION

The Direct Dynamic Refinement (DDR) method was developed and tested for a challenging problem of reflection and diffraction of a strong shock over a double ramp. For this test problem we have demonstrated that a set of error indicators developed for the DDR allow capturing strong and weak features of the complex wave structure developing in this test case.

The above described algorithms were implemented in the AUGUST code. The AUGUST code was used for a range of subsonic, transonic, and supersonic transient and steady problems. For all these conditions the AUGUST code produced robust results with the error indicators proving to be applicable for all these diverse flow regimes.

ACKNOWLEDGMENT

The work reported here was partially supported by DARPA and AFOSR under Contract #F49620-89-C-0087. The authors would like to thank Col. James Crowley and Dr. A. Nachman for their interest in this project.

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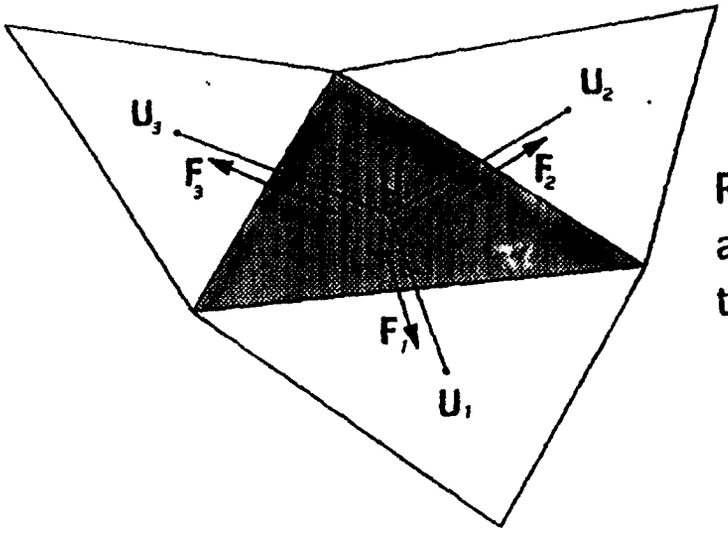


Representative triangular cell in the mesh and its neighbors showing fluxes across the edges

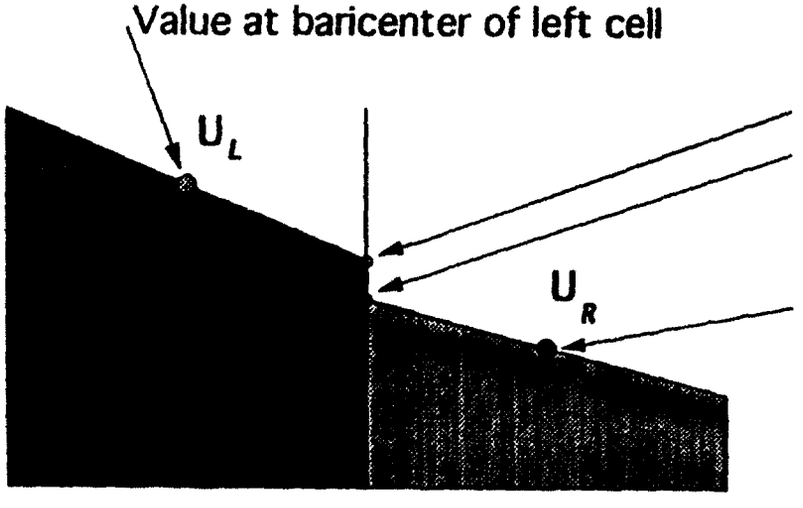
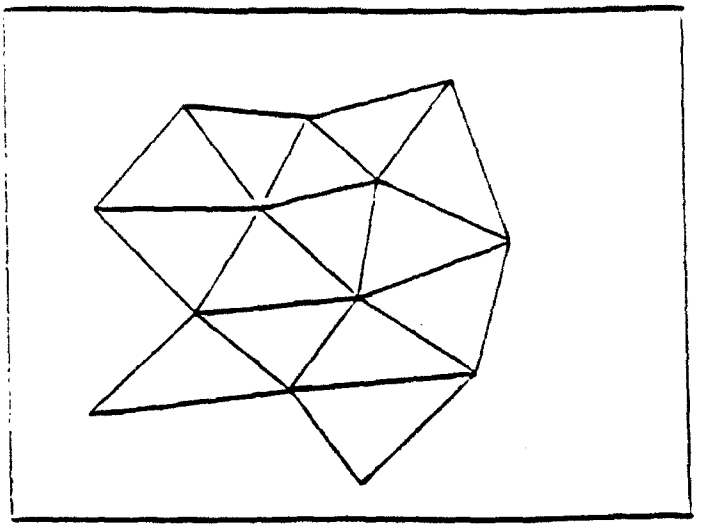
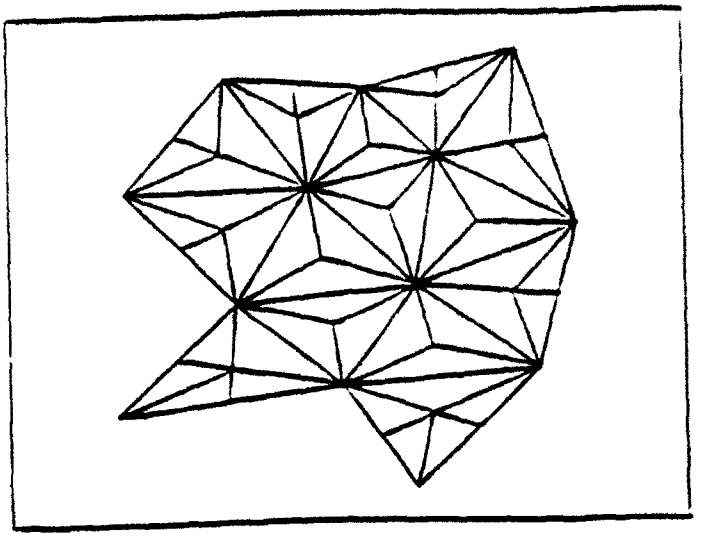


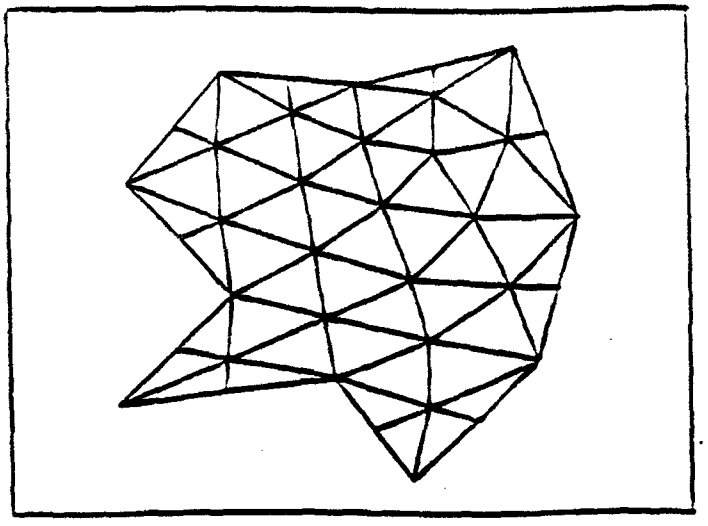
Figure 1. Representative triangular cell in the mesh showing fluxes and projected values.



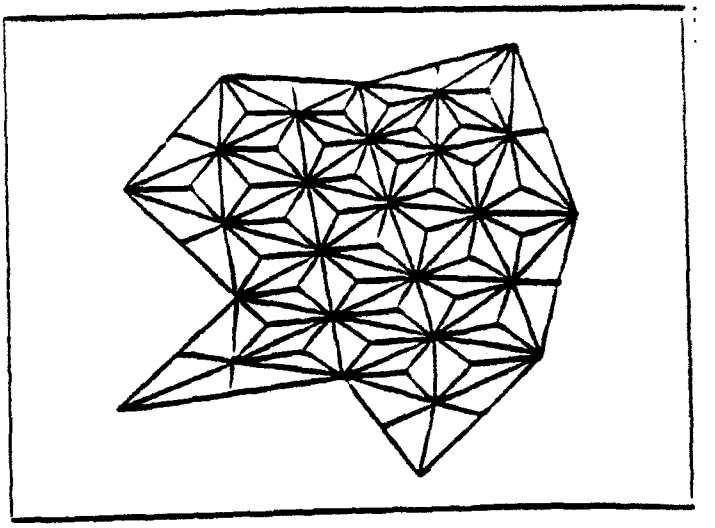
a. Original grid.



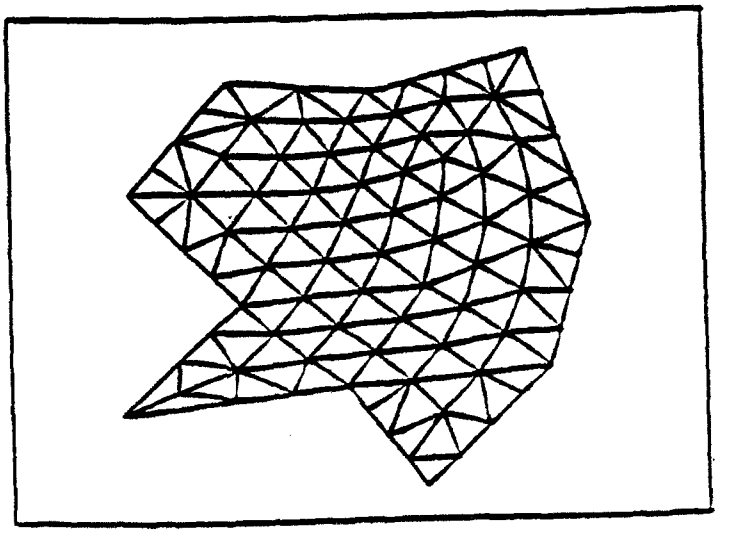
b. Grid after one refinement.



c. Grid after one refinement and one reconnection.

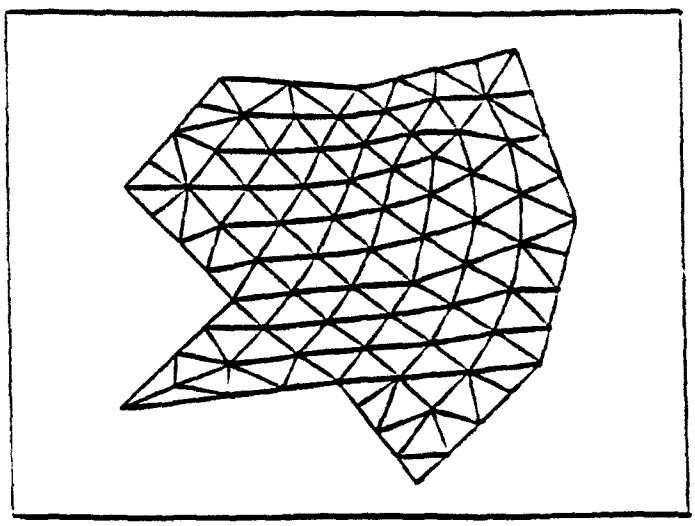


d. Second refinement.

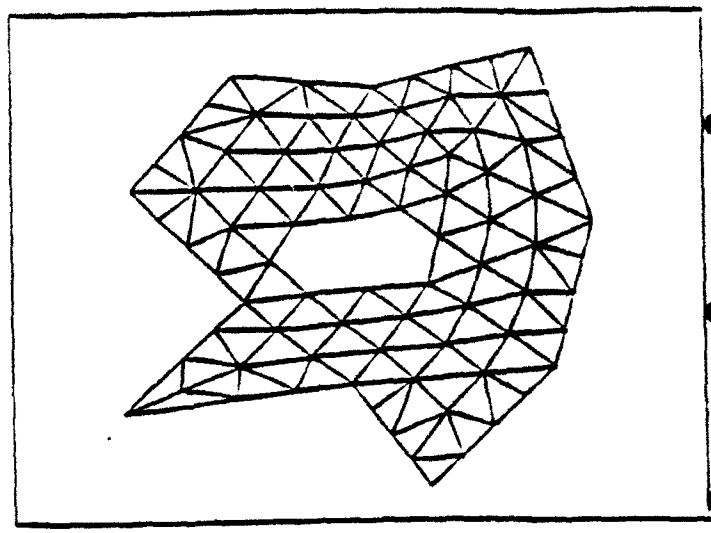


e. Second reconnection.

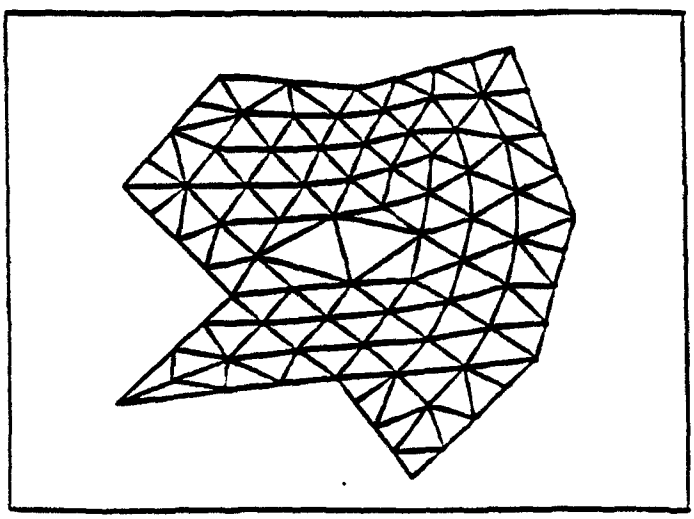
Figure 2. Illustration of the grid refinement process.



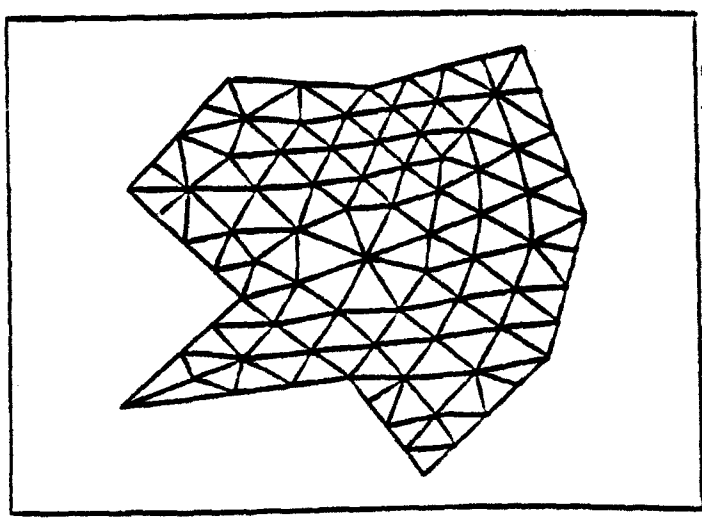
a. Original grid.



b. Point removal.



c. Constructing of new cells.



d. Grid after reconnection and relaxation.

Figure 3. Illustration of the grid coarsenning process.

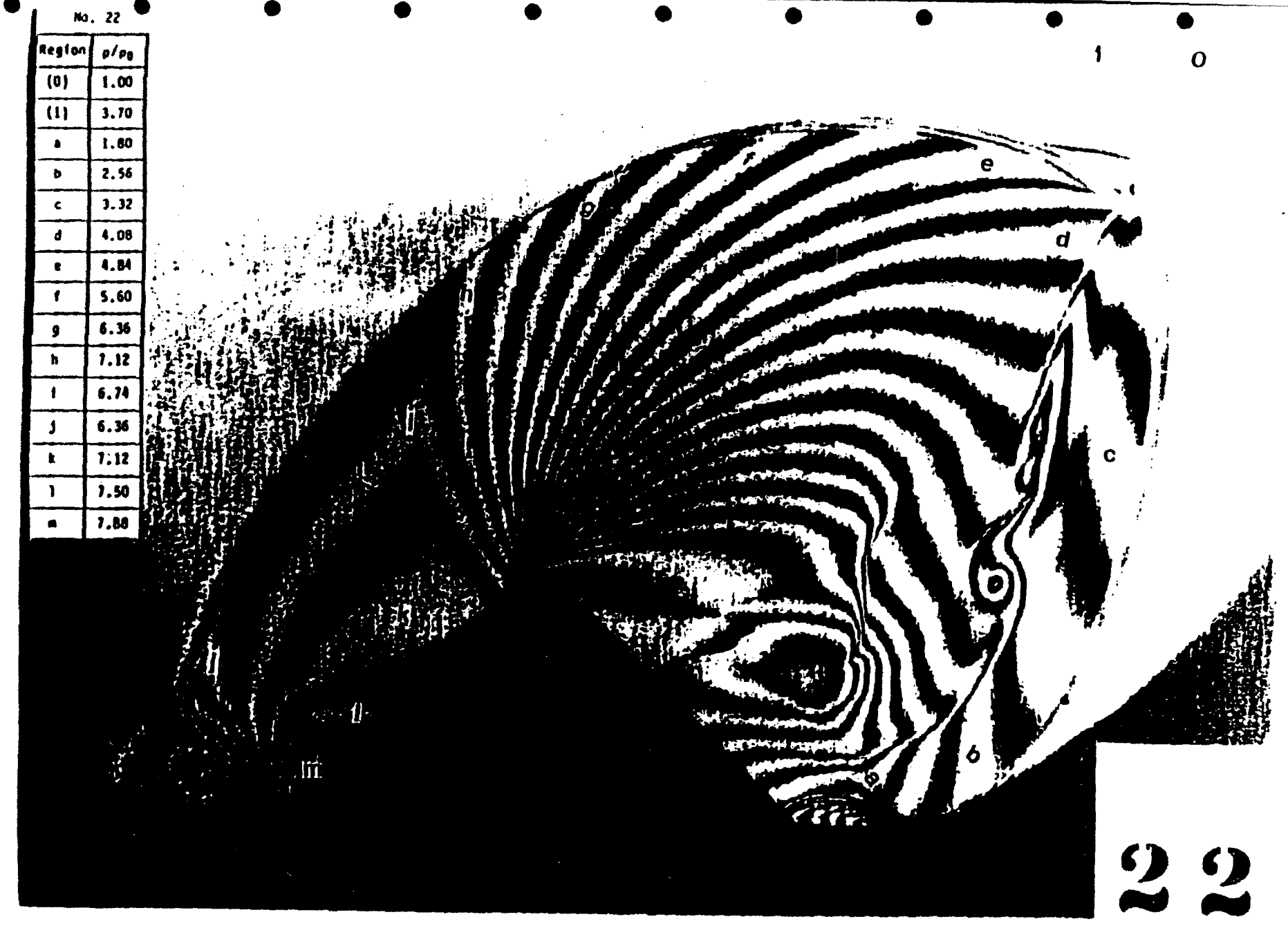


Figure 4. An experimental interferogram taken at 96 μs after shock wave hits a diamond shaped obstacle, Mach $M_s = 2.85$.

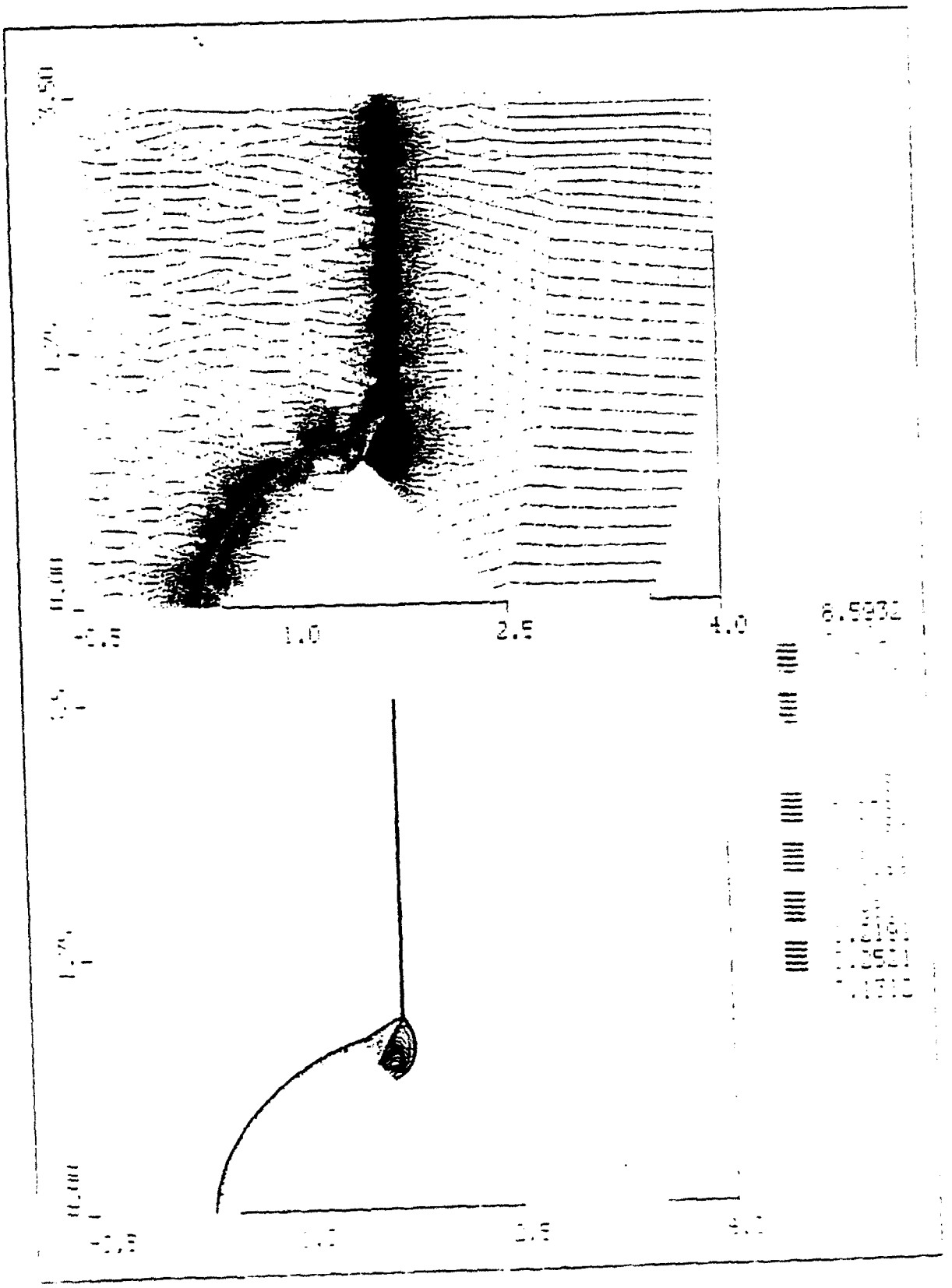


Figure 5. Computed density contours simulating flow identical to the setup of the experiment of Fig. 4. The grid is composed of 21121 vertices.

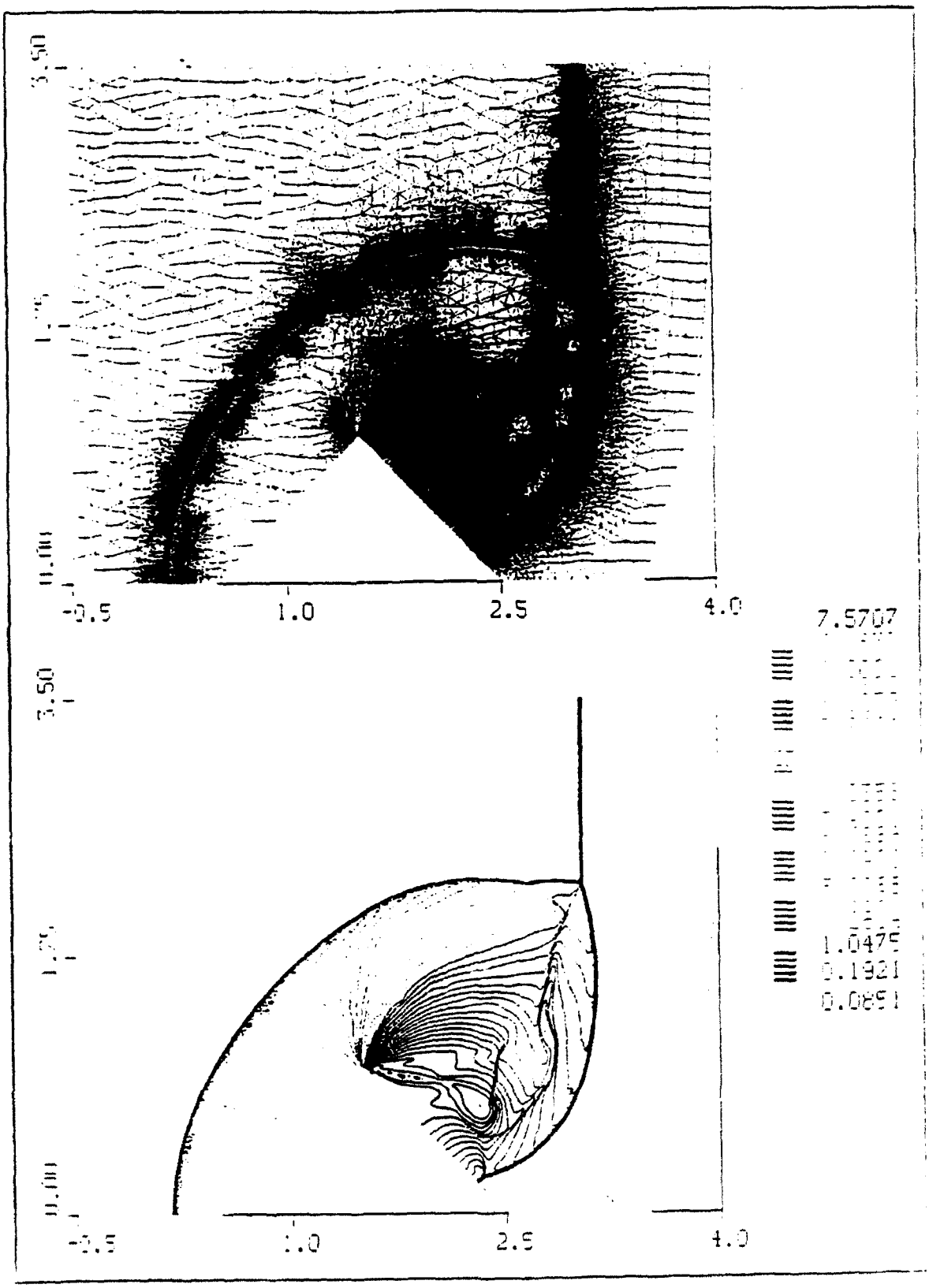


Figure 6. Computed density contours simulating flow identical to the setup of the experiment of Fig. 4. The grid is composed of 65624 vertices.

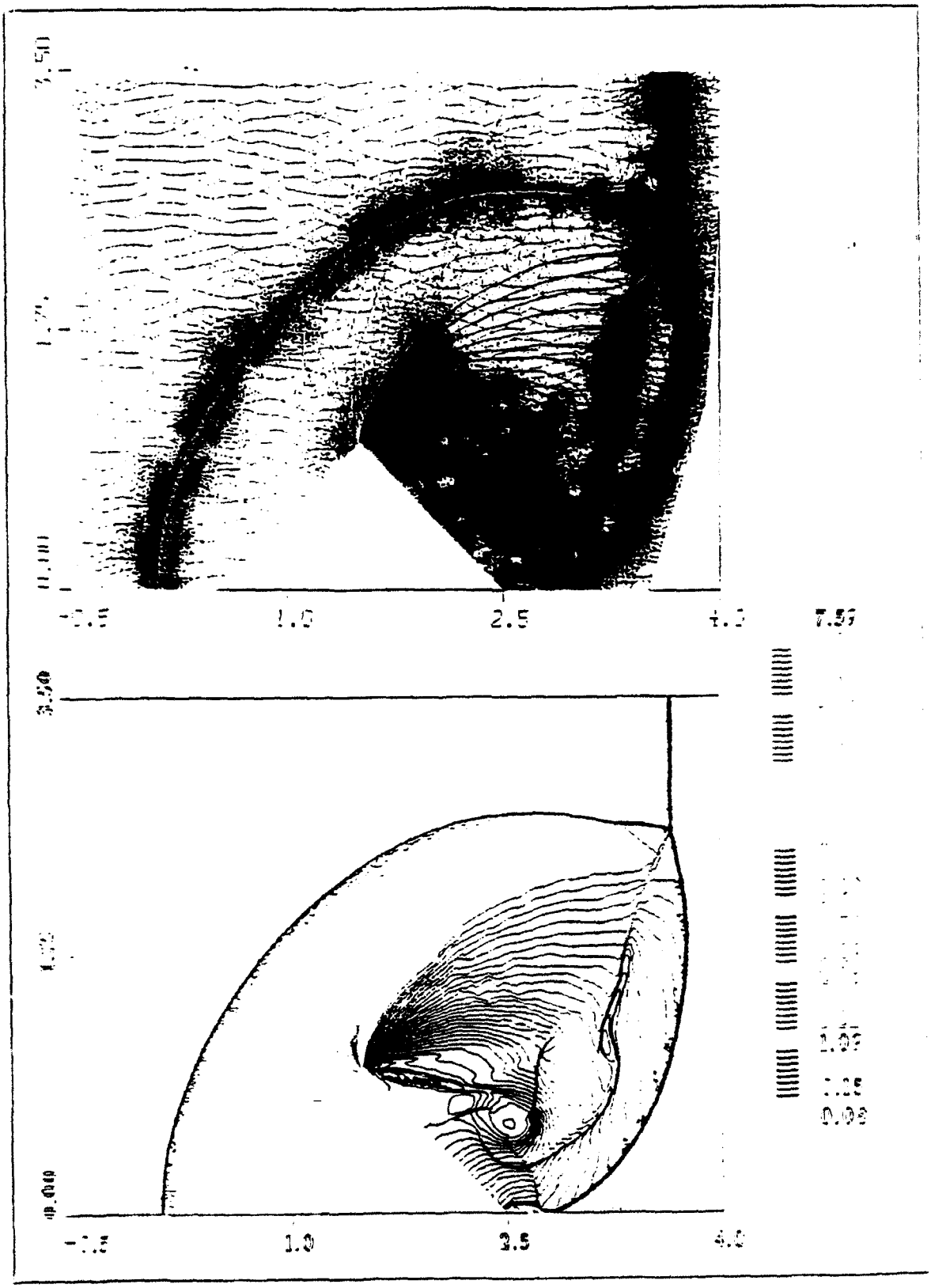


Figure 7. Computed density contours comparable to time of the experimental results shown in Fig. 4. The grid is composed of 79352 vertices.

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DECOMPOSITION BY STRUCTURED/UNSTRUCTURED COMPOSITE GRIDS FOR EFFICIENT INTEGRATION IN DOMAINS WITH COMPLEX GEOMETRIES

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Abstract

The Second Order Godunov method has been simultaneously implemented on both unstructured triangular and structured rectangular grids. This combined structured/unstructured method is a much more efficient approach to domain decomposition as compared to the separate application of each method. Application of this new technique to the complex problem of acoustic wave focusing in an ellipsoid reflector has demonstrated its advantages over both structured and unstructured methods of domain decomposition. It has been shown that the complex pattern of acoustic waves propagates seamlessly through structured/unstructured grid interfaces without reflection or distortion. The new approach provides ultimate flexibility in domain decomposition with minimum penalty in terms of memory and CPU requirements, and at the same time capitalizes on the advantages of both structured and unstructured grid methods.

Introduction

Structured rectangular grids allow the construction of numerical algorithms that perform an efficient and accurate integration of fluid conservation equations. The efficiency of these schemes results from the extremely low storage overhead needed for domain decomposition and the efficient and compact indexing that also defines domain connectivity. These two factors allow code construction based on a structured domain decomposition that can be highly vectorized and parallelized. Integration in physical space on orthogonal and uniform grids produces the highest possible accuracy of the numerical algorithms. The disadvantage of structured rectangular grids is that they cannot be used for decomposition of computational domains with complex geometries.

The early developers of computational methods realized that, for many important applications of Computational Fluid Dynamics (CFD), it is unacceptable to describe curved boundaries of the computational domain using the stair-step approximation available with the rectangular domain decomposition technique. To overcome this difficulty, the techniques of boundary-fitted coordinates were developed. With these techniques, the computational domain is decomposed on quadrilaterals that can be fitted to the curved domain. The solution is then obtained in the physical space using the geometrical information defining the quadrilaterals, or in the computational coordinate system that is obtained by transformation of the original domain into a rectangular domain. The advantage of this technique is that it employs the same indexing method as the rectangular structured domain decomposition methods that also serve to define domain connectivity. The boundary fitted coordinates approach leads to efficient codes, with approximately a 4:1 penalty in terms of memory requirement per cell as compared with rectangular domain decomposition. However, this approach is somewhat restricted in its domain decomposition capability, since distortion or large size variations of the quadrilaterals in one region of the domain lead to unwanted distortions or increased resolution in other parts of the domain. An example of this is the case of structured body fitted coordinates that are used for simulations of flows over a profile with sharp trailing edges. In this case, increased resolution in the vicinity of the trailing edge leads to increased resolution in the whole row of elements connected to the trailing edge elements.

The most effective methods of domain decomposition developed to overcome this disadvantage are those using unstructured triangular grids. These methods were developed to cope with very complex computational domains. The unstructured grid method, while efficient and powerful in domain decomposition, results in codes that must store large quantities of information defining the grid geometry and connectivity, and have large computational and storage overheads. As a rule, an unstructured grid code requires greater storage by a factor of 10, and will run about 5 times slower when compared on a per cell per iteration basis with a structured rectangular code.

Unstructured triangular meshes are designed to provide a grid that is fitted to the boundary of complex geometry. The flexibility of the unstructured mesh that allows gridding complex geometry should be weighed against the huge memory requirement needed to define the inter connectivity between the triangles. To cut down on the memory overhead, unstructured grid methods are used to their best advantage when combined with grid adaptivity. This feature usually allows the dynamic reallocation of triangles according to the physics and geometry of the problem solved, which leads to a substantial reduction in the number of cells needed for the domain decomposition. However, this advantage is highly dependent on the problem solved. Adaptive unstructured grids have an advantage over the unadaptive unstructured domain decomposition if the area of high resolution needed is around one-tenth of the global area of the computational domain. As a result, while the adaptive unstructured method may be extremely effective for simulating flow with multiple shock waves in complex geometries, it becomes extremely inefficient when high resolution is needed in a substantial area of the computational domain.

Our approach to domain decomposition combines the structured and unstructured methods for achieving better efficiency and accuracy. Under this method, structured rectangular grids are used to cover most of the computational domain, and unstructured triangular grids are used only to patch between the rectangular grids (Fig. 1), or to conform to the curved boundaries of the computational domain (Fig. 2). In these figures, an unstructured triangular grid is used to accurately define the curved internal or external boundaries and a structured rectangular grid is used to decompose the regions of the computational domain that have a simple geometry.

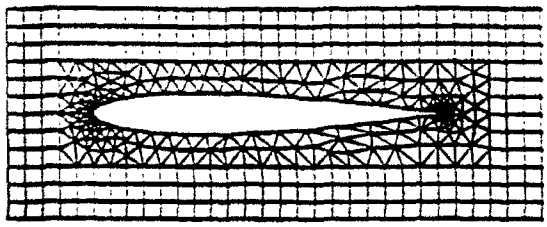

Figure 1. A possible candidate configuration for hybrid structured/unstructured domain decomposition.

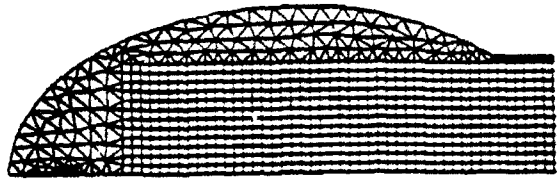

Figure 2. A possible candidate configuration for hybrid structured/unstructured domain decomposition, representing the ellipsoid reflector grid used for the numerical simulation.

Our paper will illustrate the performance gains achieved from the use of this composite grid decomposition approach. We apply the Second Order Godunov method to solve the Euler equations on both structured and unstructured sections of the grid. The challenging problem of acoustic wave focusing in an ellipsoid is used as a test case to confirm the soundness of the approach and to check its performance characteristics and accuracy.

Mathematical Model and Integration Algorithm

We consider a system of two-dimensional Euler equations written in conservation law form as:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0 \tag{1}$$

where

$$U = \begin{vmatrix} \rho \\ \rho u \\ \rho v \\ e \end{vmatrix}, \quad F = \begin{vmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(e+p) \end{vmatrix}, \quad G = \begin{vmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(e+p) \end{vmatrix}.$$

Here u, v are the x, y velocity vector components, p is the pressure, ρ is the density and e is total energy of the fluid. We assume that the fluid is an ideal gas and the pressure is given by the equation-of-state

$$p = (\gamma - 1)(e - 0.5\rho(u^2 + v^2)) \tag{2}$$

where γ is the ratio of specific heats and typically taken as 1.4 for air. It is assumed that an initial distribution of the fluid parameters is given at $t = 0$, and the boundary conditions defining a unique solution are specified for the computational domain.

The system of governing equations in Eq. (1) can be written as

$$\frac{\partial U}{\partial t} + \nabla \cdot Q = 0 \tag{3}$$

where Q represents the convective flux vector. By integrating Eq. (3) over space and using Gauss' theorem, the following expression is obtained

$$\frac{\partial}{\partial t}\int_{\Omega} U dA + \oint_{\partial\Omega} Q\, dl = 0 \tag{4}$$

where $dl = n d\mathcal{L}, n$ is the unit normal vector in the outward direction, and $d\mathcal{L}$ is a unit length on the boundary of the domain. The variable Ω is the domain of computation and $\partial\Omega$ is the circumference boundary of this domain.

Eq. (4) can be discretized for each element (cell) in the domain

$$\frac{(U_i^{n+1} - U_i^n)}{\Delta t} A_i = \sum_{j=1}^{M} Q_j^n\, n_j\, \Delta L_j \tag{5}$$

where A_i is the area of the cell; Δt is the marching time step; U_i^{n+1} and U_i^n are the primitive variables at the center of the cell at time n and at the update $n+1$ time step; Q_j is the value of the fluxes across the M boundaries on the circumference of the cell where n_j is the unit normal vector to the boundary edge j, and ΔL_j is the length of the boundary edge j. The fluxes Q_j^n are computed applying the Second Order Godunov algorithm, and Eq. (5) is used to update the physical primitive variables U_i according to computed fluxes for each marching time step Δt. The marching time step is subjected to the CFL (Courant-Frerichs-Lewy) constraint.

We seek a solution to the system of Eq. (1) in the computational domain, which is decomposed in part into triangles with arbitrary connectivity and in part into rectangles using a logically structured grid. We use the advantage of the unstructured grid (Refs. 1-4) to describe the curved boundary of the computational domain and areas that need increased local resolution. In our example, the unstructrued grid covers 10% of the total computational domain while the structured grid occupies the remaining 90%. The numerical technique for solving Euler's equation on an unstructured grid is described in Refs. 5-7, and the technique for the structured grid is described in Ref. 8. These numerical techniques apply some of the ideas that were introduced in Refs. 9-10. The structured and unstructured codes apply the center-based formulation, i.e., the primitive variables are defined in the center of the cell, which makes the cell the integration volume, while the fluxes are computed across the edges of the cell. The basic algorithmic steps of the Second Order Godunov method can be defined as follows:

1. Find the value of the gradient at the baricenter of the cell for each gas dynamic parameter U;
2. Find the interpolated values of U at the edges of the cell using the gradient values;
3. Limit these interpolated values based on the monotonicity condition (Ref. 9);
4. Subject the projected values to the characteristic's constraints (Ref. 10);
5. Solve the Riemann problem applying the projected values at the two sides of the edges;
6. Update the gas dynamic parameter U according to the conservation equations (1) applying to the fluxes computed and the current time step.

As was advocated in Ref. 7, we prefer the triangle center-based over the vertex-based version of the code. For the same unstructured grid, a triangle-based algorithm will result in smaller control volumes than a vertex-based. In addition, for the Second Order Godunov solver, implementation of the boundary conditions is more straightforward and accurate for the center-based algorithm than in the vertex-based. These two factors, along with the effects of grid connectivity, strongly affect the algorithm accuracy and

performance, and are the main reasons for the superiority of the center-based version over the vertex version.

Sound Wave Focusing in an Ellipsoid Reflector

Research relating to focusing of shock and acoustic waves is of considerable practical interest for application to Extracorporeal Shock Wave Lithotripsy (ESWL). Most of the interest in this area is related to acoustic waves in liquids; however, the basic reflection and focusing mechanisms for a given reflector geometry can be studied in air as well. For our test simulation, we chose a deep reflector shaped like an ellipsoid, which was used for ESWL by Dornier (Ref. 11) and other companies. A schematic of the cross section of this reflector is shown in Fig. 3. Strong acoustic waves are generated in the left focal point of the ellipsoid by an instantaneous release of energy and are refocused at the right focal point. Ideally, focusing should be based on waves of acoustic intensity, since the nonlinear reflections of strong shock waves lead to significant distortions in wave propagation and impair simple geometrical focusing.

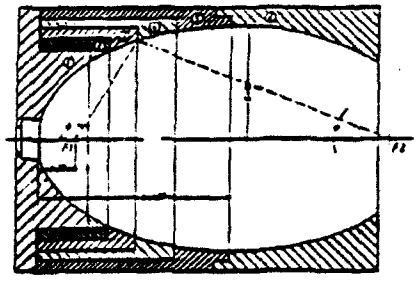

Figure 3. A schematic drawing of the center cross section of the ellipsoid reflector.

Figure 2 shows the computational domain and grid for the ellipsoid reflector example. In order to illustrate the concept of the composite structured/unstructured grid, we have shown only every 1/16 cell of the grid that was actually used for the simulation. In this example, we observe that the structured rectangular grid covers about 90% of the computational domain and the unstructured triangular grid is restricted to the curved surface of the ellipsoid and covers about 10% of the domain. The major axis of the ellipsoid is 150 mm and the minor axis is 90 mm.

The integration in the structured part of the domain is performed using a version of the split Second Order Godunov method described in Ref. 8. For the unstructured triangular grid, we used our implementation of the Second Order Godunov method that includes a compact integration stencil suitable for unstructured grids (Refs. 5-7). In the current implementation, the two sections of the grid communciate through the boundary conditions at their interfaces. According to this, the values in the mirror points at the grid interfaces for the triangular grid are taken from the computational domain of the structured grid and vice versa. These mirror values are used for calculations of the flux at the interface boundaries. For focusing problem simulations, we used 55188 triangles in the unstructured part of the grid and 141312 (736 × 192) rectangles in the structured part. It should be mentioned that in order to obtain a uniform grid (i.e., the structured and unstructured grids have the same level of refinement), the unstructured portion of the code was run with adaptivity (adding and deleting vertices). This ability enabled us to match the grid resolution based on cell areas in the structured/unstructured grids while computing the results. The initial grid had a very refined grid at the left focal point to initiate accurately the detonation. This area was coarsened later in the simulation by turning on the adaptive capability of the unstructured code.

We used the following initial condition at the time t = 0 for the simulation of the acoustic wave focusing:

a. Quiescent air in the cavity of the reflector, i.e., Pressure $P_o = 101350.$ Pa and Density $\rho_o = 1.2\,\mathrm{Kg/m^3}$.

b. Blast in the left focal point of the ellipsoid confined in a spherical volume of a radius of R = 2mm. Condition at initial blast area: Pressure $P_b = 45. * P_o$, and Density $\rho_b = 4.5 * \rho_o$.

This definition of the initial conditions guarantees that a weak blast wave will be generated, ensuring that waves of acoustic intensity will be reflected from the wall of the ellipsoid. We examined this particular reflection regime because the blast wave focusing in water occurs in acoustic mode. As it was pointed out in Ref. 11, reflection of even very weak waves in water will lead to considerable deviations from the reflection mode of a pure acoustic wave. However, the purpose of this simulation

is to demonstrate the numerical method and not to study in detail the focusing modes of the ellipsoid reflector. Therefore, we present results for one simulation following conditions outlined above.

In Fig. 4a, the simulation results are shown in the form of pressure contours at the time $t = 1.31 \times 10^{-4}$sec when the incident shock started its reflection from the reflector wall. Here we can observe that the maximum reflected pressure is no higher than 14% over the ambient pressure, which is consistent with our objective to create weak waves. Figure 4b is an enlargement of the region in the computational domain that contains structure and unstructured grids. We can also observe that the incident wave propagates seamlessly through the interface of the structured and unstructured regions. In Fig. 5, we show pressure contour plots at time $t = 2.09 \times 10^{-4}$sec. We observe that the interfaces between the two grids carry the information seamlessly.

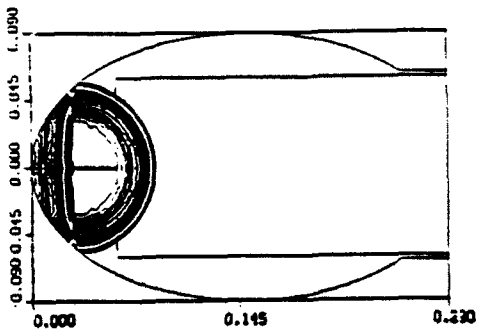

Figure 4a. Pressure contours at time $t = 1.31 \times 10^{-4}$sec showing the incident wave as reflected from the reflector's wall.

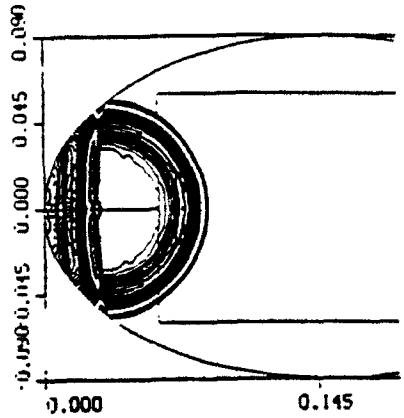

Figure 4b. Blowup of the pressure contours at time $t = 1.31 \times 10^{-4}$sec showing the matching pressure contours between the structured and the unstructured grid.

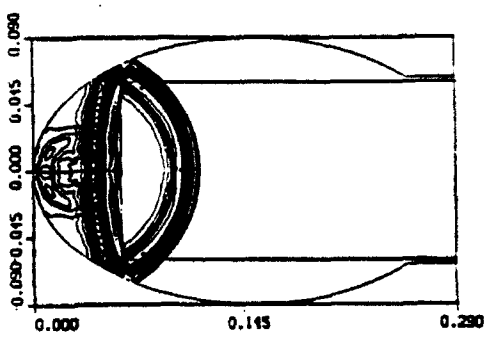

Figure 5. Pressure contours at time $t=2.09 \times 10^{-4}$sec showing the incident wave and the reflected wave pattern.

Figure 6 shows the simulation results at time $t = 4.35 \times 10^{-4}$sec. At this stage, the blast wave front that propagated to the left has undergone full reflection and the reflected wave propagates in the direction of the incident wave to the right. However, the incident and the reflected wave are both of acoustic intensity and they are propagating at the speed of sound. Therefore, the reflected wave will not be able to catch up with the incident wave at this stage of expansion. We can observe in Fig. 7, where the two waves are shown past the ellipsoid centers ($t = 5.41 \times 10^{-4}$sec), that the distance between these acoustic waves does not change as compared with Fig. 6. The reflected wave has maximum pressure in the vicinity of the axis and its value remains relatively constant (about 1.10×10^5 Pa) through the propagation process. The wave complex at the axis of symmetry consists of the incident acoustic wave front, a reflected wave that has positive followed by negative phases.

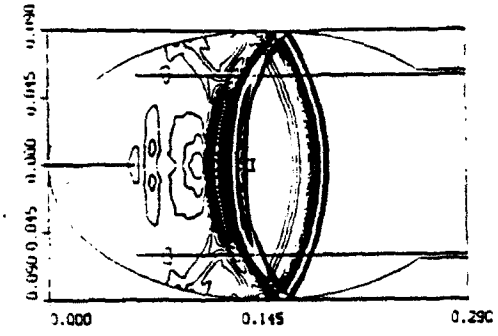

Figure 6. Pressure contours at time $t=4.35 \times 10^{-4}$sec showing the incident wave and the reflected wave pattern.

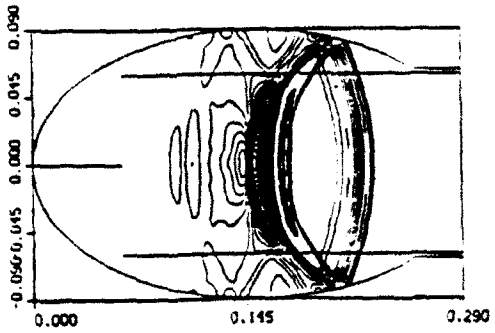

Figure 7. Pressure contours at time $t=5.41 \times 10^{-4}$sec showing the wave pattern past the center of the ellipsoid.

The enhancement of the reflected wave's amplitude starts gradually when the reflected wave is approaching the second focal point caused by the convergence of the ellipsoid. In Fig. 8, the pressure contours ($t = 8.41 \times 10^{-4}$sec) are shown at the stage that the maximum focused pressure is obtained in the system. As we can observe in Fig. 8, the incident front has left the computational domain, and the maximum pressure is obtained in small volume in the vicinity of the right focal point. In our simulation, the maximum focused pressure has reached 1.32×10^5Pa and is located 11 mm to the right of the focal point of the ellipsoid.

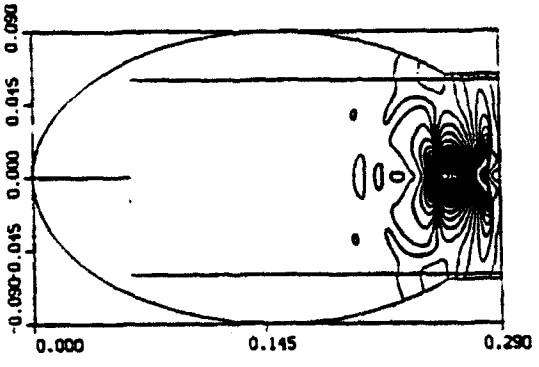

Figure 8. Pressure contours at time $t=8.41 \times 10^{-4}$sec showing the stage at which the maximum focused pressure is obtained.

In all the figures presented, the method of composite domain decomposition works extremely well, producing seamless solutions at the interfaces. We should mention here that our test problem is particularly sensitive because the main acoustic waves are weak, and any inaccuracy introduced at the grid interfaces would produce a distortion in the phase or in the intensity of the traveling waves that would be a visible disturbance evident in the results needless to mention that an adaptive scheme would have difficulty in simulating this problem due to the weakness of the wave pattern.

Conclusions

A composite method of structured/unstructured domain decomposition is introduced as an efficient technique for dealing with the computational domains of complex geometry. We have simulated a demanding acoustic wave focusing problem and have shown that our approach leads to accurate wave propagation without any reflection or distortion at the structured/unstructured grid interfaces. It should be noted that for the acoustic focusing problem as simulated and presented in this paper, both structured and unstructured methods of domain decomposition can be shown to be inadequate if used separately. The structured method has difficulty describing the curved boundaries of the computational domain, while the unstructured method is totally inefficient in describing phenomena with wide fronts that occupy a large portion of the computational domain. Our hybrid method combines the advantages of structured and unstructured methods of domain decomposition. This hybrid technique combines the efficiency of the unstructured grid to accurately represent curved walls, with the computational and memory efficiency of the structured grid in the majority of the computational domain. We also attribute the quality of the numerical result to the Second Order Godunov method, which allows a consistent, accurate and robust formulation for handling both grids and boundary conditions.

Acknowledgments

The work reported here was partially supported by DARPA and AFOSR under Contract #F49620-89-C-0087. The authors would like to thank Col. James Crowley and Dr. A. Nachman for their interest in this project.

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TWO-PHASE COMPRESSIBLE FLOW COMPUTATION ON ADAPTIVE UNSTRUCTURED GRID USING UPWIND SCHEMES

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ABSTRACT

A computer program called MPHASE for numerical study of shock wave propagation in a multi-phase, multi-component gas environment is described and applied. The mathematical model of the multi-phase, multi-component system is based on the multi-fluid Eulerian approach. Basically, we consider the two phases(i.e. gas and particle) to be interpenetrating continua: the dynamics of the flow is governed by conservation equations for each phase, and the two phases are coupled by interactive drag force and heat transfer. The code is formulated on unstructured triangular grids.

The numerical solution method is based on the Second Order Godunov Method for the gaseous medium, an upwind integration for the particles, and an implicit integration technique for the gas-particle interaction simulation. In order to produce a solution with high spatial accuracy at minimal computational cost, an adaptive procedure on the unstructured grid is used. The adaptive procedure will automatically enrich the grid by adding points in the high-gradient (or high flow activity) region and by removing points (coarsening the mesh) where they are not needed. This technique allows a detailed study of the complex two-phase shock reflection phenomena, where the effects of momentum and heat exchange between phases will significantly modify the shock structure and shock parameters.

Results will be given from the code validation study for the shock propagation in the dusty gases. The code performance will be illustrated by solving the problem of reflection and diffraction of a plan shock wave over a semicircular cylinder in a dusty gas.

1. THE MATHEMATICAL MODEL AND THE NUMERICAL SOLUTION

Conservation Equations

The mathematical model consists of conservation governing equations and constitutive laws that provide closure for the model. The basic formulation adopted here follows the gas and dilute particle flow dynamics model presented by Soo[1]. The following assumptions are used during the derivation of governing equations:

(1) The gas is air and is assumed to be ideal gas;

(2) The particles do not undergo a phase change because particles are considered as sand whose phase transition temperature is much higher than the gas temperature considered here;

(3) The particles are solid spheres of uniform diameter and have a constant material density;

(4) The volume occupied by the particles is negligible;

(5) The interaction between particles can be ignored;

(6) The only force acting on the particles is drag force and the only heat transfer between the two phases is convection. The weight of the solid particles and their buoyancy force are negligibly small compared to the drag force;

(7) The particles have a constant specific heat and are assumed to have a uniform temperature distribution inside each particle.

Under the above assumptions, distinct equations of continuity, momentum, and energy are written for each phase. The interaction effects between the two phases are listed as the source terms on the righthand side of the governing equation. The two dimensional unsteady conservation equations for the two phases can be written in the vector form in Cartesian coordinates:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = S. \tag{1}$$

Here U is the vector of conservative variables, F and G are fluxes in x and y direction, respectively, and S is the source term for momentum and heat exchange. The definition of these vectors are:

$$U = \begin{vmatrix} \rho \\ \rho u \\ \rho v \\ e \\ \rho_p \\ \rho_p u_p \\ \rho_p v_p \\ e_p \end{vmatrix}, \quad F = \begin{vmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(e+p) \\ \rho_p u_p \\ \rho_p u_p^2 \\ \rho_p u_p v_p \\ u e_p \end{vmatrix}, \quad G = \begin{vmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(e+p) \\ \rho_p v_p \\ \rho_p u_p v_p \\ \rho_p v_p^2 \\ v_p e_p \end{vmatrix}, \quad S = \begin{vmatrix} 0 \\ -f_x \\ -f_y \\ -q - u_p f_x - v_p f_y \\ 0 \\ f_x \\ f_y \\ q + u_p f_x + v_p f_y \end{vmatrix}$$

where ρ, u, v, and e are gas density, velocities, and energy, respectively; ρ_p, u_p, v_p and e_p are particle density, velocities, and energy, respectively; (f_x, f_y) and q denotes drag force components acting on the particles and heat transfer to the particles, respectively. The gas pressure p is related to ρ, u, v and e for by

$$p = (\gamma - 1)[e - 0.5\rho(u^2 + v^2)] \tag{2}$$

where γ is the specific heat ratio. The gas temperature can be found through the equation-of-state for ideal gas

$$p = \rho RT \tag{3}$$

where R is the gas constant.

The particle temperature T_p is calculated through relation

$$e_p = \rho_p c_p T_p + 0.5\rho_p(u_p^2 + v_p^2). \tag{4}$$

The source terms on the righthand side of equation (1) are momentum and heat exchange between gas and particle phases. If we let r_p and ρ_s be the particle radius and material density, respectively, then the drag forces are

$$\begin{pmatrix} f_x \\ f_y \end{pmatrix} = \frac{3}{8} \frac{\rho_p \rho}{\rho_s r_p} C_d \left[(u - u_p)^2 + (v - v_p)^2\right]^{1/2} \begin{bmatrix} u - u_p) \\ (v - v_p) \end{bmatrix}. \tag{5}$$

The particle drag coefficient C_d is a function of Reynolds number, Re, which is based on the relative velocity between the gas and particle phases. After testing the drag coefficients given by Sommerfeld[2] and by Clift *et al.*[3], the following were two adopted:

$$C_d = \frac{24}{Re}(1 + 0.15Re^{0.687}) \text{ for } Re < 800$$

and (5)

$$C_d = \frac{24}{Re}(1 + 0.15Re^{0.687}) + \frac{0.42}{1 + 42500Re^{-1.16}} \text{ for } Re > 800\ .$$

Here the Reynolds number, Re is defined as

$$Re = \frac{2\rho r_p[(u - u_p)^2 + (v - v_p)^2]^{1/2}}{\mu} \tag{6}$$

Viscosity, μ is calculated at film temperature, namely, $T_f = 0.5(T_p + T)$, and the temperature dependency of the viscosity is evaluated according to Sutherland's law

$$\mu = \mu_r \left(\frac{T}{T_r}\right)^{3/2} \frac{T_r + \Phi}{T + \Phi} \tag{7}$$

where μ_r is the dynamic viscosity of the gaseous phase at the reference temperature and Φ is an effective temperature, called the Sutherland constant.

The rate of heat transfer from gaseous phase to the particle phase is given by

$$Q = \frac{3}{2} \frac{\rho_g}{\rho_s} \frac{\mu C_p}{Pr} Nu \, (T_g - T_p) \tag{8}$$

where $Pr = \mu c_p / k_g$ is the Prandtl number, and c_p and k_g are the specific heat and thermal conductivity of gas, respectively. The Nusselt number Nu is a function of this Reynolds number and the Prandtl number as given by Drake[4]

$$Nu = \frac{2 r_p h}{R} = 2 + 0.459 Re^{0.55} Pr^{0.33}. \tag{9}$$

Initial and Boundary Conditions

The geometry of the computational domain is shown in Fig. 1. The initial conditions for gas are $\rho_o = 1.2 kg/m^3$ and $p_o = 101.3 kpa$, with a coming shock at x = -0.5. There are no particles from - 1.0 $\leq x \leq$ 0.0. From $x \geq$ 0.0, particles are initially in thermal and kinematic equilibrium with surrounding gas. The particles that are uniformly distributed in the dusty region have the following parameters for different test problems:

Mass loading, ρ_p: 0.25 kg/m^3, 0.76 kg/m^3;

Mass material density, ρ_s: 2500 kg/m^3;

Particle radii, r_p: 10 μm, 25 μm, 50 μm;

Specific heat, c_s: 766 $J/kg/K$.

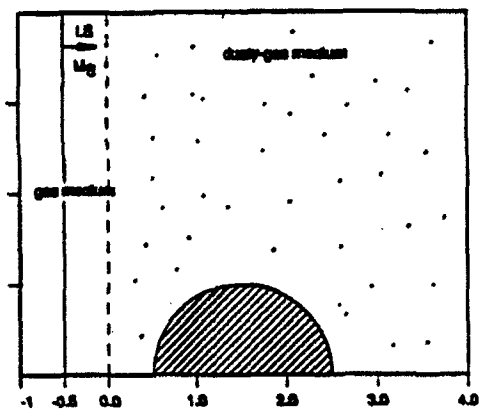

Figure 1. An illustration of the considered flow field.

The lower boundary and cylinder surface are solid walls and assumed adiabatic and impermissible. A reflecting boundary condition is assumed for both the gas and particle phase. Particles are assumed to experience a perfect elastic collision with the wall and reflect from the wall. The right and upper boundaries are open boundaries where a nonreflection boundary condition is used for the gas phase and a zero normal gradient condition is used for particle phase.

Numerical Method of Solutions

The system of partial differential equations described in the previous paragraph is integrated numerically. Equation (1) is repeated here:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = S. \tag{1}$$

In order to solve this equation numerically, an operator time-splitting technique is used. Assuming that all flow variables are known at a given time, we can calculate its advancement in time by splitting the integration into two stages.

In the first stage, the conservative part of equation (1) is solved:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0. \tag{10}$$

The Second Order Godunov method is used for the integration of the subsystem of equations describing the flow of the gaseous phase (first four components of equation (1)). The method is well documented in literature.[5,6,7] The subsystem of equations describing the particle phase flow is integrated using a simple finite difference upwind scheme. This is done because there is no shock in the particle phase and the upwind scheme leads to a robust and accurate integration scheme.

In the second stage, the source term is added and the following equation is solved:

$$\frac{\partial U}{\partial t} = S. \tag{11}$$

To integrate this equation in time, we need to obtain S as a function of U. We calculate S through equations (5) to (8).

In order to produce a solution of the high spatial accuracy at minimal computational cost, an unstructured triangular grid with adaptive procedure is used. The adaptive procedure will automatically enrich the mesh by adding points in the high gradient (or high flow activity) region of the flow field and by removing points (coarsening mesh) where they are not needed. The dynamic nature of mesh enrichment is shown in Fig. 3 for two different time frames. One can see that a very fine mesh is generated around shock fronts and other steep density gradient regions.

2. RESULTS

Model Validation for One-Dimensional Shock Wave Propagation in A Dusty Gas

To test the momentum and heat exchange mechanism for the current two-phase model, we first simulate a one-dimensional problem of a normal shock wave propagating into a dusty gas. We numerically simulate the experiments conducted by Sommerfeld[2]. In the experiments, small glass sphere particles of material density $\rho_s = 2500 kg/m^3$, specific heat capacity $c_s = 766 J/kg/K$, and average diameter of 27 μm were used as suspension particle phase. The incoming shock, and particle loading ratio $\eta = \rho/\rho_p$, are two varying parameters. The experimental results and our numerical simulation results of shock Mach number as a function of distance for two test cases are shown in Fig. 2a ($\eta = 0.63$ and Fig. 2b ($\eta = 1.4$) for comparison purpose. As one can see, the agreement between the prediction of our present model and the experimental results is very good.

Two-Dimensional Simulation Results of Pure Gas Flow

To test the accuracy of the two-dimensional computation, we compute the pure gas flow case of a shock wave reflection and diffraction over a semicircular cylinder. We then compare the simulation with experimental results. Shock wave reflection on a wedge has been extensively studied by many researchers (see e.g., review paper of Hornung[8]). Shock wave reflection by circular cylinders was numerically simulated by Yang *et al.*[9] and experiments were performed by Kaca[10]. Fig. 3a and 3b show density contours with adapted grids at two moments in time. In Figs. 4a nd 4b, the interferogram from the experiment[9] and density contours from the present simulation are compared for the same flow condition and same time. Note that the density levels are normalized by the ambient gas density in Fig. 4. As one can see from Fig. 4a and Fig. 4b, the results show an excellent quantitative as well as qualitative agreement between the numerical simulation and experimental results.

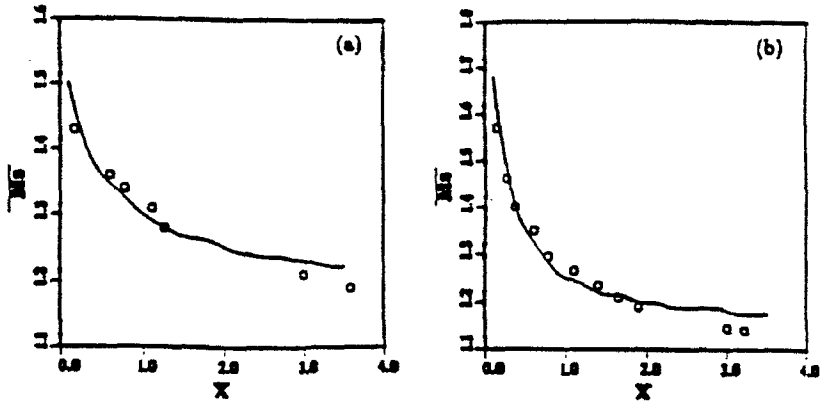

Figure 2. Comparison between computational prediction and experimental measurement of shock wave attentuation for (a) $M_\infty = 1.40$, $\eta = \frac{\rho_2}{\rho_\infty} = 0.63$ and (b) $M_\infty = 1.7$, $\eta = \frac{\rho_2}{\rho_\infty} = 1.4$ (o experiment, - calculztion).

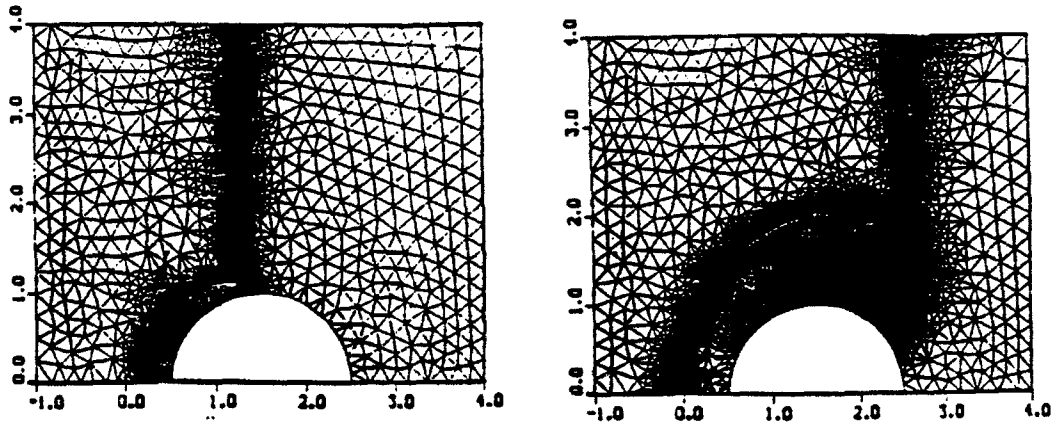

Figure 3. Computed density contours with adapted grid at two different times.

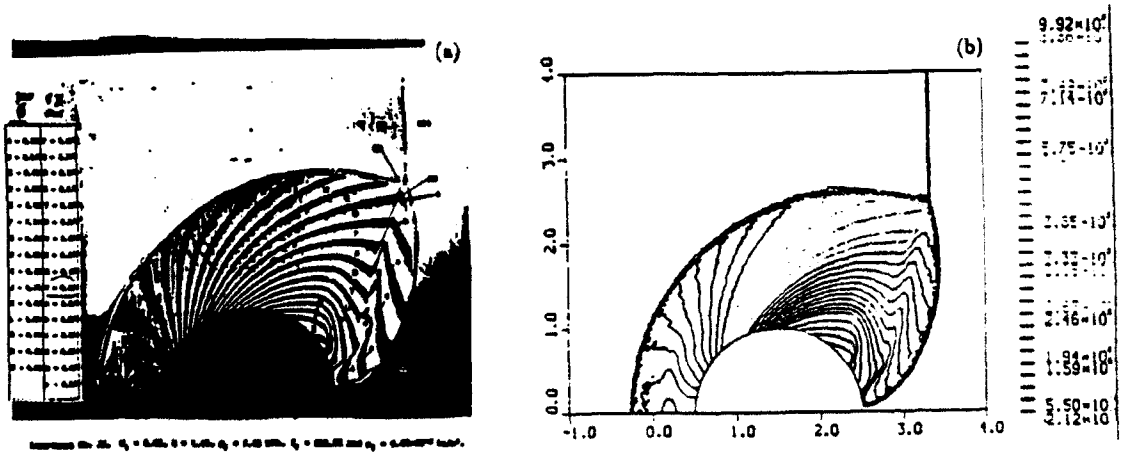

Figure 4. Comparison for $M_\infty = 2.80$ gas – only flow, (a) interferogram from experiment conducted by Kaca (1988), (b) density contours from present calculation.

Two-Dimensional Simulation Results of Two-Phase Flow

The basic setup for the two-phase simulation is shown in Fig. 1. Here the planar shock with Ms=2.3 impinges on an area of a dusty gas. The interface between clear air and dusty air is located at x=0.0 of the computational domain. The area of the dusty air contains a semicylinder with a radius of $1m$. The size of the computational domain, initial parameters of the gas, parameters of the incoming shock, size of the semicylinder and its location in the computational domain, are the same as in the reflection and diffraction simulation presented in the previous section.

The main objective of this set of simulations is to study the effects of particle size and particle loading on the parameters of the reflected and diffracted shock waves. It is also of interest to study the dynamics of reflection and diffraction in particle media. This is especially valuable since it is extremely difficult to observe these interactions experimentally in an optically thick dusty gas.

The first set of simulation results is shown for the case with dust parameters $r_p = 10\mu m$ and $\rho_p = 0.25\ kg/m^3$. The gas parameters and the parameters of the incoming shock wave are the same as in the pure gas case presented above. In Figs. 5a and 5b, particle density contours and gas density contours are shown at the stage when the incident shock wave has reached the top of the semicylinder. At this stage, particles have very little effect on the dynamics and parameters of the shock in the gas phase. The presence of the particles causes a small widening of the shock that is more noticeable for the incident shock. Also, one can observe an additional contour line at the dusty gas/pure gas interface. The particle density contours depict significant piling up of the dust particles at the leading edge stagnation point of the cylinder.

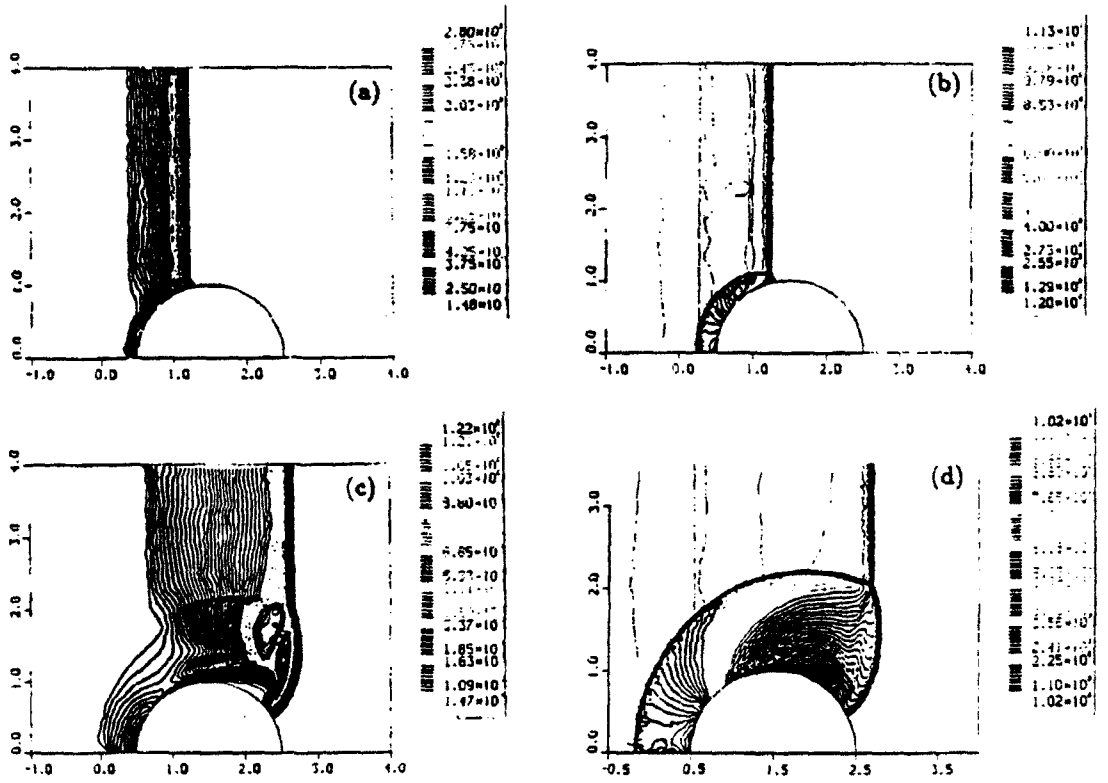

Figure 5. Density contours for the case; $M_s = 2.8$, $\rho_p = 0.25 kg/m^3$, $r_p = 10\mu m$ at two different times. (a) particle density at t_1, (b) gas density at t_1, (c) particle density at t_2, and (d) gas density at t_2.

In Figs. 5c and 5d, the particle density and gas density contours are shown at the stage where significant diffraction has taken place and the shock front is approaching the trailing edge of the cylinder. The small particle loading and small particle size leads to very small modification of the gas shock structure and parameters. One can observe further widening of the shock and some smearing of the slip

line that originates at the triple point. The particle density contours reveal that the particles piled up at the stagnation point were swept by the gas flow to the area of triple point and slip line for the gas flow, leaving a small amount of particles at the leading edge. We should note that this behavior is specific for our problem, where at t=0, the dusty gas area was located at x=0 and there is no influx of the dust from the left boundary. Also in Fig. 5c, we note that the particles reach a distinct local maxima at the distance about 25 *cm* behind the main shock front. At this maxima the particle density is 0.86 kg/m^3, which is more than three times the initial particle density. The particle density reaches a maximum value at the location of the gas slip line. We observe a significant accumulation of the particles that have been moved along the slip line by the shear flow. The larger concentration of particles in the vicinity of triple point is, in fact, the remainder of the particles that have concentrated first at the leading edge and then were swept up with the flow. It is also interesting to observe that an essentially particle- free zone is formed due to the effects of particles slipping over the top of the cylinder and the rarefaction wave behind the cylinder.

3. CONCLUSIONS

In this paper, a computer program for two-phase compressible flow computation on adaptive grids using upwind schemes is described. The following validation study and conclusion can be made.

(1) The validation study for a one-dimensional shock wave propagating in a dusty gas shows a good agreement between the prediction of our model and the results of the experiment.

(2) For a two-dimensional gas-only flow, numerical results agree well with existing experimental data qualitatively and quantitatively, indicating that the gas phase is accurately simulated by adaptive grid technique.

(3) Particles in the gas can have a profound effect on the shock wave reflection and diffraction pattern, which is a function of particle size and loading. The smaller the particle and the lesser the particle loading, the less the inference of particle on the flow field.

(4) There is a particle accumulation behind the "back shoulder" of the semicircular cylinder due to the effect of particles inertia and gas rarefaction wave.

4. ACKNOWLEDGMENTS

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PULSED DETONATION ENGINE EXPERIMENTAL AND THEORETICAL REVIEW

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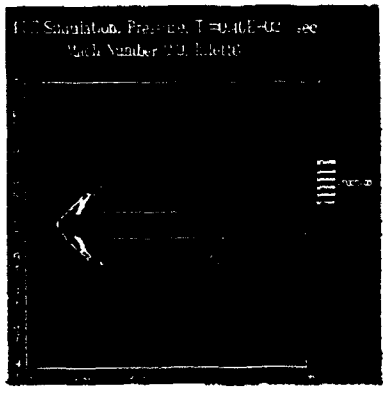

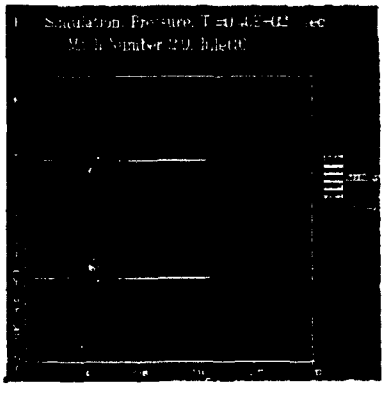

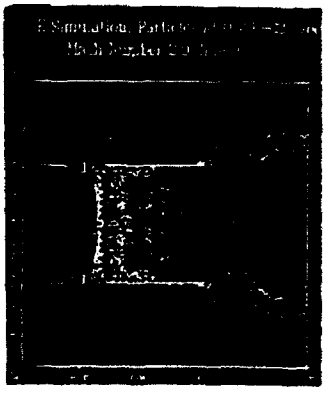

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PULSED DETONATION ENGINE
EXPERIMENTAL AND THEORETICAL REVIEW

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Abstract

A Review of past and current research on pulsed detonation engine devices connects early experimental work originating with the V1 pulsejet to recent interest in such propulsion devices. The recent interest has been, in part, stimulated by Aviation Week where sightings of aircraft contrails lead to question if some sort of PDE device has already been developed. This review summarizes what is known about PDEs, makes predictions for applications to realistic flight vehicles including missiles and full scale aircraft, and outlines what is yet required for successful PDE development.

1. Introduction

This paper reviews past and recent theoretical and experimental work related to the Pulsed Detonation Engine (PDE) concept. Such a review is timely since much interest in the PDE concept has been generated from several recent Aviation Week (AW) articles.[1,2] The AW articles, in addition to describing SAIC PDE studies, describe observations of aircraft flight and engine sound generation that are similar to what would be expected from PDE operation. These observations are intriguing since, to our knowledge, there has been no previously reported use of PDE devices in any past or recent flight vehicles. The reported observations include loud pulsing sounds at Beale AFB and photographs of high altitude contrails with "cotton ball" like beads strung on the contrails in a repetitive pattern. It is tempting to try to connect the AW reports with what we understand about PDE operation. It has come to our attention that a ground observer has identified the frequency of the pulsing sounds emanating from the vehicle that made the contrails appearing in the AW article to be of the order of 50-60 Hertz. To obtain the source (aircraft engine) frequency we must correct the observed frequency for the Doppler effect, taking into account the temperature variation between ground and flight altitude. Assuming an altitude of 45-50,000 ft. (cirrus clouds are observed behind the trails in the published photographs), a flight Mach number between one and two gives a source frequency, f, between 100 and 200 Hertz. As we show later in this paper, a PDE generating 25,000-50,000 lbs. thrust should, theoretically, operate in this frequency range. Of course we have no information concerning the subject aircraft characteristics and consequently we cannot conclude that PDEs are powering present day aircraft. On the other hand the observations appear to be consistent with expected PDE operation.

2. Early Pulsed Combustion Propulsion Devices

It is instructive to point out the differences between the PDE concept and the more commonly understood pulsejet devices. The first full scale application of pulsed propulsion devices was for the V1 flying "buzz bomb." The engine used for this vehicle was the Schmidt-Argus[3] engine and has since been generally referred to as a "pulsejet." The pulsejet for the V1 engine was based on repetitive combustion ignitions accomplished through the use of mechanical reed valves that allowed fresh air charge to be drawn into the combustion chamber. The timing of the reed valve opening was pegged to the acoustical frequency (organ pipe modes) of the combustion chamber, which consisted of a central ignition region joined to an exhaust duct. Thus, the operating parameters of the engine were fixed with engine size; only narrow ranges of thrust level variation are possible in such an engine. An increase or decrease of thrust can only be made through changes in engine internal geometry. Ever since the first occurrence of pulsejets, these engines have been considered for other applications including full scale aircraft propulsion. One of the major obstacles in the early development of the pulsejet for wider applications was the complete absence of a theoretical approach to understanding the thermodynamic process in the combustion chamber. It was assumed that the pulsejet combustion process was similar to the steady-state Lenoir constant-volume cycle and that the frequency of the combustion pulsations could be predicted by means of steady-state acoustical wave motion. However, the efficiency of the pulsejet, as determined experimentally, was much lower than a

constant-volume process would predict. We know now that the early pulsejet devices operated on an approximately constant-pressure cycle, which is known to have a lower thermodynamic efficiency than the constant-volume cycle. We have previously argued that the lack of a firm theoretical understanding of the physics and thermodynamics was primarily responsible for the failure to develop the pulsejet further for a wider range of practical applications. This argument will be discussed again later in this review.

In the meantime, the term pulsejet has become generally understood to refer to a pseudo-generic series of engines. The term "propulsive duct" is a more comprehensive descriptor encompassing a wider range of pulsed combustion engine concepts. An early series of papers by Tharjatt[4-6] described the status of work on such devices up to 1965, and provides a guide to the early attempts to understand the physics and aerodynamics of the internal gas flows in them. Even though these early investigations were seriously handicapped by a lack of knowledge of unsteady aerodynamics and the physics of repetitive combustion, it is remarkable that the conclusions offered in Tharjatt's papers are close to what we have concluded over the past several years for the PDE concept. Specifically, it was concluded that the propulsive duct engine concept should theoretically be capable of any desired level of thrust per unit area, with a corresponding reduction in specific fuel consumption. Valveless operation was also investigated and shown to offer a route to eliminating the dependency on fixed acoustical frequencies tied to a given chamber geometry. Figure 1 is representative of the valveless propulsive duct conceptualized by Tharjatt. Further, it was shown that the use of feedback techniques via multiple tube arrangements, which may not be practical from an engineering standpoint, leads to the possibility of very high frequency operation beyond the audible range. This would result in near silent operation. Finally, it was concluded that the propulsive duct should be capable of supersonic operation, and a Mach 3 engine was conceptualized; a schematic of this supersonic concept is shown in Figure 2.

Somewhat later, in a 1982 report by Kentfield,[7] the pulsejet was analyzed for predicted flight performances based on well established experimental test-stand data and available theoretical studies.[8] The results were compared against other engine alternatives suitable for small, high subsonic speed flight vehicles. The predicted performance for valveless engine configurations was shown to be highly competitive with turbojets at high subsonic Mach numbers. Actual flight tests with a drone type aircraft at Mach 0.85 showed increased performance over predicted performance values due possibly to a combination of increased air-breathing, increased intake density, and a ram effect superimposed on the pulsejet cycle. Conclusions from these studies include suggestions that valveless pulsejet performance could be comparable and, in some cases, exceed that of turbojet engines. A strong point was made concerning the low cost, simplicity and relatively high thrust-to-weight ratio of pulsejets when compared with turbojets.

The main reason for including the preceding review of pulsejets and propulsive ducts is to draw attention to the similarity between the early conclusions concerning the future performance expectations of pulsejets and the conclusions drawn to date concerning expected PDE performance. As mentioned above, we believe a primary reason that such devices have not been pursued in the past is that adequate analysis and evaluation tools did not exist at the time to help understand the complexities of pulsed operation. Modern CFD techniques now allow a comprehensive analysis of the internal and external flows associated with pulsed propulsion devices. It may well be more than just an interesting exercise to re-examine the pulsejet engines using present day CFD tools, and to compare the results with those from similar PDE studies.

3. Constant Volume Combustion and Early Pulsed Detonation Studies

Constant Volume Combustion

A constant volume combustion process is known to have a higher thermodynamic efficiency than a constant pressure combustion process. Constant volume combustion was adopted very early for use in gas turbine engine development, and the first gas turbine engines in commercial use were based on the constant volume cycle. Jet propulsion engines were one of the applications of the constant volume cycle (or explosion cycle), which was explored in the late 1940s.[8] Although the explosion cycle operates at a larger pressure variation in the combustion chamber than in a pulsejet, the cycle actually realized in these engines was not a fully constant volume one since the combustion chamber was open ended.[9] In Reference 8 the maximum pressure ratio measured in an explosion cycle engine was 3:1, whereas the pressure ratio for the same mixture under the

assumption of a constant volume cycle would be 8:1. Also, this early engine was limited by the available cycle frequency, which in turn is limited by the reaction rate. A simple calculation[8] showed that if the combustion time could be reduced in this engine from 0.006 sec to 0.003 sec, the thrust per pound of fuel-air mixture would increase 100%. Thus, a propulsion device based on an explosion-cycle has two main disadvantages:

- Constrained volume combustion (as distinguished from constant volume combustion) does not take full advantage of the pressure rise characteristic of the constant volume combustion process.

- The frequency of the explosion cycle is limited by the reaction rate, which is only slightly higher than the deflagrative combustion rate.

The main advantage of the constant pressure cycle is that it leads to engine configurations with steady state processes of fuel and oxidizer injection, combustion, and expansion of the combustion products. These stages can be easily identified and the engine designer can optimize them on the basis of relatively simple steady state considerations.

Pulsed Detonation Studies

There have been numerous attempts in the past to take advantage of detonative combustion for engine applications. The following is a brief description of some of the most relevant past experimental and analytical studies of pulsed detonation.

The Work of N. Hoffmann. The first reported work on intermittent detonation is attributed to Hoffmann[10] in 1940. Hoffmann's experiments on intermittent detonation were carried out in a long, narrow tube mounted on a test stand using acetylene-oxygen and benzine-oxygen fuel mixtures. Water vapor was added to prevent the highly sensitive acetylene-oxygen mixture from premature detonation. Hoffmann pointed out the importance of the detonation initiation (spark plug) location in reference to tube length and diffuser length. It was found that a continuous injection of the combustible mixture leads to only a narrow range of ignition frequencies that will produce an intermittent detonation cycle. These frequencies are governed by the time required for the mixture to reach the igniter, time of transition from deflagration to detonation, and time of expansion of the detonation products. Hoffmann attempted to find the optimum cycle frequency experimentally. It was discovered that detonation-tube firing occurred at lower frequencies than the spark-plug energizing frequencies, indicating that the injection flow rate and ignition were out of phase. Wartime events prevented further work by Hoffmann and his co-workers.

The Work of Nicholls and Co-Workers. A substantial effort in intermittent detonation research was made by a group headed by J. A. Nicholls[11-12] of the University of Michigan beginning in the early 50's. The most relevant work concerns a set of experiments carried out in a six foot long detonation tube.[11] The detonation tube was constructed from a one inch internal diameter stainless steel tube. The fuel and oxidizer were injected under pressure from the (closed) left end of the tube and ignited at some distance down stream. The tube was mounted on a pendulum platform, suspended by support wires. Thrust for single detonations was measured by detecting tube (platform) movement relative to a stationary pointer. For multi-cycle detonations, thrust measurement was achieved by mounting the thrust end of the tube to the free end of a cantilever beam. In addition to direct thrust measurements, the temperature on the inner wall of the detonation tube was measured. Fuel mixtures of hydrogen/oxygen, hydrogen/air, acetylene/oxygen and acetylene/air mixtures were used. The gaseous oxidizer and fuel were continuously injected at the closed end of the detonation tube and three fixed flow rates were investigated. Under these conditions, the only parameters that could be varied were the fuel/oxidizer ratio and frequency of ignition. A maximum gross thrust of ~ 3.2lb was measured in the hydrogen/air mixture at the frequency of ~ 30 detonations per second. The most promising results were demonstrated for the H_2/air mixture, where a fuel specific impulse of I_{sp} = 2100 sec was reached. The maximum frequency of detonations obtained in all experiments was 35 Hz. The temperature measurements on the inner wall showed that for the highest frequency of detonations the temperature did not exceed 800° F. This temperature is approximately the mean between the temperature of the injected gasses and the detonation wave temperature averaged over the cycle frequency.

In their later work,[13-15] the University of Michigan group concentrated on development of the Rotating Detonation Wave Rocket Motor. No further work on the pulsed detonation cycle was pursued.

The Work of L. J. Krzycki. In a setup very similar to Nicholl's, L. J. Krzycki[16] performed an

experimental investigation of intermittent detonations with frequencies up to 60 cps. An attempt was also made to analyze the basic phenomena using unsteady gas dynamic theory. Krzycki's attempt to analyze the basic phenomena relied on wave diagrams to trace characteristics, assumptions of isentropic flow for detonation and expansion, and incompressible flow for mixture injection processes. The most convincing data from the experiments are the measurement of thrust for a range of initiation frequencies and fuel mixture flow rates. Unfortunately no direct pressure measurement in the device is reported, so there is only indirect evidence of the nature of the process observed.

The basic test stand used by Krzycki is very similar to that used by Nicholls and his co-workers. The length of the detonation tube and the internal diameter were exactly the same as those in Nicholl's experiments. Figure 3 presents a schematic of the experimental apparatus containing common, generic elements of the Hoffmann-Nicholls-Krzycki experiments. A propane/air mixture was continuously injected through a reversed-flow diffuser for better mixing, and was ignited at the same distance as in the Nicholls' experiments from the injection point by an automobile spark plug. The spark frequency was varied from 1 to 60 cps. The spark plug power output was varied inversely with the initiation frequency, and at the frequency of 60 cps was only 0.65 Joule. This value is too low for direct initiation of a detonation wave by the spark, and consequently all of the experiments must have been based on transition from deflagration to detonation. According to experimental data and theory,[17] direct initiation of a mixture of propane/air at the detonability limits requires an energy release on the order of 10^6 Joules. Thus, we conclude that the required deflagration-detonation transition region length in Kryzcki's experiments would have been prohibitively large for the propane/air mixture. It follows that in all of the experiments a substantial part of the process was deflagrative. This resulted in low efficiency and negligible thrust. Krzycki repeated Nicholls' experiments using basically the same rates of injection of the detonable mixtures. Krzycki's experimental results are very well documented, allowing us to deduce a clear picture the physical processes occurring in the tube. The author arrived at the conclusion that thrust was possible from such a device but practical applications did not appear promising. It is unfortunate that, possibly based on Krzycki's extensive but misleading results, all experimental work related to the pulsed detonation engine concept stopped at this time.

Russian Work on Pulse Detonation Devices. A review of the Russian literature has not uncovered work concerning applications of pulsed detonation devices to propulsion. However, there are numerous reports of applications of such devices for other purposes such as for producing nitrogen oxide[18] (an old Zeldovich idea to bind nitrogen directly from air to produce fertilizers) and as rock crushing devices.[19]

Korovin et al.[18] provide a most interesting account of the operation of a commercial detonation reactor. The main objective of this study was to examine the efficiency of thermal oxidation of nitrogen in an intermittent detonative process as well as an assessment of such technological issues as the fatigue of the reactor parts exposed to the intermittent detonation waves over a prolonged time. The reactor consisted of a tube with an inner diameter of 16 mm and length 1.3 m joined by a conical diffuser to a second tube with an inner diameter of 70 mm and length 3 m. The entire detonation reactor was submerged in running water. The detonation mixture was introduced at the end wall of the small tube. CH_4, O_2 and N_2 comprised the mixture composition and the mixture ratios were varied during the continuous operation of the reactor. The detonation wave velocity was measured directly by piezoelectric sensors placed in the small and large tubes. The detonation initiation frequency in the reactor was 2-16 Hz. It is reported that the apparatus operated without significant maintenance for 2000 hours.

Smirnov and Boichenko[19] studied intermittent detonations of gasoline-air mixtures in a 3 m long and 22 mm inner diameter tube operating in the 6-8 Hz ignition frequency range. The main motivation for this work was to improve the efficiency of a commercial rock crushing apparatus based on intermittent detonations of the gasoline/air mixtures.[20] The authors investigated the dependence of the transitional region length from deflagration to detonation on the initial temperature of the mixture.

As a result of the information contained in the Russian reports, we conclude that reliable commercial devices based on intermittent detonations have been constructed and operated.

Pulsed Solid Explosion Studies at JPL. Work at the Jet Propulsion Laboratory (JPL) by Back, Varsi and others[21-24] concerned an experimental and

theoretical study of the feasibility of a rocket thruster based on intermittent detonations of solid explosive for propulsion in dense or high-pressure atmospheres of certain solar system planets. The JPL work was directed at very specific applications: however, these studies also addressed more general key issues concerning intermittent propulsion devices such as propulsion efficiency. In this work, a Deta sheet type C explosive was detonated inside a small detonation chamber attached to nozzles of various length and geometry. The nozzles, complete with firing plug, were mounted in a containment vessel that could be pressurized with mixtures of various inert gases from vacuum to 70 atm. The apparatus directly measured the thrust generated by single detonations of a small amount of solid explosive charge expanding into conical or straight nozzles. Thrust and specific impulse were measured by a pendulum balance system.

The results obtained from the JPL experimental study of an explosively driven rocket led to the following conclusions. First, rockets with long nozzles show increasing specific impulse with increasing ambient pressure in CO_2 and N_2. Short nozzles, on the other hand, show that specific impulse is independent of ambient pressure. Most importantly, most of the experiments obtained a relatively high specific impulse of 250 seconds and larger. This result is all the more striking since the detonation of a solid explosive yields a relatively low energy release of approximately 1000 cal/gm compared with 3000 cal/gm obtained in hydrogen oxygen combustion. Thus, it can be concluded that the total losses in a thruster based on unsteady expansion are not prohibitive and hence, in principle, very efficient intermittent detonation propulsion systems are possible.

4. Description of the PDE Concept

Basic Principles

A detonation process, due to the very high chemical reaction rate in the detonation wave, leads to a propulsion concept in which the constant volume process can be fully realized. In detonative combustion, a strong shock wave, which is part of the detonation wave, acts like a valve between the detonation products and fresh charge; the detonation wave functions at the same time as a valveless compressor between the fresh fuel/air mixture and the detonation products. The speed of the detonation wave is about two orders of magnitude higher than the speed of a typical deflagration wave. Because of this, very high power densities can be created in the detonation chamber. Each detonation can be initiated independently and, depending on the chamber geometry and external flow characteristics pertaining to a particular device, a wide range of frequencies is possible. There is no theoretical restriction on the range of operating frequencies: they are uncoupled from any acoustical chamber resonance. The independence of detonation cycle frequency is the feature that most differentiates the PDE concept from the pulsejet. It is also the feature that leads theoretically to scalability of PDE configurations for a wide range of flight applications. A key physical restriction on the range of allowable detonation frequencies arises from the rate at which the fresh fuel/air mixture can be introduced into the detonation chamber. Obviously the detonation products must be discharged from the chamber before fresh charge is injected.

First PDE Experiments

To our knowledge, the first experiments that successfully demonstrated repetitive or pulsed detonation was attainable in a propulsion-like device were carried out by Helman, Shreeve and Eidelman[25] at the Naval Postgraduate School in 1985-86. During these studies, several fundamentally new ideas were developed for pulsed detonation applications to propulsion. First, to overcome the energy requirements for detonation initiation, a pre-detonation was initiated in a small detonation tube where an oxygen rich fuel mixture could be detonated at substantially lower energies than those required for full fuel/air mixtures. Next, the experimental PDE was operated in a self-aspirating mode; the detonation exhaust gases were discharged through gasdynamic expansion and fresh air was drawn into the detonation chamber due to chamber overexpansion following detonation product exhaust. Figure 4 is a schematic of one of the variations of the PDE experimental configurations. The pre-detonation initiation tube is shown attached to a spark plug. The most important results were obtained when the fuel injection (injection was accomplished with a toroidal ring containing holes near the exhaust plane of the device) rate was timed appropriately (the lag time between the fuel/air travel to the pre-detonation port and the arrival of the pre-detonation pulse) with detonation initiation. The principle of repetitive detonation initiation and control was definitively established in these experiments. Pressure transducer traces unambigiously showed that a detonation wave was

formed in the chamber and propagated with the Mach number appropriate for the fuel-air mixture. The fuel used in the NPS experiments was ethylene and the maximum detonation frequency obtained was 25 Hz, limited only by the mechanical nature of the solenoid valve used for fuel injection control. Figures 5 and 6 are two frames from a videotape of the early NPS experiments. Figure 5 shows the experimental apparatus and Figure 6 shows the apparatus during repetitive detonation. The figures also show the fuel injector ring between the two concentric detonation chamber cylinders. It was determined that the duration of a single cycle was less than 7 msec. This means that the NPS device could have potentially operated at frequencies up to 150 Hz in the static or no flow (M = 0) case. At the time of the NPS experiments, performance extrapolations included thrust levels up to 40 lbs at 100 Hz. As described later, SAIC simulations of static operation show higher thrust levels at these frequencies due to new ideas and improvements in the PDE concept. These new ideas are incorporated in the generic PDE concept.

The Generic PDE Device

In this section, we refer to the generic PDE device, which is represented as a small engine in Figure 7. The figure shows a schematic of the basic detonation chamber attached to the aft end of a generic aerodynamic vehicle. A combustible gas mixture is injected at the closed end of the detonation chamber and a detonation wave is shown propagating through the mixture. Also shown are air injection inlets and an important part of the device that we have termed the thrust wall. The schematic suggests a small-payload aerodynamic vehicle; however, as we describe later, the concept can be extended to larger payloads simply by scaling up the size of the detonation chamber and possibly combining a number of chambers into one larger engine.

The geometry of the main detonation chamber, which determines the propulsion efficiency and the duration of the cycle (frequency of detonations), is a key issue for the PDE concept. Since the fresh charge for the generic engine is supplied from the external flow field, the efficiency of the engine depends on the interaction of the surrounding flow with the internal flow dynamics. Following is a partial list of the broad range of physical processes requiring simulation in order to model the complex flow phenomena associated with the detonation engine performance:

1. Initiation and propagation of the detonation wave inside the chamber;

2. Expansion of the detonation products from the chamber into the air stream around the chamber at flight Mach numbers;

3. Fresh air intake from the surrounding air into the chamber;

4. The flow pattern inside the chamber during post-exhaust pressure buildup, which determines the strategy for mixing the next detonation charge;

5. Strong mutual interaction between the flow inside the chamber and the external flow surrounding the engine.

All of these processes are interdependent, and interaction and timing are crucial to engine efficiency. Thus, unlike simulations of steady state engines, the phenomena described above cannot be evaluated independently. It is a challenging computational problem to resolve the flow regime inside the chamber to account for nozzles, air inlets, etc., and at the same time resolve the flow outside and surrounding the engine, where the flow regime varies from high subsonic, locally transonic and supersonic.

The single most important issue is to determine the timing of the air intake for the fresh charge that leads to repetitive detonations. It is sufficient to assume inviscid flow for the purpose of simulating the expansion of the detonation products and fresh air intake. The assumption of inviscid flow makes the task of numerically simulating the PDE flow phenomena somewhat easier than if a fully viscous flow model were employed. The effects of viscous boundary layers are negligible for the size of the generic device studied in this work, with the exception of possible boundary layer effects on the valve and inlet geometries discussed subsequently.

SAIC has performed an extensive study of the generic PDE over a wide range of operating conditions for a wide range of device configurations.[26-30] Numerical simulations of the unsteady flow and detonation processes, in addition to theoretical analysis, have resulted in an understanding and an approach to analyzing and evaluating PDE propulsion performance. Although the basic concept remains the same, there are subtle differences in the PDE manifestation for particular applications. These will be described subsequently. Details of the

numerical simulations (including assumptions used for detonation wave physics and chemistry, use of adaptive unstructured grids and Godunov methods for the Euler gasdynamic equations) are given elsewhere.[26-31] The following section is a summary of the results from numerical and theoretical studies of various applications and operating regimes for the generic PDE.

5. Operating Regimes

In this section we summarize the results of several applications and operating regimes identified in the course of our studies of the PDE concept.

M = 0 Static Operation

Under static conditions, M = 0, the PDE is completely self-aspirating. Such was the case for the early NPS PDE studies. Without an external airstream, the PDE must obtain fresh air charge as a result of the detonation chamber overexpansion immediately following exhaust of air-fuel detonation products. To the lowest approximation, the available time for chamber refill due to this overexpansion process is, for a given chamber geometry and fuel-air combination, directly proportional to its length. For M = 0 operation, we assume that the PDE configuration does not contain any air inlets other than the aft end of the device or, if inlets are present, they are closed. Simulations[26] of M = 0 PDE operation show that the time required for fresh air refill for a device with dimensions equivalent to the NPS experimental apparatus is on the order of 6-7 msec. This agrees with the NPS results and means that a maximum frequency of 150 Hz should be possible. Simulated thrust levels were higher than those estimated from scaling the NPS results. This is due to a new operating scenario that was uncovered by the simulations: detonation initiation from the aft end results in the kinetic energy of the shock wave being transferred to the thrust wall. The amount of extra thrust obtained from this mode of operation is considerably larger than that expected from gasdynamic expansion following detonation initiation at the thrust wall. The physical reason for this is found in the shock wave energetics.

The importance of M = 0 PDE performance is associated with applications of the concept for full scale aircraft propulsion, including rollout and takeoff. Simple scaling laws derived from the numerical simulation results and described later, show that M = 0 thrust levels can be large (tens of thousands of lbs.) depending on the engine cross sectional area, length and detonation frequency.

Subsonic-Transonic Operation

PDE operation in the subsonic-transonic regime differs from the static case in that the self aspiration effect decreases with increasing Mach number. This is due to the formation of a rear stagnation point behind the exhaust plane above certain Mach numbers for given geometries. The stagnation region prevents complete detonation product exhaust and subsequent fresh charge injection. For example, over the Mach number range, $0^+ < M < 0.5$, full to partial self aspiration occurs; the effect decreases rapidly for Mach numbers above 0.5, resulting in the need for some type of air inlet or air intake valve configuration. Simulations of various detonation chamber and air inlet geometries[26,28] have shown that, depending on the free-stream Mach number, appropriate shaping of the air inlet geometry and total inlet area leads to propulsion engines that are attractive for certain applications. We present here a summary of studies[28] carried out in an attempt to find a satisfactory PDE configuration for a small missile engine (the final configuration was not optimum, by any means, since all variables were not parametrically varied).

A PENAID-type missile with associated mission requirements such as range, speed, system weight, total thrust, and specific fuel consumption was used for the study. The detonation chamber dimensions were 6 cm diameter and 9 cm length with a cylindrical cross-section. A schematic of PDE integration into such a missile configuration is shown in Figure 8. The simulations showed that, for practically all cases involving simple inlets (circumferential slits around the cylindrical cross-section), the thrust data were independent of whether the inlets open intermittently (valved) or remain open during operation. This is due partially to the very short time that detonation products have to escape from the inlets thereby adding to negative thrust; this negative thrust, determined in the simulations, is negligible compared to the total integrated thrust. The thrust data do indicate a strong dependence on external flow conditions, e.g., Mach number. The Mach number plays a role in the wave drag; the details of valve and inlet configuration geometry figure prominently in the total wave drag. These studies answered an important question: can an air inlet be configured such that the inlet remains open over the full flight regime and operating conditions? The answer is "yes." Thus, at least for this regime, the PDE offers the possibility of a no-

moving-parts propulsion device. For the PENAID missile under discussion here, a configuration was found that operates between $0.2 < M < 0.9$ with open air inlets.

The following performance data were obtained for the PENAID missile configuration. For M=0.8 at sea level altitude and a detonation frequency, f=100 Hz, the PDE characteristics are:

Thrust	79 lb.
Fuel flow rate	0.025 lb./sec.
Fuel weight for 12 min	18 lb.
Oxygen weight	1.8 lb
Fuel for detonation tube	0.6 lb.
Total oxygen and fuel weight	20.4 lb.
Total engine weight	30.2 lb.
Specific fuel consumption	1.14 lb./(lb.*hr.)

Assuming the PDE device geometry is kept fixed, a higher detonation frequency will result in a linear increase in thrust and fuel flow rate at the same specific fuel consumption. For example, if the detonation frequency is increased to 200 Hz, the performance data are:

Thrust	157 lb.
Fuel flow rate	0.05 lb/sec.
Fuel weight for 12 min	36 lb.
Oxygen weight	3.6 lb.
Fuel for detonation tube	1.2 lb.
Total oxygen and fuel weight	40.8 lb.
Total engine weight	54.4 lb.
Specific fuel consumption	1.14 lb./(lb.*hr.)

At lower Mach numbers, M=0.5, the maximum operating frequencies for constant thrust will be lower since the external dynamic pressure responsible for supplying fresh air to the chamber is also lower. For the device under consideration here, the maximum frequency is 250 Hz. For a frequency of 100 Hz:

Thrust	100 lb.
Fuel flow rate	0.025 lb/sec.
Fuel weight for 12 min	18 lb.
Oxygen weight	1.8 lb.
Fuel for detonation tube	0.6 lb.
Total oxygen and fuel weight	20.4 lb.
Total engine weight	30.2 lb.
Specific fuel consumption	0.9 lb./(lb.*hr.)

Again, if the frequency is increased the thrust will increase linearly; operation at 200 Hz yields:

Thrust	200 lb.
Fuel flow rate	0.05 lb/sec.
Fuel weight for 12 min	36 lb.
Oxygen weight	3.6 lb.
Fuel for detonation tube	1.2 lb.
Total oxygen and fuel weight	40.8 lb.
Total engine weight	54.2 lb.
Specific fuel consumption	10.9 lb./(lb.*hr.)

The examples of the PDE device performance given above are based on point design conditions arising from the simulations reported earlier.[26] They cannot be extrapolated with any degree of reliability to other conditions or configurations. We conclude, however, that the performance computed for the indicated device is encouraging from the point of view of thrust, thrust control, simplicity of the device (no moving parts), and specific fuel consumption (SFC). The specific fuel consumption computed above is competitive with present day small turbojet engines. The SFC for a PDE could be significantly lower than for small turbojets (SFC's for small turbojets are in the range of 1.8-2.0 lb./(lb.*hr)). Thus, for a given mission and vehicle, a PDE propulsion unit may be more fuel efficient, resulting in increased range. Moreover, if the expected thrust control in PDE's is realizable, it may be possible to produce propulsion units that can slow down, loiter and maneuver, and finally accelerate to full thrust again rapidly. Depending on the detonation frequency, which determines the thrust for all other conditions fixed, the thrust-to-weight ratio for the PDE can be as high as 20:1. This value is certainly competitive with other propulsion concepts.

The results of the scaling studies at subsonic-transonic speeds lead to scaling laws that can be used to predict the performance of PDE's over some range of parameters, assuming that other parameters are held fixed. For example, holding the external Mach number and basic chamber and inlet geometry fixed suggests that the thrust at constant specific fuel consumption produced by the PDE scales as:

$$\text{Thrust} = T_1 * \left(\frac{v}{v_1}\right) * \left(\frac{f}{f_1}\right),$$

where T_1, (v/v_1) and (f/f_1) are the thrust computed for a chamber of volume v_1 operating at frequency f_1, the ratio of a new volume to v_1 and the ratio of the new frequency to f_1, respectively. Thus, thrust should scale linearly with the parameter $(v/v_1) * (f/f_1)$ over some range of this parameter. Departure from this linear variation may occur due to the following argument: First, since volume is proportional to the

product of cross-sectional area and length, $v \sim r^2 l$, (r ~ detonation chamber radius, l ~ chamber length) physical limits will be placed on r and l; if r is too small (less than 1 cm), a detonation will not be sustainable and if l is too small (less than 10 cm), it may be difficult to mix fuel and air effectively. Using the thrust relation established above, we make the following observations. For a PDE device producing 100 pounds thrust at 100 Hz, doubling the frequency and increasing the volume by a factor of 5 yields a thrust level of 1000 pounds. Assuming that the aspect ratio of the chamber (chamber length to radius) is fixed, this would require an engine only 25.5 cm in diameter and 25.5 cm in length. Of course, the relation between thrust and $(v/v_1) * (f/f_1)$ cannot be believed over too wide a range of parameters; but, it does serve to point out the flexibility permitted by the PDE concept.

The subsonic-transonic simulations showed that the timing of the fresh air refilling required to recharge the chamber for subsequent detonations is a strong function of the details of the valve and inlet geometry, the expansion of the combustion products, the resulting over-expansion of the chamber flow, and the external flow regime and interaction of the external flow with the internal flow. For subsonic flight, Mach 0.2-0.9, the fresh air entering the chamber comes from two separate principal flow processes; one comes from the flow through any valve or inlet and the other comes from the self-aspiration or reverse flow from the aft end of the chamber due to strong over-expansion. All these processes are interdependent and, in order to search for a given performance in a given device, require variation of many parameters. The simulation results obtained to date provide an understanding of the effects caused by variation of the above-mentioned parameters. With the information available, we conclude that a PDE propulsion unit can be optimized (although no optimization studies were carried out) for a given flight regime. The decrease in thrust with increasing Mach number has been described earlier to result from increased wave drag produced by the inlet geometry. Optimization of the inlet geometry could help to eliminate a large part of the wave drag. The simulation data can be used to determine the detonation frequency at a given Mach number yielding constant thrust. For example, for a constant thrust level of 90 pounds, the required detonation frequency varies from 84 Hz at M-0.0 to 140 Hz to M=0.8. In a similar fashion, we can obtain parametric variations of other important aspects of PDE performance, such as minimum time for refill at given Mach number as a function of air inlet opening. To find an optimum configuration that satisfies given performance over a wide flight regime requires a more extensive simulation study. It was mentioned earlier that the simulations presented here were carried out under the assumption of inviscid flow: boundary layer effects were not included. Boundary layers are only significant for the air inlets and valves.

There is an important feature of PDE operation for missiles such as the one considered here: if the expected thrust control is attainable, then the detonation frequency can be varied to produce constant thrust over a given flight envelope, or the frequency can be varied to make the missile slow down, loiter and maneuver, and finally ramp back to full thrust more or less instantaneously. Since each detonation is controlled separately, this capability should depend only on on-board electronics and power.

Supersonic-Hypersonic Operation

Numerical simulations have been carried out for PDE operation in the supersonic and hypersonic flight regimes.[29] The results of these simulations show that there are differences when compared with the lower speed regimes. The main difference, with respect to operating characteristics, is the air intake inlet must be more carefully considered. For supersonic and hypersonic flow air scoops may be required, adding to wave drag. For PDEs enclosed in a duct connected to upstream air inlets, pressure recovery from free-stream to duct inlet and finaly to PDE inlet must be accounted for. To date, several detailed studies have been carried out for the higher speed regimes; a supersonic, M = 2 PENAID missile engine simulation and a sizing analysis for a large engine operating in the supersonic to hypersonic flight regime.

Supersonic M = 2 PDE The M = 2 PENAID missile study has been reported earlier[29] and, representative simulation results are shown on the cover of this review paper. It was found that a fixed air inlet geometry could be conceptualized to operate over the Mach number range, $0.5 < M < 2$. By this is meant the timing for fresh air charge allowed a detonation frequency of 200 Hz at M = 2 and this, in turn, means that any lower frequency is allowable at any other Mach number below M = 2. Detonation frequency control may result in enhanced control over missile flight trajectory since a constant thrust, a cruise-dash-loiter-cruise or any other tailored thrust profile can be realized. We conclude that supersonic PDE operation appears possible for missile

applications. and there may also be advantages for longer range air-to-air missiles due to enhanced propulsion energy management capability.

Sizing Analysis for Large PDEs A zeroth order sizing analysis has been carried out to define and size a PDE configuration satisfying high thrust level requirements from sea level to 30,000 ft altitude and for a flight trajectory including the Mach number range, $0 < M < 4$. The nominal target thrust level was 50,000 pounds and we assume that the aircraft/engine integration requires an air inlet duct to deliver fresh air to the PDE. We sketch here an outline of the analysis and give the main results.

We use the simple scaling argument given and use the thrust data obtained from simulations of the smaller missile configurations. We also assume a nominal detonation frequency, $f = 100$ Hz. We then establish the following baseline PDE performance operating point. At 3×10^4 ft. altitude for $M = 2$ the thrust in pounds per cubic meter detonation chamber volume is 2.5×10^4 lbs/m^3. Therefore, an engine producing 5×10^4 pounds thrust requires a 2 m^3 chamber volume. The sizing study answers the following questions : what is the size and shape of the detonation chamber, required detonation chamber air inlet areas, frequency variation range, and effect of air inlet duct losses on a PDE developing the nominal target thrust?

We denote free-stream conditions by $(\,)_0$, PDE air inlet conditions by $(\,)_2$, and PDE detonation chamber conditions by $(\,)_3$. To account for air inlet duct losses we define the ratio of PDE inlet total pressure to free-stream total pressure by C or:

$$\frac{P_{t_2}}{P_{t_0}} = C. \qquad (1)$$

The simplest condition to assume for the PDE air inlet is choked flow. Although this is not valid over much of the required regime, certainly not for subsonic external flow, it will result in a pessimistic bound on the sizing parameters. Using well known gasdynamic analysis[32] the static and total pressures and density at the PDE inlet can be found as:

$$P_{t_2} = CP_0\left(1 + \frac{M_0^2}{5}\right)^{\frac{7}{2}} \qquad (2)$$

$$P_2 = P_0 C\left(\frac{5 + M_0^2}{6}\right)^{\frac{7}{2}} \qquad (3)$$

$$\rho_2 = 1.2\, C\, \rho_0\left(\frac{5 + M_0^2}{6}\right)^{\frac{7}{2}}\left(\frac{5 + M_0^2}{5}\right)^{-1} \qquad (4)$$

The mass flow rate through the engine inlet is:

$$\dot{m} = \rho_2 U_2 A_2, \qquad (5)$$

and, using equations 2-4, gives:

$$\dot{m}_2 = A_2\left(1.2\,\gamma\, C^2\left(\frac{P_0^2}{RT_0}\right)\left(\frac{5 + M_0^2}{6}\right)^{7}\left(\frac{5 + M_0^2}{5}\right)^{-1}\right)^{\frac{1}{2}} \qquad (6)$$

An equation for the area ratio A_2/A_3 can be found as:

$$\frac{A_2}{A_3} = \frac{216}{125} M_3\left(1 + \frac{M_3^2}{5}\right)^{3}, \qquad (7)$$

where M_2 has been set equal to unity. Our analysis does not include the thermodynamics of the PDE cycle; the sizing analysis is based totally on a determination of the allowable detonation frequencies in the PDE chamber. We obtain a bound on allowable flow speeds in the detonation chamber by requiring the detonation chamber to refill in the time between detonations. We further require the fuel to mix and flow with the mean speed U_3 from inlet to chamber exit, a distance equal to L, the chamber length. Thus, we obtain the relation $U_3 = f\,L$, where f is the detonation frequency. A calculation of M_3 gives:

$$M_3 = \frac{U_3}{U_3^*} = f\,L\sqrt{\frac{\rho_3}{\gamma P_3}}. \qquad (8)$$

Since the total pressure in the chamber equals the total pressure at the PDE inlet, the static pressure in the chamber as a function of chamber Mach number, given in Eq. (8), can be related to the free-stream static pressure as follows:

$$P_3 = CP_0\left(1 + \frac{M_0^2}{5}\right)^{\frac{7}{2}}\left(1 + \left(\frac{A_2}{A_3}\right) C_1 \frac{Lf}{\gamma}\frac{1}{5P_3}\right)^{\frac{-7}{2}} \qquad (9)$$

where C_1 is:

$$C_i = \left(1.2\,\gamma\, C^2 \left(\frac{P_0^2}{RT_0} \right) \left(\frac{5 + M_0^2}{6} \right)^7 \left(\frac{5 + M_0^2}{5} \right)^{-1} \right)^{\frac{1}{2}}$$

Another relation between P_3 and P_0 as a function of M_3 can be given as:

$$P_3 = CP_0 \left(1 + \frac{M_0^2}{5} \right)^{\frac{7}{2}} \left(1 + \frac{M_3^2}{5} \right)^{\frac{-7}{2}} \qquad (10)$$

Equations (7), (9) and (10) form a closed set for the variables P_3, A_2/A_3 and M_3 with parameters C, P_0, M_0, L, f, T_0, g, and R, the universal gas constant. The volume, V, of the detonation chamber is given by the product, $V = L\,A_3$. Thus, for a given volume, Equations (7), (9), and (10) can be solved for A_2/A_3 versus L or A_3. Figure 9 gives a schematic of the PDE showing the air inlet gap width "l" resulting in an inlet area of A_2, the detonation chamber length L, and the chamber cross-sectional area A_3. We choose first a square chamber cross-section; the total inlet area is therefore given by the expression $A_2 = 4l\,(A_3)^{1/2}$. Results obtained from solving Eqs. (7), (9) and (10) are presented in Figure 10 for the baseline conditions. There, the area ratio, A_2/A_3, is given versus A_3. If A_3 is chosen to be 1.2 m^2 then the length of the PDE is 1.67 m and the engine inlet opening is 15 cm. Also shown in Figure 10 is the effect of C, the pressure recovery factor. The range of values chosen for C was: $0.7 < C < 1$. The effect of C is negligible for the range studied here. More realistic estimates for duct losses resulting in much lower values of C at high Mach numbers may well have a more pronounced effect. If the cross-sectional area is held fixed, Eqs. (7), (9) and (10) yield the results shown in Figure 11. The curve cannot be extended below $M = 1$ since the assumption of choked flow at A_2 is not valid; indeed, the assumption is not valid somewhere before $M = 1$ due to duct loss effects. The results from Figure 11 can be translated into inlet gap widths as shown in Figure 12. Figure 12 shows a range of inlet openings that, when compared with the total engine length, is equivalent to 8-12% of the total engine length. Below $M = 1$, a combination of self- aspiration and recharge from air inlets must be considered depending on Mach number. For self-aspiration at $M = 0$, the ratio of A_2/A_3 is unity; the inlets are not needed. For Mach numbers between zero and say, 0.5, partial air inlet opening is required and for Mach numbers greater than 0.5, the inlets will be fully open. For a fixed PDE configuration, varying the detonation frequency changes the thrust according to the scaling law given earlier. Figure 13 shows the effect of frequency variation on A_2/A_3. Recall the design point was at f = 100 Hz. Figures 10-13 contain the answers to the questions asked during this sizing analysis: reasonable physical sizes for PDEs developing high thrust levels are predicted. A more rigorous analysis is required to validate these predictions.

To conclude this section, we show the variation of thrust as a function of chamber volume derived from the baseline conditions used above. Figure 14 gives this variation and, if a circular cross-section engine is considered, varying the baseline thrust yields engine sizes shown in Figure 15. For example, a 45,000 pound thrust engine 1.67 meters long has an engine diameter of 1.2 meters. This number is not unreasonable and compares well with sizes of current turbojet engines. As mentioned, a more detailed analysis of PDE performance is needed, including an effective "steady state" thermodynamic cycle model, to validate the PDE as a credible alternative for high thrust propulsion engines.

6. Summary and Conclusions

Past and recent studies have shown that pulsed propulsion devices theoretically offer significant advantages over steady state engines. The advantages range from the possibility of a no-moving-parts configuration to high thermodynamic efficiency constant volume cycles. Numerical simulations, theoretical analysis and scaling studies of PDE performance have shown applicability to many different flight vehicles including small missiles and full scale aircraft. Configurational flexibility offered by the PDE include non-circular cross-sectional detonation chambers allowing consideration of unique aircraft/engine integration possibilities. Thus, the numerical simulation and theoretical studies of PDE performance to date have shown interesting and important propulsion applications.

In order to realize the PDE potential, experimental data is required to validate the theoretical predictions and, most importantly, provide a proof of principle demonstration of the PDE mode of operation described in this paper, namely, detonation initiation from the exhaust end of the engine. The principle of sustained repetitive detonation has already been demonstrated in the NPS experiments, but, this took place at the inner thrust wall. The next step in the development of practical PDE devices requires a comprehensive experimental program where such key

issues as detonation initiation, air inlet design including boundary layers, fuel/air injection and mixing can be studied and understood. In addition, thrust measurements, both static and in an external flow are required to validate the numerical and theoretical predictions. Plans for such an experimental program are presently under consideration.

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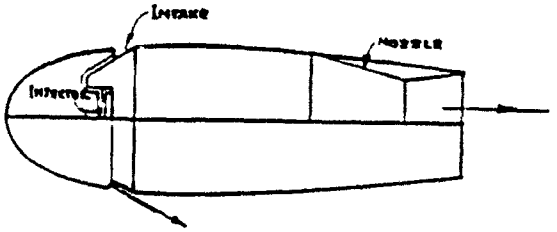

Figure 1. Valveless propulsive duct concept due to Tharjatt.

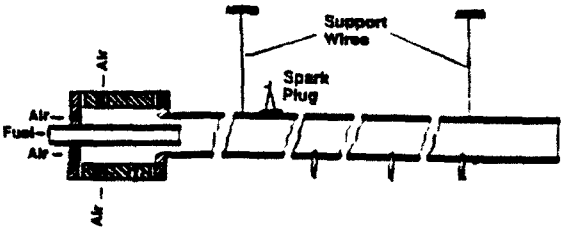

Figure 3. Schematic of the Hoffmann - Nicholls - Krzycki detonation tube experimental apparatus.

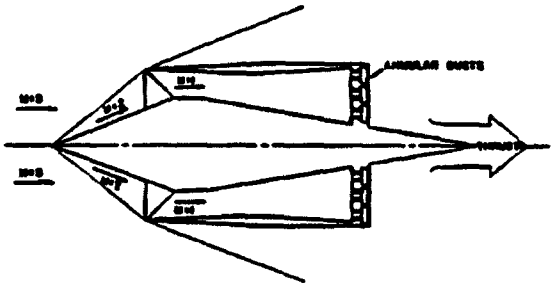

Figure 2. Supersonic, M = 3 conceptualization of the propulsive duct.

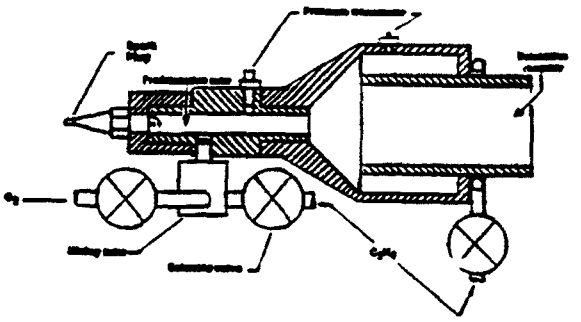

Figure 4. Schematic of the Helman, Shreeve, Eidelman PDE experimental configuration from the NPS studies.

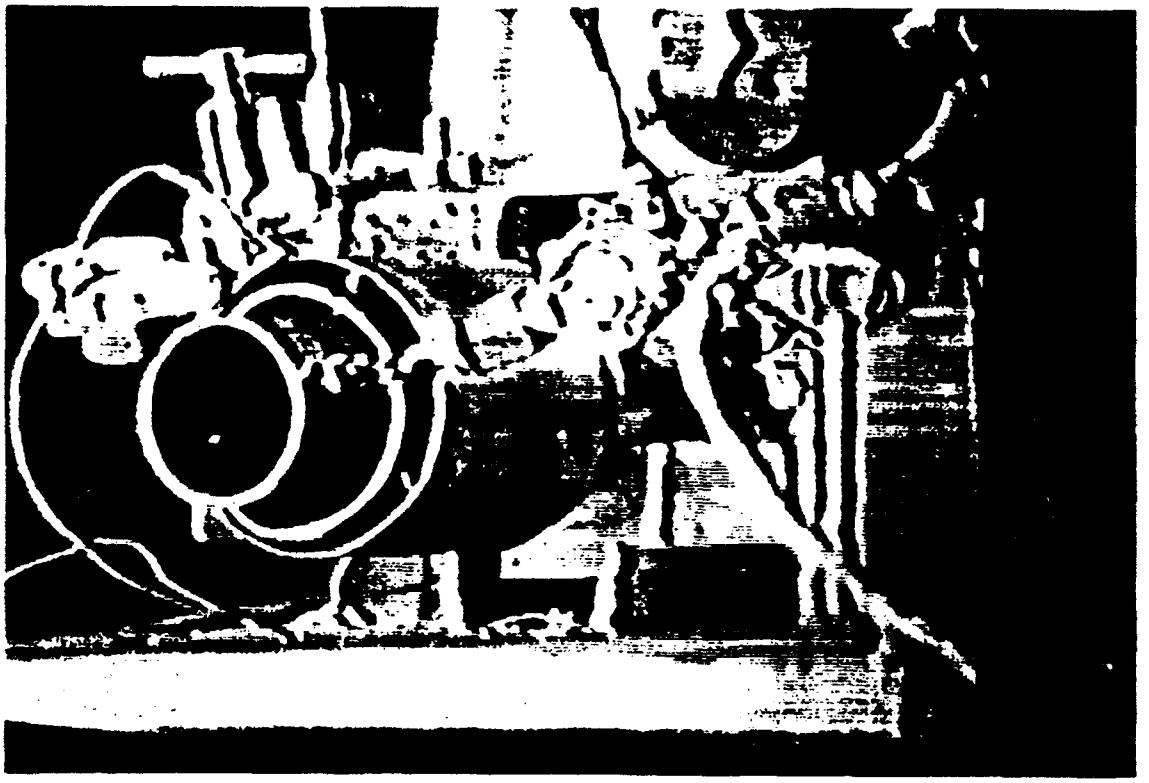

Figure 5. The PDE experimental apparatus used in the NPS studies.

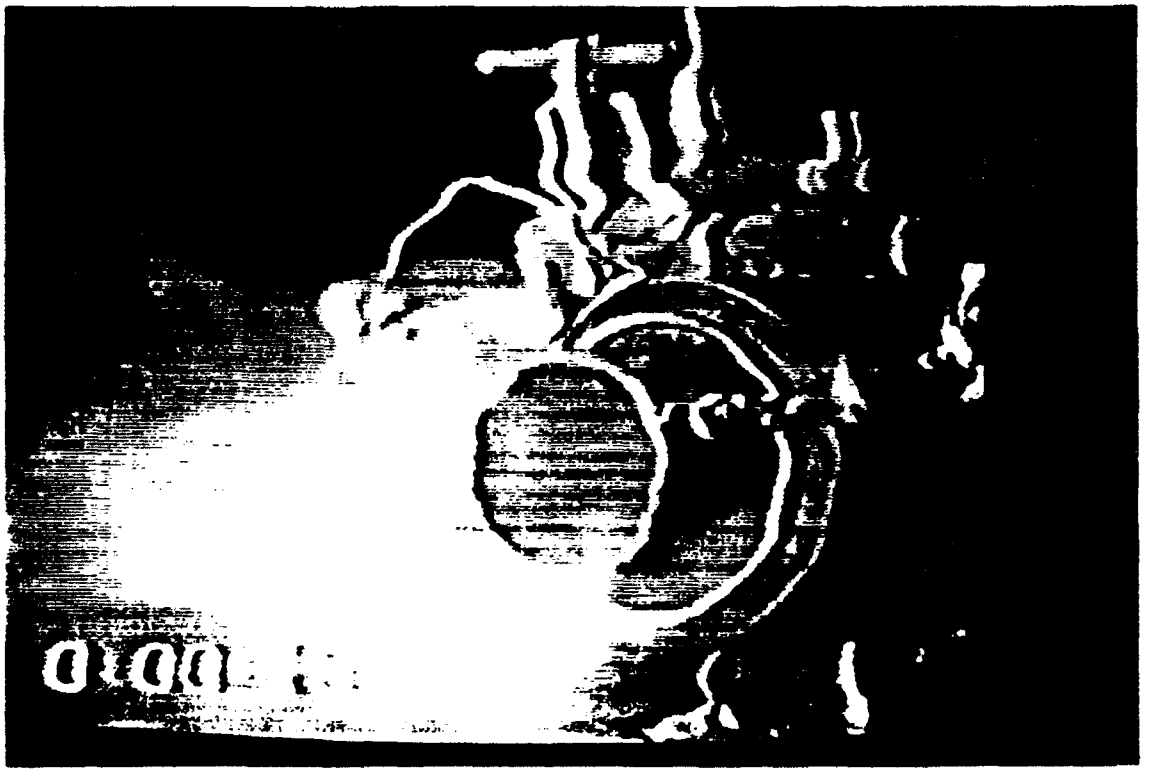

Figure 6. The PDE experiment during repetitive detonation.

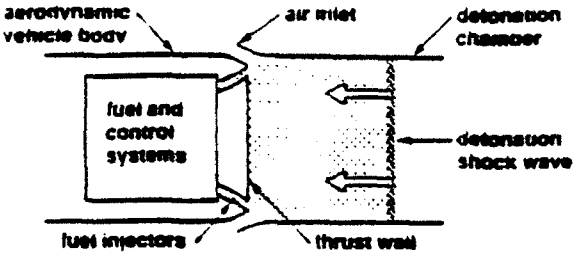

Figure 7. Schematic of the generic PDE.

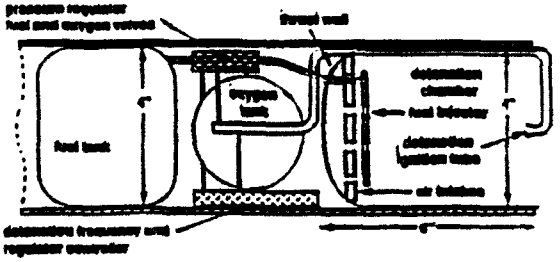

Figure 8. Schematic of PDE/PENAID missile integration.

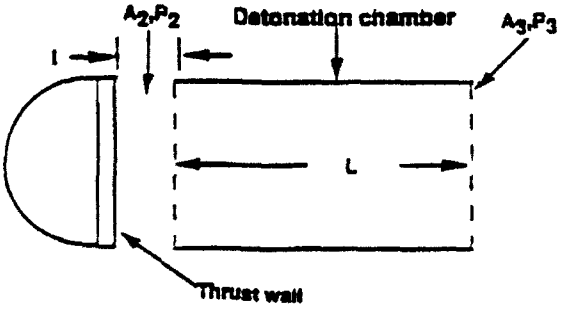

Figure 9. Schematic of PDE describing key sizing variables.

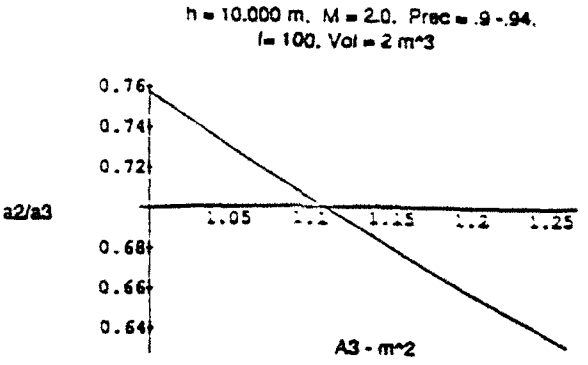

Figure 10. Results for A_2/A_3 as a function of A_3. The results are, for the chosen conditions, independent of pressure recovery.

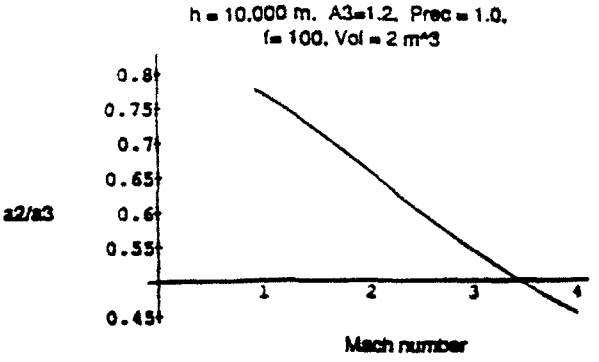

Figure 11. Results for A_2/A_3 as a function of Mach number.

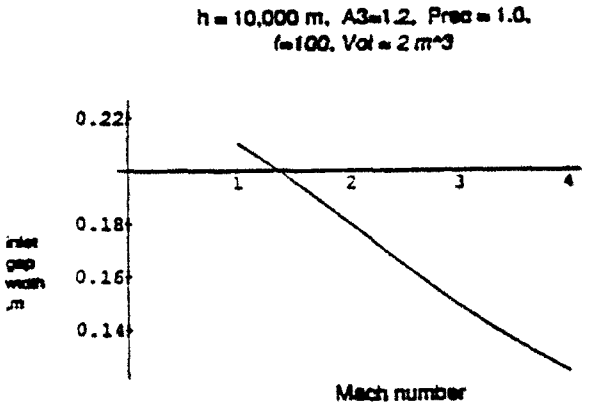

Figure 12. Results for inlet gap width, l, as a function of Mach number.

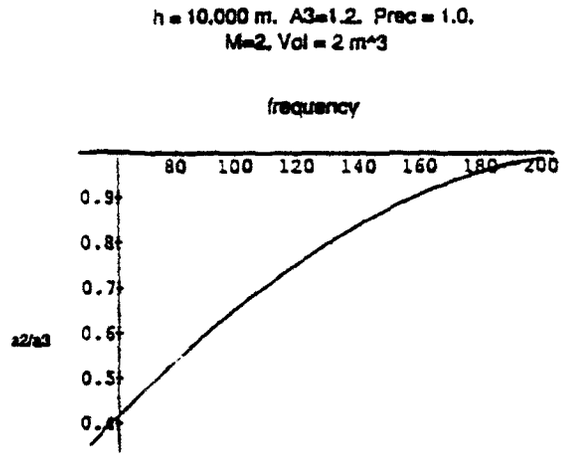

Figure 13. Results for A_2/A_3 as a function of detonation frequency.

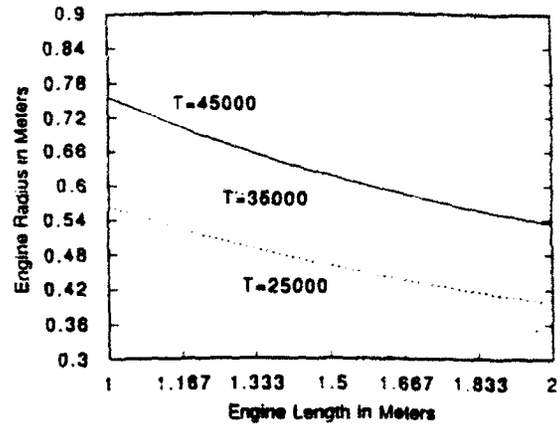

Figure 15. PDE engine radius (cylindrical cross-section) versus engine length.

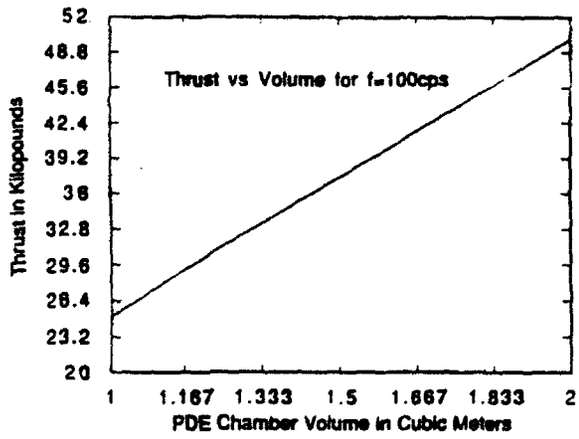

Figure 14. PDE thrust versus detonation chamber volume at a given frequency, f = 100 Hz.

Synthesis of Nanoscale Materials Using Detonation of Solid Explosives

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Abstract

Direct synthesis of nanophase materials in detonations is considered. Article discusses a number of methods that can lead to formation of super saturated states of media that in turn will presipitate as nanoscale particles when the detonation products are quenched in the expansion process. Several examples are given of reactions that will lead to production of nanophase particles of metals, oxides, diamond and other unique materials. It is shown that conditions of nucleation and growth of nanoscale material can be analysed using advanced methods of computer simulation of detonation and blast wave phenomena. A sample of this kind of simulations is given. It is concluded that detonative synthesis of nanophase material can lead to low cost technology that will produce a range of unique materials.

1. Introduction

Recent enhanced interest in nanoscale materials is merited by the discovery of a set of unconventional material properties in the form of particles that are less than 10 nm in size. Anomalous chemical activity, lower critical temperatures of oxidation and sintering, sintering of composite materials with manifold increase in tensile strength, and sintering unique semiconducting and ferromagnetic materials, have all been demonstrated for nanoscale materials. This wide range of applications makes nanosize materials an extremely interesting and important material state that is the subject of intense study by many researchers.

The synthesis of nanoscale materials is accomplished through methods such as ion-sputtering and ion-deposition, laser ablation, evaporation and condensation in a vacuum, solgel, electroprecipitation, and plasma-jet techniques. Each of these techniques has produced 2-10 nm particles of various materials; however, the yield of such processes is extremely low and the cost of materials obtained is very high.

In this article we will consider detonative synthesis, a method of nanosize materials synthesis that offers an alternative to other more costly methods of production. Detonative synthesis is extremely advantageous because it allows very high pressure and temperature conditions to be created using low cost explosive materials and simple processing equipment. The synthesis occurs directly in the plasma created by the detonation wave. Conditions for detonative synthesis can be modified by changing the physical and chemical conditions of the detonation wave and expanding detonative products. For example, for nanoscale diamond powder synthesis, rapid expansion and cooling of the detonation products are required to prevent diamond graphitization. Thus, the explosive charge and atmosphere surrounding it should be designed to create these conditions.

In the following, we will review a range of conditions necessary for nanosize material synthesis that is provided by detonative synthesis methods, and examine their applicability for specific materials.

2. Detonation Waves as Generators of High Energy Density Plasmas

Detonations are reactive wave phenomena in which a reaction is initiated by the shock waves propagating at supersonic speeds through an explosive mixture. This wave consists of a shock wave discontinuity followed by a narrow zone of homogeneous chemical reaction. The shock wave compresses the explosive from its initial state with pressure P_0 and density ρ_0 to the shocked state P_s, ρ_s, with subsequent reaction of explosive in the reaction zone that extends up to the Chapman-Jouguet (CJ) state.

Condensed Explosive Detonations

Table I gives some typical parameters for detonation waves in solid explosives. We can see from this data that temperatures of about 3000°C at pressures of 30 GPa are typical for solid explosive detonations. These parameters create extremely oversaturated conditions for some detonation products. Subsequent ultra-fast quenching can lead to synthesis of nanophase material. Behind the detonation wave reaction zone, temperatures and pressures are high and detonation products will usually contain various active chemical components. It is challenging in this environment to preserve nanosize material from further reaction.

TABLE I
Some Typical Conditions for Detonation of Solid Explosives (1)

	Pressure GPa	Temperature °K	D velocity m/sec
TNT, ρ=1.6 g/cm^3	20.6	2940	6950
RDX, ρ=1.8 g/cm^3	34.7	2590	8750
HMX, ρ=1.9 g/cm^3	39.5	2364	9160
PbN_3, ρ=4.0 g/cm^3	23.1	2660	5000

Multi-Phase Detonations

Multi-phase detonations can cover a range of conditions between gaseous and condensed material detonations. Multi-phase detonable mixtures can be composed of solid or liquid fuel particles dispersed in gaseous oxidizer, solid particles of explosive material dispersed in gas, gaseous explosive mixture mixed with the inert or reactive liquid phase (2), or explosive slurries. All these possible methods of generating detonation waves greatly extend the range of conditions available for material synthesis. It should be noted that there is a difference in the character of condensed explosive detonation and gaseous detonations. With condensed explosives, high rate decomposition reactions usually take place. For gaseous detonations, reactions can be characterized as detonative combustion. Multi-phase detonations can be based on detonative combustion, high rate decomposition, and combinations of these processes.

Nonstandard Regimes for Detonanve Reaction

A classical self-sustained detonation wave has a fixed wave structure that moves through the explosive with constant velocity. In a self-sustained detonation, a balance is achieved between the compression work of the shock wave and energy released in the reaction zone. If a self-sustained detonation is possible in a given explosive mixture at given initial conditions, it will propagate with a constant speed.

However. for many important reactive mixtures it is either very difficult or impossible to obtain a self-sustained detonation wave.

Over the last forty years, many nonstandard detonation regimes have been discovered that significantly reduce the restrictive limitations of the classical self-sustained detonation. The following is an incomplete list of the detonation regimes that significantly deviate from the classical self-sustained detonation wave:

a. Transient detonation (forms when a deflagration wave undergoes transition to detonation);
b. Overdriven detonation (compression work of the leading shock is partially sustained by an external source of energy);
c. Spinning detonation (formed by small number of detonative combustion fronts that propagate through the mixture by spinning);
d. Multi-layer detonation (propagates in layers of explosives where the detonation wave in one layer can lead to lateral initiation of an overdriven detonation wave in the adjacent layer);
e. SWACER (Shock Wave Amplification by Coherent Energy Release) detonation;
f. Light supported detonation (detonation front is supported by a laser beam heating the area behind the shock front).

All these possible regimes for initiating and sustaining detonation waves allow substantial flexibility in adapting a detonative process for the purpose of material synthesis.

3. Detonative Synthesis Chemistry for Nanophase Materials

The elementary composition of known explosives is quite limited. The most common class, CHNO explosives, produces only one condensed phase under normal thermodynamic conditions – ultra fine carbon (1):

$$C_3H_6N_6O_6(RDX) \rightarrow 3H_2O + 1.49CO_2 + 0.022 \cdot CO + 3N_2 + 1.49C_{(s)}$$
$$C_7H_5N_3O_6(TNT) \rightarrow 2.5H_2O + 1.66CO_2 + 0.188 \cdot CO + 0.001 \cdot NH_3 + 1.5N_2 + 5.15C_{(s)}$$
$$C_4H_8N_8O_8(HMX) \rightarrow 4 \cdot H_2O + 2 \cdot CO_2 + 0.008 \cdot CO + 4N_2 + 2 \cdot C_{(s)}$$

These reactions have the following yield limits for solid phase carbon: 9% for RDX or HMX, and 29% for TNT.

More "exotic" BCHNO explosives can decompose, which produces solid BN or B_2O_3. For example, the powerful explosive $B_{10}H_{100}C_{5.75}N_{15}O_{30}$, decomposes with the 26% yield of BN by weight, while less hydrogenized $B_{10}H_{18}C_{5.75}N_{15}O_{30}$ produces primarily B_2O_3 with 34% yield.

From the point of view of chemical productivity, the most promising class of explosives is presented by acetylides and azides. For example, explosive decomposition of silver acetylide ($Ag_2C_2 \rightarrow 2Ag + 2C + 87kcal/mol$) generates a 90% silver yield. A more powerful explosive decomposition of $Ag_2C_2 \cdot AgNO_3 \rightarrow 3Ag(vapor) + CO_2 + CO + 0.5N_2 + 185kcal/mol$, gives 80% silver yield but much finer dispersity is expected. The decomposition of silver acetylides is interesting to compare with a silver azide explosion, $2Ag(N_3) \rightarrow 2Ag(v) + 3N_2$, with a respective yield of silver on

the order of 72% by weight. Over two dozen metals form explosive azides, while explosive acetylides are less common. Among the most interesting azides for nanosize powder production are explosive azides of cobalt, gold, strontium, and platinum. The main challenge in producing nanophase metals by explosive decomposition of azides or acetylides will be to assure rapid quenching of nanoscale phase components of the explosive products.

Loaded Explosive Synthesis

Explosive compositions are unknown for some chemical elements, as in the case of aluminum. The most obvious solution is to mix the explosive carrier with the powder or liquid form of the desired chemical. There is already a substantial history of adding aluminum powder to explosives in order to increase their performance. It has been established that at a grain size of several microns, aluminum does not have time to sublimate in the detonation wave reaction zone; thus, it will not affect the reaction rates. On the other hand, detonation energies and temperatures are high enough to evaporate a substantial amount of additive. In order to overcome the diffusion barrier, we are considering mixing a melted explosive carrier with a liquid aluminum compound like $AlBr_3$, which has a melting point of 97°C and comparatively low evaporation energy and temperature. Aluminum azide is also a possibility.

The same approach can be implemented in the loaded explosive synthesis of the nanoscale Hf. In this case, we can use detonation mixture of $Hf(BH_4)_4$ and an explosive carrier. Similarly, Ir can be produced using an IrF_6 load: Pu using a PuF_6 load: Re using a ReF_6 load: U using an UF_6 load; W using a WCl_6 load: V using a VF_5 load; Ti by means of a $TiCl_4$ load, etc. The reduction of metals in all these cases is taking place both physically, as the result of shock-temperature dissociation of molecules, and chemically, by ionized hydrogen and, in some cases, lithium vapors.

For carbon synthesis, loading the explosives cited above with benzol (C_6H_6), 1-hexadecen ($C_{16}H_{32}$), hexacozan ($C_{26}H_{54}$), dibenzyl ($C_{14}H_{14}$) etc., can greatly increase the yield of carbon without substantially diminishing the energetic characteristics of detonation. For example, a mixture of benzol with HMX on mol to mol basis will decompose in the detonative reaction as follows:

$$C_6H_6 + C_4H_8N_8O_8 \rightarrow 7H_2O + 0.5CO_2 + 4N_2 + 9.5C_{(S)}$$

This reaction yields 30% by weight of solid carbon that has a potential to be preserved in nanoscale form.

All these examples illustrate that the loading of explosives for nanophase material synthesis expands the range of opportunities beyond the synthesis that results from the detonative decomposition of explosives.

Phase Composition of Synthesis Products

The crystalline structure of nanoscale powders obtained from detonation generally corresponds to high-pressure modifications of the solids. This is the result of high temperature and high pressure conditions in the detonation wave reaction zone and subsequent ultra-fast quenching and cooling of detonation products. In the case of carbon, diamond is formed. The phase diagram for carbon shown below easily illustrates this point. Area marked with number 1 on the phase diagram reflects parameters typical for detonation of HMX, while the area marked with 2 corresponds to detonation of TNT. It is quite obvious from Figure 1 that the detonation of TNT cannot produce diamond, while the detonation of HMX brings all condensed carbon into diamond form.

The same situation occurs with the synthesis of BN, when explosive decomposition of boron azide $B(N_3)_3$ produces hexagonal modification of BN, while powerful BCHNO explosives can produce BN with cubic sfalerite structure. Other compounds that can be obtained include interesting compositions such as ZrO_2, HfC, and WC, sometimes in their metastable modifications. Much more diverse are crystalline modifications of nanoscale metals. In cases like Gadolinium (Gd) and Samarium (Sm), five different structure modifications could be obtained as a result of different experimental conditions.

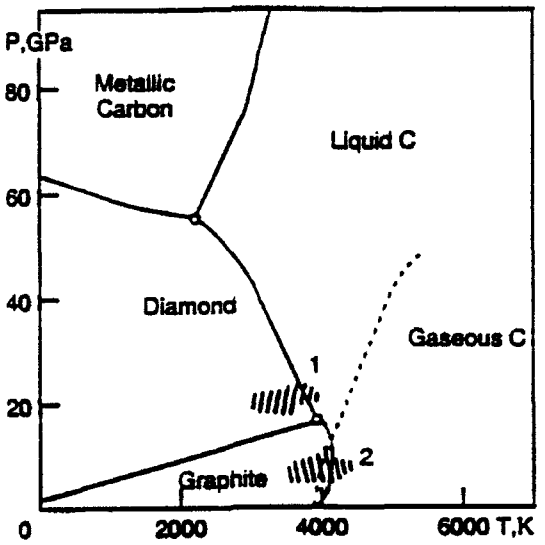

Figure 1. Carbon phase diagram schematics.

Nucleation and Growth of Nanophase Material Behind the Detonation Waves

We have discussed above the detonation wave structure in solids. We made important assumptions in our previous analysis regarding chemical equilibrium and physical stationarity of the processes on detonation front. The characteristic time of typical explosive decomposition reactions under detonation conditions in solid explosives lies in the range of $10^{-11} \div 10^{-12}$ sec. As we noted above, the characteristic time length of the reaction zone for detonations in solids is $10^{-7} \div 10^{-8}$ sec. This difference in time scales allows us to consider reactions behind the detonation front as equilibrium decompositions. Phenomenologic criteria of nucleation stationarity according to V. Shreidman (2) can be presented as follows:

$$\nu \le \left(\frac{W}{T}\right)^{-1} \rho\sigma^2 / \eta^3 \qquad (1)$$

where ν - characteristic frequency of external forces; W - activation energy of nucleation; T - temperature in energetic units; ρ and η - density and viscosity of gases; σ - surface tension coefficient for nuclei.

Following are Fo!'mer theory (3) we present activation energy through thermodynamic parameters:

$$W = \frac{16\pi}{3} \frac{\sigma^3 V^2}{(T \ln P / P_e)^2}. \qquad (2)$$

Here, P - partial pressure in gaseous precipitous phase; P_e - equilibrium pressure of saturation for condensate at given T; V - atomic volume in condensed phase.

For the conditions typical for diamond condensation in the process of detonative synthesis, the barrier of nucleation at 100 kbar pressure and 3000°k temperature behind the detonation front is W = $13 \cdot 10^{-12}$ erg. Criteria (1) in this case gives: $\nu \leq 10^{13} \div 10^{14} Hz$. Considering the time span of the detonation wave reaction zone ($10^{-7} \div 10^{-8}$ sec), we can assume stationarity of diamond nucleation. Calculations made for metals and some inorganic compounds lead to the same conclusion.

In accordance with the stationary approximation, the nucleation rate can be presented as follows (3):

$$I = \frac{2\alpha P^2 V \sigma^{1/2}}{(2\pi m T)^{1/2} T^{3/2}} \exp\left(-\frac{W}{T}\right) \quad (3)$$

α - condensation coefficient, m - atomic mass of condensate. For our reference case of diamond nucleation, calculation using equation (3) gives: $I \approx 10^{21} \frac{nuclei}{\sec \cdot cm^3}$

The diameter of critical nuclei can be estimated from activation barrier: $D = \sqrt{\frac{3W}{\pi\sigma}}$. For diamond it gives D ~ 5Å.

4. Solid Explosive Charge Detonation in a Confined Volume

Experimentally developed conditions for diamond powder synthesis rely on the multi-layered detonation of several explosives and inert material. This system undergoes a complex detonation under conditions that are overdriven for the explosive producing diamond powder, and are standard for the driver detonation with some complex multi-dimensional expansion into the surrounding media. The details of the detonation process in this system have never been studied computationally, but experimental methods indicate that very specific conditions are required. It is known that the end result of this process is extremely sensitive to conditions of the multi-layered detonation. Currently, it is not clear what variables control particle sizes, or the maximum amount of free carbon released during the detonative combustion process that can be synthesized into diamond. Experimental work in this field is sketchy; numerical analysis of this complex process will enable us to understand the sensitivity to the basic parameter variations controlling diamond synthesis. Below are the results of numerical simulation of detonation and detonation products expansion for a composite TNT/RDX charge detonated in a 1 M^3 chamber. This simulation will give the conditions of the detonative products at various stages of expansion that determines the environment prevalent in the detonative synthesis.

In Figure 2 schematics of the blast sphere cross section are shown with the solid explosive charge located at the sphere's center. The inner volume of the sphere is 1 M^3. Solid explosive is a composite charge formed from a TNT main charge with the layer of RDX around it. Detonation of a high energy RDX layer leads to the formation of an overdriven detonation wave in the main charge. Because the problem is symmetric, it is sufficient to simulate one quarter of the sphere volume to describe the full range of blast interaction that will occur for this condition. To increase the simulation's accuracy, we have divided the numerical modeling in the near field and global blast simulations. For the near field, a square grid with DR = DX = 1 mm was used to describe a region 10 cm x 10 cm containing the solid explosive charge. The simulation results from the near field region are mapped on the larger computational domain, which includes the inner wall of the blast sphere. For higher resolution and computational efficiency, we

have used structured/unstructured grids to describe the sphere's inner volume. The mathematical formulation and numerical method for the solution used in the near field are described in detail in Reference 2. These computational techniques are implemented in the MPHASE code. The model and numerical methods used for simulations in the computational domain shown in Figure 2 are described in Reference 5. These computational techniques are implemented in AUGUST code. Both MPHASE and AUGUST have been validated for the range of detonation and strong shock wave reflection and diffraction problems.(6)

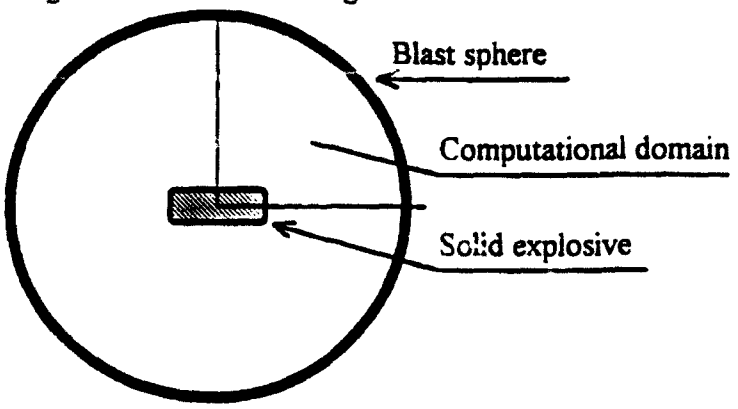

Figure 2. Schematics of the blast sphere cross section with the solid explosive charge. The computational domain is covering the upper right quadrant.

In Figure 3, simulation results for the near field region are shown as pressure density and temperature contour plots for an instant of time when the detonation wave is at 2 mm distance from the right edge of the charge. $t = 0$ is the time of detonation wave initiation in a solid explosive. Pressure and temperature contour plots are shown using a linear scale. In Figure 3 we observe propagation of the complex detonation front through the composite charge and the initial stages of detonation product expansion. The outer layer of the RDX leads to the formation of an overdriven detonation wave in the TNT charge that has shorter reaction zone, higher wave speed, higher temperatures, and higher pressures as compared with a homogeneous TNT charge detonation. The maximum temperature is reached in the air strata located in the immediate vicinity of the charge. This temperature maximum is created by a strong shock wave produced by expanding detonation products in air. The following conditions are reached at the detonation wave front in the TNT charge: $P = 62.6$ GPa; $T = 6000°C$; $\rho = 2900$ kg/m^3. It should be noted that because of high resolution of the numerical scheme we are simulating the Von Neumann spike of the detonation wave front, where the pressure is considerably higher than at the Chapman-Jouguet point.

When the shock wave reaches the edges of the computational domain for the near field simulation, the simulation results are mapped to the grid of the global domain shown in Figure 2 and are continued on larger grid. In Figure 4 pressure and temperature contour plots are shown for three consecutive instances of time for the global domain simulation. In Figure 4a results are shown at $t = 0.05$ μsec, shortly before the detonation products reached the walls of the sphere. Here we can observe significantly lower pressures as compared with Figure 3 values due to strong expansion; however, the propagating shock is leading to considerable heating of the surrounding air. In Figure 4b pressure and temperature contour plots are shown at some stage of the wave front reflection from the inner wall of the blast sphere. The average pressures and temperatures are significantly lower; however, several focus points are created during the reflection that have significantly higher pressure and temperature values. In Figure 4c, the shock wave complex is converging towards the blast sphere center, with significant amplification of the shock strength and temperature at the front. It is obvious that this system of shock waves will undergo a number of reflections. focusing, and expansions until quiescent conditions are reached in the blast sphere.

The simulations illustrated above will provide the global conditions in the blast chamber as a function of time. This information can be used for the nucleation simulations of the material behind the shock front, and estimates of possible phase transformation or reaction of the newly formed material. As a result of this multi-step approach, we can consider all the stages of the detonative synthesis process that are important for nanoscale material formation. This approach will allow us to minimize the number of experiments, understand the physics of detonative synthesis, and control the quality and yield of nanoscale materials produced experimentally.

5. Conclusions

Detonative synthesis of nanoscale material is a new technology and the nature of this process is widely unexplored. More studies should be done in addressing chemical and phase transformations under extreme and fast changing conditions in waves of detonation, shock and rarefraction. An unlimited array of elements and compounds, as well as their structural modifications (some highly metastable), is attainable through such processing.

Detonation synthesis combines the best features of traditional nanophase material technology -- the most effective generation of hot plasma and vapors, and fast quenching of a condensing product. The most unique feature of the process is the extreme density of the generated plasmas, which makes them highly supersaturated in regard to pressure and temperature.

Detonative technology has promising industrial prospects, due to very low production cost and the unique materials it yields. As a reference we can use ultra-fine carbon. In this case common nanotechnology produces carbon black; detonative synthesis diamond. These factors are completely changing the traditional view of nanomaterials applications. (7)

6. Acknowledgment

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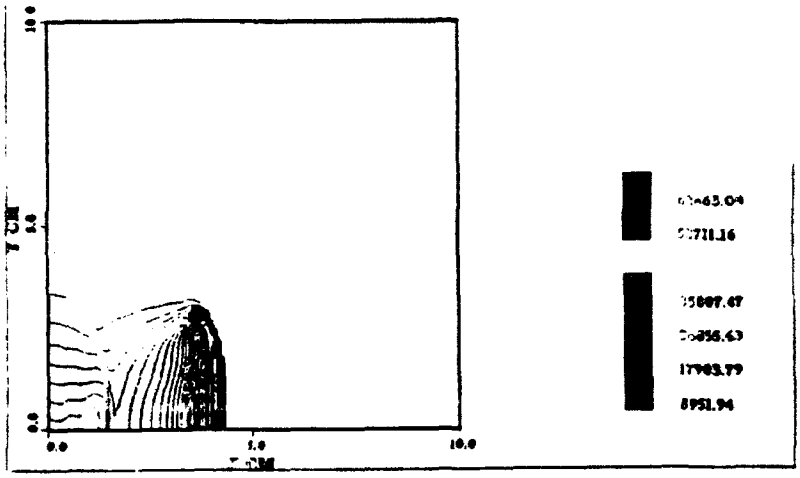
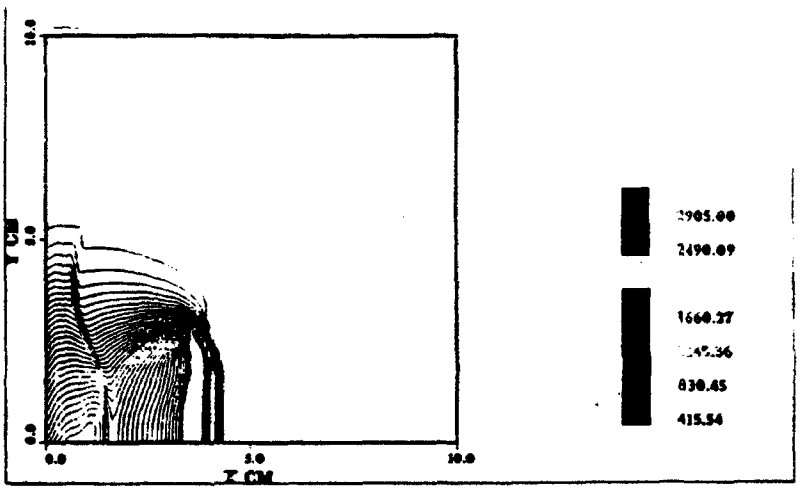
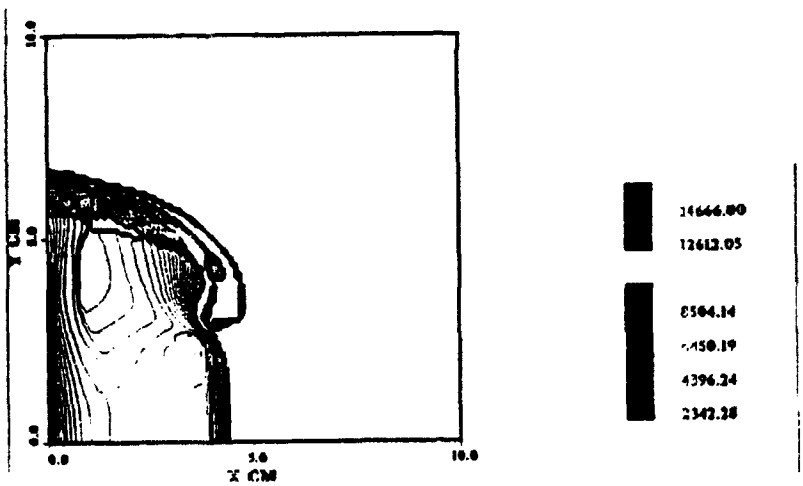


a. Pressure



b. Density

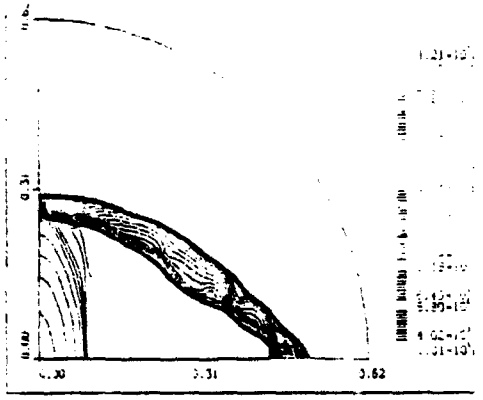


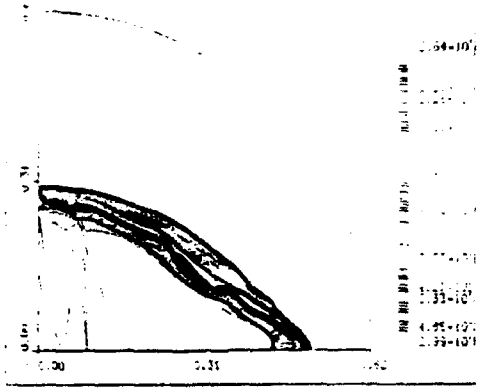
c. Temperature.

Figure 3. Pressuure, density and temperature contour plots for a composite charge detonation t = 0.01 msec.

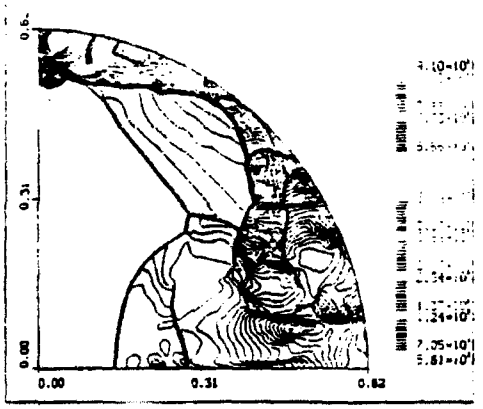
Pressure

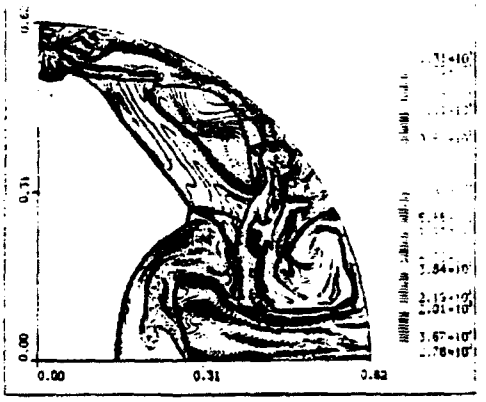
Temperature



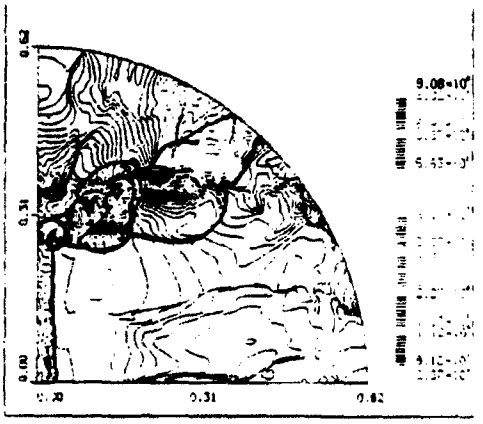


a. t = 0.05 msec





b. t = 0.2 msec



c. t = 0.3 msec

Figure 4. Simulation of blast wave reflection from the inner wave of a blast sphere.

Detonation Wave Propagation in Combustible Mixtures with Variable Particle Density Distributions

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Abstract

A mathematical model is presented describing a physical system of detonation waves propagating in a solid particle/air mixture with a wide range of solid-phase concentrations. The mathematical model was solved numerically using the Second Order Godunov method, and numerical solutions were validated for detonation waves propagating in mixtures with concentrations of solid phase from 0.75 kg/m^3 to 1000 kg/m^3. Numerical solution was obtained for detonation waves propagating in a system consisting of clouds with a small concentration of particles and a ground layer in which solid particle densities are three orders of magnitude larger than in the cloud. Three different particle concentration distributions in the ground layer were simulated and compared in terms of detonation wave structure and parameters.

Introduction

When combustible particles are intentionally or unintentionally dispersed into the air, the resulting mixture can be detonable. Formation of this potentially explosive dust environment and the properties of its detonation are of significant practical interest in view of its destructive or creative effects.

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The experimental and theoretical study of these phenomena until now has addressed only homogenous particle/oxidizer mixtures. However, intentional or accidental processes of the explosive dust dispersion will always lead to inhomogeneous particle density distribution. Some industrial methods of explosive-forming rely on detonation of explosive powder. This powder can be deposited as a thin layer over the surface area of the forming metal, with some remaining concentration in the vicinity of the layer. The phenomenology of detonation wave initiation and propagation in this environment is the main subject of this paper.

When the detonation wave is generated in a homogeneous mixture by a "direct initiation," it starts with a strong blast wave from the initiating charge. As the blast wave decays, combustion of the reactive mixture behind its shock front starts to have a larger role in support of the shock wave motion. When the initial explosion energy exceeds some critical value, transition to steady-state detonation occurs.[1–4] In explosive dust mixtures with a nonuniform distribution of particle density, the initiation dynamics are significantly more complicated. The critical initiation energy sufficient for one of the explosive particle density strata regions is not necessarily adequate for other regions. Also, when there is a significant variation in density between the different layers (regions) of the mixture, steady detonation in one layer can result in an overdriven detonation in an adjacent layer. Our paper demonstrates that the phenomenology of these interactions is distinctly different from the classical studies of multilayer detonations in gases. This is primarily because the energy content of adjacent layers in a typical multigas layer experiment[5] varies by a factor of two or four, whereas the energy content in explosive dust/air mixtures can vary by several orders of magnitude.

In this paper we use detailed numerical simulation to study the initiation dynamics and propagation phenomenology for a general case of explosive dust dispersion. We will consider particle density variation from 1000 kg/m^3 in the ground layer to 0.5 kg/m^3 or 0 for the upper edges of the cloud. The effects of variation of the cloud density on detonation wave parameters

will be examined for different cases of cloud particle density distribution. When possible, the results of computer simulations are validated in comparison with experimental and theoretical studies.

The outline of this paper is as follows. Section 2 gives a description of a mathematical model that includes governing conservation equations for two phases and the constitutive laws. We describe the model for a particle-gas interaction, combustion, and equation-of-state for gas phase. The numerical integration technique for solving the mathematical model will also be outlined. In Section 3, we present our numerical simulation results. We first validate our model by comparing one-dimensional detonation wave simulation with available experimental results. We then give the two-dimensional simulation for detonation wave propagation in combustible particles/air mixtures with variable particles density distribution. Concluding remarks are given in Section 4.

Mathematical Model and the Numerical Solution

The mathematical model consists of conservation governing equations and constitutive laws that provide closure relations for the model. The basic formulation adopted here follows the two-phase fluid dynamics model presented in the text by Kuo.[6] The approach assumes that there are two distinct continua, one for gas and one for solid particles, each moving at its own velocity through its own control volume. The sum of these two volumes represents an average mixture volume. With these assumptions, distinct equations for continuity, momentum, and energy are written for each phase. The interaction effects between the two phases are accounted for by the source terms on the right-hand side of the governing equation. The following is a short description of the two-phase flow model used in our study, with conservation equations written in Eulerian form for two-dimensional flow in Cartesian coordinates:

Continuity of gaseous phase

$$\frac{\partial \rho_1}{\partial t} + \frac{\partial(\rho_1 u_g)}{\partial x} + \frac{\partial(\rho_1 v_g)}{\partial y} = \Gamma \qquad (1)$$

Continuity of solid-particle phase

$$\frac{\partial \rho_2}{\partial t} + \frac{\partial(\rho_2 u_p)}{\partial x} + \frac{\partial(\rho_2 v_p)}{\partial y} = -\Gamma \tag{2}$$

Conservation of momentum of gaseous phase in x direction

$$\frac{\partial(\rho_1 u_g)}{\partial t} + \frac{\partial(\rho_1 u_g^2 + \phi p_g)}{\partial x} + \frac{\partial(\rho_1 u_g v_g)}{\partial y} = -F_x + \Gamma u_p \tag{3}$$

Conservation of momentum of gaseous phase in y direction

$$\frac{\partial(\rho_1 v_g)}{\partial t} + \frac{\partial(\rho_1 u_g v_g)}{\partial x} + \frac{\partial(\rho_1 v_g^2 + \phi p_g)}{\partial y} = -F_y + \Gamma v_p \tag{4}$$

Conservation of momentum of solid-particle phase in x direction

$$\frac{\partial(\rho_2 u_p)}{\partial t} + \frac{\partial(\rho_2 u_p^2)}{\partial x} + \frac{\partial(\rho_2 v_p u_p)}{\partial y} = F_x - \Gamma u_p \tag{5}$$

Conservation of momentum of solid-particle phase in y direction

$$\frac{\partial(\rho_2 v_p)}{\partial t} + \frac{\partial(\rho_2 u_p v_p)}{\partial x} + \frac{\partial(\rho_2 v_p^2)}{\partial y} = F_y - \Gamma v_p \tag{6}$$

Conservation of energy of gas phase

$$\frac{\partial(\rho_1 E_{gT})}{\partial t} + \frac{\partial(\rho_1 u_g E_{gT} + u_g \phi p_g)}{\partial x} + \frac{\partial(\rho_1 v_g E_{gT} + v_g \phi p_g)}{\partial y} =$$

$$\Gamma\left(\frac{u_p^2 + v_p^2}{2} + Echem + C_s T_p\right) - \left(F_x u_p + F_y v_p\right) - \dot{Q} \tag{7}$$

Conservation of energy of solid-particle phase

$$\frac{\partial(\rho_2 E_{pT})}{\partial t} + \frac{\partial(\rho_2 E_{pT} u_p)}{\partial x} + \frac{\partial}{\partial y}(\rho_2 E_p v_p) = \dot{Q} + (F_x v_p + F_y v_p)$$

$$-\Gamma\left(\frac{u_p^2 + v_p^2}{2} + Echem + C_s T_p\right) \tag{8}$$

Conservation of number density of solid-particle

$$\frac{\partial N_p}{\partial t} + \frac{\partial(N_p u_p)}{\partial x} + \frac{\partial(N_p v_p)}{\partial y} = 0 \tag{9}$$

In the above equations, we have the following definitions and constitutive laws:

Phase densities

$$\rho_1 = \phi\rho_g, \quad \rho_2 = (1-\phi)\rho_p \tag{10a}$$

and fractional porosity

$$\phi = 1 - \frac{N_p M_p}{\rho_p} = \frac{\text{Volume of void}}{\text{total volume}} \tag{10b}$$

where M_p is the mass of each particle and ρ_p is the solid-particle density.

Total internal energy of gaseous phase

$$E_{gT} = E_g + \frac{1}{2}(u_g^2 + v_g^2) \quad \text{and} \quad E_g = E_g(p_g, \rho_g) \tag{11}$$

where $E_g(p_g, \rho_g)$ is the equation-of-state for gas phase, which will be discussed later.

Total internal energy of solid-particle phase

$$E_{pT} = E_p + \frac{1}{2}(v_p^2 + v_p^2) \quad \text{and} \quad E_p = E\text{chem} + C_s T_p \tag{12}$$

In order to close the above system of conservation equations, it is necessary to define certain criteria and interaction laws between the two phases, which include mass generation rate, Γ, drag force between particles and gas, F_x, F_y, and the interphase heat transfer rate $\dot{Q}$. The model for particle and gas interaction and particle combustion that results in the constitutive relation for the conservation equations is explained in detail in the next subsection.

Model for a Particle Gas Interaction and Combustion

Presently, the physics of the energy release mechanisms in solid-particles/air mixtures is not clearly understood. This can be attributed to the obvious difficulties of making a direct nonobtrusive measurement in the optically thick environment typical for this system. In the experimental and theoretical work done for the grain dust detonation conditions,[7] it was demonstrated that the volatile components released by the particle heated behind the shock front play a major role in determining the detonability limits of the mixture. Eidelman and Burcat[8] successfully applied a combination of fast evaporation and aerodynamic shattering mechanisms to simulate a two-phase detonation process.

The chemical processes of a single particle combustion, which mainly occur in the gaseous phase, are significantly faster than the physical processes of particle gasification or disintegration. Thus, in the multiphase mixtures, the rate of energy release will be mostly determined by physics of particle disintegration. It is very difficult to describe the details of particle disintegration in the complex environment prevalent behind the shock or detonation wave. For example, Reinecke and Waldman[9] defined five different disintegration regimes for a relatively simple environment of water droplets passing through a weak shock. Fortunately, in most cases of multiphase detonation, only the main features of the particle disintegration dynamics need to be captured to describe the phenomena. For example, Eidelman and Burcat[10] used simple models for particle evaporation and shattering to obtain simulation results that compared very favorably with experimental data. Because of

our inability to resolve the particle disintegration problem in all its complexity, the validation of the model against known experimental data is essential.

In this paper, we consider solid particles consisting of explosive material. Explosive material contains fuel and oxidizer in a passive state at low temperature; however, when the temperature rises the fuel and oxidizer react, leading to detonation or combustion. The intiation of reaction for explosives occurs at relatively low temperature. For example, TNT will detonate when heated to the temperature[11] of 570°C. Only particles larger than a critical detonation size can detonate directly when initiated by a shock wave. Here, consider particles smaller than 4 mm in diameter that will not detonate when heated, but will burn when the temperature on the particle surface reaches a critical value. Since the heat conduction inside the explosive material is relatively slow, the process of particle heating needs to be resolved in detail. Our simulations numerically solve the temperature field in the particles at every step of numerical integration of the global conservation equations. The explosive particle combustion model examined in this paper assumes that the fraction of the particle that reaches the critical temperature will burn instantaneously.

Energy transfer by convection and conduction is simulated by solving the unsteady heat conduction equation in each computational cell at each time step. Assuming a particle's temperature to be a function of time and radial position only, the unsteady heat conduction equation may be transformed to:

$$\frac{d^2w}{dr^2} = \frac{1}{\alpha}\frac{dw}{dt} \tag{13}$$

subject to the boundary conditions:

$$w = 0 \quad \text{at} \quad r = 0, \quad t > 0$$

$$k\frac{dw}{dr} + (h - \frac{1}{R})\, w = hRT_g \quad \text{at} \quad r = R, t > 0 \tag{14}$$

where

$w(r,t) = rT(r,t)$
r = radial position
$T(r,t)$ = temperature
R = particle radius
T_g = temperature of surrounding gas
k = thermal conductivity of particle
h = convective heat transfer coefficient

The Nusselt number, used to find h, is given by an empirical relation given by Drake.[12] The gas viscosity is derived from Sutherland's Law. The gas thermal conductivity is calculated by assuming a constant Prandtl number. Finally, the boiling temperature at a given pressure is derived from the Clapeyron-Clausius equation under the following assumptions: 1) phrasing-constant latent enthalpy of phase-change; 2) the vapor obeys the ideal equation-of-state; and 3) the specific volume of the solid/liquid is negligible compared to that of the vapor. A critical temperature is also employed to serve as an upper limit to the boiling point, regardless of pressure.

Equation 13 with boundary condition 14 can be numerically integrated using either implicit or explicit schemes.

Since the particle radius R becomes very small due to evaporation, the implicit Crank-Nicolson algorithm is used because of its stability properties and its second order temporal and spatial accuracy. Using the Crank-Nicolson scheme to predict the particle temperature profiles at times t_1 and t_2 permits easy calculation of the total energy exchange $\dot{Q}$ between t_1 and t_2, due to convection and conduction.

Knowledge of the particle temperature profile also allows the precise determination of the quantity of the mass to transfer from the particle to the gas Γ. Once any point at a radial location $0 \leq r \leq \mathrm{R}$ has a temperature exceeding the boiling temperature, the entire mass between r and R is transferred to the gas phase in one time step. In so doing, an energy equal to the product of the mass lost and the particle intrinsic energy is transferred by the particle to the gas.

The interphase drag force Fx, Fy is determined from the experimental drag for a sphere, as presented by Schlichting.[13]

$$F_x = \left(\frac{\pi}{8}\right) N_p \rho_g C_D |\mathbf{V}_g - \mathbf{V}_p| (u_g - u_p) R^2 \tag{15}$$

where

$$C_D = \begin{cases} \frac{24}{Re}\left(1 + \frac{Re^{2/3}}{6}\right) & \text{for Re} < 1000; \\ 0.44 & \text{for Re} > 1000 \end{cases} \tag{16}$$

and $Re = \frac{2R|V - V_p|}{\mu_g}$, R is radius of particle, and μ_g is gas viscosity at temperature of $T_{film} = \frac{1}{2}(T_g + T_p)$.
Similarly, the formulae for Fy is

$$Fy = \frac{\pi}{8} N_p \rho_g C_D |\mathbf{V}_g - \mathbf{V}_p| (v_g - v_p) R^2 \tag{17}$$

Equation-of-State for Detonation Products

To close the system of governing equations, one needs a constitutive relation between pressure, temperature, and energy for gas phase, which is an equation-of-state. This study uses the Becker-Kistiakowsky-Wilson (BKW) equation-of-state,[14,15] that is,

$$p_g V_g / \bar{R} T_g = 1 + x e^{bx} \tag{18}$$

where

V_g = volume of gas phase
p_g = pressure of gas phase
T_g = temperature of gas phase
$\bar{R}$ = universal gas constant
$x = k/V_g(T + \Theta)^a$
$k = K \Sigma_j X_i k_i$

with empirical constants a, b, K, Θ, and k_i. The constants k_i, one for each molecular species, are covolumes. The covolumes are multiplied by their mole fraction of species X_i and are added to find an effective volume for a mixture. For a particular explosive, if we know the composition of detonation products, a, b, Θ, K, and all k_is can be found in Ref. 15.

The internal energy is determined by thermodynamics relation

$$\left(\frac{\partial E_g}{\partial V_g}\right)_T = T_g\left(\frac{\partial p_g}{\partial T_g}\right)_V - p_g \tag{19}$$

Integration of this equation for a fixed composition of the detonation products will allow us to calculate the energy of the detonation products as a function of temperature and volume. For each component, its thermodynamic properties as functions of temperature were calculated from the NASA tables compiled by Gordon and McBride.[16]

The BKW equation-of-state is the most commonly used and well-calibrated of those equations-of-state used to calculate the properties of detonation products. The detailed discussion and review of the BKW equation-of-state can be found in Ref. 15.

Numerical Method of Solutions

The system of partial differential equations described in the previous paragraph is integrated numerically. The Second Order Godunov method is used for the integration of the subsystem of equations describing flow of gaseous phase material and is described in Ref. 17. In the following, we will elaborate only on some specifics of its application to simulations of detonation products. The subsystem of equations describing the flow of particles is integrated using a simple upwind integration. This is done because our mathematical model neglects the pressure of interparticle interaction, and that prevents formulation of a Second Order Godunov scheme for particles.

The physical system under study will have concentrations of solid explosive powder ranging from 1000 kg/m^3 near the

ground to 0.75 kg/m^3 or less in the cloud. Detonation of this mixture will create detonation products with effective γ ranging from 3 to 1.1. To describe the flow of detonation products, we use the BKW equation-of-state described above. Since the Second Order Godunov method uses primitive variables to calculate Riemann problems at the edges of the cells, its implementation for non-ideal EOS is difficult. In our simulations, we have resolved this problem by using direct and inverse equations-of-state. After integrating a system of gas conservation laws, we use the direct BKW equation-of-state to calculate pressure, gamma, and temperature as functions of thermal energy, density, and mixture composition. After this step, we have a complete set of parameters allowing calculation of the fluxes in the Second Order Godunov method as well as interaction of the multiphase processes. The "inverse" EOS calculates internal energy as a function of density, pressure, and mixture composition. In our code, we use the "inverse" EOS to calculate the fluxes of conserved variables after calculation of the flux of primitive variables.

For the multiphase system under study, dx=dy=1mm was used to allow explicit integration of the gasdynamic and physical processes of evaporation and heat release. When a mismatch occurred between the physical and gasdynamical characteristic times, the time step was adjusted by some fraction to assure stability. However, this did not result in a significantly smaller time step than the one calculated using CFL criteria. For larger cell sizes, this approach will be impractical. Recently, we implemented a scheme in which multiphase processes are calculated implicitly; however, this will be reported elsewhere.

The numerical method is implemented in a code named MPHASE, which is fully vectorized and supported by number of graphics and diagnostics codes.

Results

Model Validation for One-Dimensional Detonation Wave Problem

The main advantage of our particle combustion model is its description of the phenomenology of detonation for a wide

Table 1 One-dimensional validation result

D[m/sec] - Detonation wave velocity,
P_{CJ}[Pa] - Pressure at Chapman-Jouguet Point
P_p[Pa] - Peak pressure; ρ_p[kg/m^3] - Peak density

RDX density (kg/m^3)	Parameters	Present calculations	Expt'l Ref. 1	Tiger calculations - Ref. 2	BKW calculations Ref. 1	Soviet experiments Ref. 3
1000 kg/m^3	D	6156	5881		6128	
	P_{CJ}	1.230×10^{10}			1.86×10^{10}	1.00×10^{10}
	P_p	2.57×10^{10}				
	ρ_p	1936				
500 kg/m^3	D	6051		6000		
	P_{CJ}	0.905×10^{10}		0.80×10^{10}		0.82×10^{10}
	P_p	1.95×10^{10}				
	ρ_p	1722				
400 kg/m^3	D	4800		4640		
	P_{CJ}	0.370×10^{10}		0.36×10^{10}	0.3×10^{10}	
	P_p	0.625×10^{10}				
	ρ_p	926				
250 kg/m^3	D	4040		3660		
	P_{CJ}	0.2476×10^{10}		0.13×10^{10}		
	P_p	0.4536×10^{10}				
	ρ_p	552				
100 kg/m^3	D	3496				
	P_{CJ}	0.5063×10^9				
	P_p	0.7656×10^9				
	ρ_p	230				
0.75 kg/m^3	D	1632	1410*	1670*		
	P_{CJ}	0.35×10^7	0.200×10^{7}*	0.26×10^{7}*		
	P_p	0.484×10^7				
	ρ_p	8				

Ref. 1 - Mader, C., Numerical Modeling of Detonations, (University of California Press, Ltd., 1979) p. 47. Ref. 2 - Wiedermann, A., "An Evaluation of Extended Layer Loading Effects," UTRI Report, Feb. 1990. Ref. 3 - Stanyukovich, K. P., "Physics of Explosion" (in Russian), Nauka, 1975.

range of explosive particle sizes and densities. We will demonstrate this capability on a set of one-dimensional test problems. For these test problems, we simulated the initiation and propagation of the detonation waves in a shock tube-like setting, where the explosive particles are distributed uniformly through the shock tube volume.

Results of these simulations are summarized in Table 1, which shows detonation wave velocity, peak pressure, and peak density given as a function of the average density of the solid explosive. Here, the explosive two-phase mixture is composed from RDX particle and air, where RDX particle concentration varies from 0.75 kg/m^3 to 1000 kg/m^3. This concentration variation covers a whole range of solid explosive concentrations of interest to our problem. The simulations performed with the MPHASE code were compared with the experimental results[15,18] and calculations done with the TIGER code that are presented in Ref. 19.

From Table 1, it is clear that our simulation results compare favorably with other simulation results and experimental data. The maximum deviation between our results and referenced results is no greater than 15% for the entire range of explosives densities. Considering that our results were obtained with a single model for particle combustion applied to the extreme range of densities, our model gives an excellent prediction of the detonation wave parameters.

Two-Dimensional Simulation Results

Figure 1 shows a setup for a typical simulation with a computational domain of 25 cm $\times$ 25 cm. The explosive powder density is distributed according to the 4th power law of vertical distance, starting from the ground where the density is 1000 kg/m^3, to 1.2 cm, where the density is 0.75 kg/m^3. From this point to 25 cm height, the density is constant and equal to 0.75 kg/m^3. The density distribution in the direction of the "x" axis is uniform. The boundary conditions for the computational domain shown in Fig. 1 are specified as follows: solid wall along the "x" axis, symmetry conditions along the "y" axis, supersonic outflow for upper boundary, and at the

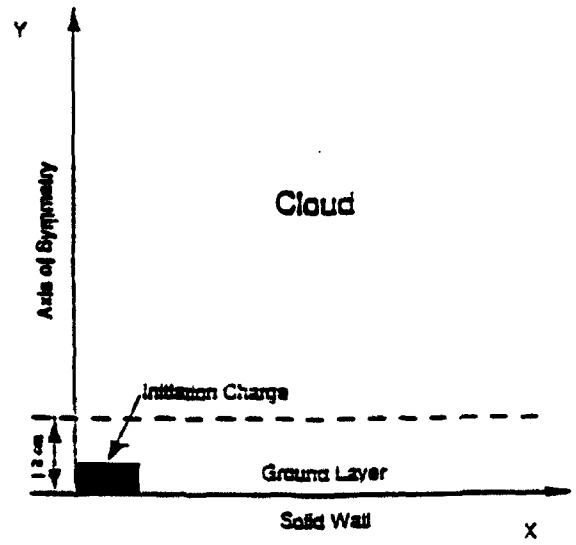


Fig. 1 Computational domain and boundary conditions.

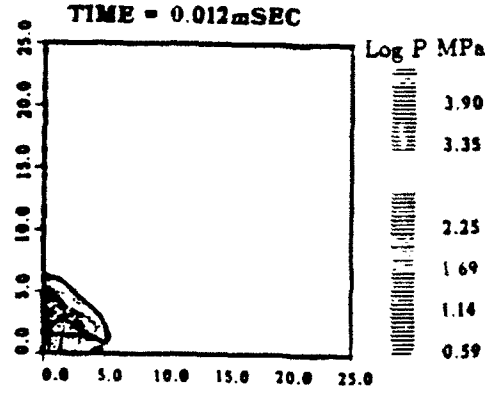
right of the computational domain. The mixture consists of RDX powder and air at ambient conditions, and it is assumed to be quiescent at the time of initiation.

The simulation starts at t=0 when the mixture is initiated at the lower left corner of the computational domain, as shown in Fig. 1. The energy released by the initiating explosion leads to formation of the detonation wave propagating through the multiphase media. Figure 2a shows pressure contours for the propagating detonation wave at the time of t=0.012 msec after initiation. The pressure contour levels are shown on the logarithmic scale in MPa. The maximum pressure value of 7940 MPa is observed in the layer of condensed explosive located near the ground. The pressure in the layer is two to three orders of magnitude higher than pressure behind the detonation wave in the 0.75 kg/m^3 RDX cloud and air located above the distance of 1.2 cm from the ground. Figure 2a demonstrates that the detonation wave in the cloud is overdriven, since the pressure behind the shock continuously rises and reaches its maximum in the layer. From this figure, we also observe that the overdriven wave propagates faster in the cloud than in the layer. This is explained by the fact that it is easier to compress air that is very lightly loaded with particles and located above the ground layer than it is to compress air heavily loaded with a particle mixture near the ground. It is interesting to note a discontinuous pressure change between the yellow contours and the light blue and green contours behind the detonation front. This discontinuity is overemphasized by our presentation of contour lines on the logarithmic scale; however, further examination of our simulation results indicates this feature is real and is similar in nature to barrel shocks observed for strong jets.

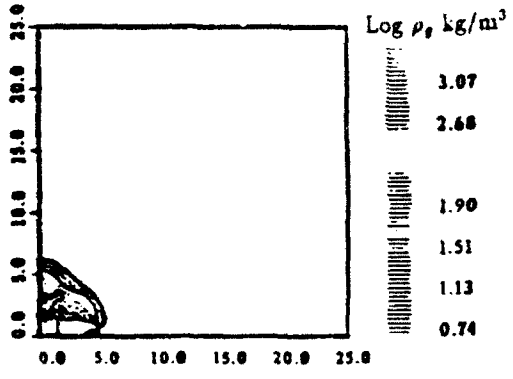
In Fig. 2b, gas-phase density contours are shown for the time t=0.012 msec. Here the contour lines are distributed on the logarithmic scale. The main features of the shock wave structure are very similar to those observed in the pressure contours figure. We see that a jet of high-density gases reflects from the center of symmetry axis. which will create a contact discontinuity that we will observe at later times. The barrel

shock is clearly visible in this figure. In Fig. 2c, the particle density contour plots are shown for t=0.012 msec. The contour levels in Fig. 2c are given on the logarithmic scale and the initial deposition of the explosive material in the ground layer of the computational domain can be clearly observed. The white contour line delineates the beginning and the end of the reaction zone in the cloud. To the left of these contours lies an area with combustion products and to the right are unburned particles in the cloud. The reaction zone length is of the order of 1 cm.

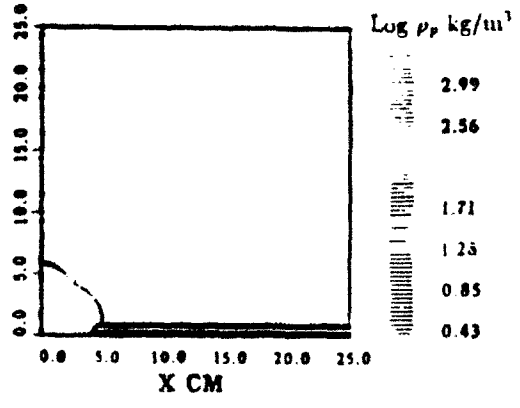
Figure 2d shows pressure contours for the same simulation for the time t=0.055 msec, just before the detonation wave leaves the computational domain. In this figure, we see that the global structure of the wave did change slightly from Fig. 2a. We observe that the barrel shock wave is fully developed and has a half-ellipse shape. The detonation wave in the cloud is still overdriven; however, part of the shock wave front that propagates vertically weakened because it gets further away from the detonation front in the layer. Another noticeable feature is the increase in distance between the detonation front in the layer and in the cloud area close to the layer. This is a result of the fact that the lightly loaded two-phase media above the layer can be compressed much more easily than the particle-heavy ground layer. In Fig. 2e, temperature contours are shown for t=0.055 msec. Comparing this figure with an early stage of the wave propagation, we observe a significant cooling of the front area propagating upwards, which indicates transition from the overdriven detonation regime to a self-sustained detonation. We also observe in Fig. 2a clear development of two detonation fronts, one moving vertically in the cloud and another moving horizontally in the layer. Because the energy density of the explosive powder in the layer is about three orders of magnitude larger than in the cloud, the vertical parts of the front represent an overdriven detonation wave in the cloud. Even though the vertical front has slowed down compared with the horizontal front, its speed and parameters far exceed those typical for detonation waves in a cloud. In fact, the self-sustained detonation regime in the cloud will



a) Pressure.

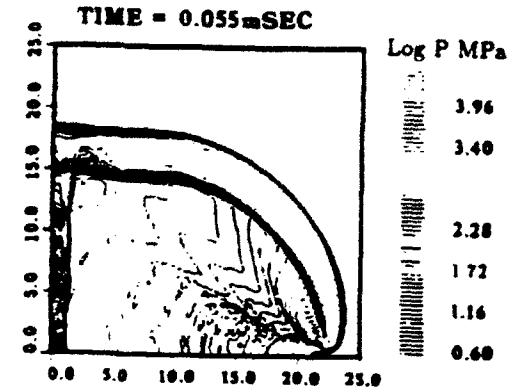


b) Gas Density.

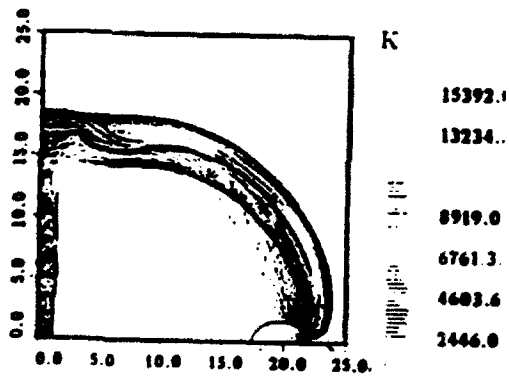


c) Particle Density.

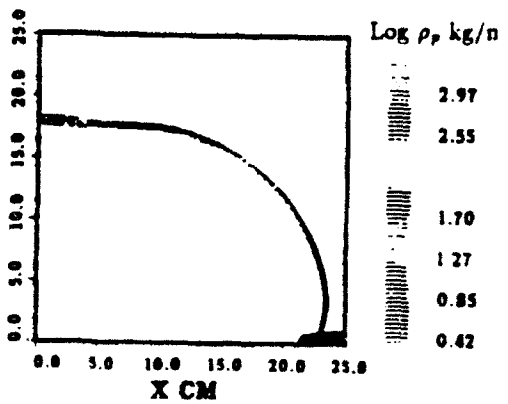
Fig. 2 Fourth power layer distribution; maximum density in the layer 800 kg/m^3; density in the cloud 0.75 kg/m^3; time 0.012 m/s and 0.055 m/s after initiation.



d) Pressure.



e) Temperature.



f) Particle Density.

Fig. 2 (continued) Fourth power layer distribution: maximum density in the layer 800 kg/m^3; density in the cloud 0.75 kg/m^3; time 0.012 m/s and 0.055 m/s after initiation.

develop at the distance of about 3 m from the layer. The area of the front close to the detonation wave in the layer will remain hot and overdriven, since it is located very close to the detonation front in the layer. In Fig. 2f, particle density contours are shown on a logarithmic scale. We can clearly observe the reaction zone delineated by black contour lines. In this case, the reaction zone length in the cloud is about 1 cm. Consistent with the gradual transition from overdriven to self-sustained detonation, the reaction zone length is larger for the vertical part of the detonation front. The detonation wave velocity observed in our simulation is approximately 4048 msec, which is significantly lower than the detonation wave velocity observed in RDX with a density of 860 kg/m^3 (see Table 1), the highest density in the ground layer. This can be explained by high gradient of particle density distribution in the layer, where the density drops rapidly from 860 kg/m^3 at the bottom of the layer to 1 kg/m^3 at the top strata of the layer at 12 mm above the ground.

To further explore properties and phenomenology of the detonation waves propagating in the layer/cloud systems, we simulated additional cases in which explosive powder density distribution was different from the case reported above, although total weight of fuel per unit area remained the same.

In Fig. 3, results are shown for the case of a uniform 2.5 cm-thick layer of RDX with a density of 100 kg/m^3 and a 0.75 kg/m^3 cloud initiated under the same conditions as in the previous example. Figures 3a, 3b, and 3c show pressure, gas density, and particle density contour plots at t=0.066 msec. We observe that because the layer has considerably smaller density compared to the case reported above, the precursor effect of the detonation wave in the cloud preceding the wave in the layer is less pronounced. Also, one can observe a significant difference in the shape of the strong contact discontinuity in the region of the shock front close to the layer. In Fig. 3b, we can clearly distinguish two contact surfaces. One is between condensed explosive detonation products in the layer and in the cloud, and another is between the detonation products from

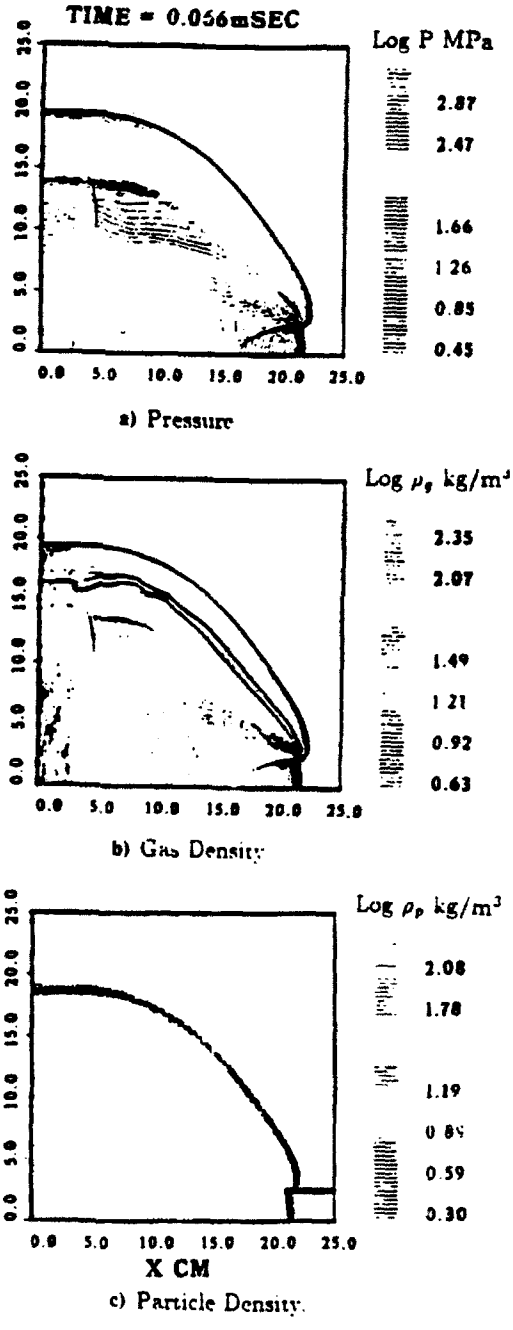


Fig. 3 Constant density 2.5-cm-thick layer; maximum density in the layer 100 kg/m^3; density in the cloud 0.75 kg/m^3; time 0.055 m/s after initiation.

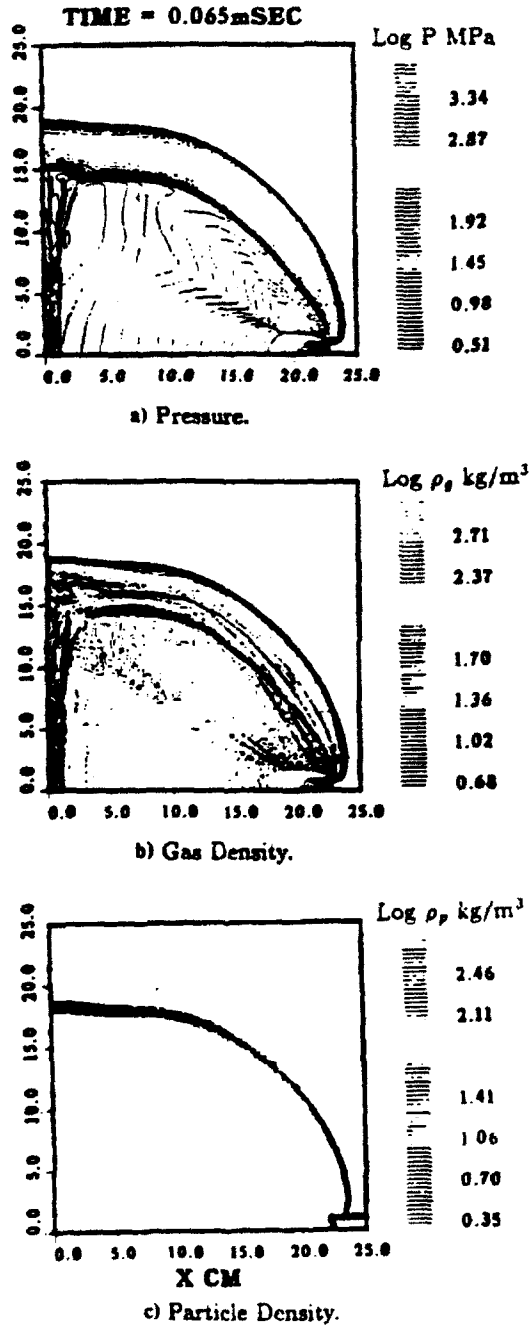


Fig. 4 Constant density 1.2-cm-thick layer; maximum density in the layer 250 kg/m^3; density in the cloud 0.75 kg/m^3.

layer explosive detonation and from cloud particle detonation. We should note that these contact surfaces are overemphasized by the logarithmic display of the contour plot levels. The maximum pressure observed in this simulation is 955 MPa, which is about one order of magnitude smaller than in previous simulation. This is consistent with the one order of magnitude difference in the maximum density of the ground layer in the two cases. The detonation wave speed in the case presented in Fig. 3 is 3407 msec. That is only slightly lower than the speed predicted by one-dimensional simulations presented in Table 1, which reflects the influence of the two-dimensional expansion on the detonation wave propagation.

Figure 4 presents results for the case of a uniform density of 250 kg/m^3 in 1.2 cm ground layer. All other parameters are the same as in the previous two cases. In Figs. 4a, 4b, and 4c, pressure, gas density, and particle density contour plots are shown at the time t=0.066 msec after initiation of the detonation wave. Here, the detonation wave propagates faster than in the previous cases U=3660 msec. This is about 400 msec slower than in the case of parabolic density distribution. Maximum pressure on the ground is 2150 MPa, which is consistent with the increase of powder density in the layer. The basic structure of the detonation front and the contact surfaces is similar to the case of parabolic density distribution.

Conclusions

We have presented a mathematical model and numerical solution for the simulation of initiation and propagation of the detonation waves in multiphase mixtures consisting of solid combustible particles and gas. Using this model, we studied detonations in mixtures of solid RDX particles and air, with the objective of examining the effects of wide variation in particle density distribution on the dynamics and structure of detonation waves. We considered a physical system of solid particle clouds in air, in which a significant amount of particles settle on the ground and the condensed-phase concentrations in the particle/air mixture range from 0 to 1000 kg/m^3. This range of solid-phase densities necessitated development of the

model and its numerical implementation for a wide range of particle concentrations. Our validation study has shown good agreement between the simulations and referenced results for the whole range of particle concentrations.

Two-dimensional simulations were done for the system of low particle density concentration clouds and ground layers formed by high concentrations of the RDX powder. We examined three cases of ground layer density distribution: a fourth power distribution within 12 mm above ground with a maximum density on the ground of 860 kg/m^3; a uniform 25 mm-thick layer with a density of 100 kg/m^3; and a 12 mm-thick uniform layer with a density of 250 kg/m^3. In all these cases, the weight of condensed phase per unit area was the same, which allowed examination of the effects of the particle density distribution on detonation wave parameters.

In all examined two-dimensional cases, the detonation wave in the cloud in the computational domain was significantly overdriven and did not play an important role. We estimated that the self-sustained regime of the detonation wave in the cloud for the examined cloud concentrations can occur only at the distances of 2–3 m above ground. At the same time, the particle density distribution in the layer determines the dynamics of the detonation wave as well as pressure on the ground.

In all three two-dimensional simulations, we observed a very distinct shape of the detonation wave front in the vicinity of the layer. In this area, the overdriven detonation in the cloud is preceding the detonation wave in the ground layer. This feature of the detonation front can be explained by the fact that the energy released in the detonation wave in the ground layer produces a faster shock wave in the dilute cloud than in those heavily loaded with solid particle stratas from the ground layer. However, these structures were not observed experimentally, and more studies are needed to examine their parameters.

The maximum pressure affecting the ground was directly related to the maximum particle density in the lower strata of the layer. However, the detonation front velocity for the fourth

power distribution case was considerably lower than calculated for a one-dimensional case with 860 kg/m^3 particle density, reflecting the significant effect of two-dimensional expansion. Two other cases with 250 kg/m^3 and 100 kg/m^3 maximum densities had the detonation wave velocity only slightly lower than the one-dimensional simulations of the same RDX/air concentrations. It is interesting to compare the simulation of the fourth power density distribution case and 250 kg/m^3 case. In both cases, the same amount of explosive was distributed in the same physical space; however, the parameters of developed detonations were vastly different. Existence of the high-density strata at the bottom of the ground layer in the fourth power case significantly increased the maximum pressure at the ground and produced higher detonation wave velocity.

Using a variable density layer, one can reach a combination of pressure and velocity conditions outside of Chapmen-Jougett limitations. The range of conditions that can be obtained in the variable density system and the parametrics for this range need a more systematic study. In this article, we introduced only the mathematical formulation and numerical simulation method validated for the range of conditions of interest. In addition, we have given some examples of its application for two-dimensional simulations. However, this methodology should be linked to an experimental study for a more in-depth analysis of the phenomenology discussed here.

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Detonation Wave Propagation in Combustible Particle/Air Mixture with Variable Particle Density Distributions

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Abstract—A mathematical model is presented describing a physical system of detonation waves propagating in a solid particle/air mixture with a wide range of solid phase concentrations. The mathematical model was solved numerically using the Second Order Godunov method, and numerical solutions were validated for detonation waves propagating in mixtures with concentrations of solid phase from 0.75 kg/m^3 to 1000 kg/m^3. Numerical solution was obtained for detonation waves propagating in a system consisting of clouds with a small concentration of particles and a ground layer in which solid particle densities are three orders of magnitude larger than in the cloud. Three different particle concentration distributions in the ground layer were simulated and compared in terms of detonation wave structure and parameters.

Key words. detonation wave, two-phase flow, numerical simulation

1. INTRODUCTION

When combustible particles are intentionally or unintentionally dispersed into the air, the resulting mixture can be detonable. Formation of this potentially explosive dust environment and the properties of its detonation are of significant practical interest in view of its destructive or creative effects. The experimental and theoretical study of these phenomena until now has addressed only homogenous particle/oxidizer mixtures. However, intentional or accidental processes of the explosive dust dispersion will always lead to inhomogeneous particle density distribution. Some industrial methods of explosive forming rely on detonation of explosive powder. This powder can be deposited as a thin layer over the surface area of the forming metal, with some remaining concentration in the vicinity of the layer. The structure of the detonation waves and the phenomenology of their initiation and propagation in these environments are the main subjects of this paper.

When the detonation wave is generated in a homogeneous mixture by a "direct initiation," it starts with a strong blast wave from the initiating charge. As the blast wave decays, combustion of the reactive mixture behind its shock front starts to have a larger role in support of the shock wave motion. When the initial explosion energy exceeds some critical value, transition to steady state detonation occurs (cf. Eidelman *et al.*, 1976; Burcat *et al.*, 1978; Oved *et al.*, 1978; Eidelman and Burcat, 1980). In explosive dust mixtures with a nonuniform distribution of particle density, the initiation dynamics is significantly more complicated. The critical initiation energy sufficient for one of the explosive particle density strata regions is not necessarily adequate for other regions. Also, when there is a significant variation in density between the different layers (regions) of the mixture, steady detonation in one layer can result in an overdriven detonation in an adjacent layer. Our paper demonstrates that the phenomenology of these interactions is distinctly different from the classical studies of multi-layer detonations in gases. This is primarily because the energy content of adjacent layers in a typical multi-gas layer experiment varies by a factor of two or four (Liu *et al.*, 1990), whereas the energy content in explosive dust/air mixtures can vary by several orders of magnitude.

In this paper we use detailed numerical simulation to study the initiation dynamics and propagation phenomenology for a general case of explosive dust dispersion. We will consider particle density variation from 1000 kg/m^3 in the ground layer to 0.75 kg/m^3 for the upper edges of the cloud. The effects of the cloud density variation on detonation wave parameters will be examined for different cases of cloud particle density distribution. When possible, the results of computer simulations are validated in comparison with experimental and theoretical studies.

The outline of this paper is as follows. Section 2 gives a description of mathematical model that includes governing conservation equations for two phases and the constitutive laws. We describe the model for a particle gas interaction, combustion and equation-of-state for gas phase. The numerical integration technique for solving the mathematical model will also be outlined. In Section 3, we present our numerical simulation results. We first validate our model by comparing one dimensional detonation wave simulation with available experimental results. We then give the two dimensional simulation for detonation wave propagation in combustible particles/air mixtures with variable particle density distribution. Concluding remarks are given in Section 4.

2. THE MATHEMATICAL MODEL AND THE NUMERICAL SOLUTION

The mathematical model consists of conservation governing equations and constitutive laws that provide closure relations for the model. The basic formulation adopted here follows the two-phase fluid dynamics model presented in the text by Kuo (1990). The approach assumes that there are two distinct continua, one for gas and one for solid particles, each moving at its own velocity through its own control volume. The sum of these two volumes represents an average mixture volume. Furthermore, particles in their own control volume are assumed monodisperse and they are moving with the same velocity. With these assumptions, distinct equations for continuity, momentum and energy are written for each phase. The interaction effects between the two phases are accounted as the source terms on the right hand side of the governing equation. The following is a short description of the two phase flow model used in our study, with conservation equations written in Eulerian form for two dimensional flow in Cartesian coordinates.

Conservation Equations

Continuity of gaseous phase:

$$\frac{\partial \rho_1}{\partial t} + \frac{\partial(\rho_1 u_g)}{\partial x} + \frac{\partial(\rho_1 v_g)}{\partial y} = \Gamma; \tag{2.1}$$

Continuity of solid particle phase:

$$\frac{\partial \rho_2}{\partial t} + \frac{\partial(\rho_2 u_p)}{\partial x} + \frac{\partial(\rho_2 v_p)}{\partial y} = -\Gamma; \tag{2.2}$$

Conservation of momentum of gaseous phase in x-direction:

$$\frac{\partial(\rho_1 u_g)}{\partial t} + \frac{\partial(\rho_1 u_g^2 + \phi p_g)}{\partial x} + \frac{\partial(\rho_1 u_g v_g)}{\partial y} = -F_c + \Gamma u_p; \tag{2.3}$$

Conservation of momentum of solid particle phase in y-direction:

$$\frac{\partial(\rho_1 v_g)}{\partial t} + \frac{\partial(\rho_1 u_g v_g)}{\partial x} + \frac{\partial(\rho_1 v_g^2 + \phi p_g)}{\partial y} = -F_y + \Gamma v_p; \tag{2.4}$$

Conservation of momentum of solid particle phase in x-direction:

$$\frac{\partial(\rho_2 u_p)}{\partial t} + \frac{\partial(\rho_2 u_p^2)}{\partial x} + \frac{\partial(\rho_2 v_p u_p)}{\partial y} = F_x - \Gamma u_p; \tag{2.5}$$

Conservation of momentum of solid particle phase in y-direction:

$$\frac{\partial(\rho_2 v_p)}{\partial t} + \frac{\partial(\rho_2 u_p v_p)}{\partial x} + \frac{\partial(\rho_2 v_p^2)}{\partial y} = F_y - \Gamma v_p; \tag{2.6}$$

Conservation of energy of gas phase:

$$\frac{\partial(\rho_1 E_{gT})}{\partial t} + \frac{\partial(\rho_1 u_g E_{gT} + u_g \phi p_g)}{\partial x} + \frac{\partial(\rho_1 v_g E_{gT} + v_g \phi p_g)}{\partial y} =$$

$$\Gamma\left(\frac{u_p^2 + v_p^2}{2} + E_{chem} + C_s \bar{T}_p\right) - \left(F_x u_p + F_y v_p\right) = \dot{Q}; \tag{2.7}$$

Conservation of energy of solid particle phase:

$$\frac{\partial(\rho_2 E_{pT})}{\partial t} + \frac{\partial(\rho_2 E_{pT} u_p)}{\partial x} + \frac{\partial}{\partial y}(\rho_2 E_{pt} v p = \dot{Q} + (F_x v_p + F_y v_p)$$

$$-\Gamma\left(\frac{u_p^2 + v_p^2}{2} + E_{chem} + C_s \bar{T}_p\right); \tag{2.8}$$

Conservation of number density of solid particle:

$$\frac{\partial N_p}{\partial T} + \frac{\partial(N_p u_p)}{\partial x} + \frac{\partial(N_p v_p)}{\partial y} = 0. \tag{2.9}$$

In the above equations, $\phi = 1 - \frac{N_p M_p}{\rho_p}$, $\rho_1 = \phi \rho_g$, $\rho_2 = (1 - \phi)\rho_p$, where N_p and M_p are the number density of particles and mass of each particle, respectively, and ρ_g and ρ_p are the material density of gas and particle densities, respectively. u_g, v_g, p_g are gas phase x-velocity, y-velocity and pressure, respectively; u_p, v_p, $\bar{T}_p$, are x-velocity, y-velocity and average particle temperature, respectively. C_s is the solid particle specific heat, and $E_{chem} = E_{comb} - E_{evap}$, where E_{comb} is heat of combustion and E_{evap} is heat of evaporation. Γ is the rate of phase change from solid to gas and Q is heat transfer between the two phases: F_x, F_y are drag force between the two phases in x and y directions, respectively.

Equations (2.2) and (2.9) are linked through the relation $\rho_2 = N_p M_p$. In the case of a reactive solid phase, M_p decreases due to combustion. The mass of a single particle at any point can be obtained from $M_p = \rho_2(x, y)/N_p(x, y)$, and the diameter of a particle at any spatial location is $D(x, y) = [6M_p(x, y)/\pi\rho_p]1/3$. The total internal energy of gaseous phase

$$E_{gT} = E_g + \frac{1}{2}(u_g^2 + v_g^2) \quad \text{and} \quad E_g = E_g(p_g, \rho_g) \tag{2.10}$$

where $E_g(\rho_g, \rho_g)$ is the equation-of-state for gas phase, which will be discussed later.

The total internal energy of solid particle phase is

$$E_{pT} = E_p + \frac{1}{2}(u_p^2 + v_p^2) \quad \text{and} \quad E_p = E_{comb} + C_s \bar{T}_p. \tag{2.1}$$

In order to close the above system of conservation equations, it is necessary to define certain criteria and interaction laws between the two phases, which include mass generation rate, Γ, drag force between particles and gas, F_x, F_y and the interphase heat transfer rate $\dot{Q}$. The model for particle and gas interaction and particle combustion that results in the constitutive relation for the conservation equations, is explained in detail in the next subsection.

Model for a Particle Gas Interaction and Combustion

Presently the physics of the energy release mechanisms in solid particles/air mixtures is not clearly understood. This can be attributed to the obvious difficulties of making a direct non-obtrusive measurement in the optically thick environment typical for this system. In the experimental and theoretical work done for the grain dust detonation conditions (Kauffman *et al.*, (1979), it was demonstrated that the volatile components released by the particle heated behind the shock front play a major role in determining the detonability limits of the mixture. Eidelman and Burcat (1981) successfully applied a combination of fast evaporation and aerodynamic shattering mechanisms to simulate a two-phase detonation process.

The chemical processes of a single particle combustion, which mainly occur in the gaseous phase, are significantly faster than the physical processes of particle gasification or disintegration. Thus, in the multi-phase mixtures, the rate of energy release will be mostly determined by physics of particle disintegration. It is very difficult to describe the details of particle disintegration in the complex environment prevalent behind the shock or detonation wave. For example, Reinecke and Waldman (1975) defined five different disintegration regimes for a relatively simple environment of water droplets passing through a weak shock. Fortunately, in most cases of multi-phase detonation, only the main features of the particle disintegration dynamics need to be captured to describe the phenomena. For example, Eidelman and Burcat (1980) used simple models for particle evaporation and shattering to obtain simulation results that compared very favorably with experimental data. Because of our inability to resolve the particle disintegration problem in all its complexity, the validation of the model against known experimental data is essential.

In this paper we consider solid particles consisting of explosive material. Explosive material contains fuel and oxidizer in a passive state at low temperature; however, when the temperature rises the fuel and oxidizer react, leading to detonation or combustion. The initiation for explosives will occur at a relatively low temperature. For example, TNT will detonate when heated to the temperature of 570°C. Only particles larger than a critical detonation size can detonate directly when initiated by a shock wave. We consider here particles smaller than 4mm in diameter that will not detonate when heated, but will burn when the temperature on the particle surface reaches a critical value. Since the heat conduction inside the explosive material is relatively slow, the process of particle heating needs to be resolved in detail. Our simulations numerically solve the temperature field in the particles at every time step of numerical integration of the global conservation equations. The explosive particle combustion model examined in this paper assumes that the fraction of the particle that reaches the critical temperature will burn instantaneously. Energy transfer by convection and conduction is simulated by solving the unsteady heat

conduction equation in each computational cell at each time step. Assuming a particle's temperature T_p to be a function of time and radial position only, the unsteady heat conduction equation may be transformed to:

$$\frac{d^2w}{dr^2} = \frac{1}{\alpha}\frac{dw}{dt}, \tag{2.12}$$

subject to the boundary conditions:

$$w = 0 \; at \; r = 0, \; t > 0$$

$$k\frac{dw}{dr} = (h - \frac{1}{R})w = hRT_g \; at \; r = R, t > 0 \tag{2.13}$$

where:

$w(r,t)$	=	$rT_p(r,t)$
r	=	radial position
T(r,t)	=	temperature
R	=	partial radius
T_g	=	temperature of surrounding gas
k	=	thermal conductivity of particle
h	=	convective heat transfer coefficient.

The Nusselt number, used to find h, is given by an empirical relation given by Drake (1961). The gas viscosity is found from Sutherland's Law. The gas thermal conductivity is calculated by assuming a constant Prandtl number. Lastly, the boiling temperature at a given pressure is found from the Clapeyron-Clausius equation under the assumptions of: 1) constant latent enthalpy of phase change, 2) the vapor obeys the ideal equation-of-state, and 3) the specific volume of the solid/liquid is negligible compared to that of the vapor. A critical temperature is also employed to serve as an upper limit to the boiling point, regardless of pressure.

Equation (2.12) with boundary condition (2.13) can be numerically integrated using either implicit or explicit schemes, which will be explained later.

Knowledge of the particle temperature profile also allows us to determine, Γ, the rate of phase change from solid particle to gas. Once any point at a radial location $0 \leq r \leq R$ has a temperature exceeding the boiling temperature, the entire mass between r and R is transferred to the gas phase in one time step. In so doing, an energy equal to the product of the mass lost and the particle combustion of heat minus heat of evaporation energy is transferred from the particle to the gas.

The interphase drag forces (Fx, Fy) are determined from the experimental drag for a sphere, as presented by Schlichting (1983).

$$F_x = \left(\frac{\pi}{8}\right) N_p \rho_g C_D |\mathbf{V_g} - \mathbf{V_p}|(\mathrm{u_g} - \mathrm{u_p})\mathrm{R}^2 \tag{2.14}$$

where

$$C_D = \begin{cases} \frac{24}{Re}\left(1 + \frac{Re^{2/3}}{6}\right) & for \; Re < 1000; \\ 0.44 & for \; Re > 1000. \end{cases} \tag{2.15}$$

and $Re = \frac{2R|V - V_p|}{\mu_g}$, R is the radius of the particle and μ_g is gas viscosity at a temperature of $T_{film} = \frac{1}{2}(T_g + \bar{T}_p)$. Similarly, the formula for F_y is

$$F_y = \frac{\pi}{8} N_p \rho_g C_D |v_g - v_p| (v_g - v_p) R^2. \tag{2.16}$$

Equation of-State for Detonation Products

To close the system of governing equations, one needs a constitutive relation between density, pressure, temperature, and energy for gas phase, which is an equation-of-state. This study uses the Becker-Kistiakowsky-Wilson (BKW) equation-of-state (cf. Cowan and Fickett, 1956; Mader, 1979), which is,

$$p_g V_g / \bar{R} T_g = 1 + x e^{bx}. \tag{2.17}$$

where V_g = volume of gas phase
p_g = pressure of gas phase
T_g = temperature of gas phase
$\bar{R}$ = universal gas constant
$x = k / F_g (T + \Theta)^a$
$k = K \sum_i X_i k_i$

with empirical constants a, b, K, Θ and k_i. The constants k_i, one for each molecular species, are co-volumes. The co-volumes are multiplied by their mole fraction of species, X_i, and are added to find an effective volume for a mixture. For a particular explosive, if we know the composition of detonation products a, b, Θ, K, and all k_i's can be found in the book by Mader (1979).

The internal energy is determined by thermodynamics relation

$$\left(\frac{\partial E_g}{\partial V_g}\right)_T = T_g \left(\frac{\partial p_g}{\partial T_g}\right)_V - p_g. \tag{2.18}$$

Integration of this equation for a fixed composition of the detonation products will allow us to calculate the energy of the detonation products as a function of temperature and volume. The thermodynamic properties as functions of temperature were calculated for each component from the NASA tables compiled by Gordon and McBride (1976).

The BKW equation-of-state is the most used and well calibrated of those equations-of-state used to calculate the properties of detonation products. The detailed discussion and review of the BKW equation-of-state can be found in the literature (cf. Cowan and Fickett, 1956; Mader, 1979).

Numerical Method of Solutions

The system of partial differential equations described in the previous paragraph is integrated numerically. Equations (2.1)—(2.9) can be written in the following vector form:

$$\frac{\partial \Phi}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = \Omega. \tag{2.19}$$

In order to numerically solve this equation, an operator time-splitting technique is used. Assuming that all flow variables are known at a given time, we can calculate its advancement in time by splitting the integration into two stages.

In the first stage, the conservative part of Eq. (2.19) is solved:

$$\frac{\partial \Phi}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0. \tag{2.20}$$

The Second Order Godunov method is used for the integration of the subsystem of equations describing the gaseous phase flow. The method is well documented in the literature (cf. Eidelman *et al.*, 1984; Colella, 1985; Colella and Glaz, 1985). In the following we will elaborate only some specifics of application of the method with BKW equation-of-state to simulate detonation product.

The physical system under study will have concentrations of solid explosive particle ranging from 1000 kg/m^3 near the ground to 0.75 kg/m^3 in the cloud. Detonation of this mixture will create detonation products with effective γ ranging from 3 to 1.1. To describe the flow of detonation products, we use the BKW equation-of-state described previously. Since the Second Order Godunov method uses primitive variables to calculate Riemann problems at the edges of the cells, its implementation for non-ideal EOS is difficult. In our simulations, we have resolved this problem by involving a local parameterization of EOS and by using direct and inverse equations-of-state. After integrating a system of gas conservation laws, we use the direct BKW equation-of-state to calculate pressure, gamma, and temperature as functions of thermal energy, density, and mixture composition. After this step, we have a complete set of parameters allowing calculation of the fluxes obtained from solving the Riemann problem (Colella and Glaz, 1985). The "inverse," EOS calculates internal energy as a function of density and pressure. In our code we use the "inverse" EOS to calculate the fluxes of conserved variables after calculation of the flux from Riemann problem of primitive variables.

The subsystem of equations describing the particle phase flow is integrated using a simple finite difference upwind scheme. This is done because there is no shock in the particle phase and the upwind scheme leads to a robust and accurate integration scheme.

In the second stage, the source term is added and the following equation is solved:

$$\frac{\partial \Phi}{\partial t} = \Omega. \tag{2.21}$$

To integrate this equation in time, we need to obtain Ω as a function of Φ. To do this, we first solve the particle heat conduction and heat transfer equation (2.12) with a boundary condition (2.13) that gives the temperature distribution as a function of particle radius and time using a local particle grid. Since the particle radius, R, will become very small due to evaporation, the implicit Crank-Nicolson algorithm is used because of its stability properties and its second order temporal and spatial accuracy. Using the Crank-Nicolson scheme to predict the particle temperature profiles at times t_1 and t_2 permits easy calculation of the total energy exchange, Q, between t_1 and t_2, due to convection and conduction. Knowing the temperature distribution inside the particle, we can calculate gas generation rate Γ, drag force F_x, F_y, and heat exchange Q, between two phases and hence, Ω of Eq. (2.21). After obtaining the source term, we can integrate Eq. (2.21) by an explicit scheme.

For the multiphase system under study, $\Delta_x = \Delta_y = 1mm$ was used to allow explicit integration of the gasdynamic and physical processes of evaporation and heat release. When a mismatch occurred between the physical and gasdynamical characteristic times, the time step was adjusted by some fraction to assure stability. However, the resulting time step was not significantly smaller than that calculated by CFL criteria. For larger cell sizes, this approach will be impractical.

The numerical method is implemented in a code named MPHASE, which is fully vectorized and supported by number of graphics and diagnostics codes.

Table I.
One Dimensional Validation Result

D[m/sec]—Detonation wave velocity,
P_{CJ}[Pa]—Pressure at Chapman-Jouguet Point
P_p[Pa]—Peak pressure: ρ_p[kg/m^3]—Peak density

RDX Density (kg/m^3)	Parameters	Present Calculation	Expt'l Ref. 1	Tiger Calculation Ref. 2	BKW Calculation Ref. 1	Soviet Experiments Ref. 3
1000 kg/m^3	D	6155	5981		6128	
	P_{CJ}	1.220×10^{10}			1.08×10^{10}	1.00×10^{10}
	P_p	2.57×10^{10}				
	ρ_p	1936				
860 kg/m^3	D	6031		5900		
	P_{CJ}	0.986×10^{10}		0.88×10^{10}		0.82×10^{10}
	P_p	1.95×10^{10}				
	ρ_p	1722				
466 kg/m^3	D	4800		4500		
	P_{CJ}	0.379×10^{10}		0.30×10^{10}	0.3×10^{10}	
	P_p	0.625×10^{10}				
	ρ_p	924				
250 kg/m^3	D	4049		3600		
	P_{CJ}	0.2478×10^{10}		0.13×10^{10}		
	P_p	0.4538×10^{10}				
	ρ_p	552				
100 kg/m^3	D	3495				
	P_{CJ}	0.5013×10^{9}				
	P_p	0.7658×10^{9}				
	ρ_p	220				
0.75 kg/m^3	D	1622	1410*	1870*		
	P_{CJ}	0.25×10^{7}	0.284×10^{7}*	0.26×10^{7}*		
	P_p	0.484×10^{7}				
	ρ_p	8				

Ref. 1—Mader, C., "Numerical Modeling of Detonation," (University of California Press, Ltd., 1979), p. 47.

Ref. 2—Wiedermann, A., "An Evaluation of Bimodal Layer Loading Effects," IITRI Report, Feb., 1990.

Ref. 3—Stanukovitch, K.P., "Physics of Explosion" (in Russian), Nauka, 1975.

3. RESULTS

Model Validation for a One Dimensional Detonation Wave Problem

The main advantage of our particle combustion model is its description of the detonation phenomenology for a wide range of explosive particle sizes and densities. We will demonstrate this capability on a set of one dimensional test problems. For these test problems we have simulated the initiation and propagation of the detonation waves in a shock tube-like setting, where the explosive particles are distributed uniformly through the shock tube volume.

Results of these simulations are summarized in Table I, which shows detonation wave velocity, peak pressure, and peak density given as a function of the average density of the

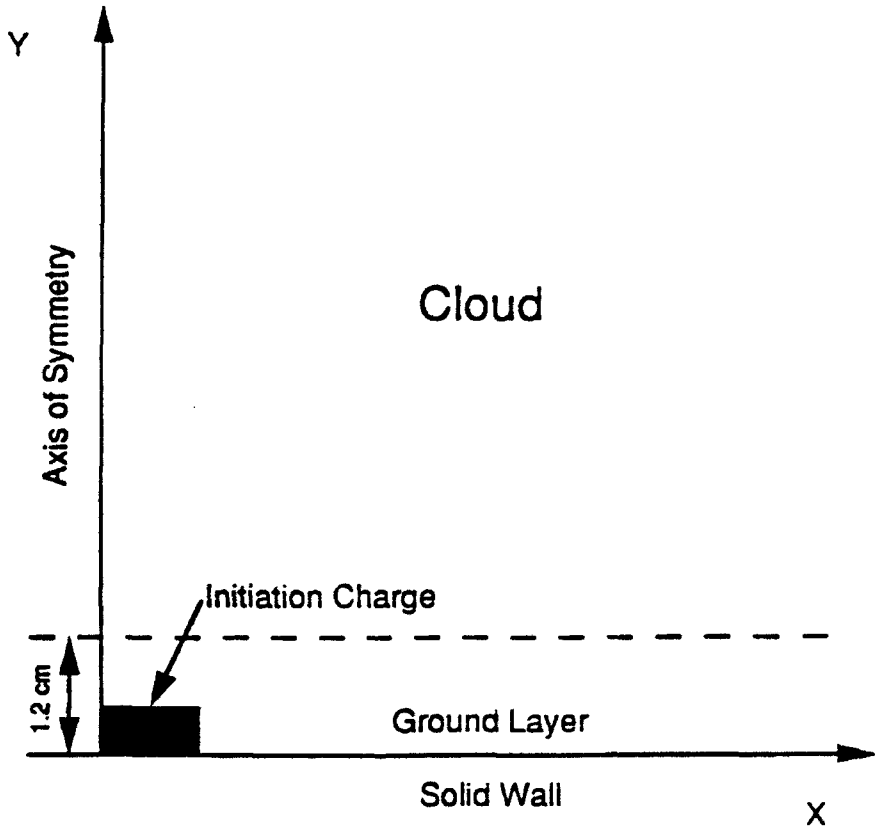

FIGURE 1 Computational domain and boundary conditions.

solid explosive. Here the explosive two-phase mixture is composed from RDX particle and air, where RDX particle concentration varies from 0.75 kg/m^3 to 1000 kg/m^3. This concentration variation covers the whole range of solid explosive concentrations of interest to our problem. The simulations performed with the MPHASE code were compared with the experimental results (Mader, 1979; Stanukovitch, 1975), and calculations were done with the TIGER code presented by Wiedremann (1990).

From Table I, it is clear that our simulation results compare favorably with other simulation results and experimental data. The maximum deviation between our results and referenced results is no greater than 15% for the entire range of explosives densities. Considering that our results were obtained with a single model for particle combustion applied to the extreme range of densities, our model gives an excellent prediction of the detonation wave parameters.

Two Dimensional Simulation Results

Figure 1 shows a setup for a typical two dimensional simulation. Here the computational domain is 25cm × 25cm. The explosive powder density is distributed according to the 4th power law of vertical distance, starting from the ground where the density is 800 kg/m^3, and rising to 1.2cm, where the density is 0.75 kg/m^3. From this point to 25cm height, the density is constant and equal to 0.75 kg/m3. The density distribution in the

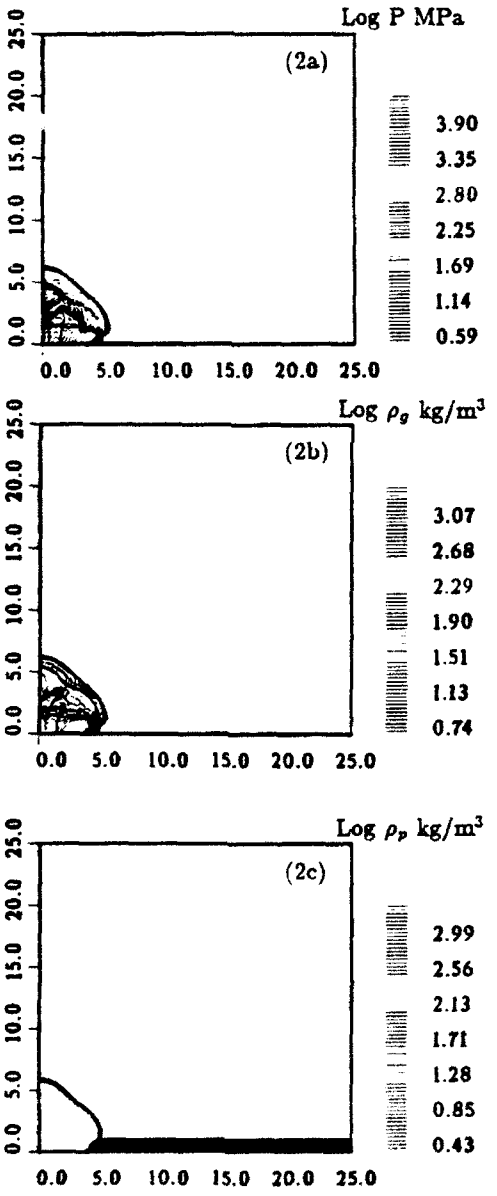

FIGURE 2 *Fourth power distribution of particle density in the layer.* The maximum density in the layer is 800 kg/m^3. (2a), (2b), and (2c) are gas pressure, gas density, and particle density at 12 μsec, respectively. See COLOR PLATE IV.

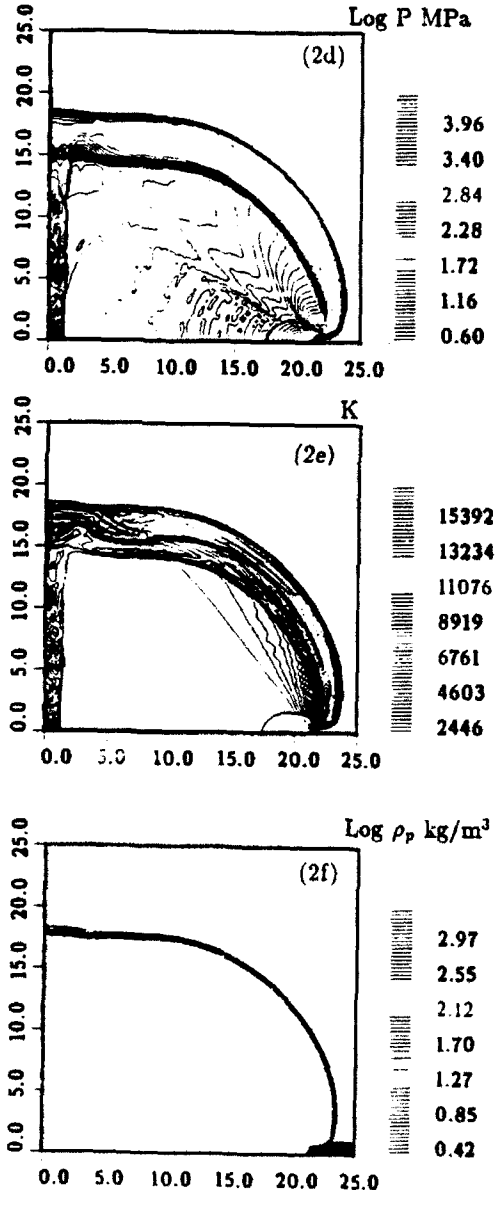

FIGURE 2 (Continued) (2d), (2e), and (2f) are gas pressure, temperature, and particle density at 55 μsec, respectively. See also COLOR PLATE IV.

direction of the "x" axis is uniform. The boundary conditions for the computational domain shown in Fig. 1 are specified as follows: solid wall along the "x" axis; symmetry conditions along the "y" axis; supersonic outflow for upper boundary and at the right of the computational domain. The mixture consists of RDX powder and air at ambient conditions and it is assumed to be quiescent at the time of initiation.

The simulation starts at t = 0 when the mixture is initiated at the lower left corner of the computational domain by an initiating charge, as shown in Fig. 1. The initiating charge is 6 mm × 10 mm, with pressure of 4 GPa and density of 450 kg/m^3. The energy released by the initiating explosion leads to formation of the detonation wave propagating through the multiphase media. Figure 2a shows pressure contours for the propagating detonation wave at the time of t = 12 μsec after initiation. Here the pressure contour levels are shown on logarithmic scale in MPa. The maximum pressure value of 7940 MPa is observed in the layer of condensed explosive located near the ground. The pressure in the layer is two to three orders of magnitude higher than pressure behind the detonation wave in the 0.75 kg/m^3 RDX cloud and air located above the distance of 1.2cm from the ground. Figure 2a demonstrates that the detonation wave in the cloud is overdriven, since the pressure behind the shock continuously rises and reaches its maximum in the layer. From this figure, we also observe that the overdriven wave propagates faster in the cloud than in the layer. This is explained by the fact that it is easier to compress air that is very lightly loaded with particles and located above the ground layer, than it is to compress air heavily loaded with a particle mixture near the ground. It is interesting to note a discontinuous pressure change between the yellow contours and the light blue and green contours behind the detonation front. This discontinuity is over-emphasized by our presentation of contour lines on the logarithmic scale; however, further examination of our simulation results indicates this feature is real and is similar in nature to barrel shocks observed for strong jets.

In Fig. 2b, gas phase density contours are shown for the time t = 12 μsec. Here the contour lines are distributed on logarithmic scale. The main features of the shock wave structure are very similar to those observed in the pressure contours figure. Here we see that a jet of high density gases reflects from the center of symmetry axis, creating a contact discontinuity that we will observe at later times. The barrel shock is clearly visible in this figure. In Fig. 2c, the particle density contour plots are shown for t = 12 μsec. The contour levels in Fig. 2c are given on the logarithmic scale and the initial deposition of the explosive material in the ground layer of the computational domain can be clearly observed. The black contour lines delineate the beginning and the end of the reaction zone in the cloud. To the left of these contours lies an area with combustion products and to the right unburned particles in the cloud. Here we can see that the reaction zone length is of the order of 1cm.

Figure 2d shows pressure contours for the same simulation for the time t = 55 μsec just before the detonation wave leaves the computational domain. In this figure we see that the global structure of the wave did change slightly from Fig. 2a. We observe that the barrel shock wave is fully developed and has a half ellipse shape. The detonation wave in the cloud is still overdriven; however, part of the shock wave front that propagates vertically becomes weaker as it gets further away from the detonation front in the layer. In Fig. 2e, gas temperature contours are shown at t = 55 μsec. In this case, it is interesting to note that the highest temperatures are observed behind the front of the overdriven cloud detonation wave in immediate vicinity of the layer's upper strata. Very high temperatures in this region can be explained by the high pressure generated from the detonation of the explosive material in the layer and by relatively low density of cloud strata in the layer's immediate vicinity. Here, as in the pressure contours graph, the area of barrel shock can be clearly identified.

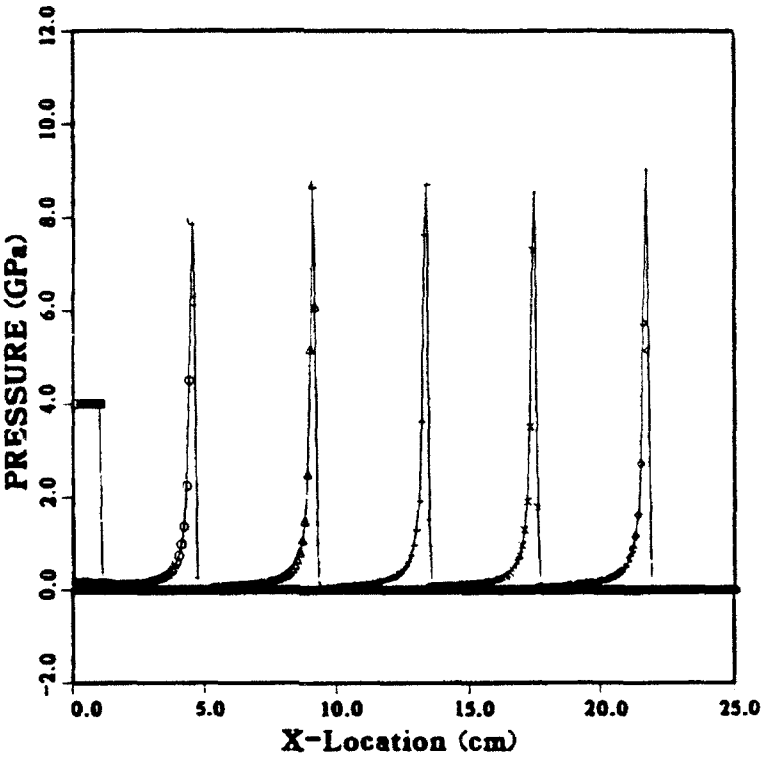

FIGURE 3 History of pressure distribution on the ground from initiation to steady detonation: □ - 0 μsec, o - 12 μsec, △ - 24 μsec, + - 34 μsec, x - 44 μsec and ◇ - 55 μsec.

We also observe in Fig. 2 a clear development of two detonation fronts, one moving vertically in the cloud and another moving horizontally in the layer. Because the energy density of the explosive particle in the layer is about three orders of magnitude larger than it is in the cloud, the vertical parts of the front represent an overdriven detonation wave in the cloud. Even though the vertical front has slowed down compared with the horizontal front, its speed and parameters far exceed those typical for detonation waves in a cloud. In fact, the self-sustained detonation regime in the cloud will develop at the distance of about three meters from the layer. The area of the front close to the detonation wave in the layer will remain hot and overdriven, since it is located very close to the detonation front in the layer. In Fig. 2f, particle density contours are shown on a logarithmic scale. We can clearly observe the reaction zone delineated by black contour lines. In this case, the reaction zone length in the cloud is about 1cm. Consistent with the gradual transition from overdriven to self-sustained detonation, the reaction zone length is larger for the vertical part of the detonation front. The detonation wave velocity observed in our simulation is approximately 4048 m/sec, which is significantly lower than the detonation wave velocity observed in RDX with a density of 860 kg/m^3 (see Table I), which is the highest density in the ground layer. This can be explained by a high gradient of particle density distribution in the layer, where the density drops rapidly from 800 kg/m^3 at the bottom of the layer to 0.75 kg/m^3 at the top strata of the layer at 12 mm above the ground.

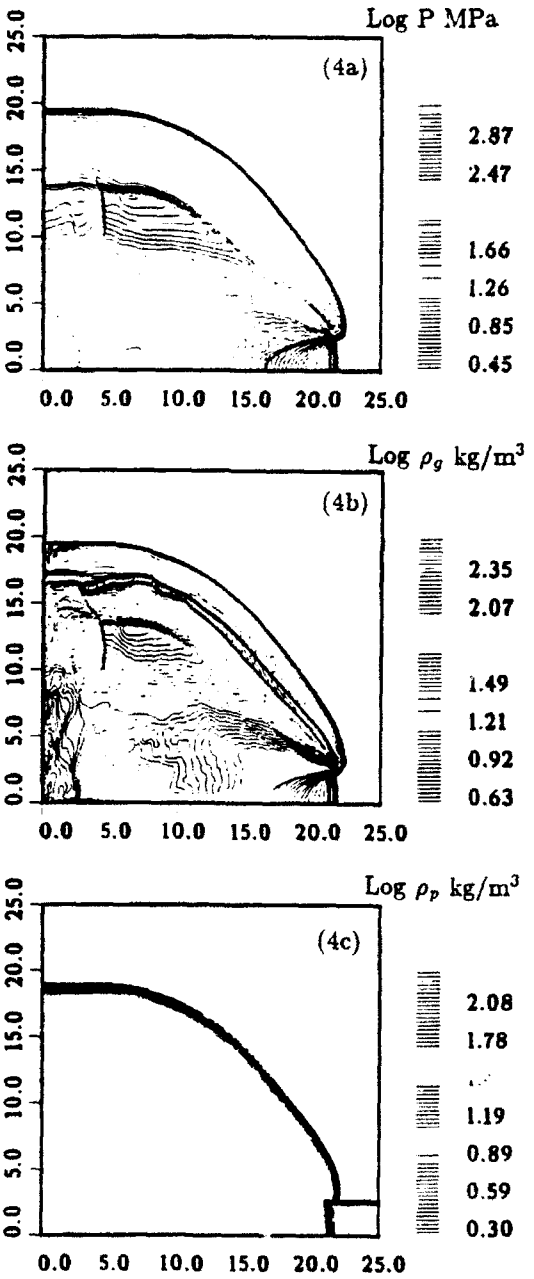

FIGURE 4 2.5 cm thick layer at constant density of 100 kg/m^3. Density in the cloud is 0.75 kg/m^3. (4a), (4b), and (4c) are gas pressure, gas density, and particle density at 66 μsec, respectively. See COLOR PLATE V.

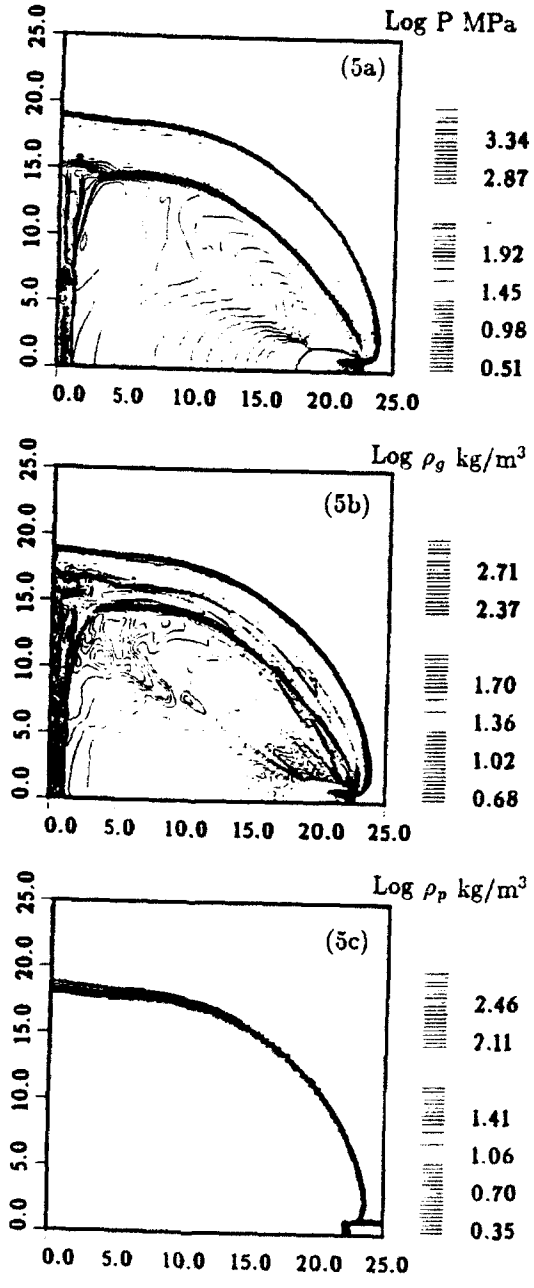

FIGURE 5 1.2 cm thick particle layer at constant density of 250 kg/m^3. Particle density in the cloud is 0.75 kg/m^3. (5a), (5b), (5c) are gas pressure, gas density, and particle density at 65 μsec, respectively. See COLOR PLATE VI.

To show the transient process from initiation to steady-state detonation, we plot the pressure-distance profiles at six separate times after ignition (Fig. 3). Here the pressure is taken on the ground. Examining the profiles, we observe that the steady detonation is reached after 10cm. For each profile, we see that the pressure distribution is characterized by a strong detonation front followed by a fast expansion wave because of lateral expansion.

To further explore properties and phenomenology of the detonation waves propagating in the layer/cloud systems, we simulated additional cases in which explosive powder density distribution was different from the case reported above, although total weight of particle per unit area remained the same.

In Fig. 4, results are shown for the case of a uniform 2.5 cm thick layer of RDX with density of 100 kg/m^3, and a 0.75 kg/m^3 cloud initiated under the same conditions as in the previous example. Figures 4a, 4b, and 4c show pressure, gas density, and particle density contour plots at t = 66 μsec. Here we observe that because the layer has much less density than the case reported above, the precursor effect of the detonation wave in the cloud preceding the wave in the layer is less pronounced. We also observe a significant difference in the shape of the strong contact discontinuity in the region of the shock front close to the layer. In Fig. 4b, we can clearly distinguish two contact surfaces, one between condensed explosive detonation products in the layer and in the cloud, and another between the detonation products from layer explosive detonation and from cloud particle detonation. We should note that these contact surfaces are over-emphasized by the logarithmic display of the contour plot levels. The maximum pressure observed in this simulation is 955 MPa, which is about one order of magnitude smaller than in the previous simulation. This is consistent with one order of magnitude difference in the maximum density of the ground layer in the two cases. The detonation wave speed (3407 m/sec) for the case presented in Fig. 4, which is only slightly lower than the speed predicted by the one dimensional simulations presented in Table I, reflects the influence of the two dimensional expansion on the detonation wave propagation.

Figure 5 presents results for the case of a uniform density of 250 kg/m^3 in a 1.2 cm ground layer. All other parameters are the same as in the previous two cases. In Figs. 5a, 5b, and 5c, pressure, gas density, and particle density contour plots are shown at the time t = 65 μsec after detonation wave initiation. Here, the detonation wave propagates faster than in the previous cases U = 3660 m/sec. This is about 400 m/sec slower than in the case of fourth power density distribution. Maximum pressure on the ground is 2150 MPa, which is consistent with the increase of powder density in the layer. The basic structure of the detonation front and the contact surfaces is similar to the case of fourth power density distribution.

4. CONCLUSIONS

We presented a mathematical model and numerical solution for the simulation of detonation wave initiation and propagation in multiphase mixtures consisting of solid combustible particles and gas. Using this model, we studied detonations in mixtures of solid RDX particles and air, with the objective of examining the effects of wide variation in particle density distribution on the dynamics and structure of detonation waves. We considered a physical system of solid particle clouds in air where a significant amount of particle can settle on the ground and the particle phase concentrations in the particle/air mixture can range from 0 to 1000 kg/m^3. This range of solid phase densities necessitated development of the model and its numerical implementation for a wide range of particle concentrations. Our validation study has shown good agreement between the simulations and referenced results for the whole range of particle concentrations.

Two dimensional simulations were done for the system of low particle density concentration clouds and ground layers formed by high concentrations of the RDX powder. We examined three cases of ground layer density distribution: a fourth power distribution within 12 mm above ground with a maximum density on the ground of 800 kg/m^3; a uniform 25 mm thick layer with a density of 100 kg/m^3; a 12 mm thick uniform layer with a density of 250 kg/m^3. In all these cases, the weight of condensed phase per unit area was the same, which allowed examination of the effects of the particle density distribution on detonation wave parameters.

In all examined two dimensional cases, the detonation wave in the cloud in the computational domain was significantly overdriven and did not play an important role. We estimated that the self-sustained regime of the detonation wave in the cloud for the examined cloud concentrations can occur only at the distances of 2–3 M above ground. At the same time, the particle density distribution in the layer determines the dynamics of the detonation wave as well as the pressure on the ground.

We observed in all three two dimensional simulations a very distinct shape of the detonation wave front in the vicinity of the layer. In this area, the overdriven detonation in the cloud is preceding the detonation wave in the ground layer. This feature of the detonation front can be explained by the fact that the energy released in the ground layer detonation wave produces a faster propagating shock wave in the dilute cloud than in the ground layer which is heavily loaded with solid particles. However, these structures were not observed experimentally, and more studies are needed to examine their parameters.

The maximum pressure affecting the ground was directly related to the maximum particle density in the lower strata of the layer. However, the detonation front velocity for the fourth power distribution case was considerably lower than calculated for a one dimensional case with 860 kg/m^3 particle density, reflecting the significant effect of two dimensional expansion. Two other cases with 250 kg/m^3 and 100 kg/m^3 maximum densities had detonation wave velocity only slightly lower than the one dimensional simulations of the same RDX/air concentrations. It is interesting to compare the simulation of the fourth power density distribution case and the 250 kg/m^3 case. In both, the same amount of explosive was distributed in the same physical space; however, the parameters of developed detonations were vastly different. Existence of the high density strata at the bottom of the ground layer in the fourth power case significantly increased the maximum pressure at the ground, and produced higher detonation wave velocity.

Using a variable density layer, we can reach a combination of pressure and velocity conditions outside of the Chapmen-Jougett limitations. The range of conditions that can be obtained in the variable density system and its parametrics needs a more systematic study. In this article, we introduced only the mathematical formulation and numerical simulation method validated for the range of conditions of interest. In addition, we have given some examples of the method's application for two dimensional simulations. However, this methodology should be linked to an experimental study for a more in-depth analysis of the phenomenology discussed here.

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Computation of Shock Wave Reflection and Diffraction Over a Semicircular Cylinder in a Dusty Gas

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COMPUTATION OF SHOCK WAVE REFLECTION AND DIFFRACTION OVER A SEMICIRCULAR CYLINDER IN A DUSTY GAS

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Abstract

The unsteady shock wave reflection and diffraction generated by a shock wave propagating over a semicircular cylinder in a dusty gas are studied numerically. The mathematical model is a multi-phase system based on a multi-fluid Eulerian approach. A Second Order Godunov scheme is used to solve the gas phase Euler equations and an upwind scheme is used to solve the particle phase conservation equations on an unstructured adaptive mesh. For the validation of the model, the numerically predicted one dimensional shock wave attenuation is compared with experimental results. Shock wave reflection and diffraction over a semicircular cylinder in a pure gas flow is simulated first to show the excellent agreement between the present computation and the experimental results. For a shock wave reflection and diffraction in a dusty gas, the effects of particle size and particle loading on the flow field are investigated. Gas and particle density contour plots are presented. It has been shown that the shock wave configuration differs remarkably from pure gas flow depending on the particle parameters. The difference is explained as the result of momentum and heat exchange between the two phases.

Introduction

Shock wave propagation into a gas particle suspension medium has attracted great attention in recent years due to its many engineering applications. Some of these applications include blast wave propagating over a dusty surface, exhaust from a solid propellant rocket, and coal or grain dust detonation. Many studies dealing with two phase environment can be found in literature. A general description and theoretical analysis of such flow can be found in review papers by Marble[1] and by Rudinger,[2] and in a book by Soo.[3] Numerical models for dilute gas-particle flows were reviewed by Crown.[4] Numerical studies of gas-particle flow in a solid rocket nozzle can be found in *Refs.* 5 and 6. Miura and Glass [7] theoretically and numerically studied the oblique shock waves in a dusty-gas flow over a wedge. The one-dimensional unsteady structure of shock waves propagating through a gas-particle mixture was investigated both experimentally and numerically by Sommerfeld.[8] Recently, Kim and Chang[9] illustrated a *numerical simulation of shock* wave propagation into a dusty gas and the reflection of the wave from a wedge. Shock wave ignition of different reactive dust is experimentally investigated by Sichel *et al.*[10] and comprehensive model for the structure of dust detonations is also described by Fan and Sichel.[11]

In this paper, we study shock wave reflection and diffraction over a semicircular cylinder in a dusty gas. We numerically simulate the problem of a shock wave initiated in a pure gas section moving into a dusty region and impinging on a semicircular cylinder. We first formulate the compressible two-phase flow on the basis of a Eulerian multi-fluid formulation. We consider the two phases (i.e., gas and particle) to be interpenetrating continua. The dynamics of the flow are governed by conservation equations of each phase and the two phases are coupled by interactive drag force and heat transfer. We solve the system of conservation equations numerically on an unstructured adaptive grid. The objectives of the study are: (a) to solve the two-phase compressible flow field and compare the simulation with available experimental results; (b) to observe and investigate the reflection and diffraction wave patterns when a shock wave propagates over a semicircular cylinder in a dusty gas, with particle radius and loading as parameters.

The outline of this paper is as follows. Section 2 gives a description of the mathematical model and method of numerical solution, including governing conservation equations for two phases, the constitutive laws, the initial and boundary conditions, and particle parameter. A brief outline of numerical schemes and the adaptive unstructured grid is also given. In Section 3, we present our numerical simulation results. We validate our model by comparing a one-dimensional simulation of a shock wave propagating into a dusty gas with available experimental results. We also show the excellent agreement between our two-dimensional gas-only simulation with existing experimental results. Results for reflection and diffraction of shock wave over a semicircular cylinder are given for different particle parameters. Concluding remarks are given in Section 4.

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Mathematical Model and the Numerical Solution

Conservation Equations

The mathematical model consists of conservation governing equations and constitutive laws that provide closure for the model. The basic formulation adopted here follows the gas and dilute particle flow dynamics model presented by Soo.[3] The following assumptions are used during the derivation of governing equations:

(1) The gas is air and is assumed to be ideal gas;

(2) The particles do not undergo a phase change because for particles considered here (sand) phase transition temperature is much higher than the temperatures typical for the simulated cases;

(3) The particles are solid spheres of uniform diameter and have a constant material density;

(4) The volume occupied by the particles is negligible;

(5) The interaction between particles can be ignored;

(6) The only force acting on the particles is drag force and the only heat transfer between the two phases is convection. The weight of the solid particles and their buoyancy force are negligibly small compared to the drag force;

(7) The particles have a constant specific heat and are assumed to have a uniform temperature distribution inside each particle.

Under the above assumptions, distinct equations of continuity, momentum, and energy are written for each phase. The interaction effects between the two phases are listed as the source terms on the righthand side of the governing equation. The two-dimensional unsteady conservation equations for the two phases can be written in the vector form in Cartesian coordinates:

$$\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}=S. \tag{1}$$

Here U is the vector of conservative variables, F and G are fluxes in x and y direction, respectively, and S is the source term for momentum and heat exchange. The definition of these vectors are:

$$U=\begin{vmatrix}\rho\\ \rho u\\ \rho v\\ e\\ \rho_p\\ \rho_p u_p\\ \rho_p v_p\\ e_p\end{vmatrix},\quad F=\begin{vmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ u(e+p)\\ \rho_p u_p\\ \rho_p u_p^2\\ \rho_p u_p v_p\\ u e_p\end{vmatrix},\quad G=\begin{vmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ v(e+p)\\ \rho_p v_p\\ \rho_p u_p v_p\\ \rho_p v_p^2\\ v_p e_p\end{vmatrix},$$

$$S=\begin{vmatrix}0\\ -f_x\\ -f_y\\ -q-u_p f_x-v_p f_y\\ 0\\ f_x\\ f_y\\ q+u_p f_x+v_p f_y\end{vmatrix}$$

where ρ, u, v, and e are gas density, velocities, and energy, respectively; ρ_p, u_p, v_p and e_p are particle density, velocities, and energy, respectively; (f_x, f_y) and q denotes drag force components acting on the particles and heat transfer to the particles, respectively. The gas pressure p is related to ρ, u, v and e for by

$$p=(\gamma-1)[e-0.5\rho(u^2+v^2)] \tag{2}$$

where γ is the specific heat ratio. The gas temperature can be found through the equation-of-state for ideal gas

$$p=\rho RT \tag{3}$$

where R is the gas constant.

The particle temperature T_p is calculated through relation

$$e_p=\rho_p c_p T_p+0.5\rho_p(u_p^2+v_p^2). \tag{4}$$

The source terms on the righthand side of Eq. (1) are momentum and heat exchange between gas and particle phases. If we let r_p and ρ_s be the particle radius and material density, respectively, then the drag forces are

$$\begin{pmatrix}f_x\\ f_y\end{pmatrix}=\frac{3}{8}\frac{\rho_p\rho}{\rho_s r_p}C_d\left[(u-u_p)^2+(v-v_p)^2\right]^{1/2}\begin{bmatrix}(u-u_p)\\ (v-v_p)\end{bmatrix}. \tag{5}$$

The particle drag coefficient C_d depends on relative Reynolds number, Re and relative Mach number, M_r. In the present study, since the relative Mach number is small ($M_r < 0.5$), the effect of M_r on C_d is neglected. The Reynolds number, Re, is based on the relative velocity between the gas and particle phases. After testing the drag coefficients given by Sommerfeld[8] and by Clift *et al.*,[12] the following two were adopted:

$$C_d=\frac{24}{Re}(1+0.15Re^{0.687}) \text{ for } Re<800.$$

and

$$C_d=\frac{24}{Re}(1+0.15Re^{0.687})+\frac{0.42}{1+42500Re^{-1.16}} \quad \text{for } Re>800\ . \tag{6}$$

Here the Reynolds number Re is defined as

$$Re = \frac{2\rho r_p[(u-u_p)^2+(v-v_p)^2]^{1/2}}{\mu} \quad (7)$$

Viscosity, μ, is calculated at film temperature, namely, $T_f = 0.5(T_p + T)$, and the temperature dependency of the viscosity is evaluated according to Sutherland's law

$$\mu = \mu_r \left(\frac{T}{T_r}\right)^{3/2} \frac{T_r + \Phi}{T + \Phi} \quad (8)$$

where μ_r is the dynamic viscosity of the gaseous phase at the reference temperature and Φ is an effective temperature, called the Sutherland constant.

The rate of heat transfer from gaseous phase to the particle phase is given by

$$Q = \frac{3}{2}\frac{\rho_p}{\rho_s}\frac{\mu C_p}{Pr} Nu\,(T - T_p) \quad (9)$$

where $Pr = \mu c_p/k_g$ is the Prandtl number, and c_p and k_g are the specific heat and thermal conductivity of gas, respectively. The Nusselt number Nu is a function of Reynolds number and the Prandtl number as given by Drake[13]

$$Nu = \frac{2r_p h}{R} = 2 + 0.459 Re^{0.55} Pr^{0.33}. \quad (10)$$

Initial and Boundary Conditions

The geometry of the computational domain is shown in Fig. 1. The initial conditions for gas are $\rho_o = 1.2 kg/m^3$ and $p_o = 101.3 kpa$, with a coming shock at x = -0.5. There are no particles from -1.0 $\leq x \leq$ 0.0. From $x \geq$ 0.0, particles are initially in thermal and kinematic equilibrium with surrounding gas. The particles that are uniformly distributed in the dusty region have the following parameters for different test problems:

Mass loading, ρ_p: 0.25 kg/m^3, 0.76 kg/m^3;
Mass material density, ρ_s: 2500 kg/m^3;
Particle radii, r_p: 10 μm, 25 μm, 50 μm;
Specific heat, c_s: 766 $J/kg/K$.

The lower boundary and cylinder surface are solid walls and assumed adiabatic and impermeable. A reflecting boundary condition is assumed for both the gas and particle phase. Particles are assumed to experience a perfect elastic collision with the wall and reflect from the wall. The right and upper boundaries are open boundaries where a nonreflection boundary condition is used for the gas phase and a zero normal gradient condition is used for particle phase.

Numerical Method of Solutions

The system of partial differential equations described in the previous paragraph is integrated numerically. Equation (1) is repeated here:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = S. \quad (1)$$

In order to solve this equation numerically, an operator time-splitting technique is used. Assuming that all flow variables are known at a given time, we can calculate its advancement in time by splitting the integration into two stages.

In the first stage, the conservative part of Eq. (1) is solved:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0. \quad (11)$$

The Second Order Godunov method is used for the integration of the subsystem of equations describing the flow of the gaseous phase (first four components of Eq. (1)). The method is well documented in literature.[14,15,16] The subsystem of equations describing the particle phase flow is integrated using a simple first order finite difference upwind scheme[17]. This is done because there is no shock in the particle phase and the upwind scheme leads to a robust and accurate integration scheme.

In the second stage, the source term is added and the following equation is solved:

$$\frac{\partial U}{\partial t} = S. \quad (12)$$

To integrate this equation in time, we need to obtain S as a function of U. We calculate S through Eqs. (5) to (10).

In order to produce a solution of the high spatial accuracy at minimal computational cost, an unstructured triangular grid with adaptive procedure is used. The adaptive procedure will automatically enrich the mesh by adding points in the high gradient (or high flow activity) region of the flow field and by removing points (coarsening mesh) where they are not needed. The dynamic nature of mesh enrichment is shown in Fig. 4 for three different time frames. One can see that a very fine mesh is generated around shock fronts and other steep density gradient regions.

Results

Model Validation for One-Dimensional Shock Wave Propagation in Dusty Gas

To test the momentum and heat exchange mechanism for the current two-phase model, we first simulate a one-dimensional problem of a normal shock wave propagating into a dusty gas. We numerically simulate the experiments conducted by Sommerfeld.[8] In the experiments, small glass spherical particles of material density $\rho_s = 2500 kg/m^3$, specific heat capacity $c_s = 766 J/kg/K$, and average diameter of 27 μm

were used as the suspension particle phase. The incoming shock Mach number M_s and particle loading ratio $\eta = \rho_p/\rho$, are two varying parameters. The experimental results and our numerical simulation results of shock Mach number as a function of distance for two test cases are shown in Fig. 2a ($\eta = 0.63, M_s = 1.49$) and Fig. 2b ($\eta = 1.4, M_s = 1.7$) for comparison purposes. It is clear that the agreement between the prediction of shock wave attenuations from our present model and the experimental results is very good.

Two-Dimensional Simulation Results for Pure Gas Flow

To test the accuracy of the two-dimensional computation, we first compute the pure gas flow case of a shock wave reflection and diffraction over a semicircular cylinder. We then compare the simulation with experimental results. Shock wave reflection on a wedge has been extensively studied by many researchers (see e.g., review papers of Ben-Dor and Dewey[18] and Hornung[19]). Shock wave reflection over circular cylinders was numerically simulated by Yang *et al.*[20]. Recently, Glass *et al.*[21] using high order Godunove scheme numerically simulated the shock wave reflection over a half diamind and semicircular cylinder and compared the simulation with experimental results obtained by Kaca.[22]. Figure 3 is a schematic sketch to show four stages of a shock wave reflection over a semicircular cylinder and terminologies which will be used to describe the flow fields. Figures 4a, 4b and 4c show the calculated density contours at three moments in time. When the planar shock wave propagates and encounters the cylinder, it first experiences a head-on collision with the front stagnation point of the semicylinder and then immediately reflects from the first quarter of the cylinder, forming a regular reflection (RR), which is shown in Fig. 4a. The regular reflection consists of two shocks, i.e., the incident shock and reflected shock, both originating from a common point on the cylinder wall. As the shock wave propagates up the cylinder, the angle between the incident shock and the tangent of the cylinder becomes larger and the regular reflection changes into a Mach Reflection (MR) as shown in Fig. 4b. The MR is characterized by three waves, incident shock (I), reflected shock (R), and Mach stem (M). All three shocks intersect at one common point called triple point (T). For Mach reflection, one can further observe both Simple Mach Reflection (SMR) and Complex Mach Reflection (CMR). Later, as the incident shock wave passes over the top of the semicircular cylinder, it experiences a rarefaction on the back side of the cylinder. The shock wave system grows upward and rightward with a curved Mach stem and forms a slipline(S) or a contact discontinuity (CD) as shown in Fig. 4c. In Figs. 5a and 5b, the interferogram from the experiment[22] and density contours from the present simulation are compared for the same flow condition and same time. Note that the density levels are normalized by the ambient gas density. Fig. 5. As one can see from Fig. 5, the results show an excellent quantitative as well as qualitative agreement between the numerical simulation and experimental results.

Two-Dimensional Simulation Results of Two-Phase Flow

The basic setup for the two-phase simulation is shown in Fig. 1. Here the planar shock with $Ms = 2.8$ propagates into an area of a dusty gas and impinges on a semicircular cylinder. The interface between pure air and dusty air is located at $x = 0.0$ of the computational domain. The area of the dusty air contains a semicylinder with a radius of $1m$. The size of the computational domain, initial parameters of the gas, parameters of the incoming shock, size of the semicylinder and its location in the computational domain, are the same as in the reflection and diffraction simulation presented in the previous section.

The main objective of this set of simulations is to study the effects of particle size and particle loading on the parameters of the reflected and diffracted shock waves. It is also valuable to study the dynamics of particle media, since it is extremely difficult to observe these interactions experimentally in an optically thick dusty gas.

The first set of simulation results is shown for the case with dust parameters $r_p = 10\mu m$ and $\rho_p = 0.25\ kg/m^3$. The gas parameters and the parameters of the incoming shock wave are the same as in the pure gas case presented above. In Figs. 6a and 6b, particle density contours and gas density contours are shown at the stage when the incident shock wave has reached the top of the semicylinder. At this stage, the largest difference of velocity and temperature between the two phases exists and the nonequilibrium between the two phases causes extensive heat and momentum exchange between particles and the gas. The presence of the particles causes a widening of the shock that is more noticeable for the incident shock. Also, an additional contour line is observed at the dusty gas/pure gas interface. Comparing gas density for pure gas flow field shown in Fig. 4b and the dusty gas density of Fig. 6b, we see that Mach stem and contact discontinuity resulting from Mach reflection are smeared in the dusty gas flow due to the presence of the particle. The particle density contours depict significant piling up of the dust particles at the leading edge stagnation point of the cylinder.

In Figs. 6c and 6d, the particle density and gas density contours are shown at the stage where significant diffraction has taken place and the shock front is

approaching the trailing edge of the cylinder. Further widening of the shock and some smearing of the slip line that originates at the triple point is evident. The particle density contours reveal that the particles were swept by the gas flow to the area of triple point and slip line for the gas flow, leaving a small amount of particles at the leading edge. We should note that this behavior is specific for our problem, where at $t = 0$, the dusty gas area was located at $x = 0$ and there is no influx of the dust from the left boundary. Also in Fig. 6c, we note that the particles reach a distinct local maxima at the distance about 25 cm behind the incident shock front. At this maxima the particle density is 0.86 kg/m^3, which is more than three times the initial particle density. The particle density reaches a maximum value at the location of the gas slip line. We observe a significant accumulation of the particles that have been moved along the slip line by the shear flow. The larger concentration of particles in the vicinity of triple point is, in fact, the remainder of the particles that were swept up with the flow. It is also interesting to observe that an essentially particle-free zone is formed due to the effects of particles slipping over the top of the cylinder and the rarefaction wave behind the cylinder.

To study the influence of particle loading on the dynamics of reflection and diffraction, we have simulated the case with a dust density of $\rho_p = 0.76$, and with $r_p = 10\mu m$. The results for this simulation are shown in Figs. 7a and 7b in the form of particle and gas density contour plots. In Fig. 7a, the particle density contours are shown at the diffraction phase. Here we can observe two local maxima for particles accumulated in the regions along the slip line characteristic for the shock diffraction process. It should be noted here that in our problem the conditions behind the incident shock wave and its structure are in constant flux. At higher loading, dust will have a profound effect on the gasdynamics of reflection and diffraction. Figure 7b shows gas density contours for the reflection stage corresponding to the particle density contours shown in Fig. 7a. We observe from Fig. 7b that the incident shock wave is significantly smeared and the triple point cannot be clearly identified. Because of the widening of the incident shock, the area where the reflected and incident shock join is spread over 50 cm distance. From Fig. 7a, we see that the high density particle region is spread wider than in the previous case, and the particle density reaches its maximum at about 25 cm behind the front. There is a visible maximum in gas density in the area where the reflected shock is interacting with the area of maximum particle density behind the incident shock. A part of the reflected shock front that is moving to the left side of the computational domain is not affected by the dust since it is propagating into an area with little dust concentration. The parameters and structure of this part of the front remain basically the same as in the case of pure gas flow.

To examine the effect of particle size on the reflection-diffraction process, we simulated a case where the particle loading and gas flow conditions are the same as in the previous case with particle density $\rho_p = 0.76$. However, the particle size is $r_p = 50\mu m$. In Figs. 8a and 8b, results for this simulation are illustrated by particle density and gas density contours correspondingly. The particle contour plots depict a significantly wider particle relaxation zone than in the previous case. The longer relaxation zone is caused by the larger inertia of larger particles. The maximum particle density of 2.64 kg/m^3 is reached 50 cm behind the incident shock front. This value is significantly lower than 4.01 kg/m^3 reached behind the shock in calculation with 10 μm particles. Larger particles skip above the apex of the cylinder creating a void where particle density is very small. Also, because of larger particle size, the maxima of particle concentration that has been created by a slip surface of the reflected Mach stem is indistinct. The main reason for this is that the particles do not follow the gas flow as closely as they did in the previous case due to the inertia of large particles. The maximum particle density is reached here at the slip line behind the Mach stem.

Comparing gas density of Fig. 8b to the previous case shown in Fig. 7b, we observe that the slip line behind the curved Mach stem becomes less distinguishable in Fig. 7b. This result is expected, since at fixed particle loading, smaller particles have a larger surface/volume ratio and the larger surface/volume ratio increases momentum and heat exchange between the two phases.

One general comment regarding all three cases presented above: Due to the heat and momentum exchange between the two phases, the shock is decaying as it traverses the cylinder. Ultimately, it will reach a new equilibrium state as suggested by Fig. 2. It should be noted that the shock considered in the previous three cases is still in the process of transition in the gas-particle mixture.

Conclusion

In this paper, numerical study for a two-phase compressible flow is performed for the reflection and diffraction of a shock wave propagating over a semicircular cylinder in a dusty gas. The following conclusions can be made:

(1) The validation study for a one-dimensional shock wave propagating in a dusty gas shows a good agreement between the prediction of our model and the results of the experiment;

(2) For a two-dimensional gas-only flow, numerical results agree well with existing experimental data quali-

tatively and quantitatively, indicating that the gas phase is accurately simulated by the adaptive grid technique;

(3) Particles in the gas can have a profound effect on the shock wave reflection and diffraction pattern. which is a function of particle size and loading. The lesser the particle loading, the less the influence of particle on the flow field:

(4) In the three simulation cases, there is a particle accumulation behind the "back shoulder" of the semi-circular cylinder due to the effect of particle inertia and gas rarefaction wave;

(5) For different particle size at fixed particle loading, the larger particle will have a longer relaxation zone and less accumulation at "back shoulder" and behind incident shock. The gas density contours show a less distinguishable slip line in small particle case than in the large particle case.

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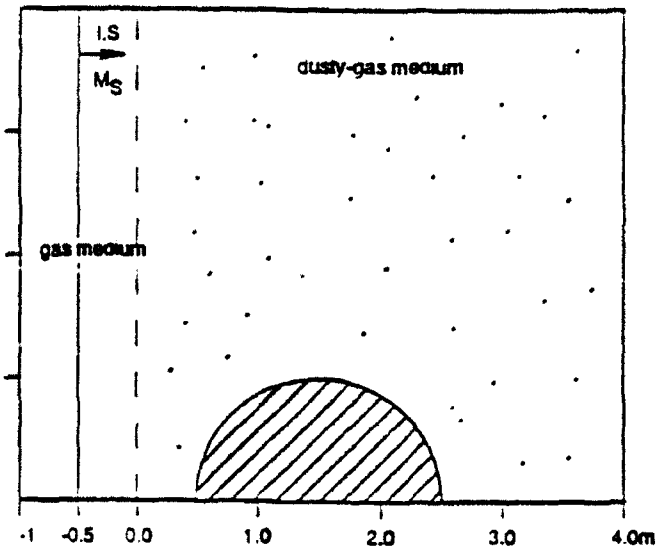


Figure 1. An illustration of the considered flow field.

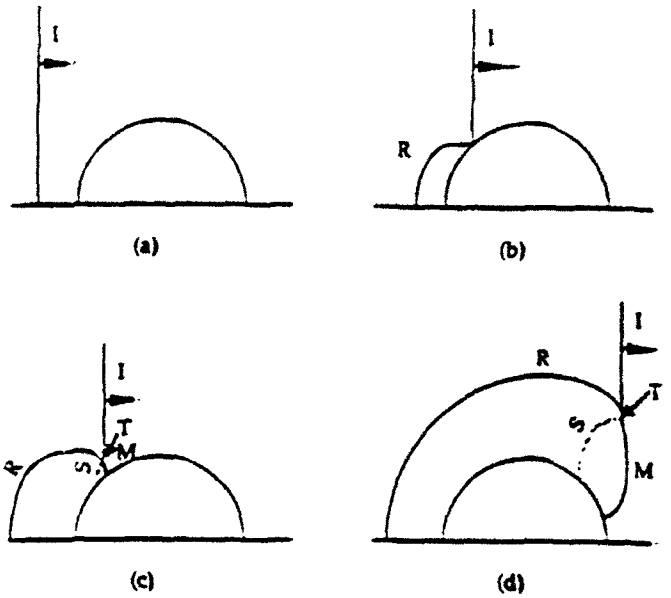
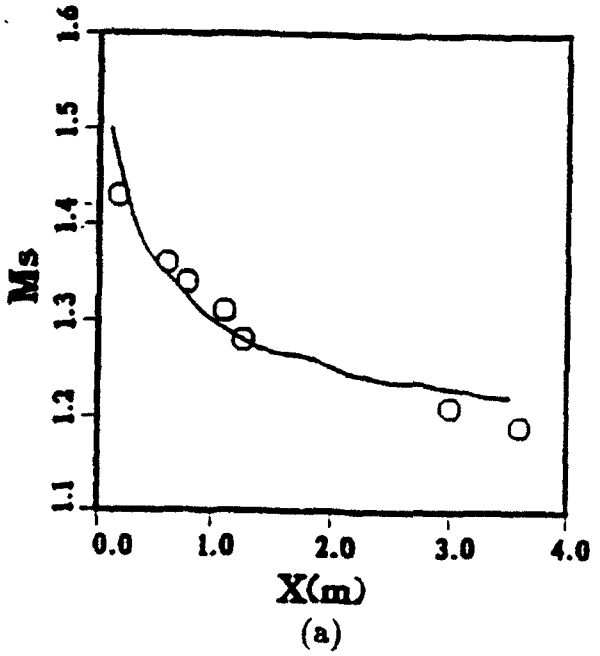


Figure 3. Stages of shock wave reflection over a semicircular cylinder, (a) before collision, (b) regular reflection, (c) Mach reflection, (d) well developed Mach reflection.



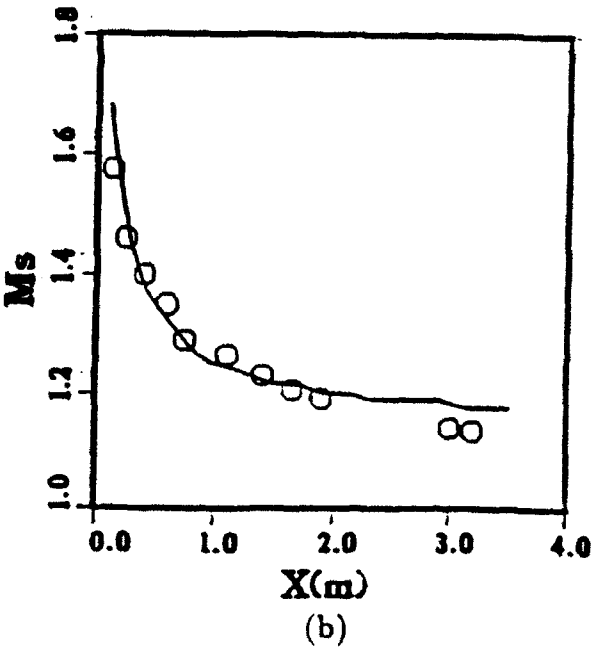
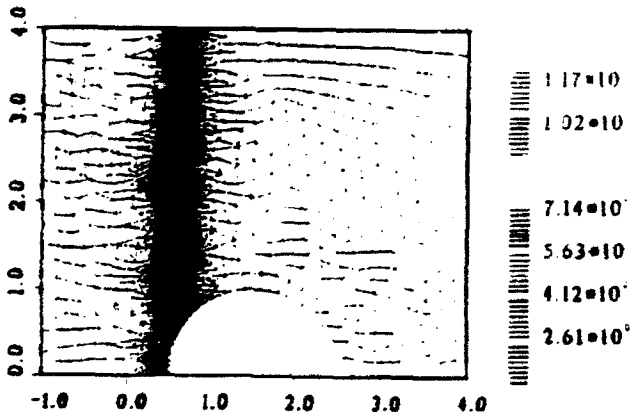
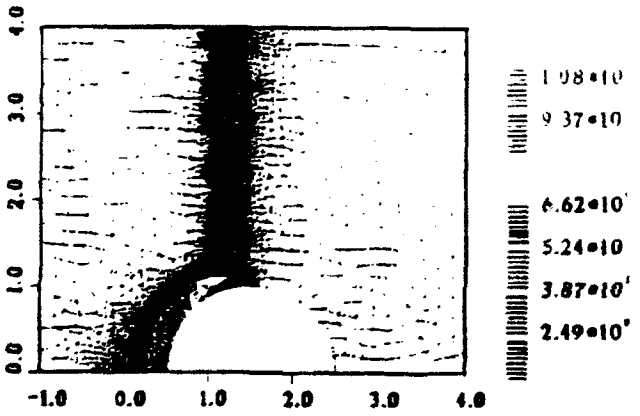


Figure 2. Comparison between computational prediction and experimental measurement of shock wave attenuation for (a) $M_s = 1.49$, $\eta = \frac{\rho_2}{\rho_0} = 0.63$ and (b) $M_s = 1.7$, $\eta = \frac{\rho_2}{\rho_0} = 1.4$ (o experiment, - calculation).



(a)



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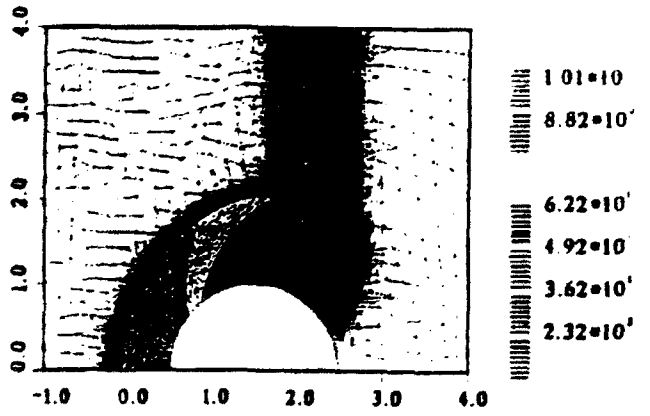
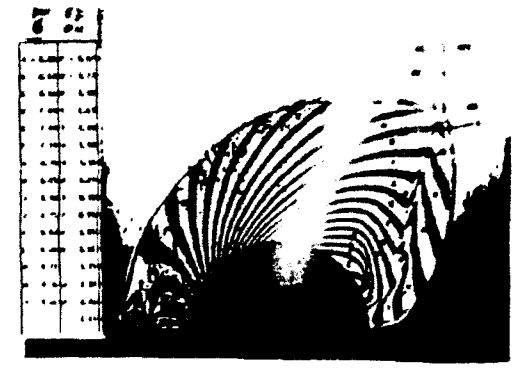
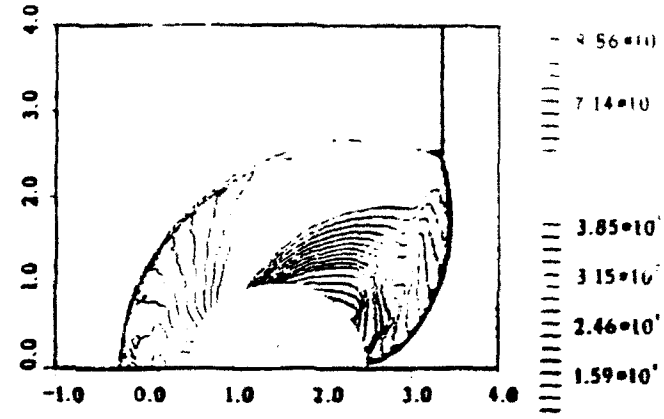


(c)

Figure 4. Computed density contours with adapted grid at three different times: (a) regular reflection (RR), (b) Mach reflection (MR) and (c) diffraction with slipline (S).

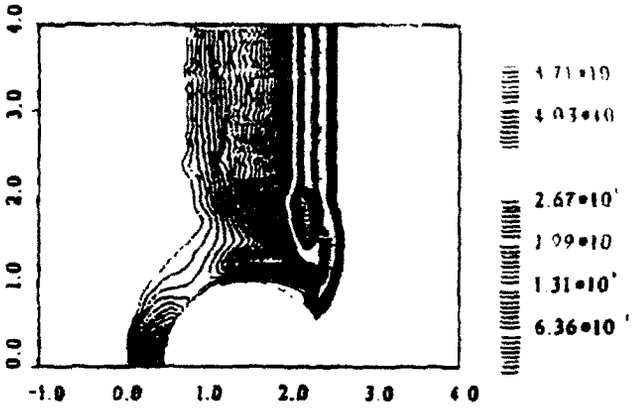


(a)

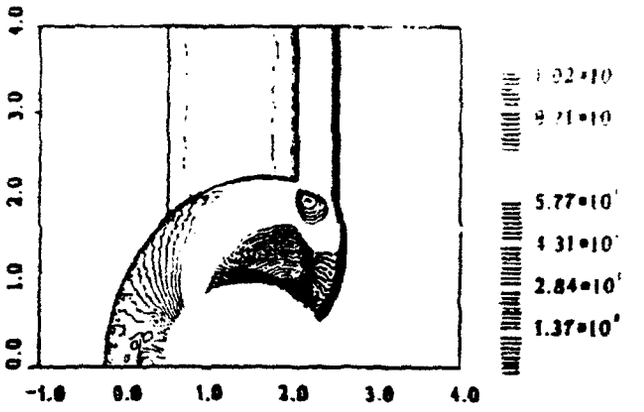


(b)

Figure 5. Comparison for M_s = 2.80 gas - only flow. (a) interferogram from experiment conducted by Kaca (1988), (b) density contours from present calculation.

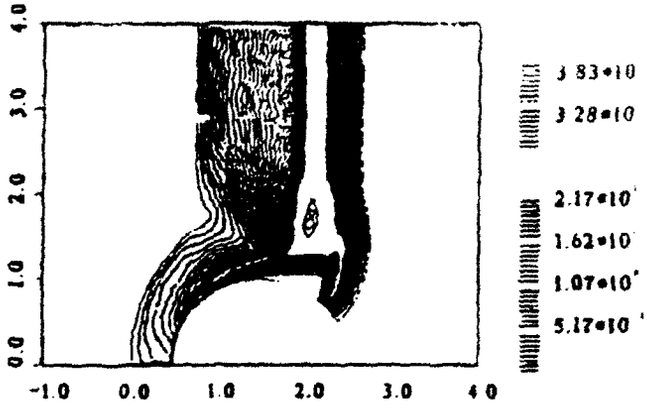


(a)

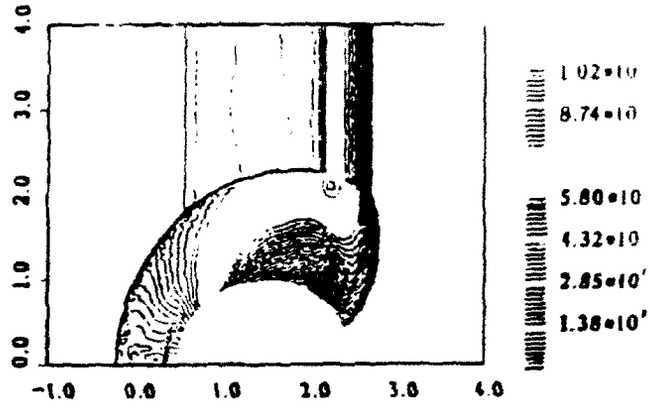


(b)

Figure 7. Density contours for the case: $M_s = 2.8$, $\rho_p = 0.76$ kg/m^3 and $r_p = 10\mu$m, (a) particle density and (b) gas density.



(a)



(b)

Figure 8. Density contours for the case: $M_s = 2.8$, $\rho_p = 0.76$ and $r_p = 50\mu$m, (a) particle density and (b) gas density.

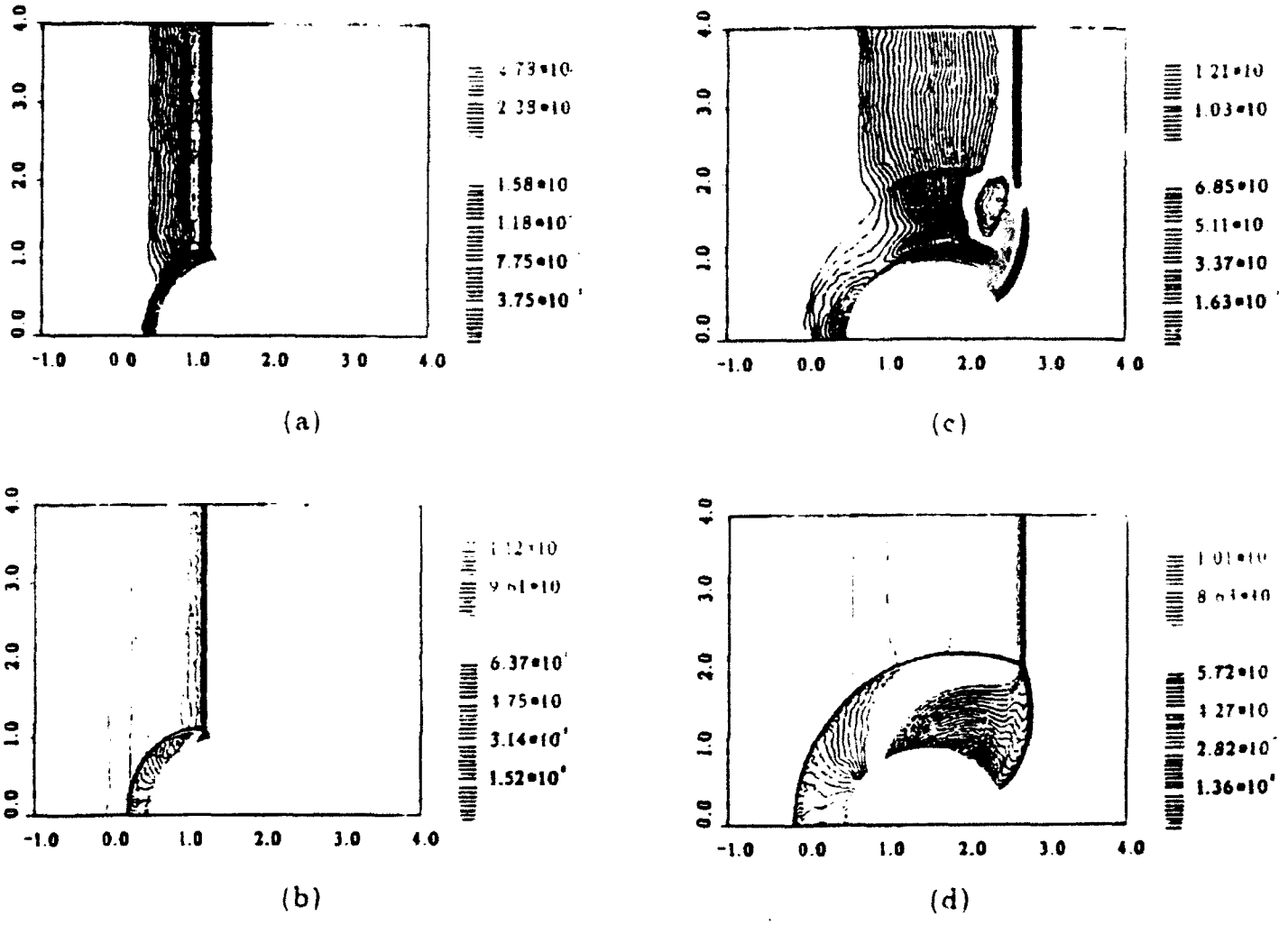


Figure 6. Density contours for the case: $M_s = 2.8$, $\rho_p = 0.25$ kg/m^3, $r_p = 10\mu$m at two different times, (a) particle density at t_1, (b) gas density at t_1, (c) particle density at t_2, and (d) gas density at t_2.

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ACOUSTIC WAVE FOCUSING IN AN ELLIPSOIDAL REFLECTOR FOR EXTRACORPOREAL SHOCK-WAVE LITHOTRIPSY

by

Itzhak Lottati* and Shmuel Eidelman†
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Abstract

Simulations of acoustic wave focusing in an ellipsoidal reflector for extracorporeal shock-wave lithotripsy (ESWL) are presented. The simulations are done on a structured/unstructured grid with a modified Tait equation of state for water. The Euler equations are solved by applying a second-order Godunov method. The computed results compare very well with the experimental results.

Introduction

Research relating to focusing of shock and acoustic waves is of practical interest for extracorporeal shock-wave lithotripsy (ESWL). A considerable body of work is dedicated to this subject (see e.g., review in Ref. 1), and numerical simulations play a prominent role in research on these devices. It is conceivable that real-time numerical simulation can be used for better assessment of shock-wave impact on the targeted areas and more effective focusing. Requirements for these real-time simulations in terms of robustness, accuracy and efficiency are very stringent, and can be satisfied only with the most advanced numerical methods.

Structured rectangular grids allow the construction of numerical algorithms that integrate the fluid conservation equations efficiently and accurately. The efficiency of these schemes results from the extremely low storage overhead needed for domain decomposition and the efficient and compact indexing, which also defines domain connectivity. These two factors allow code construction based on a structured domain decomposition that can be highly vectorized and parallelized. Integration in physical space on orthogonal and uniform grids produces numerical algorithms with the highest possible accuracy. The disadvantage of structured rectangular grids is that they cannot be used to decompose computational domains with complex geometries. Thus it is difficult to represent computationally a complex computational domain with the curved boundaries characteristic of typical reflectors used in ESWL devices.

The early developers of computational methods realized that, for many important applications of Computational Fluid Dynamics (CFD), it is unacceptable to describe curved computational domain boundaries using the stair-step approximation available with the rectangular domain decomposition technique. To overcome this difficulty, the techniques of boundary-fitted coordinates were developed. With these techniques, the computational domain is decomposed on quadrilaterals that can be fitted to the curved domain. The solution is then obtained in physical space using the geometrical information defining the quadrilaterals, or in the computational coordinate system that is obtained by transformation of the original domain into a rectangular domain. The advantage of this technique is that it employs the same indexing method as the rectangular structured domain decomposition methods that also serve to define domain connectivity. The boundary fitted coordinate approach leads to efficient codes, with approximately a 4:1 penalty in terms of memory requirement per cell as compared with rectangular domain decomposition. However, this approach is somewhat restricted in its domain decomposition capability, since distortion or large size variations of the quadrilaterals in one region of the domain lead to unwanted distortions or increased resolution in other parts of the domain. An example of this is the case of structured body-fitted coordinates used to simulate flows over a profile with sharp trailing edges. In this case, increasing the resolution in the vicinity of the trailing edge increases resolution in the whole row of elements connected to the trailing edge elements.

The most effective methods of domain decomposition developed to overcome this disadvantage are those using unstructured triangular grids. These methods were developed to cope with very complex computational domains. The unstructured grid method, while efficient and powerful in domain decomposition, results in codes that must store large quantities of information defining the grid geometry and connectivity, and have large computational and storage overheads. As a rule, a code with an unstructured grid requires greater storage by a factor of 10, and will run about 5 times slower on a per cell per iteration basis than a structured rectangular code.

Unstructured triangular meshes are designed to pro-

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vide a grid that is fitted to the boundary of complex geometry. The flexibility of the unstructured mesh that allows complex geometry to be gridded should be weighed against the huge memory requirement needed to define the interconnectivity of the triangles. To cut down on the memory overhead, unstructured grid methods are used to their best advantage when combined with grid adaptivity. This feature usually allows the dynamic reallocation of triangles according to the physics and geometry of the problem solved, which leads to a substantial reduction in the number of cells needed for the domain decomposition. However, this advantage is highly dependent on the problem solved. Adaptive unstructured grids have an advantage over nonadaptive unstructured domain decomposition if the area of high resolution needed is around one-tenth of the global area of the computational domain. As a result, while the adaptive unstructured method may be extremely effective for simulating flow with multiple shock waves in complex geometries, it becomes extremely inefficient when high resolution is needed in a substantial area of the computational domain.

Our approach to domain decomposition for ESWL applications combines the structured and unstructured methods to achieve better efficiency and accuracy. Under this method, structured rectangular grids are used to cover most of the computational domain, and unstructured triangular grids are used only to patch between the rectangular grids (Fig. 1) or to conform to the curved boundaries of the computational domain (Fig. 2). In these figures, an unstructured triangular grid is used to accurately define the curved internal or external boundaries and a structured rectangular grid is used to decompose the regions of the computational domain that have a simple geometry.

Mathematical Model

We consider a system of two-dimensional Euler equations written in conservation law form:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0 \tag{1}$$

where

$$U = \begin{vmatrix} \rho \\ \rho u \\ \rho v \\ e \end{vmatrix}, \quad F = \begin{vmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(e+p) \end{vmatrix}, \quad G = \begin{vmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(e+p) \end{vmatrix}.$$

Here u, v are the x, y velocity vector components, p is the pressure, ρ is the density, and e is total energy of the fluid.

The equation of state for water was adopted from Ref. 2. The actual pressure and density $\tilde{p}, \tilde{\rho}$ in water are modified and then applied in the Euler solver. The modified pressure and density are given as

$$p = \tilde{p} + B, \tag{2}$$

$$\rho = \tilde{\rho}/(1 + \tilde{p}/B)^n, \tag{2a}$$

where B = 2955 bar and n = 7.44 to adjust the velocity of sound to that for water (a_0 = 1483 m/sec).

The initial pressure distribution $\tilde{p}(r)$ in the left focal point is chosen as

$$\tilde{p}(r) = 1.0 \text{ bar } + \Delta p \exp\left[-(r - r_0)/(a_0 \tau)\right], \tag{2b}$$

where Δp is the intensity of the blast, τ is a time scale and a_o is sound speed in water ($\tau = 3\mu$sec).

It is assumed that an initial distribution of the fluid parameters is given at $t = 0$, and the boundary conditions defining a unique solution are specified for the computational domain.

Integration Algorithm

The system of governing equations (1) can be written in the following form:

$$\frac{\partial U}{\partial t} + \nabla \cdot \mathbf{Q} = 0, \tag{3}$$

where Q represents the convective flux vector. By integrating Eq. (3) over space and using Gauss' theorem, we obtain the following expression:

$$\frac{\partial}{\partial t} \int_\Omega U dA + \oint_{\partial\Omega} \mathbf{Q} \cdot d\mathbf{l} = 0, \tag{4}$$

where $d\mathbf{l} = \mathbf{n} dl$, n is the unit normal vector in the outward direction, and dl is the element of length on the boundary of the domain. The variable Ω is the domain of computation and $\partial\Omega$ is the domain boundary.

Equation (4) can be discretized for each element (cell-triangle) of the domain:

$$\frac{(U_i^{n+1} - U_i^n)}{\Delta t} A_i = \sum_{j=1}^{3} \mathbf{Q}_j^{n+\frac{1}{2}} \mathbf{n}_j \Delta l_j, \tag{5}$$

where A_i is the area of the cell; Δt is the marching time step; U_i^{n+1} and U_i^n are the primitive variables at the center of the cell at time n and at the updated $(n+1)st$ timestep; $\mathbf{Q}_j^{n+\frac{1}{2}}$ are the value of the fluxes across the three boundaries edges on the circumference of the cell, where $\mathbf{n}_j$ is the unit normal vector to edge j of the boundary, and Δl_j is the length of the boundary edge

j. Equation (5) is used to update the physical primitive variables U_i according to computed fluxes for each timestep Δt. The time step is subjected to the Courant-Fredrichs-Levy (CFL) constraint.

To ensure a second order spatial accuracy, the gradient of each primitive variable is computed in the baricenter of the cell. This gradient is used to define the projected values of primitive variables at the two sides of the cell edge, as shown in Fig. 3. The gradient is approximated by a path integral

$$\int_{\Omega} \nabla U_i^{\text{cell}} dA = \oint_{\partial\Omega} U_j^{\text{edge}} d\mathbf{l} \,. \tag{6}$$

The notation is similar to the one used for Eq. (5), except that the domain Ω is a single cell and U_i^{cell} and U_j^{edge} are values at the baricenter and on the edge respectively. The gradient is estimated as

$$\nabla U_i^{\text{cell}} = \frac{1}{A} \sum_{j=1}^{3} \tilde{U}_j^{\text{edge}} \mathbf{n}_j \Delta l_j, \tag{7}$$

where $\tilde{U}_j^{\text{edge}}$ is an average value representing the primitive variable value for edge j.

The gradients that are computed at each baricenter are used to project values for the two sides of each edge by piecewise linear interpolation. The interpolated values are subjected to monotonicity constraints.[3] The monotonicity constraint assures that the interpolated values are not creating new extrema.

The monotonicity limiter algorithm can be written in the following form:

$$U_{\text{pro}}^{\text{edge}} = U_i^{\text{cell}} + \phi \nabla U_i \cdot \Delta \mathbf{r}, \tag{8}$$

where Δr is the vector from the baricenter to the point of intersection of the edge with the line connecting the baricenters of the cells over the two sides of this edge. ϕ is the limiter coefficient that limits the gradient ∇U_i.

First, we compute the maximum and minimum values of the primitive variable in the i's cell and its three neighboring cells that share common edges (see Fig. 3):

$$\left.\begin{aligned} U_{\text{cell}}^{\text{max}} &= \max\left(U_k^{\text{cell}}\right) \\ U_{\text{cell}}^{\text{min}} &= \min\left(U_k^{\text{cell}}\right) \end{aligned}\right\} k = i, 1, 2, 3 \,. \tag{9}$$

The limiter can be defined as:

$$\phi = \min\left\{1, \phi_k^{lr}\right\}, \; k = 1, 2, 3, \tag{10}$$

where the superscript lr stands for left and right of the three edges (6 combinations altogether). ϕ_k^{lr} is defined by:

$$\phi_k^{lr} = \frac{\left[1 + \text{Sgn}\left(\Delta U_k^{lr}\right)\right] \Delta U_{\text{cell}}^{\text{max}} + \left[1 - \text{Sgn}\left(\Delta U_k^{lr}\right)\right] \Delta U_{\text{cell}}^{\text{min}}}{2\Delta U_k^{lr}}$$

$$k = 1, 2, 3, \tag{11}$$

where $\Delta U_k^{lr} = \nabla U_i^{lr} \cdot \Delta \mathbf{r}_k$ and

$$\left.\begin{aligned} \Delta U_{\text{cell}}^{\text{max}} &= U_{\text{cell}}^{\text{max}} - U_i^{\text{cell}} \\ \Delta U_{\text{cell}}^{\text{min}} &= U_{\text{cell}}^{\text{min}} - U_i^{\text{cell}} \end{aligned}\right\} . \tag{12}$$

To obtain second-order accuracy in space and time, we subject the projected values of the left and right side of the cell edge to characteristic constraints following Ref. 4. The one-dimensional characteristic predictor is applied to the projected values at the half timestep $t^n + \Delta t/2$. The characteristic predictor is formulated in the local system of coordinates for the one dimensional Euler equation. We illustrate the implementation of the characteristic predictor in the direction of the unit vector $\mathbf{n}_c$. The Euler equations for this direction can be written

$$W_t + A(W) W_{n_c} = 0, \tag{13}$$

where

$$W = \begin{Bmatrix} \tau \\ u \\ p \end{Bmatrix}; \; A(W) = \begin{pmatrix} u & -\tau & 0 \\ 0 & u & \tau \\ 0 & \rho c^2 & u \end{pmatrix}, \tag{14}$$

where $\tau = \rho^{-1}$, ρ denotes density, and u, p are the velocity and pressure. The matrix $A(W)$ has three eigenvectors $(l^{\#}, r^{\#})$ (l for left and r for right, where $\#$ denote $+,0,-$) associated with the eigenvalues $\lambda^+ = u + c$, $\lambda^0 = u$, $\lambda^- = u - c$.

An approximation of the value projected to an edge, accurate to second order in space and time, can be written

$$\begin{aligned} W_{i+\Delta r}^{n+1/2} &\approx W_i^n + \frac{\Delta t}{2} \frac{\partial W}{\partial t} + \Delta r \frac{\partial W}{\partial r_{n_c}} \\ &\approx W_i^n + \left[\Delta r - \frac{\Delta t}{2} A(W_i)\right] \frac{\partial W}{\partial r_{n_c}} \end{aligned} . \tag{15}$$

An approximation for $W_{i+\Delta r}^{n+1/2}$ can be written as

$$W_{i+\Delta r}^{n+1/2} = W_i + (\Delta \mathbf{r}_i - \frac{\Delta t}{2}(M_x M_n)\mathbf{n}_c).\nabla W_i, \tag{16}$$

where

$$(M_x M_n) = \begin{cases} \text{Max}(\lambda_i^+, 0) & \text{for cell left to the edge} \\ \text{Min}(\lambda_i^-, 0) & \text{for cell right to the edge} \end{cases} . \tag{17}$$

The gradients ied in the process of computing the projected values at $t^n + \Delta t/2$ are subjected to the monotonicity limiter.

Following the characteristic predictor described above, the full Riemann problem is solved at the edge. The solution of the Riemann problem defines the flux $Q_j^{n+\frac{1}{2}}$ through the edge. The fluxes through the edges of triangles are then integrated (Eq. 5), thus updates the variables at t^{n+1}. One of the advantages of this algorithm is that calculation of the fluxes is done over the largest loop in the system (the loop over edges) and can be carried out in the vectorized or parallelized loop. This makes the algorithm efficient.

The algorithm presented is a modification of the algorithm of Ref. 5, which was derived for a structured mesh. The present algorithm has been applied to simulate a wide range of flow problems and has been found to be very accurate in predicting the features of the physics. The performance of the algorithm is well documented in Refs. 6-9. The algorithm for the rectangular cells are identical except the cell has four edges (Eq. 5).

Sound Wave Focusing in an Ellipsoidal Reflector

For our simulations, we chose a deep reflector shaped like an ellipsoid, which was used for ESWL by Dornier and other companies. A schematic of the cross section of this reflector is shown in Fig. 4. Strong acoustic waves are generated in the left focal point of the ellipsoid by an instantaneous release of energy and are refocused at the right focal point. Ideally, a reflector should employ waves of acoustic intensity, since the nonlinear reflections of strong shock waves lead to significant distortions in wave propagation and impair simple geometrical focusing.

Figure 2 shows the computational domain and grid for the ellipsoidal reflector that we used in our study. In order to illustrate the concept of the composite structured/unstructured grid, we have shown only every sixteenth cell of the grid that was actually used for the simulation. In this example, we observe that the structured rectangular grid covers about 90% of the computational domain, and the unstructured triangular grid is restricted to the curved surface of the ellipsoid and covers about 10% of the domain. The major axis of the ellipsoid is 150 mm and the minor axis is 90 mm.

Two simulations were conducted with two different Δp values to study how the intensity of the blast affects focusing of waves in the reflector. The first simulation was done with $\Delta p = 725$ bar and $\tau = 3\mu$s where $|r - r_0| < 10$ mm. The other simulation was done by using pressure three times larger than in first simulation.

In Figs. 5a-5d simulation results for the $\Delta p = 725$ bar conditions are shown in the form of pressure contour plots. Figure 5a shows pressure distribution for the initial stage of wave propagation before the wave front has reached the surface of the reflector. The contour plots are shown at t=1.10 $\times 10^{-5}$sec. At this time the maximum pressure in the wave has dropped to 173 bar. In Fig. 5b pressure contours are shown at t=3.32 $\times 10^{-5}$sec. Here we observe that the wave reflected from the surface of the reflector has maximum pressure about five times than that of the incident wave. However, both wave fronts propagate through the water with a constant speed equal to the speed of sound, and the phase shift observed in Fig. 5b holds through the calculation. In Fig. 5c the simulation results are shown at the stage when the incident wave is crossing the center of symmetry of the reflector. Here $t = 8.88 \times 10^{-6}$sec. It is interesting to note that the value of the overpressure at this location was used in Ref. 1 as a normalizing value for presentation of the experimental and computational results. In our case for the initialization with $\Delta p = 725$ bar the incident pressure at the center of the ellipsoid is $p = 11.1$ bar. In Fig. 5d simulation results are shown at $t = 19.2 \times 10^{-5}$sec, when maximum focusing of the reflected wave take place. The pressure values in the focal point reaches 188 bar. This maximum is immediately followed by a negative phase with a minimal pressure of 163 bar. This strong pressure variations can cause disintegration of the stones by the ESWL apparatus.

In Figs. 6a-6b simulation results are shown for the second case of $\Delta p = 2175$ bar. As we can see in Fig. 6a, this value of the initial overpressure produces an incident wave with about 33 bar, which is a bit higher than the 29 bar value observed in Ref. 1. The wave structure at the time of focusing is shown in Fig. 6b. Here we can observe that for this case the maximum pressure reaches 494 bar, followed by a 371 bar minimum. Comparing this case with that reported above, we conclude that the amplification at the focal point is smaller in the second case.

The waves observed in the system are of acoustic intensity and are propagating at the speed of sound. The reflected wave will therefore not be able to catch up with the incident wave. Except for some compressibility effects in the initiation and focusing stages when pressures are high, the fluid will behave as incompressible. Figure 7 shows the density contour for the first case ($\Delta p = 725$ bar). As expected, the compressibility effect is negligible.

In Fig. 8 the simulation results are compared with the experimental results in a plot of normalized pressures as function of distance from the focal point. In this figure the simulation results for the case of initiation with $\Delta p = 725$ bar and $\Delta p = 2175$ bar are shown by the curves marked with triangles and rectangles respectively. The experimental results for the 29-bar incident pressure

(which most closely fits our second simulation) are shown by the curve marked by circles. In Fig. 8 we see that the maximum reflection factor is achieved for weaker waves, which is consistent with the results reported in Ref. 1. The simulation results are very close to the experimental ones in the case of $\Delta p = 2175$ bar initiation for focal point location and pressure amplification factor, which validates the simulation methodology.

In all the figures presented, the method of composite domain decomposition works extremely well, producing solutions with no seams at the interfaces. We should mention here that our test problem is particularly sensitive because the main acoustic waves are weak, and any inaccuracy introduced at the grid interfaces would produce a distortion in the phase or in the intensity of the traveling waves that would be a visible disturbance evident in the results.

Conclusions

A composite method of structured/unstructured domain decomposition is introduced as an efficient technique for dealing with the computational domains of complex geometry. We have simulated a demanding acoustic wave focusing problem and have shown that our approach leads to accurate wave propagation without any reflection or distortion at the structured/unstructured grid interfaces. Note that for the acoustic focusing problem as simulated and presented in this paper, both structured and unstructured methods of domain decomposition can be shown to be inadequate if used separately. The structured method has difficulty describing the curved boundaries of the computational domain, while the unstructured method is totally inefficient in describing phenomena with wide fronts that occupy a large portion of the computational domain. Our hybrid method combines the advantages of structured and unstructured methods of domain decomposition. This hybrid technique combines the efficiency of the unstructured grid, which accurately represents curved walls, with the computational and memory efficiency of the structured grid in the majority of the computational domain. We also attribute the quality of the numerical result to the Second Order Godunov method, which allows a consistent, accurate and robust formulation for handling both grids and boundary conditions.

Acknowledgment

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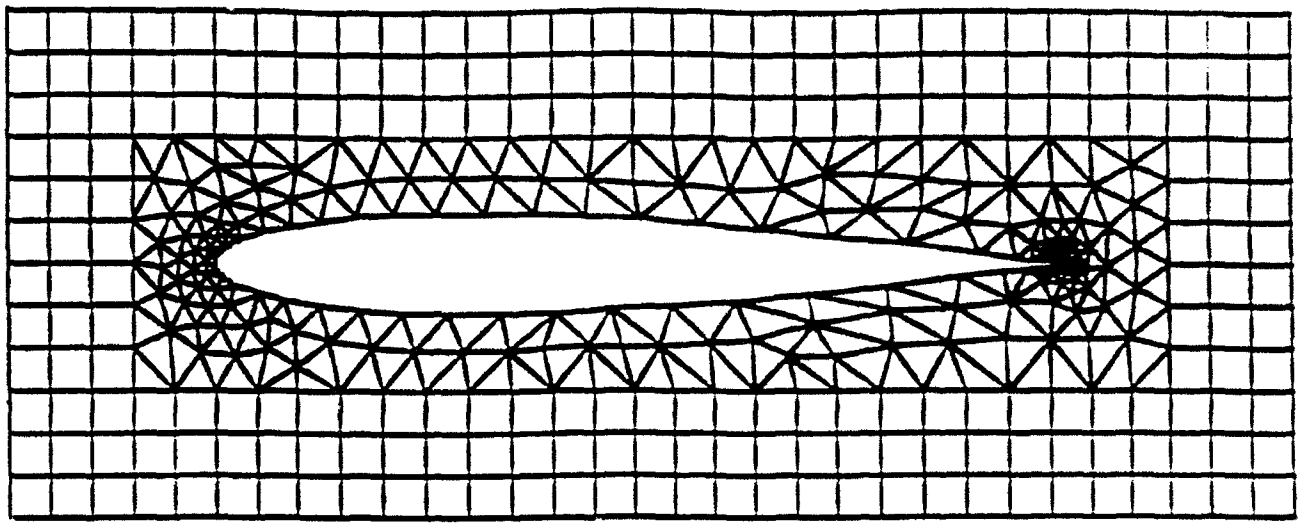


Figure 1. A possible candidate configuration for hybrid structured/unstructured domain decomposition.

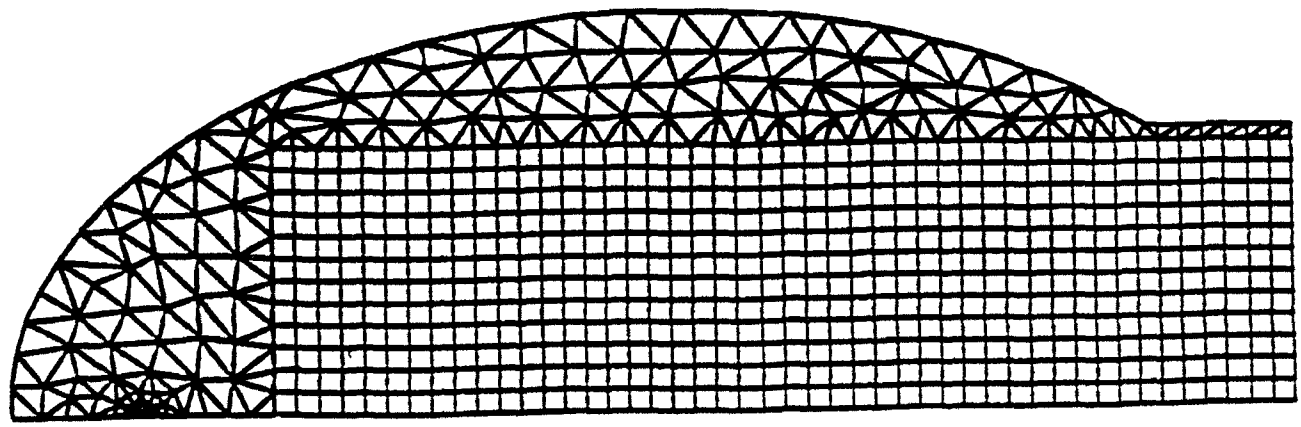


Figure 2. A possible candidate configuration for hybrid structured/unstructured domain decomposition, representing the ellipsoid reflector grid used for the numerical simulation.

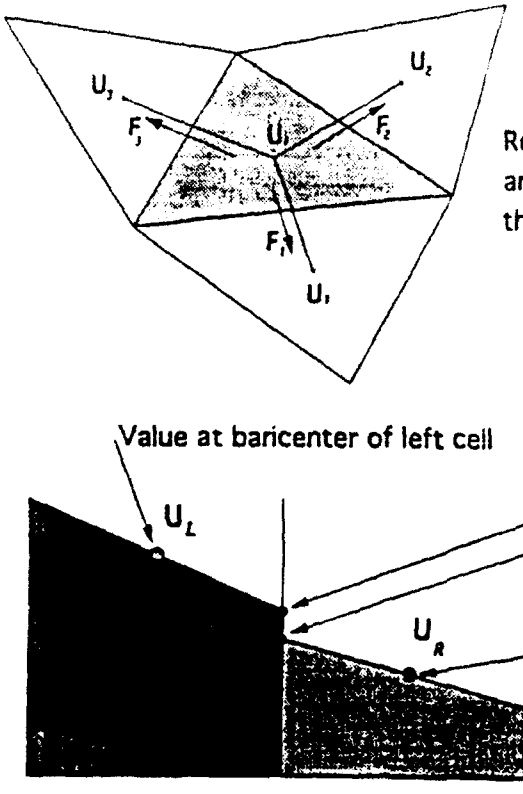


Figure 3. Second order triangular based flux calculation.

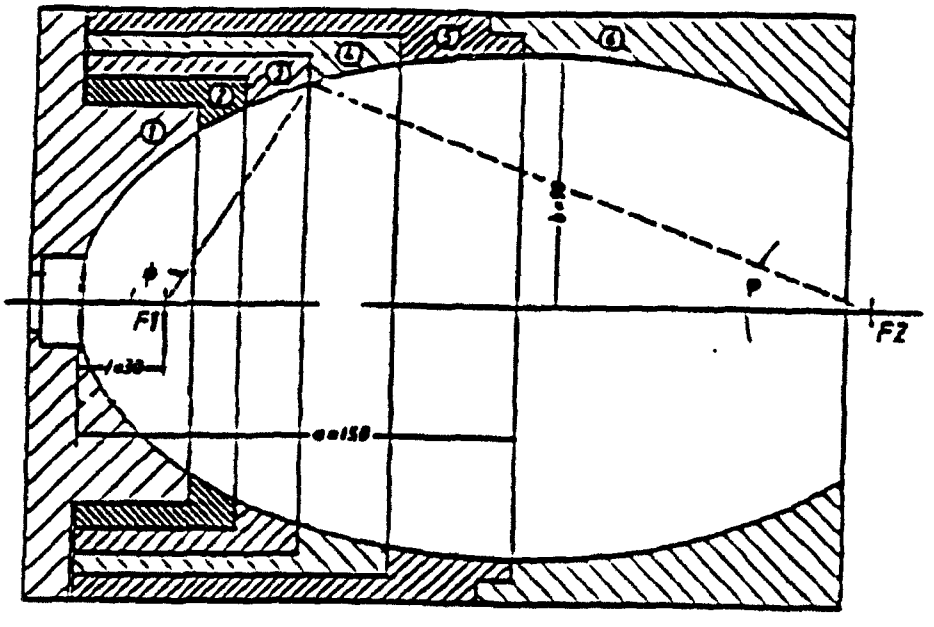
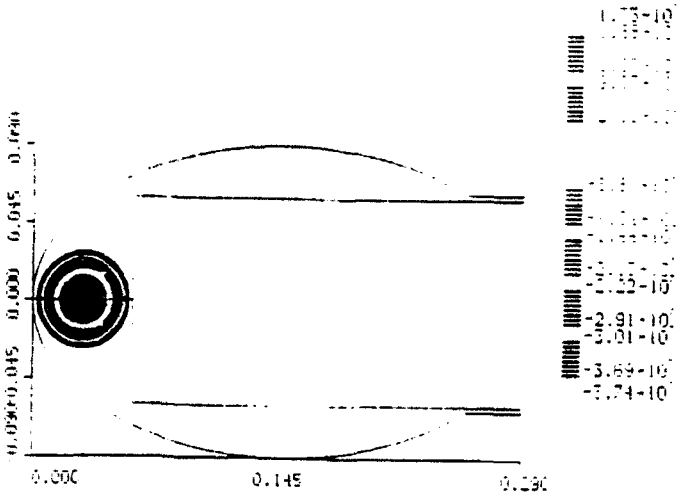
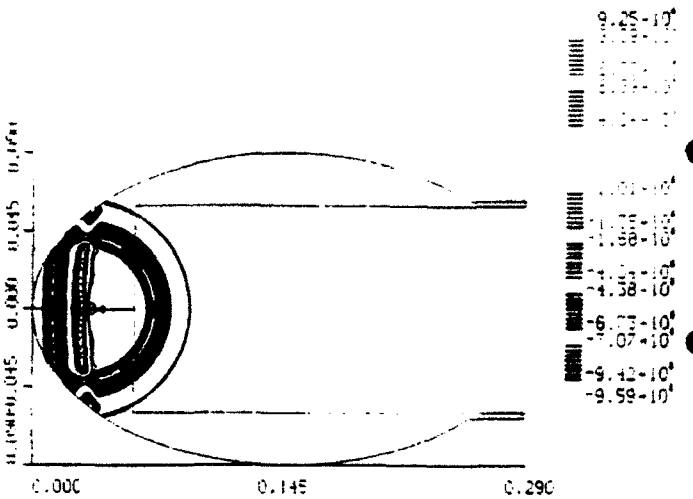


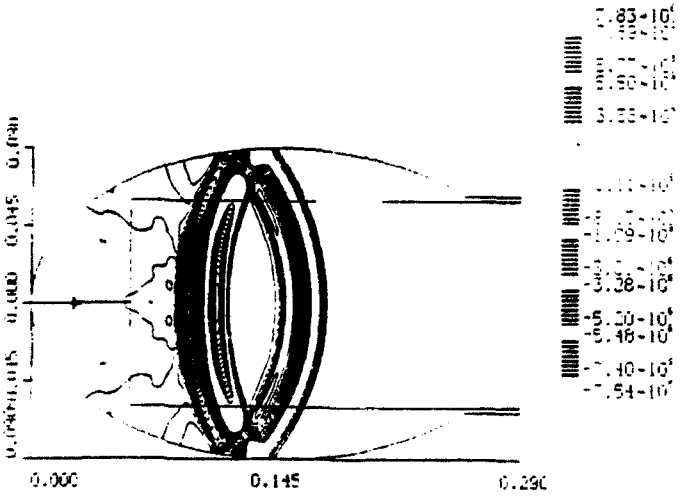
Figure 4. A schematic drawing of the center cross section of the ellipsoid reflector.



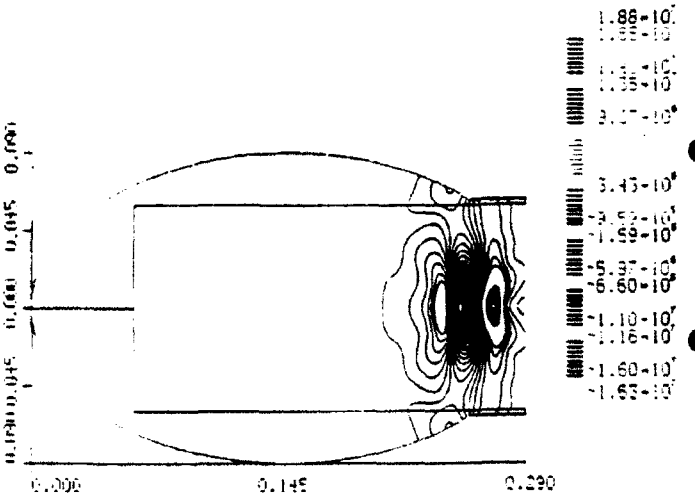
a. Time = 1.10×10^{-5}sec



b. Time = 3.32×10^{-5}sec

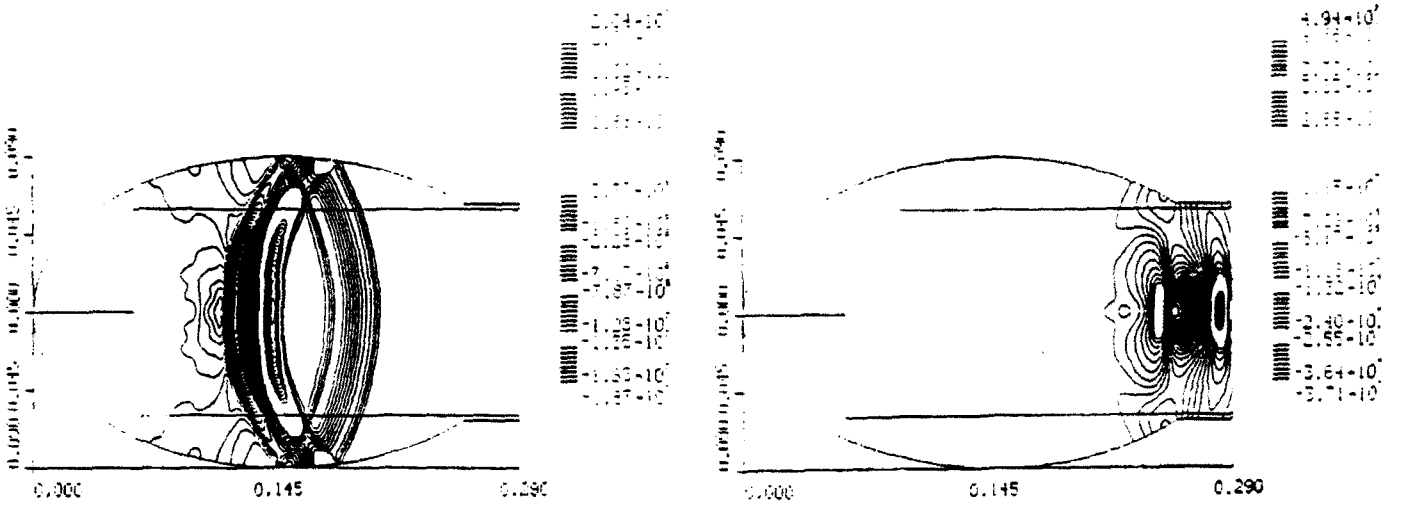


c. Time = 8.88×10^{-5}sec



d. Time = 1.92×10^{-4}sec

Figure 5. Pressure contours showing the incident wave and the reflected wave pattern for $\Delta p = 725$ bar.



a. Time = 1.08×10^{-4}sec

b. Time = 1.96×10^{-4}sec

Figure 6. Pressure contours showing the incident wave and the reflected wave pattern for $\Delta p = 2175$ bar.

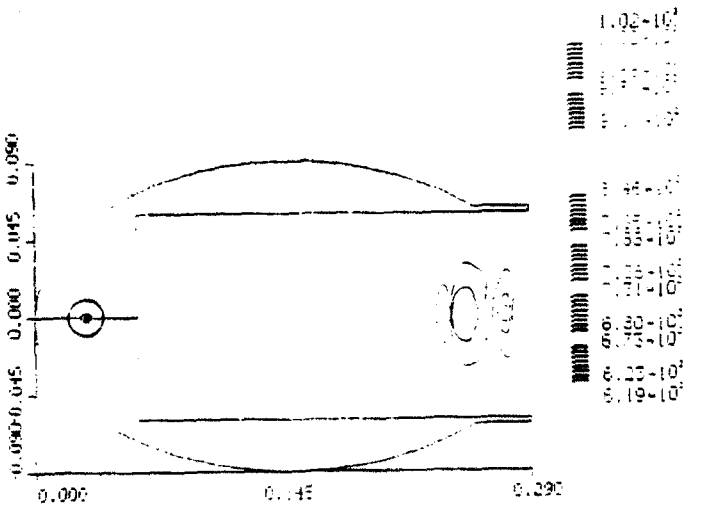


Figure 7. Density contours emphasizing the fact that the compressibility effect is negligible ($\Delta p = 725$ bar at t = 1.92×10^{-4}sec).

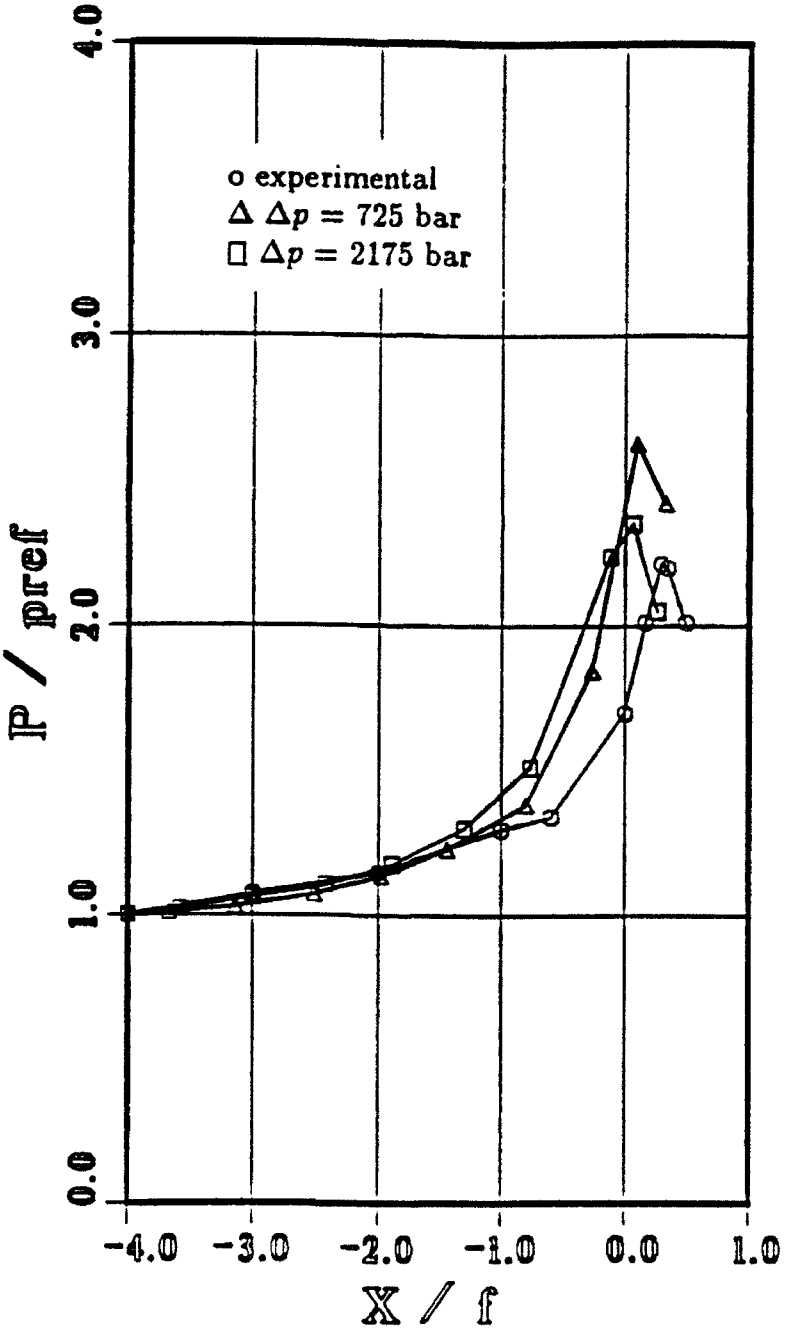


Figure 8. Normalized maximum pressure distribution on the axis of symmetry. A comparison between computed and experimental results.