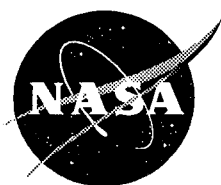
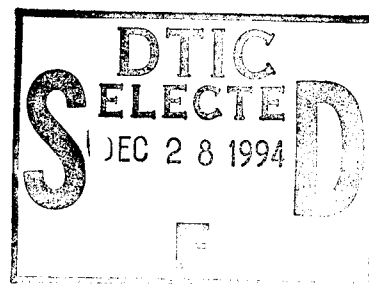


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ICASE

SEMIANNUAL REPORT



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INTRODUCTION

The Institute for Computer Applications in Science and Engineering (ICASE) is operated at the Langley Research Center (LaRC) of NASA by the Universities Space Research Association (USRA) under a contract with the Center. USRA is a nonprofit consortium of major U. S. colleges and universities.

The Institute conducts unclassified basic research in applied mathematics, numerical analysis, fluid mechanics, and computer science in order to extend and improve problem-solving capabilities in science and engineering, particularly in the areas of aeronautics and space research.

ICASE has a small permanent staff. Research is conducted primarily by visiting scientists from universities and industry who have resident appointments for limited periods of time as well as by visiting and resident consultants. Members of NASA's research staff may also be residents at ICASE for limited periods.

The major categories of the current ICASE research program are:

- Applied and numerical mathematics, including numerical analysis and algorithm development;
- Theoretical and computational research in fluid mechanics in selected areas of interest to LaRC, including acoustics and combustion;
- Experimental research in transition and turbulence and aerodynamics involving LaRC facilities and scientists;
- Computer science.

ICASE reports are considered to be primarily preprints of manuscripts that have been submitted to appropriate research journals or that are to appear in conference proceedings. A list of these reports for the period April 1, 1994 through September 30, 1994 is given in the Reports and Abstracts section which follows a brief description of the research in progress.

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RESEARCH IN PROGRESS

APPLIED AND NUMERICAL MATHEMATICS

SAUL ABARBANEL

Issues in Long-time Integration

It was shown previously that long time integration of systems of p.d.e's (such as the Euler or the Navier-Stokes Equations) may lead to errors with exponential temporal growth. This may adversely effect the treatment of problems in acoustics, unsteady motion of aerodynamic surfaces, direct simulation of turbulence and other time-dependent phenomena. These effects are particularly marked when one uses high order of accuracy (four and above) spatial discretizations due to the difficulties of constructing stable boundary closures. Previous work with Gottlieb and Carpenter started our research in these areas.

One issue concerns the deterioration of accuracy due to Runge-Kutta temporal integration (ICASE Report 93-83). Recently we have succeeded in prescribing the correct posing of boundary conditions, at the intermediate stages of the R-K integrator, not only in the linear case but also for the nonlinear case of conservation laws. An ICASE report has been written and will be issued shortly.

Work has also continued on improving the cell-Reynolds-number restriction which results from the interaction between the advection and diffusion terms in the Navier-Stokes equations.

NATALIA ALEXANDROV

Development of a Program in Multidisciplinary Design Optimization

Multidisciplinary Design Optimization (MDO) is a methodology for the design of complex, coupled engineering systems, such as aircraft, automobiles and other mechanisms, the behavior of which is determined by interacting subsystems. MDO is also applicable to a larger class of problems, such as design in general, control, and parameter identification. MDO has recently emerged as a distinct field of research and practice that has brought together many previously separate disciplines and tools of engineering and applied mathematics. Although the potential of MDO for improving the design process and reducing the manufacturing cost of complex systems is widely recognized by the engineering community, the extent of practical application of the methodology is not as high as it could be, due to a shortage of easily applicable MDO technology. That is why it is important to identify promising research areas and to define a systematic program in applied mathematics for the development of techniques that would facilitate wider implementation of the MDO methodology.

The areas of research identified in applied mathematics that will be of importance to the MDO technology include the following: the development of nonlinear optimization algorithms (including algorithms for large scale constrained optimization and algorithms for nonlinear mixed integer programming); analysis of the optimization algorithms (convergence, complexity, and robustness);

development of optimization algorithms designed especially for problems with very expensive function evaluations; analysis of the MDO formulations (optimality conditions, equivalence, applicability); perturbation and sensitivity analysis; modeling and approximation concepts; incorporation of simulations and optimization into a single framework. The work on the development and analysis of the optimization algorithms has been in progress since March and on the analysis of MDO formulations has been in progress since March 1994.

In order to obtain a clear direction for the development of an MDO program, an ICASE/LaRC MDO workshop has been organized to take place in March of 1995. The workshop will provide information on the state-of-the-art in MDO and on the promising and useful research opportunities.

Multilevel Algorithms for Nonlinear Constrained Optimization

From the point of view of an optimizer, MDO problems can be viewed as large-scale nonlinear programming problems in which the majority of constraints are equality constraints that represent the analyses of MDO that are the contributions of the disciplines to the system. The discipline analyses in MDO represent a naturally occurring small number of large blocks of constraints. Large-scale optimization problems, in general, and MDO problems, in particular, require algorithms that allow for decomposition of the original problem into a number of smaller ones. Therefore, in developing our methods, we consider the general nonlinear constrained optimization problem.

We have extended the multilevel algorithm for equality constrained optimization proposed by the author last year to a class of multilevel optimization algorithms for solving the general large-scale nonlinear equality constrained optimization problem and square and underdetermined systems of nonlinear equations. The class is inspired by the local Brown-Brent methods for nonlinear systems and is based on the trust-region approach to constrained optimization. The constraints of the problem can be partitioned into blocks in any manner suitable to an application, without any assumption on the separability structure of the problem. The algorithm then solves progressively smaller dimensional subproblems to arrive at the trial step. The methods belong to the class of out-of-core methods—they require access only to the currently processed block of constraints and, thus, are expected to be well suited to very large problems, as, theoretically, there is no limit to the size of the problem they can handle. The computed trial steps are required to satisfy very mild conditions, both theoretically and computationally. In fact, the contributing substeps can be computed by different optimization algorithms, which is of practical importance because in applications like MDO various constraint blocks originate from different disciplines and will require different approaches to solving the subproblems. The algorithms are proven to converge under reasonable assumptions. The methods have elicited interest in the engineering community, both at NASA and in academia. Part of this work has been done jointly with John Dennis of Rice University.

The work on local convergence analysis and on practical implementation of the class is now in progress. The algorithms are expected to be useful at all stages of MDO formulations and decomposition. They will be tested for applicability and robustness in various MDO formulations.

Algorithms for General Multilevel Nonlinear Optimization

The problem of general multilevel optimization (MLO) is as follows: find a (possibly constrained) minimum of an objective function, subject to the result being a (possibly constrained) minimum of another objective function, subject to the result being a minimum of another function,

and so on. One of the main objectives in the definition and study of the multilevel problem is to provide a classification and analysis to the numerous multilevel formulations already in wide use in engineering. These tend to be erratically successful, and the proponents of these formulations at NASA Langley have requested that a formal analysis of the formulations be done to determine their applicability. Our general interest is also based on that any design problem is multiobjective in nature. However, the multiobjective (or multicriteria, or vector) optimization problem is ill-posed. Existing methods, such as objective function synthesis and goal programming, require introduction into the optimization procedure of predetermined quantities, such as weights on the contributing objectives and goals. Our aim is to regularize the ill-posed problem without having to introduce a priori estimates.

We have stated problem MLO in a way that encompasses all multilevel formulations in use today. Initial analysis of the bilevel and multilevel problems has been completed. We have not made the assumptions of convexity and separability that usually are made in existing treatments of bilevel optimization. We stated two algorithms for solving the general, constrained multilevel problem, based on the multilevel algorithms for equality constrained optimization, described above. The trial step in each of the algorithms is again computed in a sequence of solving progressively smaller dimensional subproblems. If a multilevel problem exhibits some separability structure, then the algorithms can be stated in parallel form. Part of this work has been done jointly with John Dennis of Rice University.

We plan to implement the algorithms, provide global and local convergence theory, and test them first on a multilevel test package written at NASA Langley, and then on a number of realistic problems.

Theoretical Foundations of MDO Formulations

The MDO problem can be formulated in a number of ways, which are important for the practical effectiveness of the methodology. Work on formulations has been done by researchers from Rice University, NASA Langley, and Boeing. Interest has been expressed at NASA to obtain thorough analysis of MDO formulations, their equivalence and applicability to various problems.

Analysis of the optimality conditions for various formulations is being conducted.

We plan to evaluate the formulations in cooperation with J. Sobieski of NASA Langley.

JUSTIN R. APPEL

The Efficient Solution of Discretized Flow Control Problems

Flow control problems are constrained optimization problems in which the constraints are systems of partial differential equations. Thus, in a discrete setting, the number of constraint equations is very large so that an important research issue is the efficient solution of constrained optimization problems with a large number of constraints. The aim of our research is to apply the algorithm developed by Dr. Natalia Alexandrov to a flow control problem such as a drag minimization problem or flow matching. We will take a flow control code developed at Virginia Tech and apply Dr. Alexandrov's algorithm to solve the discretized optimization problem. In the flow control setting we will study the relative efficiency of her algorithm to the current algorithms being used in the flow control codes.

In this study we chose a coupled solid/fluid temperature control problem for flow through a channel. The fluid in the channel is governed by the incompressible Navier-Stokes equations and the temperature in the whole domain is governed by the energy equations. Due to certain assumptions about the flow we are able to uncouple the mechanical equations from the thermal equations. The flow is solved using Taylor-Hood finite elements and the thermal equations are solved using quadratic finite elements based on an isoparametric triangulation. The code was developed at Virginia Tech by Max Gunzburger and Hyung C. Lee. In applying Dr. Alexandrov's algorithm, it was first necessary to reduce the system to block form consisting of four regions: fluid, solid, interface, and control regions. The algorithm is based on restricting the optimization problem to different hyperplanes corresponding to the different blocks of the system. Originally, the algorithm was developed using LU factorizations to solve the linear systems. The amount of work can be reduced somewhat by applying a new iterative method for solving systems with multiple right hand sides. We are still in the early stages of testing the relative efficiency of the algorithm.

From the work accomplished this summer and further work to be done we hope to publish a paper. In the future it is our aim to continue working with Dr. Alexandrov's algorithm to make it more efficient. Also, since we now have the system in block form we can apply other algorithms for solving constrained optimization problems to study their efficiency. Another goal is to remove the assumptions on the flow so that the mechanical equations can not be uncoupled from the thermal equations. This will result in a much larger and inheritantly more difficult problem to solve. This work has been done in collaboration with and under the advisement of Dr. Max Gunzburger, Interdisciplinary Center for Applied Mathematics and Department of Mathematics at Virginia Tech, and Dr. Natalia Alexandrov, ICASE staff scientist. Dr. Gunzburger is also a consultant for ICASE.

KURT BRYAN

Sensitivity Analysis for an Inverse Problem in Thermal Imaging

Thermal imaging is a technique of wide utility in non-destructive testing (NDE). The technique is used to recover information about the internal condition of an object by applying a heat flux to its boundary and observing the resulting temperature response on the object's surface. From this information one attempts to determine the internal thermal properties of the object. The technique has been much investigated as a method for detecting damage or corrosion in aircraft parts and structural members.

We investigate the problem of determining changes in the boundary profile of a two-dimensional sample via thermal imaging. The changes in the boundary could represent corrosion or some other departure from an ideal or desired boundary profile. The problem is formulated as an inverse problem for the unknown boundary. Our analysis is based on a linearization of the original problem, and we prove uniqueness and continuous dependence results for the the linearized inverse problem. We also propose an efficient algorithm for solving the inverse problem and study the behavior of the algorithm when applied to simulated data sets.

Up to this point we have studied only the two-dimensional inverse problem on a region with a simple geometry. We intend to extend our results to more general regions and to full three

dimensional regions, as well as investigate convergence results and methods for regularizing this ill-posed inverse problem.

This research was conducted jointly with Lester Caudill of the department of chemistry at Princeton University.

JENNIFER M. DEANG

Computational Data for the Stokes Equations using a Least-Squares Finite Element Method

My work has been an extension of the work of Pavel B. Bochev from the Department of Mathematics and Interdisciplinary Center for Applied Mathematics at Virginia Tech involving a first-order velocity-vorticity-pressure system in a square channel. The convergence rates were determined for the velocity boundary conditions (IBC1) with a weighted least-squares functional, and the pressure-normal velocity boundary conditions (IBC2) without the use of weights. One goal for this additional computation study was to see if weights were necessary in four different cases of mixed boundary conditions involving IBC1 and IBC2. A second numerical study involved cutting out a portion of the square channel and thus introducing a corner in the fluid flow field where the "true" solution has a singularity.

As in the previous computational study, all numerical results were computed by the use of piecewise quadratic finite element spaces based on a uniform or refined triangulation. With mixed boundary conditions, several conclusions were drawn from this computed data: 1) With the presence of additional IBC2 conditions, the need for the weighted least-square procedure was decreased, as expected. 2) If the two IBC2 conditions were parallel to the x and y axis, this configuration yielded better convergence results compared to positioning of IBC2 conditions parallel to the x axis only. For the second study, work was done to calculate a function, Φ , with a singularity. If the velocity $\mathbf{u}$ was the only variable affected by the Φ function, results involving the refined grid versus a unrefined grid were more favorable and the convergence rates with the refined grid were similar to the previous square channel example. If the Φ function was used in the equations for all four variables: $\mathbf{u}, \leq, p$, the obtained results were below normal and sometimes the algorithm did not even converge for $\leq$ and p in the iteration steps allowed.

Thus, the influence of Φ is quite evident and at this point we are trying to develop a method that will yield the expected convergence rates. We also plan to research the ability to prove theoretically the *need* for a weighted least-squares functional in the case of mixed boundary conditions, based on the numerical data.

PAUL FISCHER

Spectral Element Methods for Computational Fluid Dynamics

Efficient solution of the Navier-Stokes equations in complex domains is dependent upon the availability of fast solvers for sparse linear systems. We seek to improve existing spectral element methods through further development of deflation based iterative solvers for the pressure.

Deflation is a general approach to improving the convergence rate of iterative methods for solving $A\mathbf{x} = \mathbf{b}$ in which the solution is expressed as $\mathbf{x} = \bar{\mathbf{x}} + \tilde{\mathbf{x}}$, where $\bar{\mathbf{x}}$ is some readily computed

projection of $\underline{x}$ onto a subspace $\chi \subset \mathbb{R}^n$. The remainder, $\tilde{x}$, is computed via conjugate-gradient iteration restricted to $\chi^\perp$, the orthogonal complement of χ , w.r.t. $\|\cdot\|_A \equiv (A\cdot, \cdot)^{\frac{1}{2}}$. It is desirable that χ nearly contain the eigenspace associated with A 's extreme eigenvalues and/or that it nearly contain $\underline{x}$. We have developed two complementary strategies for selecting χ which help to overcome the slow convergence frequently encountered in the presence of extreme refinement or high-aspect ratio elements. The first is to extend prior coarse grid bases for χ from piecewise constant to piecewise linear functions; this has resulted in a two-fold reduction in the pressure iteration count for difficult computations of high Reynolds number flow past a cylinder. The second is to augment χ with the Krylov spaces of residuals from previous time steps; this results in as much as a five-fold *additional* reduction in iteration count, to the point where the number of required iterations is often less than ten.

The enrichment of the coarse grid space comes at the price of a larger system to be solved directly. We will work with Alex Pothén on the incorporation of sparse matrix technology for both serial and parallel computations. In addition we will investigate the possibility of deflating more modes in certain areas while retaining fewer modes in regions where piecewise constants suffice.

DANIELE FUNARO

A Spectral Element Code

I am in the process of writing an extensive and detailed report on the use of spectral elements for the approximation of boundary value problems, with a particular attention to elliptic type equations with high transport terms and small diffusion.

The algorithm described is based on a preconditioned iterative method to solve the matching equations at the interfaces between the various subdomains. An iterative preconditioned procedure is also used inside each subdomain for the solution of the corresponding collocation problem. The set of collocation nodes is obtained by modifying the usual Legendre grid in the up-wind direction, in a way depending on the magnitude of the transport terms in relation to the one of the diffusive terms.

Applications are expected to be developed for the discretization of the incompressible Navier-Stokes equations, using a splitting algorithm to decouple velocity and pressure, with the aim of obtaining a reliable and fast solver whose performances are independent of the Reynolds number and the polynomial degree used for the approximation.

MAURICE HOLT

Review of Godunov Methods

Godunov's method for solving unsteady problems in Gas Dynamics is described and discussed at length in the second edition of my monograph "Numerical Methods in Fluid Dynamics", which appeared in 1986. In the succeeding decade several extensions of the method have been proposed which increase its accuracy to second order while retaining the properties in the original method of Monotonicity and absence of oscillations in shock capturing. The contributions most clearly related to the first Godunov scheme, notably by Colella and Woodward, Roe and van Leer are reviewed and

added to the earlier account. At the time of writing the monograph, these contributions had either not been completed or not yet recognized as Godunov extensions. The revised chapter in this book (to appear as a third edition) will include these extensions and the present report is a preliminary version of this coverage.

The extensions treated specifically are the MUSCL (Monotonic Upstream-centered Scheme for Conservation Laws) scheme of van Leer, the Piecewise Parabolic Method (PPM) of Colella and Woodward and the characteristic based scheme of Roe. This report firstly deals with these methods as originally presented. Thus PPM is described only in application to the unidirectional wave equation, with indication of its extension to the Eulerian Gas Dynamic Equations. The MUSCL scheme, as developed by van Leer is applied to the one dimensional Lagrangian equations. Roe's scheme, freer than the other schemes of algebraic details, is presented in general form. In a further discussion of extensions the methods in question are treated in a more general manner, with attention given to their connection with Godunov methods. The MUSCL scheme was proposed as an extension of the original Godunov scheme by requiring unknowns in successive computational cells to be varying linearly across each cell rather than the constant. In this way the scheme was upgraded to second order accuracy. The PPM scheme claimed to attain third order accuracy by permitting quadratic rather than linear variation of unknown across each computational cell. The Roe scheme does not require specification of variation in the unknown within each cell and is adapted to the use of approximate solution of Riemann problems rather their exact analytic solutions. All the extended Godunov schemes claim to satisfy the monotonicity requirements and a discussion follows of the relation between this and the requirements of TVD (Total Variation Diminishing) and ENO (Essentially Non-Oscillatory Schemes). Finally an updated explanation of the Random Choice version of Glimm's scheme by Wiglin is given.

All the above extension of Godunov methods to second order accuracy are based on shock capturing. In consequence they are complex, especially in terms of maintaining satisfaction of the monotonicity condition. It would be useful to investigate shock fitting schemes, updated, for example, from Godunov's second scheme, as alternatives.

GRAHAM HORTON

Numerical Solution of Markov Chains

Markov chains are an important tool in the reliability and performance modelling of computer and other technical systems. They are represented by a large indefinite system of equations, or alternatively, as an eigenvalue problem often with tens or hundreds of thousands of degrees of freedom. Since Markov chain solvers are integrated into interactive modelling tools, there is substantial motivation for fast solution methods. Following the development of our original multi-level method in 1993, we have concentrated on improving and refining the algorithm and on experimental evaluation for various classes of Markov chains known from the literature.

During two visits to ICASE in March/April and in August 1994, research into the new multi-level solution algorithm for Markov chains developed last year at ICASE was pursued. The original technical report was accepted and presented as a full paper at the SIGMETRICS conference at Nashville in May. It was shown that the multi-level scheme can be put into correspondence with a classical multigrid method in which the inter-grid transfer operators become solution-dependent.

Experimental evaluations of the method using adaptive smoothing and applied to nearly decomposable Markov chains were carried out and the method was found to perform very well in both cases. Both have been submitted to the forthcoming Numerical Solution of Markov chains conference in January 1995. We are currently investigating the combination of the multi-level scheme with the iterative aggregation method of Koury, McAllister and Stewart, which carries a greater promise of parallelism and superior efficiency in a paged virtual memory environment. Journal versions of these studies are in preparation.

Four directions for future research are envisaged. We intend to test the scheme on reliability models of the type used to model complex aerospace systems. The applicability of the approach to PDEs will be studied, in particular in cases where solution values are constrained to lie within a bounded interval. Parallel implementation of the scheme, already performed at Erlangen University, will be pursued on machines of interest to NASA Langley. In addition, the application of a multi-level approach to the simulation of more general stochastic processes will be considered.

LELAND JAMESON

WOFD Applied to Combustion

The wavelet-optimized finite difference (WOFD) method is a numerical method which mimics the good part of a full wavelet method while avoiding the pitfalls. That is, wavelet methods when viewed from the physical space have a finite-difference equivalent. WOFD uses wavelets in their finite-difference form thereby facilitating evaluation of nonlinear terms and implementation of boundary conditions, which are, by the way, the two most difficult issues encountered when one considers constructing a wavelet-based numerical method which can be applied to a large class of partial differential equations.

In a joint project with T.L. Jackson and M.Y. Hussaini WOFD has been applied to problems in combustion where the challenging issue is resolution of the very thin reaction zone. The numerical results obtained with WOFD are consistent with linear stability analysis and asymptotic analysis, whereas previously published results by others are not consistent.

Future plans are to apply WOFD to more challenging combustion problems in higher dimensions.

Adaptive-ENO and Conservation Laws

WOFD is a numerical method which chooses a grid based on wavelet analysis, and on this wavelet-defined grid one can perform calculations with point values. For conservation laws, on the other hand, a wavelet-based mechanism similar to that used by WOFD can be applied to choose cells instead of grid points. On this adapted set of cells one can apply ENO.

In a joint effort with R.B. Bauer this type of adaptive ENO method was applied to the simple test problem of the inviscid Burgers' equations with periodic boundary conditions. The initial condition is a sine wave such that a moving shock develops. In short, the the adaptive ENO achieved the same answer, the maximum pointwise difference was .0001, as the uniform-cell ENO while only using 7 sec of CPU time whereas the uniform-cell ENO used 173 sec of CPU time.

Due to the remarkable savings in CPU time, research into applying the adaptive ENO in higher dimensions is under way and will continue.

DAVID A. KOPRIVA

Spectral Multidomain Methods for Compressible Flows

Multidomain methods for the solution of compressible flows that have been developed to date do not yet have all the features that would be desirable for a general method: Geometric flexibility, conservation, time accuracy, and efficient parallelization. Our old method was developed for steady-state problems and is limited to first order accuracy in time. It is geometrically flexible, but complex topologies would require complex coding to treat the special cases that occur at the intersections of multiple subdomains. Those special cases also inhibit parallel efficiency because of communication of corner point information. Finally, the method is not conservative, which is necessary if shocks are to be captured. We have been developing a new family of multidomain spectral methods for compressible flow problems that will have the desired features that are now lacking. The new method is based on a staggered grid, analogous to fully staggered grids often used in finite difference methods. In the spectral case, however, the solutions are defined at the nodes of a Gauss quadrature rule, while the fluxes are evaluated at the nodes of a Gauss-Lobatto rule. In the multidomain context, the fluxes, but not the solution unknowns, are needed at interfaces. This allows the use of flux vector splitting or a Riemann solver to determine the characteristic decomposition. In two space dimensions, the method does not include (the Gauss rules being open) the corners of subdomains. The staggered grid concept has many advantages. First it is conservative, even through subdomain interfaces. Thus, it should be possible to apply shock capturing techniques to the approximation. As in a finite volume scheme, only flux values, not derivatives, are required at interfaces. This allows discontinuous (and even singular) changes in the Jacobians of the mappings between the subdomains and the unit square on which the approximation is actually computed. Since fluxes are only required at faces and not at corners, the coding of the method has no special cases at corners, so any number of subdomains can meet at a point. Thus, geometric flexibility is obtained. The interface condition can be computed to the same temporal accuracy as are the interiors. Finally, communication between subdomains is only through faces, which means (in 2D) that there are at most four neighbors. This should enhance the parallel efficiency over the old collocation scheme where a subdomain could have up to eight communicating neighbors in two space dimensions.

HEINZ-OTTO KREISS

Asymptotic Multiple Time Scale Analysis of Compressible Homogeneous Turbulent Shear Flows

A recent analysis of compressible homogeneous turbulent shear flows has revealed new small scale structures which are qualitatively different from those found in incompressible flows. An understanding of these differences will serve to improve future subgrid-scale models. In particular, one finds a system of waves whose fronts lie at a shallow angle with the streamwise direction. These form a system which couples pressure and dilatation which is probably controlled by a one-dimensional wave equation.

We have developed an asymptotic development of the Navier-Stokes equations specialized to homogeneous shear flows valid on a long time scale. This was necessary since the spatial structures results were in a structural equilibrium. To lowest order we find that the Navier-Stokes equations

are unchanged except for the removal of the pressure gradient in the streamwise direction (in a coordinate reference frame in which the flow appears to be exactly homogeneous). Furthermore, scalings appear in the direction normal to the shear which indicates that the flow has a qualitatively different behaviors in that direction.

We propose to conduct some numerical simulations of these reduced set of equations and compare the results with the DNS of the full Navier-Stokes equations. If the results are comparable, the reduced set of equations will serve as a point of departure for further analysis.

R. W. MACCORMACK

Development of a Low Dissipation Flux Vector Splitting Method

Numerical dissipation is an essential ingredient in all stable numerical procedures. Excess numerical dissipation, above that required for maintaining stability, is a destruction mechanism affecting solution accuracy. Flux-vector and flux-difference vector splitting procedures introduce dissipation through the use of upward difference approximations. Some procedures introduce too much dissipation and are unsuitable for use in the solution of the Navier-Stokes equations where viscous effects are important and can be masked by numerical dissipation.

A flux vector splitting procedure has been developed that limits numerical dissipation to regions containing pressure gradients only. Density, velocity and energy gradients, by themselves, introduce no numerical dissipation. Numerical dissipation will be strong at shock waves and weak within boundary layers and across contact discontinuities. Numerical production of entropy should be small.

The procedure will be tested in a two dimensional Navier-Stokes computer program for calculating the flow about sphere-core bodies at supersonic speeds. The results will be compared with other known solutions to assess the performance of the new procedure.

ROBERTO MARSILIO

3D Shock/Vortex Interaction

The interactions between 3-D shock waves and vortices are fundamental fluid dynamics problems, (these are a simple prototype of a shock/turbulence interaction). Shock/Vortex interactions, like shock/boundary layer interactions or the vortex breakdown problem in the compressible domain are just two examples of the fundamental and practical importance of this subject. There has been very little research conducted on this topic and, consequently very little is known about the interactions of shock waves and 3-D vortices. Therefore, in order to gain a better physical understanding of the phenomenon and to provide a numerical data set that can be used for turbulence modelling, a numerical study, in collaboration with G. Erlebacher, has been initiated.

The numerical procedure developed is based on the time-dependent integration of the Euler equations. The governing equations written in the quasi-linear form are integrated using a 6th order compact scheme (for the spatial derivatives) and a 4th order Runge-Kutta scheme for the time integration. A three dimensional shock-fitting procedure has been developed in which the shock is

seen like a moving internal boundary separating the two contiguous , upstream and downstream, regions.

Future work will consist to validate the code using appropriate analytical/numerical solutions. The final goal of this work is to better understand the behaviour of the turbulence with particular regard to the shock-turbulence interaction.

DIMITRI MAVRIPLIS

Unstructured Multigrid Techniques for the Navier-Stokes Equations

The overall objective of this work is to develop efficient solution procedures for the Navier-Stokes equations on unstructured meshes involving low memory overhead and with eventual application to parallel machines.

Multigrid methods offer a promising approach to achieving rapid convergence of the Navier-Stokes equations without incurring large memory overheads. For unstructured meshes, the construction of coarse mesh levels is non trivial. A first approach operates on a set of non-nested coarse and fine meshes, and transfers variables between the various meshes of the sequence using linear interpolation. This non-nested multigrid approach has been demonstrated for the three-dimensional Reynolds-averaged Navier-Stokes equations (using a single field equation turbulence model) on high-lift swept wing configurations with very fine grids of 2 million points or 10 million tetrahedra. Convergence to steady stage for such cases can be obtained in 200 to 400 multigrid cycles, which can be performed in 1.25 hours using all 16 processors of the CRAY-C90.

Although the non-nested multigrid approach has proved successful from a numerical standpoint, the requirement of generating multiple coarse grid levels for a single solution is cumbersome. The agglomeration multigrid approach relies on a graph algorithm to automatically construct coarse level graphs given an initial fine mesh, upon which governing equations are discretized and solved. The coarse agglomerated grids are no-longer simplicial grids, and alternate discretization techniques must be considered. Similarities of the agglomeration technique with algebraic multigrid techniques have been investigated as well. For the 3D Euler equations, convergence rates of the agglomeration multigrid algorithm which are competitive with the non-nested unstructured mesh multigrid algorithm have been demonstrated. These rates are also competitive with the best structured multigrid Euler codes available. For the two-dimensional Navier-Stokes equations, the agglomeration multigrid has been shown to converge only slightly more slowly than the corresponding non-nested unstructured mesh multigrid algorithm. The agglomeration multigrid work is done jointly with V. Venkatakrishnan.

The agglomeration algorithm is being incorporated into a 3D Navier-Stokes solver. Additionally, better coarsening strategies for highly stretched meshes and anisotropic equations are being investigated. Further similarities between the agglomeration and algebraic multigrid approaches will be investigated, and a more algebraic formulation of the current approach will be sought.

LISA MESAROS

Multidimensional Fluctuation Splitting Schemes

In the past few years a substantial effort has been put into the development of a truly multi-dimensional upwind method for approximating solutions to systems governed by hyperbolic conservation laws, specifically the Euler Equations. The goal is to develop a scheme that will have the same success in two and three dimensional flows as that obtained in one-dimension via upwind Riemann Solvers. The latest direction of the project is to incorporate preconditioning techniques that decompose the system of equations into canonical forms, similar to those of Ta'asan. In breaking the system into convective equations and a wave-like elliptic system, appropriate distribution schemes can be used for each. This work is done under the direction of Phil Roe (University of Michigan).

While at ICASE, much of my time was spent working with Bram van Leer (University of Michigan), Eli Turkel (Tel Aviv University) and Chang-Hsien Tai (Chung Cheng Institute of Technology, Taiwan) on the development of more robust preconditioners that provide the necessary equation decoupling. Problems with the original van Leer-Lee-Roe preconditioner caused by the extreme sensitivity of the preconditioner to the streamline direction in near stagnation point regions was overcome, with the development of a new family of preconditioners. The importance of this in the context of multidimensional schemes is that the new preconditioner which determines the distribution of fluctuations within grid elements, does not change rapidly between adjoining cells thus hindering convergence. With the new, more robust decoupling, a numerical model was implemented and several test cases analyzed. The cases computed consisted of flow over a NACA0012 airfoil at freestream Mach numbers ranging from 0.01 to 1.2. The solutions obtained demonstrate the low numerical dissipation generated by the scheme in smooth regions coupled with its ability to sharply capture non-oscillatory shocks even when lying oblique to the grid.

We plan to continue along the current path with further analysis being done for the discrete scheme used to approximate the elliptic system representing the acoustic behavior in subcritical flow. Although accurate solutions are being obtained, convergence is still slow. A detailed study in collaboration with Shlomo Ta'asan on the use of a Lax Wendroff scheme to solve an elliptic system, such as the Cauchy-Riemann equations, will be performed in hopes of achieving better convergence rates while maintaining accuracy.

ERIC MORANO

Coarsening Strategies for Unstructured Multigrid Techniques with Application to Viscous Flows

The following work was done in collaboration with Dimitri Mavriplis and V. Venkatakrishnan.

When solving the equations that represent viscous flows, such as the Navier-Stokes equations, it is important to take into account the presence of a boundary layer and/or other phenomena associated with the flow such as vortices. The use of a very fine and very stretched grid is part of the requirements for a correct discretization of the equations on the domain to be studied. The use of such grids lead to extremely long time of computation. One cure may be the use of multigrid methods. Yet, multigrid methods have shown limitations when used with very stretched grids.

Indeed, the gain in performance is generally much lower than in the case of inviscid flows and the difficulties remain in the production of the different coarse grids, assuming that the initial fine grid is fine enough to represent the flow. Therefore, the purpose of this work is to analyze and to cure the loss of performance of the multigrid scheme and to propose an easier and faster way to produce grids of good quality in order to restore an "ideal" convergence rate.

In order to simplify the approach, it has been decided first to work on the Laplace equation on a square:

$$\begin{cases} \Delta u = 0 \\ \text{with } u(0, y) = 1, u(x, 1) = 2, u(1, y) = 3 \text{ and } u(x, 0) = 4. \end{cases}$$

Two types of discretization have been considered: a finite-volume formulation on quadrangular unstructured meshes and a finite-element Galerkin formulation on triangular unstructured meshes. A weighted Jacobi relaxation is used as a smoother/solver:

$$U^{\alpha+1} = U^{\alpha} - \omega D^{-1}(AU - f)$$

In our case U is the solution vector, A is the matrix resulting from the discretization, D its diagonal, and f is equal to zero. The work focuses on the Galerkin formulation, the transfers between the grids are linear interpolation for the solution and the corrections, and linear distribution for the residuals. Since the purpose is not to optimize the relaxation parameter ω , it is arbitrarily chosen equal to 0.85. It has been decided to perform 2-grid experiments rather than multigrid experiments: in this case the coarse grid is converged up to a residual value of less than 10^{-10} . Two-grid experiments represent the ideal behavior toward which a multigrid code must tend, since the coarse grid is completely converged resulting in completely damped low frequency error modes. Various meshes have been produced from regular non-stretched meshes to highly stretched Chebyshev meshes. In the case of regular non-stretched meshes, the best strategy to produce a coarse grid is to apply a full-coarsening method where the overall number of nodes is decreased by a factor 4. In this case, with 1 Jacobi sweep on the fine grid per cycle, a convergence rate of 0.33 was achieved. For stretched meshes, however, a regular full-coarsening method results in a slow convergence rate equal to 0.88. A method used to cure this problem is the use of a semi-coarsening algorithm. In spite of the increase in complexity of a basic cycle (20 %), the convergence rate may be proved equal to 0.41, resulting in a much more effective algorithm. In the case of a 1-directional stretching, with a constant aspect-ratio, a semi-coarsened mesh is easily obtained from the fine mesh by removing every second vertex in the normal direction to the stretching. Yet, when the distribution of nodes in the normal direction is no longer linear but exponential, removing every second vertex will only locally improve the quality of the mesh, and, in some area, will even worsen the aspect ratio. Actually, stretched meshes lead to a discretization where the value of the matrix coefficient is very low when associated to the stretching direction, resulting in a poor dissipative scheme. A usual semi-coarsening tends to correct this problem by increasing the value of this coefficient on the coarse grid. Hence the idea of a coarsening code. The coarsening procedure relies on the value of the matrix coefficient. It is decided to remove the neighbor (in terms of connectivity) of a selected node that has the highest value of its associated matrix coefficient. This procedure results in a semi-coarsening method, in the sense that every second vertex is eliminated, hopefully in the direction normal to the stretching. An algorithm developed by V. Venkatakrishnan, for his

agglomeration technique, is modified. It relies on a distance function for selecting the nodes to be kept in the coarse mesh. This algorithm has produced a coarse grid in the case of regular stretched meshes almost identical to the grid where every second vertex is removed “manually”, hence an identical convergence rate of 0.41. The more versatile characteristic of this code, compared to a manual coarsening, provides a coarse grid for any kind of mesh. This code was used on a grid where the distribution of nodes in the direction normal to the stretching is exponential. In this case the resulting convergence rate, although not tremendously better than the one obtained with a manually coarsened mesh (0.46), was obtained equal to 0.43. In the case of Chebyshev meshes where no manual semi-coarsening can be achieved, the algorithm has resulted in a coarse grid that once used in the multigrid solver achieved a convergence rate of 0.35, to be compared to 0.73 achieved with a fully coarsened mesh.

The main feature of the coarsening algorithm is that it should be capable of generating optimal coarse meshes for any type of initial fine mesh. Therefore, it is interesting to use this algorithm in order to provide the sequence of grids needed for unstructured computations. Yet, a new difficulty arises in this particular case. Indeed, the set of nodes resulting from the coarsening algorithm has to be re-triangulated. A very robust re-triangulation method relies on a Delaunay triangulation. This triangulation has already proved its effectiveness in the case of meshes used for inviscid flows, where the overall aspect ratio of the triangles is very close to 1. In the case of stretched meshes this approach is generally not satisfactory and another criterion must be used in order to build the new triangulation. This difficulty could also be avoided by the use of an agglomeration technique. When this difficulty is overcome then this technique may be applied for solving the Navier-Stokes equations or any equations requiring stretched meshes with very high aspect-ratio.

IJAZ PARPIA

Fractional Step Methods on Unstructured Meshes for Incompressible Flow

The objective of this work is to develop efficient fractional-step schemes with finite-difference and finite-volume spatial discretizations on unstructured meshes for the simulation of viscous incompressible flows.

In order to minimize storage requirements, a face-based data structure is used, and the flow variables are co-located at the vertices of the mesh. It is well known that naive discretizations on unstaggered structured grids leads to odd-even decoupling in the pressure solution. A similar problem carries over to unstructured-mesh schemes whenever the Laplacian in the Poisson equation for the pressure is differenced in a manner consistent with the discretization of the pressure gradient in the momentum equation. An effective way to overcome this problem is to relax the requirement of consistent differencing, which is equivalent to the addition of an artificial source term in the discrete continuity equation. A method using this approach has been developed and tested.

The codes developed during this study will be extended to simulate non-Newtonian fluid flow, including time-dependent fluids such as polymers and biological fluids.

JAMES QUIRK

Large Realistic Simulations of Shock Wave Phenomena

Two detailed computational studies were conducted so as to shed light on fundamental shock wave phenomena that are not fully understood. One study examined the interaction of a planar shock wave with an isolated gas inhomogeneity that took the form of a cylindrical bubble (work with S. Karni, NYU), while the other looked at the reflection of a detonation wave from a ramp (work with J.E. Shepherd and R. Akbar, CALTECH).

The shock-bubble interaction is representative of a mechanism that has been proposed to ensure rapid mixing of air and fuel in supersonic combustion systems. The present numerical results reveal several subtleties of the interaction process that were not apparent from earlier experimental work. It also exposes flaws in recently proposed analytic models for the amount of vorticity produced by a shock-bubble interaction. This study has been written up and will appear as an ICASE report.

The numerical study for the reflection of a detonation wave highlights the phenomenological complexity of reactive fronts and thus far it has raised more questions than it has answered. However, progress is being made and soon it is hoped that this study will bridge the gap between current theories and experimental observations.

Both of the present numerical studies faithfully reproduce the complex mechanisms that have been observed experimentally. Given the disparate physical scales involved, this would not have been possible without the use of a sophisticated adaptive mesh refinement algorithm. Previous simulations in the literature were under-resolved and so prone to misinterpretation. The resolution of the present fully-resolved simulations has, however, exposed slight weaknesses in modern shock-capturing schemes and so work is planned to see if these weaknesses can be removed.

ROLF RADESPIEL

Multigrid for Chemically Reacting Flows

Previous work on the solution of the Euler and Navier-Stokes equations for a calorically perfect gas indicated that the combination of multigrid algorithms and explicit multistage time stepping schemes is effective for both upwind and central-difference spatial discretizations. However, many external aerodynamics problems and internal flows require to model the relevant chemical reactions which often yields stiff systems of equations. The appropriate numerical treatment of the source terms within the framework of existing multigrid methods and an assessment of the benefits of multigrid for flow problems with strong chemical reactions is the objective of the present work.

In order to overcome the stiffness introduced by strong chemical source terms some implicit treatment of these terms is needed. Hence we have rederived the elements of the Jacobian matrix of the source terms with respect to all conserved flow variables for generalized chemical reactions. The treatment of strong source terms within a multigrid algorithm is studied with a newly developed 1-D code for reacting mixtures of air and hydrogen. Various chemical models have been simulated which range from dissociating air to a 9 species model for reacting air and hydrogen. Point-implicit treatment of the source terms is used so that the time step is evaluated according to the fluid dynamics wave speeds, only. Our numerical results confirm that current practice in NASA's

existing multidimensional combustion codes, which is to neglect the partial derivatives of the source terms with respect to temperature is valid in smooth flow regions with combustion. In contrast, the complete Jacobian is needed for efficient computation of flows where significant chemical reactions are initiated by shock waves. Using a combination of simple explicit multistage time stepping schemes and standard multigrid, converged flow solutions for supersonic hydrogen combustion were obtained within less than one tenth of the iterations needed by the single-grid computation. The computational saving by multigrid is a factor of about 4 which is obtained for first and second order spatial discretizations. Multigrid computations for test cases with shock-induced dissociation of oxygen are underway. These additional test cases have been chosen to represent typical reentry aerodynamics problems. The work has been done in collaboration with R.C.Swanson and R.Gaffney from NASA.

Our future plans include a study of the benefits gained from preconditioning the reacting flow equations in order to cluster the speeds of acoustic and convective waves. This is a well-known means to improve the damping characteristics of multistage schemes used as the smoother in the multigrid algorithm. Use of the aforementioned 1-D multigrid code seems appropriate here in order to better understand the effects of preconditioning at strong shocks.

CHI-WANG SHU

High Order Methods for Shocks

High order methods are important for problems with both discontinuities and rich smooth region structure. We study such methods both theoretically and numerically.

Jointly with Harold Atkins at NASA Langley, we are starting the project of applying the discontinuous Galerkin finite element method, analyzed by Cockburn and Shu since 1989, to computational fluid dynamics and computational acoustics problems. The first step is to obtain a testing code for second order scheme solving the Euler equations. The structure of the code will be carefully studied to maximize performance. Jointly with Gordon Erlebacher and Yousuff Hussaini, we are continuing our investigation of shock vortex interaction problems. Results of shock fitting, linear theory and shock capturing approaches are being compared.

Research will be continued for high order methods in finite difference, finite elements and spectral schemes.

DAVID SIDILKOVER

Genuinely Multidimensional Scheme for the Compressible Euler equations

The search for the genuinely multidimensional schemes for the compressible Euler equations was motivated mainly by the expectation that such schemes will provide a possibility to construct very simple, robust and efficient steady-state multigrid solvers.

Some high-resolution genuinely two-dimensional schemes for scalar advection were developed already several years ago. Their remarkable property is that the Gauss-Seidel relaxation, which is a very efficient and simple smoother, is stable when applied directly to the resulting discrete equations. However, extending the genuinely multidimensional approach to the systems of equations

appeared to be a difficult problem. Finally, such a scheme for the compressible Euler equations was developed. Gauss-Seidel relaxation is stable when applied directly to these high-resolution schemes. This allowed us to develop a very simple and efficient multigrid steady-state solver.

Future plans include further improvement of the constructed solver's efficiency. Another future direction is to extend this approach to the steady-state compressible Navier-Stokes equations. The extension of the multidimensional scheme suitable for solving time-dependent problems is planned as well.

RALPH SMITH

Implementation of Distributed Parameter Control Techniques for Structural Acoustic Systems

The success of PDE-based control techniques for reducing vibration and noise levels in structural acoustic systems has recently been demonstrated both theoretically and through extensive numerical simulations. In the applications under consideration, unwanted noise is generated by a vibrating structure, and control is implemented through the excitation of surface-mounted piezoceramic patches which generate in-plane forces and/or bending moments in response to an applied voltage. The modeling, development and implementation of control methods using this technology in structural acoustic systems is being investigated in collaboration with H.T. Banks (North Carolina State University), D.E. Brown, V.L. Metcalf, R.J. Silcox (Acoustics Division, LaRC) and Y. Wang (Brooks Air Force Base).

A current focus of this research involves the development of techniques for experimentally implementing the resulting PDE-based control methods. Initial efforts have centered around the estimation of physical parameters and implementation of control in a structural system involving a circular plate with surface-mounted piezoceramic patches. A specific issue being considered in the parameter estimation studies concerns the modeling and effect of "almost" clamped boundary conditions since perfectly fixed boundary conditions are impossible to obtain in laboratory situations and physical applications. The implementation of control has involved the development of an effective state estimator which reconstructs the state from strain or acceleration measurements at isolated locations on the plate. This reconstructed state is then used in the feedback loop to determine appropriate controlling voltages to the patches. Initial experiments performed in the acoustics laboratory have demonstrated a significant reduction in vibration levels in response to the controlling voltage and we are currently working to refine these results and extend the techniques to the case involving persistent excitation of the plate.

Upon completion of the experiments involving the circular plate, we will begin experiments with a hardwalled structural acoustic system with a vibrating plate at one end. We will also continue extending the analysis and numerical techniques to models in which the structure enclosing the acoustic cavity is a vibrating shell.

HILLEL TAL-EZER

K-Spectra and Non-normal Matrices

Spectrum analysis is an essential tool in applied mathematics and engineering. When the matrix is normal, the spectrum of a matrix is the domain in the complex plane which plays an essential

role in the analysis and behavior of related algorithms. It is well known that when the matrix is far from being normal, eigenvalues do not tell all the story and in extreme cases can be misleading. In this present research we address the question: what is the right domain in the complex plane one should consider when dealing with non-normal matrices. Knowing the right domain, we would be able to develop efficient algorithms for solving large-scale systems iteratively and to choose the most suitable time-step in time-dependent algorithms.

Mathematical simulation of engineering and industrial problems, frequently results in the need to deal with finite-dimension operators (matrices). A set of $n \times n$ linear or non-linear equations maybe the most frequently addressed problem. Another example is the numerical solution of ODE's or PDE's. When designing an algorithm for these problems one should carry out a careful analysis of the related matrices. It is known that the knowing the domain in the complex plane which includes all the eigenvalues of the matrix is not enough in the non-normal case. In the present research, we have shown that for non-normal matrices, one should consider a domain which is larger than the spectra and smaller than the field of values of the matrix. The domain depends on a parameter k and thus, we name it K-SPECTRA. We were able to prove that the widely used, general purpose, iterative algorithm GMRES(k), stagnates if and only if zero is in the K-SPECTRA.

We will continue researching the K-SPECTRA. We have observed, numerically, that polynomial approximation of functions of matrices can be characterized by the quality of approximating the scalar function in the K-SPECTRA. We would like to try to prove it. Based on this deeper understanding, we are planning to develop an efficient, general iterative algorithm which would not suffer from stagnation.

CHRISTOPHER TAM

Computational Aeroacoustics

Computational aeroacoustics (CAA) is a relatively new sub-area of research. The primary objective is to solve aeroacoustics problems, in the sense of providing an understanding of the noise generation mechanisms and the prediction of the intensity and characteristics of the radiated sound field, by computational methods. Development of CAA is of interest to NASA. The nature and characteristics of aeroacoustics problems are distinctly different from those of the traditional aerodynamics and fluid dynamics problems. Because of this, methods developed for computational aerodynamics and standard CFD are not necessarily suitable for aeroacoustics problems. Our work is to provide a critical review of the computational issues relevant to aeroacoustics. The review is to become the core part of an invited paper entitled "Computational aeroacoustics: issues and methods" to be presented at the AIAA Aerospace Sciences Meeting, January 1995.

Aeroacoustics problems are, by definition, time dependent. Usually they involve very large bandwidth of frequencies. The magnitude of the radiated sound is, however, very small; many orders of magnitude smaller than that of the flow field which generates the noise. These characteristics are the basic cause of many of the computational difficulties encountered at CAA. The following are some of the computational issues relevant to CAA which we have identified: (1) Large spectral bandwidth, (2) Acoustics mean-flow disparity, (3) Long propagation distance (numerical dispersion and dissipation), (4) Nonlinearity, (5) Distinct and well separated length scales, (6) Radiation and overflow boundary conditions, (7) Wall boundary conditions.

Computational methods and boundary treatments specifically designed to address some of the above issues have been developed during the last several years. Our effort on methods development will continue. At the same time, applications of those newly developed methods to important aeroacoustics problems, such as supersonic jet noise, fan jet inlet noise and airframe noise are anticipated to begin real soon.

ELI TURKEL

Preconditioning Methods

For inviscid flow the speeds of the waves are u and $u + c$. For high Reynolds flows the viscous terms do not appreciably change this situation. For low speed flows, or near stagnation points u is much smaller than the speed of sound, c and so there is a large difference between the speeds of the different waves. This results in the use of a time step that is appropriate for some of the waves in the system but not others. In addition to low speed flow there are many problems that contain both high speed and low speed regions within the same problem. One example is a low speed nozzle with transonic flow at the throat. Another example would be low speed aircraft at a high angle of attack. In all these cases it is necessary to use the conservation form of the equations while still being able to handle low speed flow.

We introduce a preconditioning matrix which changed the time history of the flow. In particular we multiply the time derivatives by a nonsingular matrix. When the Euler equations are written in symmetric form the preconditioner should also be symmetric and positive definite or at least symmetrizable. The purpose of the preconditioner is to change the eigenvalues of the system (speed of the waves) so that they are as equal as possible. At a Mach number of zero it is possible to equalize all the speeds through the use of a preconditioner. However, the condition number of the system will always be infinite at the sonic line. It is possible to choose the preconditioner so as to reduce the rate at which the condition number approaches infinity. In addition we change the form of the equations so that we now update the continuity equation for the pressure rather than the density. This enables the code to resemble an incompressible code in the limit of zero Mach number.

This preconditioning has been implemented in both the two dimensional and three dimensional versions of the central difference Runge-Kutta schemes. With these modifications we are able to solve for the inviscid flow around a NACA0012 at a Mach number of 0.01 with convergence rates similar to that of transonic flow. Similar results were obtained for viscous flow about a RAE airfoil using a Baldwin-Lomax turbulent model. In both cases the convergence rate for transonic cases was not reduced and in some cases even improved. Finally the changes were made in TLNS3D and similar improvements in both convergence rate and accuracy were obtained for inviscid flow about an ONERA M6 wing at very low Mach numbers

Future work will stress the inclusion of viscous effects in the preconditioner. We also hope to apply the code to three dimensional viscous problems.

BRAM VAN LEER

Stability of Preconditioned Euler Schemes in a Stagnation Point

Local preconditioning of the Euler equations designed to equalize the characteristic speeds has been used to obtain a number of desirable properties in discrete schemes: faster convergence to steady solutions, preservation of accuracy for low Mach numbers, decoupling of the equations as needed for fluctuation splitting, and optimal high-frequency damping as needed for multi-grid relaxation. There are two distinct classes of preconditioners in use today: those derived from the symmetric Van Leer-Lee-Roe matrix and those derived from the asymmetric Turkel matrix. The symmetric preconditioner has the advantage that it decouples the convective from the acoustic equations; its disadvantage is that it appears to lead to instability or lack of convergence near a stagnation point. This makes it impossible to obtain steady Euler solutions on all but the coarsest grids, if a stagnation point is present in the flow.

In order to overcome this instability we looked for a cause in the form of undesirable limit values of certain matrix elements for $M \rightarrow 0$, and then searched through a large family of matrices for a member that did not have this flaw. This work was done in close collaboration with Eli Turkel, Chang-Hsien Tai and Lisa Mesaros (all at ICASE) and Jeff White (NASA). It turns out that, among all preconditioning matrices that achieve the optimal characteristic condition number, there is no symmetric matrix that has the proper limit form for $M \rightarrow 0$; one has the choice between switching to Turkel's matrix or a sub-optimal symmetric matrix. In the latter case the lowest characteristic condition number one can achieve for slow flow is 2.

Numerical experiments by Tai with a structured flux-based finite-volume code showed that the sub-optimal symmetric preconditioner allows the computation of low-speed airfoil flow solutions previously unattainable. Mesaros experienced the same with her unstructured multi-dimensional fluctuation-split scheme. There are still some robustness issues related to the use of conservative variables and the lack of dissipation near stagnation points; these probably can be treated with an adjustment of the artificial dissipation similar to Harten's "entropy fix". Extension to three dimensions appears straightforward, but numerical tests have not yet been carried out.

JOHN VAN ROSENDALE

Floating Shock-Fitting by Lagrangian Adaptive Refinement

There are two basic approaches to computation of compressible flows, shock-capturing and shock-fitting. Shock-capturing, in which one applies a well chosen difference scheme throughout the flow field, is effective and reliable. However, such schemes smear shocks over several mesh cells, limiting the accuracy and resolution obtainable.

The alternative is shock-fitting, in which the shocks are treated as internal boundaries in the flow across which one applies the Rankine-Hugoniot jump conditions. Shock-fitting algorithms can achieve an arbitrarily high order of accuracy, though properly locating shocks is difficult, especially for flows containing complex embedded shocks.

In recent work we formulated a new approach to compressible flow simulation, combining the advantages of shock-fitting and shock-capturing. Starting with a MUSCL-style discretization based on Roe's approximate Riemann solver, we warp the mesh to align cell-faces with shocks and other

discontinuities. Since Roe scheme imposes the exact Rankine-Hugoniot jump conditions on edges aligned with shocks, the result is effectively a shock-fitting scheme. However, since we retain a conservative Roe scheme discretization, this is also still a “shock-capturing” algorithm, retaining the robustness and generality of the “shock-capturing” approach.

Our algorithm has now been validated on a sequence of two dimensional problems, including generation of N-waves from airfoils of various shapes. Using a new variant of the Van Albada limiter, we achieve second order accurate solutions without clipping extrema, and with perfectly sharp shocks. On supersonic airfoil problems, these sharp shocks are retained all the way to the far-field boundaries, unlike most CFD algorithms, which diffuse weak shocks over many mesh cells. Moreover, extension of this algorithm to 3D is straight forward. This will be our next step, since calculation of the sonic boom profile of supersonic aircraft is an important practical problem we should be able address.

V. VENKATAKRISHNAN

Solution Techniques for Unsteady Flow Simulations over Complex Geometries

Solution algorithms for time-accurate computations in aerodynamics have lagged behind those used for computing steady flows, especially on unstructured grids. For many physical time-dependent phenomena of interest, such as aeroelasticity and buffeting, the time steps allowed by explicit schemes are much smaller than the physical time scales of interest. The purpose of this work is to devise efficient implicit algorithms that allow for arbitrarily large time steps. This allows the time step to be chosen purely based on the flow physics. This work is being done jointly with Dimitri Mavriplis.

We have shown earlier that the agglomeration multigrid strategy can be used to solve for steady flows over complex geometries in two and three dimensions. The approach adopted here is to use the agglomeration multigrid as an inner loop at each time step. This implicit scheme does not suffer from storage requirements associated with implicit schemes that solve linear systems. Hence, we expect this method to be readily extendable to three dimensions. After discretizing the time derivative using 3-point backward differencing, the resulting system of nonlinear equations is solved by using the agglomeration multigrid strategy. For time-dependent flows, after discretization in space, one obtains a system of coupled ordinary differential equations, coupled through the mass matrix. Thus, even with an explicit method, one has the formidable task of inverting the mass matrix. It is not clear if the technique called “lumping”, whereby the mass matrix is replaced by an identity matrix, preserves second-order accuracy in space. In our framework, however, we are able to accomplish the inversion of the mass matrix indirectly during the multigrid procedure. In fact, we have found that the convergence of the system is enhanced when the mass matrix is included. We notice, however, that the solutions obtained with the mass matrix and the lumped mass matrix exhibit only slight differences. We allow for movement of the control surfaces in airfoil-type geometries to enable us to simulate phenomena, such as flutter and flap-deployment.

We are currently studying algorithms for adapting the mesh to large scale motion of the control surfaces. Mechanisms to add and delete grid points are also being considered. Incremental agglomeration algorithms, which are efficient when the grid changes only in a local region, are being investigated.

FLUID MECHANICS

ALVIN BAYLISS

Numerical Study of a Flexible Surface Excited by Jet Noise

J. L. McGreevy, L. Maestrello and I are studying the role of jet noise in exciting a flexible surface such as an aircraft panel. The goal is to model panel vibration and the ensuing acoustic radiation in response to panel excitation by jet noise. The primary emphasis at present has been on the role of sound generated from instability waves in the jet as a mechanism for panel excitation. Our methodology is to solve the nonlinear Euler equations on both sides of the panel. On one side of the panel the flow field includes the jet flow exiting from a nozzle while on the other side of the panel we solve the Euler equations without any imposed flow field.

In progress to date, we have computed both the panel response and the resulting acoustic radiation into the far field for an assembly consisting of two flexible panels connected by a rigid extension. We have determined the spectral content of the incident pressure on the panels and on the reflected pressure. We have also shown that the location of the panels relative to the jet exit is crucial in determining panel response. An ICASE report on this work has been written and submitted a journal.

In the future, work is to be extended to account for the forward motion of the jet. We will consider both jets in uniform motion and jets in accelerated motion. We are also considering the effect of multiple panels.

Numerical Study of Acoustic Radiation from a Flexible Surface

A. Frendi, L. Maestrello, J. Robinson and I have studied the problem of plane wave excitation of a flexible panel at or near a resonant frequency. We consider this problem in three dimensions. The goals of this research are (i) to determine nonlinear modes of panel response, (ii) to determine the effect of acoustic damping on panel response and radiation and (iii) to compare with experimental measurements. The problem is solved by coupling the nonlinear Euler equations describing the near and far field radiation to an equation for the evolution of the flexible surface. The pressure difference across the surface acts as a source term. The far field acoustic pressure can exhibit nonlinear effects.

In previous work we have studied this problem in two dimensions. We have determined bifurcations from linear to nonlinear response and exhibited windows of quasi-periodic behavior. This has resulted in an ICASE report which has been accepted for publication in the Journal of Sound and Vibration. Results have also shown that details of the panel fabrication can lead to significant differences in the nonlinear response of the panel. At present we are performing detailed comparisons with experiments.

In the future we plan to consider techniques to control the panel response, and to quantify the effects of nonlinear wave propagation on the far field acoustic response.

STANLEY A. BERGER

Vortex Breakdown

Vortex breakdown is the name given to the sudden change in the structure of a tightly wound vortex with a significant axial velocity component, often characterized by the appearance of a stagnation point on the axis. It arises in various vortical flow situations, ranging from aerodynamic to industrial, and its effects may correspondingly be beneficial or harmful. Among the harmful effects are degradation of aerodynamic performance and structural integrity of high-speed high-angle-of-attack aircraft. Potential benefits are the increased rate of dissipation of the trailing vortex wake behind large transport aircraft- and the resulting ability to lower aircraft separation at congested airports- and the confinement, and, or, mixing of chemical reactants in chemical reactors and mixers. In spite of decades of theoretical and experimental investigations, the basic mechanism causing breakdown is still elusive. Numerical simulations, all using finite-differences, have not resolved the issue, in part since they are controversial because the breakdowns that are calculated have a very pronounced tendency to move up to the first computational cell, thereby raising the issue of the validity of the simulations. We have been trying to uncover the origin of this phenomenon so as to allow valid calculations of breakdown to be carried out.

We have developed a model of breakdown based on the Navier-Stokes equations simplified appropriately for the physics of breakdown. Analysis of these equations shows that in spite of the apparent strongly parabolic nature of the problem, there is a subtle ellipticity introduced by the normal momentum equation. To allow analysis, a still further simplified model was developed. Analytical and numerical solution of this model exhibits the phenomenon of upward migration of the breakdown and the source of the difficulty, suggesting ways in which it might be overcome. (This work was done with Dr. Gordon Erlebacher.)

Our future plans include extensions of this model. We have also been validating the model by comparing it with the database from a full Navier-Stokes simulation of breakdown provided to us by R.E.Spall and T.B.Gatski. We are also doing full numerical simulations of breakdown using a code for the full Navier-Stokes equations developed by G.Kuruvila and M.D.Salas.

Turbulence Modeling

We have been considering the problem of modeling the interaction of turbulence with a free surface. This would have potential application to a wide variety of problems in fluid mechanics. Most of the existing modeling of this interaction has used the Reynolds-averaged Navier-Stokes equations, and various models of different degrees of complexity to account for the turbulent stresses. None of these agree quantitatively, or even fully qualitatively, with measurements. In particular, and most importantly, in general they do not capture the reverse energy cascade-energy moving from larger to smaller wave numbers-that is known to result from the interaction of the turbulence with the two-dimensional free-surface. A large-eddy simulation does not correct this difficulty, since neither the traditional Smagorinsky model nor the more recent dynamic subgrid-scale models for the subgrid-scale stresses in LES correctly reproduces the reverse energy cascade. We have been looking at approaches that might correctly capture this phenomenon.

Together with Charles Speziale, I have been evaluating, in the context of a Reynolds-averaged Navier-Stokes equations approach, the use of the very recent algebraic stress model of Gatski and

Speziale. This model is far superior to the standard k-epsilon model and shows great promise for modeling complex turbulent flows. We are investigating the use of such a model, in either its original form, or with slight modifications, in a RANS calculation of turbulence/free-surface interaction. We are also looking into the use of LES for this problem, in particular how to extend the work of Gatski and Speziale to obtain an explicit algebraic expression for the full subgrid-scale stress tensor, in the hope that this may model complex turbulent flows in a LES simulation more accurately than does a simple Smagorinsky-type model.

MICHAEL BOOTY

Modulation of a Fast Flame

The one-dimensional unsteady propagation of a deflagration wave which has a Mach number $M = O(1/E)$ can be described by a leading order asymptotic model in the limit of large activation energy, $E \gg 1$. The reactants are premixed and the reaction rate is strongly dependent on the temperature, with a dependence given by the Arrhenius factor $\exp(-E/T)$.

This flame structure is subsonic but fast compared to the diffusional-thermal category. Asymptotic methods based on the largeness of E are used to resolve the structure of the narrow flame zone, which is then replaced by a discontinuity across which jump conditions must be satisfied by small-amplitude variations in the (outer) flow field away from the flame. For the fast flame considered, the outer equations are the semilinear hyperbolic system of reactive acoustics, and must be solved numerically. Variation of the flame's propagation speed arises from its interaction with "sound" waves and the effects of weak chemical activity ahead of the flame. At some instant, a singularity forms in the small-amplitude outer equations and propagates, indicating the birth of a different class of wave which may take the form of an unsteady weak detonation.

Numerical studies were made for the case where the flame is situated between a piston, which drives the flow, and a preceding, reactionless shock wave. The effect of parameters and initial conditions, particularly temperature profiles immediately ahead of the flame, on the flame speed, singularity path, and type of singularity were considered. In the future, different physical configurations will be studied, in addition to the consideration of different Mach number-activation energy regimes and multidimensional effects. This work has been done in collaboration with J.F. Clarke of Cranfield Institute of Technology.

THOMAS M. BROWN, III

Counterflow Diffusion Flames

Work continues on the investigation of counterflow diffusion flames as models of turbulent, non-premixed H_2 - Air reaction zones. Further investigations are required due to deviations from flamelet theory. Investigations continue to use the NASA LaRC developed opposed jet burner (OJB) which is capable of producing controllable stretched laminar flamelets.

This work includes both experimental and numerical investigations. Species and temperature measurements along with extinction measurements have been taken in the OJB and 1-D stretched laminar flame simulations have been calculated and compared. Recent work has also included

velocity measurements of the OJB made at NASA LaRC using laser doppler velocimetry (LDV) and particle imaging velocimetry (PIV). These measurements are currently being analyzed and compared to 1-D simulations.

Unsteady stretch is currently the topic of much investigation in the combustion community because of its relevance to turbulent diffusion flame modeling. Several recent modeling efforts have been made but as yet no experimental results have been presented. We are currently developing an unsteady flow system to enable investigations of unsteady stretch in the opposed jet burner configuration.

DAVID A. CASTANON

Multidisciplinary Design Optimization Research

This research was conducted with Sanjoy K. Mitter. Multidisciplinary Design Optimization (MDO) is an interdisciplinary approach aimed at producing improved airframe designs which capture the performance requirements and constraints imposed by diverse disciplines such as structures, aerodynamics, controls, acoustics, electromagnetics and computational fluid dynamics. The basis for MDO is to use high-performance computing to create an environment where appropriate tools and models representing the required design expertise in the various disciplines can be integrated into a general design and analysis framework.

The purpose of our visit to ICASE was to become familiar with NASA Langley's work on MDO, and to identify opportunities for collaborative research and make suggestions for further development of their research. In particular, we tried to understand how control design issues could be incorporated in current work on MDO. Our primary point of contact at NASA was Dr. Tom Zang. During our visit, we held numerous technical discussions with Dr. Zang, we reviewed NASA's FIDO project, and held discussion with Dr. Sobieski, Dr. Neuman and the Flight Dynamics and Controls group.

As the result of our visit, we have a better appreciation of why it has been difficult to merge control design ideas into MDO approaches. We have prepared a brief document summarizing our views about MDO for Dr. Zang and Dr. Hussaini.

THOMAS C. CORKE

Use of Glow Discharge Actuators to Excite Helical Mode Instability in the Boundary Layer on a Cone at Mach 3.5

The objective of this work is to develop an experiment to study boundary layer instabilities at high Mach numbers in which the disturbance initial conditions are known, and which quantitative measurements of the spatial disturbance field can be made for a direct comparison to theory or computation. The method for introducing disturbances must be capable of exciting helical mode pairs of equal-opposite wave numbers, with controllable wave angles, frequencies and initial amplitudes. The measurement technique must be capable of measuring time-resolved fluctuations in temperature (T) and mass flux (ρU) at different spatial locations within and outside the boundary layer. Lastly, the experiment needs to be run in a low-disturbance environment so that the input disturbance levels needed to overcome background fluctuations can be small enough to satisfy

the linear instability assumptions. To accomplish these objectives we selected as a basic flow the boundary layer on a 7° half-angle cone with a sharp tip. The cone is a hollow, thin-walled design which is instrumented with 20 pressure ports and thermocouples for documenting the basic flow characteristics ($\bar{T}(x)$ & $\bar{P}(x)$). The tip of the cone is removable. Located downstream of the tip is an azimuthal array of 30 glow discharge actuators. Their position in the flow direction (x) places them upstream of Branch I of the linear neutral-growth curve for the most amplified frequencies in the operation-range of stagnation pressures. The number and spacing of the actuators is designed to be able to excite helical mode pairs with angles which bracket the range of most amplified. For spatial measurements, a 3-D traversing mechanism was designed. The traverse mounts on the sting arm which holds the cone. It is motorized for three axis of motion (wall-normal, y , axial, x and azimuthal, γ). The traverse holds a hot-wire sensor. The hot-wire would be traversed through the boundary layer to sample different spatial positions. At each of these, different overheat settings would be used to decompose the voltage fluctuations into the fluctuating components of T and ρU .

All of the experiment is controlled by a digital computer which simultaneously outputs the voltage time series to excite the glow actuators, acquires the voltage time series from the hot-wire, controls the traversing mechanism and hot-wire overheat.

The size of the cone and traverse were designed to be placed inside the nozzles of the Mach 3.5 and Mach 6 "quiet" supersonic tunnels at NASA LaRC. These are the only facilities which have disturbance levels which are documented to be low enough for controlled instability experiments.

The experiment was conducted in the Mach 3.5 flow over a period of 2 weeks. It represented a number of milestones. It was the first time that an array of actuators would be used in any supersonic flow, and it was the first time a traversable hot-wire would be placed near a model in this facility. The first objective was to determine if the tunnel would "start" (i.e., if a supersonic flow could be established in the nozzle) with the presence of the cone and traversing mechanism, and remain started at the stagnation pressures used to set the instability conditions which dictated the design of the actuator array. In the initial runs, we found that we were not able to start the tunnel. The problem was that the location of the vertical strut which supports the cone sting in our initial configuration, caused the bell-mouth inlet to the tunnel diffuser to be placed too far from the exit of the nozzle. A considerable effort was made to improve the design of the nozzle, but none of these modifications proved to be sufficient. Finally, the location of the vertical was moved upstream on the sting. This required the machining of an adaptor sleeve. This modification reduced the distance between the nozzle exit and diffuser bell-mouth by 50%. With this change, the tunnel easily started.

Under the started condition, the traversing mechanism was fully tested and proved to work well. Also the hot-wire sensor proved to be durable and work well. The glow discharge actuators were tested in two configurations. The first was with no flow. In this case, the pressure in the tunnel was lowered to the value of the static pressure over the cone at Mach 3.5. Under this condition, the 30 actuators performed perfectly. With flow at Mach 3.5, we were also able to operate the actuators, but found them to require more power than in the static case. Investigating this more closely, we found a large build-up of static charge on the cone. By design, the cone was electrically isolated from earth ground in order to reduce the potential for the glow actuators to arc to the cone body. The static charging of the cone body was an unforeseen problem. We focused on possible passive methods to dissipate the charge (which could reach several hundred volts). These involved

connecting the cone body to earth ground through various resistive and capacitance networks. None of these proved completely satisfactory.

We will be looking at various active approaches to dissipate the static charge build-up on the cone. We have planned the next experiment to be conducted in October in the Mach 6 facility. At this Mach number, we expect to primarily focus on the second mode instability. These measurements are expected to be performed over a period of 4 weeks. The processing of the hot-wire time series is expected to take approximately 3-4 months. Here we will focus on determining linear amplification rates and streamwise and spanwise wave numbers for comparisons to linear stability estimates. We will also run conditions with large enough initial amplitudes to lead to the nonlinear regime and possibly transition to turbulence. For these, we will also investigate different nonlinear models for transition. The next entry in the tunnel is expected to follow that period.

WILLIAM O. CRIMINALE

Initial Value Problems to Shear Flows

The central topic of research dealt with initial-value problems in shear flows. This means well established basic flows are subjected to prescribed disturbances at an initial instant and the ensuing dynamics are to be determined. The strategy employed was not that of classical normal expansions but rather a combination of analytical and numerical means for solution. For the analytical work, modeling of the basic flow was involved; the numerics dealt directly with the integration of the governing partial differential equations. The results provide explicitly both the early period transients and the long time asymptotic behavior of any perturbation. With this knowledge it is then possible to devise means for flow control and it is possible to either delay or enhance disturbances as the need may be.

Three classes of problems were probed using the strategy outlined: (1) three-dimensional vortex, (2) family of free shear flows consisting of the jet, wake, and mixing layer, (3) viscous channel flows. The basic vortex investigated is one that is under favorable or adverse strain and is a non-parallel flow. Complete closed form solutions for three-dimensional perturbations to this problem were found and the full dynamics determined. The free shear flows are those that can be examined in an inviscid fluid, thereby allowing some simplification in the system. Here it was possible to significantly delay the perturbations in both the jet and wake but enhancement in the mixing layer was only marginally feasible. Viscous channel flows were examined under a large class of possible perturbations, including two and three-dimensional inputs, sub-critical and critical disturbances, and even Reynolds numbers up to one million. In this problem, as indeed the other two as well, the details of the flow field are important to understanding the dynamics. Most notably the perturbation vorticity plays a large role.

Future plans will include viscous pipe flow and the very important boundary layer. The first problem has remained an enigma in such studies but is known from experimental observations to break down. The boundary layer is a greater challenge because the questions of receptivity and bypass transition are major central issues in the general field of fluid mechanics.

All work was done in collaboration with T.L. Jackson and D.G. Lasseigne.

ANDREW DANDO

Wavenumber Selection for Small-Wavelength Görtler Vortices in Curved Channel Flows

Following the success of phase-equation methods in predicting pattern formations for convection problems, these ideas have now begun to be applied to boundary layer instabilities. This joint work, with Prof. Philip Hall, is an initial study on wavenumber selection for Görtler vortices. The ultimate objective of this work is to provide a theoretical explanation for effects, such as vortex splitting/merging and deformed vortex structures, which have been observed in experimental work.

We assume that the phase variable of these Görtler vortices varies on slow spanwise and time scales. Carrying out an asymptotic analysis of the flow we obtain, in addition to the governing nonlinear equations for the vortex, a partial differential equation for the vortex wavenumber via a second order solvability condition and the phase conservation equation. We also consider the effects, on the structure of the vortices, of the outer wall varying on the same slow spanwise scale as the vortex wavenumber.

This study is to be submitted as an ICASE report when numerical work on the wavenumber P.D.E. is completed.

A. O. DEMUREN

Pressure Diffusion in Non-Homogeneous Shear Flows

Reynolds stress models are required for calculating turbulent flows in which body forces are important or the anisotropy of the turbulence field plays a dominant role, such as flow in streamwise corners. In the development of Reynolds stress models the assumption of homogeneity is made, but very close to a wall the turbulence is highly inhomogeneous, so that such models are not valid. The objective of the present work is to develop and validate models based on the elliptic relaxation concept which will allow Reynolds stress models to be integrated all the way down to the wall in many practical flows.

A non-local model is presented for approximating the pressure diffusion in calculations of turbulent free shear and wall boundary layer flows. It is based on the solution of an elliptic relaxation equation which enables local diffusion sources to be distributed over lengths of the order of the integral scale. The pressure diffusion model was implemented in a boundary layer code within the framework of turbulence models based on the k-e-v2 system of equations, and also full Reynolds stress equations. Model computations were performed for mixing layers and wall boundary layer flows. In each case, the pressure diffusion model enabled the well-known free-stream edge singularity problem to be eliminated.

The model will now be applied to predict free-stream turbulence effects in flat plate and curved boundary layers, and to the general problem of relaxation of turbulent shear layers after reattachment or removal of curvature.

PETER DUCK

The Effect of Three-dimensional Disturbances on the Supersonic Flow Past a Wedge

In this study, the work of Duck, Lasseigne & Hussaini (ICASE report 93-61) is being extended into the three-dimensional context. The effect of small amplitude three-dimensional freestream disturbances (which may take the form of acoustic, vorticity or entropy waves) on a shock wave attached to a wedge in a supersonic flow is being considered, the aim being to understand the flow downstream of the shock wave. This work is joint with Drs. Hussaini and Lasseigne.

The investigation is strongly suggesting that disturbances can be amplified downstream, leading to an unstable flow situation, with the shock location and associated physical flow quantities becoming unbounded, at least within the linearized stability analysis employed. Indeed, somewhat independent, linearized stability analysis confirms this possibility. This situation is markedly different from the two-dimensional situation considered previously, in which what may be regarded as somewhat fortuitous, cancellations lead to boundedness of all physical quantities.

The plan is to extend this work to include detonation waves, using simple, but well-tested chemistry models. We also plan to extend some computations that have been made involving flows past cones with attached shock waves to detonation waves.

GORDON ERLEBACHER

Direct Numerical Simulation of a Turbulent Supersonic Boundary Layer

The high Reynolds number supersonic turbulent boundary layer is an important stepping stone for the development of compressible turbulence models. High quality data is required to calibrate new algebraic and second order turbulence closures. This data will also serve to elucidate some of the physical mechanisms in turbulent boundary layers for the development of more sophisticated models.

The 5th order code of M. Rai has been modified to simulate the development of a spatial turbulent boundary layer $M = 2.5$ flow with no embedded shocks. Viscous terms are discretized with a symmetric stencil. The free-stream is modeled as a symmetry plane, so that we are really simulating a very wide channel. Compressibility effects allow us to consider a boundary-layer of $Re_\theta = 6000$. Wall blowing and suction provide the mechanism via which the flow quickly transitions to a turbulent state. Turbulent statistics are only considered sufficiently downstream of the transition transients. Initial results indicate the presence of a log wall layer. Profiles of Reynolds stress across the boundary layer qualitatively agree in shape and value with incompressible experimental results.

The code is undergoing parallelization to run on the SP-2 at NASA Langley. This will permit a simulation at a higher resolution to be performed which is necessary to fully resolve the smallest scales of the flow, and extend the physical domain sufficiently downstream to insure that the memory of the transition region has been erased

JAMES GEER

Periodic Basis Functions with Built-In Discontinuities

Series expansions of functions, such as Fourier series, perturbation series, etc., are often useful in developing numerical or semi-numerical, semi-analytical algorithms for the solution of differential equations. However, when only a partial sum of such as series is used, some “undesirable” effects (such as the Gibbs phenomena) may be present, or the partial sum may have “difficulty” approximating certain features of the solution, such as boundary layers, internal layers, or various discontinuities.

Several new classes of periodic basis functions which have “built-in” singularities have been defined and some of their fundamental properties have been studied. In particular, it has been shown that, for a certain class of functions $f(x)$, the combination of a finite sum of these functions, along with a finite Fourier series, leads to sequence of approximations which converges exponentially to f , even though f may have a finite number of discontinuities. In particular, these approximations eliminate the Gibbs phenomena.

These new (basis) functions will be studied within the context of developing some “new” spectral methods for systems of ODE’s and PDE’s. In particular, they will be applied to several model problems which either have discontinuities in the initial data and/or develop discontinuities (or “near-discontinuities”) as time increases.

Hybrid Pade-Galerkin Techniques

The practical usefulness of perturbation solutions to physical problems are often limited, either because the expansion parameter has to be restricted to “very small” values, or because the solutions are not uniformly valid. In addition, the radius of convergence of perturbation series is sometime determined by mathematical singularities which are not relevant to the physical problem of interest (e.g., singularities corresponding to *complex* values of the expansion parameter may limit the convergence of the series, but these singularities may have no direct physical “meaning”).

A three-step hybrid analysis technique, which successively uses the regular perturbation expansion method, the Pade expansion method, and then a type of Galerkin approximation, is being developed and studied. Currently, it is being applied to several model problems which develop boundary layers as a certain parameter becomes large. These problems involve ODE’s, PDE’s, and integral equations. In particular, the technique appears to simulate these boundary layers by producing approximate solutions with real or complex singularities which lie just outside the domain of interest.

The hybrid Pade’ Galerkin technique will be applied to and studied in the context of some ODE’s and elliptic PDE’s which develop internal layers, as well as boundary layers, and also to two classes of integral equations of the first kind.

SHARATH S. GIRIMAJI

Scalar Dissipation Model for Use in LES of Turbulent Scalar Mixing

Large Eddy Simulation (LES) is a possible means of computing complex turbulent flows of mixing and reaction. One of the major terms that needs closure modeling, in this approach, is the

mean scalar dissipation. Efforts to develop a model for this term began in the last half-year and continued through this half-year. This work is being performed with Y. Zhou of ICASE.

Using the successive subgrid elimination procedure, closure expressions for the distant interaction type terms and backscatter terms in the mean scalar dissipation are being developed. This model represents a major improvement over models currently used, which only account for the distant-interaction terms and even that in a very approximate manner. A paper of the above title has been completed and submitted for publication.

Future plans, in this area, include further refinement of this model and development of closure expressions for other terms that need modeling using the same procedure.

Modified Restricted Euler Equations for Turbulent Flows with Mean Velocity Gradients

In order to better understand the turbulence energy cascade and other small scale phenomena (including scalar mixing), we need a better understanding of the behavior of fluctuating velocity gradients. This project is also continued from the last half-year and is being performed in collaboration with C. Speziale.

A dynamical system of equations for the velocity gradients has been developed from the Euler equations. This equation, called the 'Modified restricted Euler equation', has been analyzed numerically. Preliminary results indicate that the model captures several features of the velocity gradients known from the direct numerical simulations of anisotropic homogeneous turbulent flows.

Detailed comparison with DNS data of anisotropic turbulent flows is being planned. The ultimate goal is to utilize this equation to develop better models of small-scale processes in turbulence.

Role of the Velocity Field in Turbulent Scalar Mixing

Despite the reasonably rapid progress made recently in the field of turbulent scalar mixing, the effect of the velocity field on this process is not well understood. The understanding of this effect is important for accurate modeling of turbulent mixing and, hence, merits a detailed study.

This study is just underway. Scalar-mixing DNS data is being analyzed to yield valuable insight into the process. The study is rendered difficult by the rather large statistical variations in the DNS data.

A strategy to overcome this difficulty and glean useful results is being planned.

CHESTER E. GROSCH

Numerical Experiments in Stability and Transition

The velocity field created by shallow bumps or hollows on surfaces are of interest as a means of creating transition or modifying the transition process by interacting with Tollmien-Schlichting waves. I had previously analyzed the results of some experiments designed to study these velocity fields. The object of the current research is to numerically simulate the flow field generated by a shallow bump in a boundary layer.

This work has been carried out with R.D. Joslin. Using a code provided by him we have been simulating this flow. In particular, the spanwise spectrum of the disturbance showed the rapid growth of a low wavenumber component. The simulation used a 661 by 61 by 20 grid. The disturbance was imposed using linearized boundary conditions at the wall, periodic spanwise

boundary conditions and a no-disturbance free stream condition. Calculations were carried out until the domain had reached steady state. Preliminary analysis of the results show good qualitative agreement with the experimental results including velocity profiles of u in the normal and spanwise directions and the downstream evolution of the spectrum of u . The low frequency component grows although the total kinetic energy decays outside of the neighborhood of the bump. The v and w components are large near the bump and decay rapidly with x . There is a transfer of energy between the components as well as between the spanwise components of u .

Quantitative comparisons of the experimental and computational results are being carried out. We hope to extend the computation by simulating the interaction of a TS wave with the bump. This can be done by introducing a 2-D or 3-D TS wave at inflow of the domain. In addition to the computations, this could also be done experimentally as an extension to the GGJ experiment. These computations and experiments should increase our understanding of the interaction of TS waves with surface imperfections and guide further theoretical developments such as the importance and treatment of nonparallel effects. The effect of bump shape and size should also be examined, but this may not be possible.

PHILIP HALL

Phase Equation Approach to Boundary Layer Transition

Transition to turbulence in boundary layers is a highly nonlinear process. Several modes of instability are possible and boundary layer growth causes the local wavenumber or frequency of a disturbance to evolve. The aim of this project is to provide a rational framework for the description of the processes involving wavenumber changes associated with the breakdown of TS waves and the splitting/merging of vortices.

The evolution of fully nonlinear wave or vortex systems in a fluid flow can usually only be described by Navier Stokes simulations. The calculations are computationally intensive and often can only be carried out by making an assumption of periodicity in one or more of the spatial variables. A phase equation approach to such problems typically reduces the computational task by an order of magnitude and enables nonparallel effects to be taken care of in a rational manner. The approach also shows how ad-hoc numerical methods such as PSE can be made less arbitrary by the derivation of a wavenumber evolution equation. We have shown that monochromatic waves in subsonic and supersonic boundary layers are always modulationally unstable. Thus for example there is no such thing as a stable 2D TS wave in a boundary layer flow. We have also shown that some TS waves are subcritically unstable in supersonic flows.

The work will be developed further for supersonic flows and three-dimensional modulation equations for three-dimensional flows will be found. The methods will also be applied to inviscid instability problems.

PAUL HAMMERTON

Propagation of Sonic Booms Through Stratified Atmosphere

Accurate predictions of shock overpressure and shock rise-time are important in determining the subjective annoyance of sonic booms produced by supersonic aircraft. The shock structure for propagation through a stratified viscous medium has been investigated using asymptotic methods, but for a real atmosphere it is believed that relaxation effects associated with internal vibration of polyatomic molecules plays an important role in determining the shock structure. Since relaxation times for air are highly sensitive to the presence of moisture, the relative humidity of the atmosphere is likely to have a significant effect on shock rise-times.

A governing equation is derived taking account of exponential density stratification, the effect of relaxation processes and the cylindrical spreading associated with a supersonic body in freespace. In general the shock rise-time is small compared with the overall pulse duration, and hence an analysis based on the method of matched asymptotic expansions is possible, at least when a single relaxation mode dominates the medium. It is well-known that in a relaxing medium, shocks can either be fully-dispersed, that is the whole profile is controlled by relaxation processes, or partly-dispersed in which case relaxation alone is insufficient to support the shock, and a narrow sub-shock arises controlled by other mechanisms such as thermoviscous diffusion. For propagation through a stratified medium, it is found that even when only one relaxation mode is present, the evolution of the shock profile can be very intricate. In particular it is found that the structure of the relaxation shock can change from fully-dispersed to partly-dispersed, corresponding to the appearance of a shorter width scale within the shock. During this visit to ICASE, attention was focussed on obtaining numerical results covering regimes when the shock region is narrow as well as regimes when the shock may start to thicken. Ideally any numerical scheme should be able to resolve the narrow shock regions to allow detailed comparison with asymptotic theory. This has now been accomplished, and the drastic changes in shock rise-time, predicted by asymptotic theory, are confirmed numerically.

For air, relaxation modes associated with the internal vibration of both O_2 and N_2 are significant. Asymptotic theory for multiple relaxation modes runs into serious problems, in that the leading order shock description can only be obtained numerically. The code now developed can easily be modified to include more relaxation modes, and work is in progress towards obtaining predictions of shock overpressure and shock rise-time for real conditions. In the long term, the goal of this project is to extend the analysis to allow for more realistic variations of atmospheric density stratification. In this case the ray paths must be determined numerically, before the variation of the shock structure is analyzed.

M.S. HOWE

Studies Related to Airframe Noise

An important component of airframe noise is produced by the turbulent boundary layer flow over the fuselage. Sound is generated directly by "quadrupole" sources in the boundary layer turbulence and transmitted into the cabin and radiated to the sides of the aircraft flight path. In addition, since the fuselage structure typically has an elastic panel with a frame-stringer construction, non-acoustic components of the boundary layer pressure field are *scattered* at structural irregularities

producing both sound and structural vibrations. The sound generated by these mechanisms is a dominant component of the cabin noise of a jet transport in steady cruise.

An analytical investigation is being made of a model problem that exhibits many of the characteristics of the boundary layer-structure interactions responsible for the generation of airframe noise. The model involves a line vortex adjacent to an elastic plate which has a concentrated line discontinuity in mechanical properties. The vortex translates across the discontinuity under the influence of "images" in the plate, and part of the kinetic energy of the vortex flow is converted into sound and plate vibrations as a result of the interaction of the vortex pressure field with the structural inhomogeneity. The sound and structural excitation are being calculated.

It is proposed to use the results of this idealized analysis to validate a numerical simulation of the interaction. Work on this later phase of the project is expected to start in October 1994.

FANG Q. HU

Computational Methods For Aeroacoustics

Accurate and efficient time advancing schemes for acoustic problems have been considered (work in collaboration with M. Y. Hussaini, ICASE, and J. Manthey, graduate student Old Dominion University). For acoustic problems, non-dissipative and non-dispersive properties are desired. It is found that if the traditional third or fourth order Runge-Kutta schemes were used for time advancing in central difference schemes, time steps greatly smaller than that allowed by the stability limit are necessary. An optimization of the Runge-Kutta schemes has been carried out by either reducing the formal order of accuracy for a given number of stages or increasing the number of stages for a given formal order. As a result much larger time step can be used, which increases the computational efficiency. The optimized Runge-Kutta schemes have been applied to the proposed Benchmark Problems (ICASE Workshop, 24-25 Oct.).

THOMAS JACKSON

Instabilities in Various Flows

Due to the projected use of the scramjet engine and the observed phenomenon of increased flow stability at high Mach numbers, the investigation of stability characteristics of compressible mixing layers continues to be an active area of research. All previous investigations on the stability of mixing layers, either reacting or non-reacting, have assumed equal molecular weights for the gases above and below the splitter plate. Furthermore, if the flow is assumed to be reactive, all previous analysis employed a simplified kinetic model consisting of a one-step, irreversible Arrhenius reaction. We are currently extending previous results to determine the effects (i) of multi-component gases and (ii) various reduced mechanisms have on the stability characteristics of compressible mixing layers. This work is in collaboration with C.E. Grosch, D.G. Lasseigne and F. Kozusko (Old Dominion University).

In collaboration with W. Criminale (University of Washington) and D.G. Lasseigne (Old Dominion University), work is continuing on the evolution of disturbances in viscous shear flows. This work offers a means whereby completely arbitrary initial input can be specified and the resulting

temporal behaviour, including both early time transients and the long time asymptotics, can be determined. The bases for the analysis are: (a) linearization of the governing equations; (b) Fourier decomposition in the plane and streamwise direction of the flow; and (c) direct numerical integration of the resulting partial differential equations. This method is currently under investigation for viscous channel flows, and in the near future will be extended to include boundary layer flows.

ASHWANI K. KAPILA

Regularization of Multi-phase Models in Combustion

Combustion of granular materials which gasify during burning is modeled by two-phase balance equations. For the important case of high-speed combustion, where diffusive effects are relatively unimportant, the model is hyperbolic but not in conservation form. Unlike ordinary gasdynamics, a sufficient number of Rankine-Hugoniot conditions are unavailable for the determination of end states behind discontinuities. In fact, one must solve the problem of discontinuity structure (usually a differential system of at least second order) to connect states across discontinuities. This has serious implications for numerical algorithms designed to capture discontinuities, and the present research explores ways in which the governing equations can be regularized (through addition of appropriate dissipative terms involving higher derivatives).

Previous work by Dold and Kapila has given a mathematical description of events that lead to the creation of detonations in initially quiescent materials. This work was confined to situations where energy is released through a single high-activation energy reaction. Preliminary work suggests an entirely different scenario for branched-chain kinetics. The problem is being explored numerically in collaboration with J. Quirk and M. Short.

Propagation of flames through nonuniform media is a fundamental problem in combustion theory. To date the problem has been tractable only for the so-called slowly-varying flames for which the scale of nonuniformities is broader than the flame thickness; the flame then behaves in an essentially quasisteady manner, sensing only the state immediately ahead. In collaboration with T. Jackson and L. Jameson, a numerical study is being undertaken for the important case of nonuniformities whose scale is comparable to the flame thickness. Initially, flame responses to step, pulse, and wavetrain disturbances are being sought.

GLENN LASSEIGNE

Wedge Supported Detonations

This work was done in collaboration with P. Duck and M.Y. Hussaini.

To characterize the response of detonations attached to a wedge apex to disturbances in the freestream or to movement of the wedge itself. Application to the Oblique Detonation Wave Engine is a direct result.

The linearized Euler equations in the region between the wedge surface and the detonation are solved. The boundary conditions applied at the detonation and the wedge surface correspond to known prescribed disturbances and wedge motions. The solution is investigated for parametric trends as well as decomposing the solution to study the different responses of a supported *vs.*

unsupported detonation. The supported detonation is subject to reflections from the wedge surface and is required to be attached to the apex; both make a significant contribution to the far field solution which is quantified and could be compared to numerical solutions.

Identified the normal Mach number behind the detonation as the most relevant parameter to consider in characterizing the response. Identified and quantified the decaying portion of the far field solution and its parametric dependence. Identified a "shadow region for certain wavelength disturbances. Comparisons are also made between response of wedge supported and unsupported detonations and shocks.

To do the full numerical calculations in order to compare finite thickness detonations with the theory which considers an infinitesimal thickness. Also, new work which considers three dimensional disturbances would be an excellent test problem for a three-dimensional numerical code.

Finite Activation Energy Flame Stability

This work was done in collaboration with T.L. Jackson and C.E. Grosch.

To develop the theory for premixed flame stability valid for finite activation energies. Incorrect application of the infinite activation energy results by those doing numerical simulations in the published literature made it essential that this theory be developed so that the correct comparisons can be made.

The equations governing a pre-mixed flame are linearized about a numerically computed steady state. The growth rate of disturbances are computed using the Compound Matrix method and the results are compared to high activation energy results and to published numerical results as well as to new results computed by L. Jameson. These results apply for all Lewis number, and not just for near unity Lewis numbers.

Resolved the discrepancy between numerical solutions and the high activation energy theory by providing the appropriate theory for finite activation energies. Extended theory to all Lewis number.

To add other physical phenomena to the model which affect the stability of flames such as heat release.

Interaction of Vortex and Shock

To develop the code for calculation of the linear theory of vortex and shock interactions (or entropy spots and shock interactions). This would provide a means of calculating the acoustic disturbance analytically to compare with numerical simulations

The Fourier transform of the incoming disturbance is used to calculate the transfer coefficients and thus the Fourier transform of the transmitted disturbance is known. The inverse of the transform is taken by formally (numerically) calculating the appropriate integrals.

Adaptive Mesh Refinement (parallel computation)

To develop the expertise to use the AMR code created by J. Quirk which has been parallelized to run on workstation clusters on the many different problems where mesh refinement would improve the efficiency of the numerical code.

Instability of Reacting Mixing Layers

This work was done in collaboration with T.L. Jackson, C.E. Grosch, and F. Kozusko.

Due to the projected use of the scramjet engine for the propulsion of hypersonic aircraft and the observed phenomenon of increased flow stability at high Mach numbers, the investigation of stability characteristics of compressible mixing layers continues to be an active area of research. All previous investigations on the stability of mixing layers, either reacting or non-reacting, have assumed equal molecular weights for the gases above and below the splitter plate. Furthermore, if the flow is assumed to be reactive, all previous analysis employed a simplified kinetic model consisting of a one-step, irreversible Arrhenius reaction. For a review of past work, see Jackson (1992) and Grosch (1994). The objective of this work is to investigate the effects of (i) multi-component gases and (ii) complex kinetics on the instability characteristics of compressible mixing layers.

The Euler equations are linearized about a mean flow and, assuming a normal mode analysis, the resulting system yields Rayleigh's equation. For the case of a multi-component gas, the gas law takes into account differing gases. For the case of a complex kinetic model, the species equations must be included. Rayleigh's equation is then solved numerically to determine the phase speeds and spatial growth rates. The neutral subsonic phase speeds are determined by the Lees-Lin regularity condition.

Preliminary results suggest that differing molecular weights can have a significant effect on the phase speeds and spatial growth rates of an incompressible, non-reacting mixing layer. In addition, by using certain reduced mechanisms for the modeling of combustion processes in reacting mixing layers, we found that many of the stability features are the same as for the simple one-step model.

We plan to complete the work within the next several months.

The Initial-value Problem for Shear Flows

This work was done in collaboration with T.L. Jackson and W.O. Criminale.

Classical hydrodynamic stability theory has been successful in demonstrating the stability characteristics of any particular shear flow. This is done by assuming a separable normal mode solution in the form of traveling waves and then establishing the existence of at least one unstable eigenvalue. No attention was directed to any particular initial-value or the transient period of the dynamics. This work offers a means whereby completely arbitrary initial input can be specified and the resulting temporal behaviour, including both early time transients and the long time asymptotics, can be determined.

The bases for the analysis are: (a) linearization of the governing equations; (b) Fourier decomposition in the plane and streamwise direction of the flow; and (c) direct numerical integration of the resulting partial differential equations.

Various mean flows have been considered. For jets and wakes, disturbances can be enhanced or delayed depending on the choice of symmetric or asymmetric vorticity initial conditions (Criminale, Jackson and Lasseigne, 1994). For plane Poiseuille and plane Couette flows, transient dynamics for both subcritical and supercritical values of the Reynolds number can be determined.

These concepts will be extended to include Blasius boundary layer. In addition, effects such as compressibility and spatial evolution are also currently under investigation.

Vortex Perturbation Dynamics

This work was done in collaboration with T.L. Jackson and W.O. Criminale.

An initial value approach is used to examine the dynamics of perturbations introduced into a vortex under strain. Both the basic vortex considered and the perturbations are taken as fully three-dimensional.

Instead of seeking stability criteria per se, an initial-value problem is both posed and solved. The results are general can be expressed in closed form, and contain both the early period transients as well as the asymptotic fate of disturbances explicitly. A Green's function approach is developed as well as solving for spatially distributed initial disturbances. The importance of the spatial distribution on the evolution is thus determined.

ALEX MAHALOV

New EDQNM Formulation for Rotating Turbulence

The interest in the effects of rotation is reflected in the large body of theoretical, experimental, and numerical work documenting them. As the effects are both multifold and subtle, the development of models which account for the effects of rotation on turbulence requires an understanding of the processes occurring in these flows.

One relevant issue is the dependence on rotation of the spectral transfer rate of energy from large scales to small scales. Rotation is known to reduce the transfer rate by scrambling the phase coherence necessary for the turbulence cascade to transfer energy to the small scales and to decrease the rate of dissipation of the turbulence. The rotation interferes with the energy-cascade mechanism resulting in changes in the energy spectrum. We have been attempting to describe these processes. We have formulated an EDQNM model for flows subjected to a background rotation. The novelty of the approach is that the EDQNM is applied to the Poincare transformed equations and therefore neglecting the Coriolis term in the third order moments equations is no longer required to make the problem tractable. This further obviates the need for a heuristic approximation for the effects of rotation in the third order moment equations. The model is consistent with the Orszag (1971) EDQNM description of non-rotating turbulent flows.

We plan to compare our model with the EDQNM description of Cambon and Jacquin (1989). We also plan to compare its performance with available experimental/numerical data available for turbulent flows subjected to a background rotation. The work is expected to culminate in an expression for the effects of rotation on the dissipation which can then be incorporated into dissipation equation models. This work is being done in collaboration with R. Ristorcelli and Y. Zhou.

S. R. OTTO

Centrifugal Instabilities in Curved Mixing Layers

There have many been experimental studies of the instability of mixing layers, and some of these articles have concerned themselves with the effect that the centerline's curvature has on the

problem. As the mixing layer curves into the faster stream a longitudinal vortex is found to be a viable mode of instability.

In Hu, Otto & Jackson (In the proceedings of the ICASE workshop, on Transition, Turbulence and Combustion) we discuss the high Görtler number form of this problem and were able to show that the presence of the curvature rendered the situation unstable to spanwise periodic modes. If the mixing layer curved into the slower stream it was shown that the situation is stable to inviscid Görtler modes. With this degree of curvature there was found to be very little effect on the inherent Kelvin-Helmholtz modes. In Otto, Jackson & Hu we solved the parabolic partial differential equations governing the evolution of linear vortices in situations with order one Görtler numbers. As might be expected the vortices persisted for a finite distance downstream and their behaviour was found to depend strongly on the initial conditions which were used. As the calculation advanced downstream the characteristics of the modes coalesced and it is in this régime that it is applicable to use a parallel analysis. One slightly surprising result that was obtained, is that the case in which the mixing layer curved into the slower stream was also found to support the vortices (for greatly reduced streamwise distances and with smaller growth rates). The code still predicted that the inviscid vortices would be stable as in the previous article.

There are many factors which affect the evolution of instabilities. In the near future we hope to be able to deal with the role of compressibility, crossflow, receptivity and nonlinearity. The nonlinear problem will be initially tackled in the far downstream régime, which will allow us to make significant analytical progress.

This work was completed in collaboration with T.L. Jackson, F.Q. Hu, and S.O. Seddougui.

Nonlinear Receptivity of Görtler Vortices

In Bassom & Hall (93-58) the receptivity of Görtler vortices was discussed. It was found, as is to be expected, that the shape of the hump is crucial in determining the form of the mode's linear evolution. The perturbations are shown to grow for a finite downstream distance, and it is likely that during this time nonlinear effects will come into play.

The equations given in Bassom & Hall are solved in order to give the initial conditions for a simulation of the nonlinear problem. The parabolic evolutionary equations are evolved forward using a combination of finite difference and spectral methods.

We hope to be able to determine how various other physical phenomena will affect this mechanism, for example suction and blowing. It will also be interesting to determine the effect that a three-dimensional flow has on the receptivity.

This work was completed in collaboration with A.P. Bassom (University of Exeter, UK).

The Effect of Pressure Gradients and Crossflows on Görtler Vortices

Many flow problems have flows in more than one direction, for example the flow over a swept wing. The flow over a concave plate is known to be susceptible to centrifugal vortices, but the question is how does the flow form effect this?

The pressure gradient is taken to have a form conducive to a similarity solution, and the solutions are given by a Falkner-Skan-Cooke profile. The linear parabolic governing equations are solved numerically and the growth of the modes are tracked downstream. The results seem to indicate that a favourable pressure gradient will enhance the Görtler mechanism, this is in contradiction to

previous parallel flow work. The numerical work is compared with the far-downstream asymptotic structure and agreement is obtained, Otto & Denier (94-19).

The effect that a pressure gradient has on the receptivity of the situation is being studied and also its effect on the nonlinear problem.

This work was completed in collaboration with J.P. Denier (UNSW, Sydney, Australia).

The Secondary Stability of Vortex Structures

As vortex structures evolve downstream they render the flow profile highly inflectional. It is conjectured that this can lead to severe secondary instabilities. Although the vortices evolve spatially we seek secondary temporal instabilities for both Görtler and crossflow vortices.

The underlying vortex states are found from both reduced asymptotic forms of the equations and linearized Navier-Stokes formulations. The resulting flows are analyzed using a secondary instability solver. This involves solving a three-dimensional form of the Rayleigh equation. In Otto & Streett (1994, In proceedings of the ICASE workshop, on Transition, Turbulence and Combustion) we showed that modes obtained from a three-dimensional Orr-Sommerfeld equation are prone to secondary instabilities once they have a suitable amplitude. In Otto & Denier (93-46) we discussed the secondary instability of the most unstable Görtler vortex, and it was found that prior to the nonlinear breakdown of the mode a secondary instability attained a significant growth rate. This particular mode had a significant second harmonic component.

We hope to be able to analyse crossflow vortices obtained from a linearized Navier-Stokes solver and also perform secondary analysis on nonlinear Görtler vortices in three-dimensional boundary layers.

This work was completed in collaboration with J.P. Deneir and C.L. Streett.

The Stability of a Time Dependent Situation

Most of the studies of the stability of spatially evolving layers involve reducing the equations in some manner so that the ellipticity of the problem is somehow removed. In the temporal problem the situation is already parabolic in its evolutionary equation. It has been shown that the so-called Rayleigh problem is prone to Tollmien-Schlichting modes (Otto 93-73), the triple deck approach has been compared with the Orr-Sommerfeld solutions in the régime of common validity, that is high Reynolds number.

In Webb, Otto & Lilley (94-30) the nonlinear evolution of Tollmien-Schlichting modes was discussed. Period fitting techniques were used in order to reduce the cost of the calculation and the inadequacy of the Orr-Sommerfeld equation was demonstrated.

It will be interesting to extend this incompressible problem into the compressible régime and to discuss the associated acoustic radiation.

This work was completed in collaboration with J.C. Webb, G.M. Lilley, and F.Q. Hu.

DEMETRIUS T. PAPAGEORGIOU

Breakup of Liquid Jets and Related Flows

Liquid jets and their stability are fundamental flows occurring in numerous applications. Examples include, but are not limited to, ink-jet printing and related manufacturing processes, materials

processing in both ground and space-based processes, injection and spray technologies, extrusion processes in optical fibre manufacture. It is important to understand the fundamental dynamics which lead to breakup of jets into droplets in order to predict theoretically efficient operational regimes or controls for the systems.

The theoretical approach is a strongly nonlinear stability theory based on two related analyses. Firstly, the physics of breakup indicates an appropriate asymptotic reduction of the phenomenon into coupled nonlinear partial differential systems of simpler equations than the original ones, which are then used to predict breakup which manifests itself as a finite-time singular solution of the equations with the jet radius vanishing at a point in space and time. The local theory provides scaling functions which are used in the continuation of the dynamics beyond breakup by incorporation of overall momentum and mass balance arguments. The second approach, which produces identical results, looks for terminal states of the original governing equations (Euler, Navier-Stokes or Stokes) directly in order to derive asymptotically dominant scaling functions at breakup. The theory has been applied to the breakup of circular jets in air which are an example of a single-phase jet flow.

The theory is fundamental enough to be applied to other problems of industrial interest. The main directions we envision this research to take, is the modification of the dynamics by external agents such as surface active agents or electrical double layers which are of considerable interest in microgravity processing of materials. In addition an extension is under way to include the stability of two-fluid jets where the outer annular fluid can be chosen to control the instabilities of the primary core fluid. We will also model extensions of this theory to compressible fluids with the main application being combustion of mixtures.

Instabilities in Swirling Jets

The objective of this project is to study theoretically the stability of jets which contain a swirl component. This problem has numerous applications but of particular interest is the development of a theoretical basis which can be utilized in the possible enhancement or suppression of fundamental instabilities in fuel/combustion systems for example.

Both compressible and incompressible flows are considered which in their unperturbed state are exact solutions of the three-dimensional Euler equations (they are in fact weak solutions). The stability analysis is carried out in two regimes, linear and nonlinear. The questions of interest in the linear regime include the dominance of absolute or convective instability, effects of the swirl on the stability of the flow and effects of capillary forces on the Kelvin-Helmholtz instability. Nonlinear theory is approached in two ways: first by a strongly nonlinear long-wave approximation and by weakly nonlinear models in the high Mach number limit.

Future work will extend to the analysis of high swirl compressible flows where a vacuum may form at the center and a coupling of instability waves is possible. Another case, which has received little attention is the stability of multi-fluid swirling jets and we also plan to consider such problems.

Nonlinear Stability of Core-Annular Flows and Related Dynamical Systems

Interfacial instabilities in multi-fluid flows manifest themselves in a variety of industrial and natural phenomena. Their study offers a promising interdisciplinary interface between the modeling of such flows with their (in many cases) dissipative nonlinear dynamical systems characteristics. We are considering extensions of well-studied model equations to include physical problems with

additional effects. In particular we are considering the stability of two-fluid viscous flows when the system possesses an underlying background time harmonic forcing; examples are oscillatory two-phase Couette flow and pulstile two-phase core-annular flow.

The theoretical approach is a combination of modeling coupled with numerical experiments using dynamical systems ideas. For instance, extensions of the Kuramoto-Sivashinsky equation to include time-periodic coefficients have led to some interesting results on quasi-periodic routes to chaos. On the linear stability side, we have analyzed the effect of background modulations on growth or decay enhancement of perturbations with a possible view in the control of instabilities by oscillatory modulations. Some mathematical aspects of the Kuramoto-Sivashinsky equation, such as nonlinear modulational stability, have also been addressed.

Future work in this direction will involve more complete numerical studies of the linearized equations of motion of two-fluid oscillatory systems in order to identify parameters which may completely stabilize the system (this has been confirmed in the limit of long waves). An extensive study of Kuramoto-Sivashinsky equations with time periodic coefficients is also envisioned and in particular the inclusion into such systems of dispersive effects which enter due to viscosity differences between the two phases for instance.

J. R. RISTORCELLI

Compressible Turbulence Modeling

Fundamental issues involving the Reynolds stress and $k - \varepsilon$ turbulence models at speeds in which the compressibility of the fluid is important are being studied. Our primary concern is with producing suitable models for the effects of compressibility; the idea being that most of the terms requiring modeling in turbulence closures can be accounted for using incompressible turbulence models and that terms specifically related to compressible effects can be identified and treated independently of the terms already modeled using incompressible turbulence models. These effects include variable inertia effects associated with variations in the mean density, the mass flux, effects due to the non-zero fluctuating dilatation, the dilatational covariances, and changes in the viscosity due to variations in temperature. To date our investigations have focussed on the first two effects.

In this last semiannual period the focus of our investigations in compressible turbulence area has been on the the effects of compressibility as manifested through the fluctuating dilatation. Specifically on the pressure dilatational covariance, $\langle pd \rangle$, which exchanges energy between the fluctuating pressure and velocity fields and the dilatational dissipation covariance, $\frac{4}{3}\nu \langle dd \rangle$, which acts as an additional source of dissipation of the turbulence energy. A substantial portion of the time has been spent developing a theory using ideas from acoustics, singular perturbation theory and statistical fluid mechanics which produces explicit expressions for these quantities.

A "pseudo-sound" aeroacoustic theory has been formulated. In essence small M_t expansion of the equations have been used to produce constitutive relations for $\langle pd \rangle$, $\langle dd \rangle$. These dilatational covariances are found to be functions of the pressure field, its time derivatives, the velocity field and its covariance with gradients of the fluctuating pressure. With only a few of the frequently employed assumptions, homogeneity and quasi-normality, and the assiduous application of the machinery of statistical fluid mechanics, *analytic* expressions can be produced for both $\langle pd \rangle$ and $\langle dd \rangle$. Expressions for both of the unknown covariances in two different and important

flow situations have been obtained: turbulence without a production mechanism and turbulence undergoing an arbitrary three-dimensional mean deformation. Scalings of the phenomena with respect to M_t , k , and ϵ and the mean shear and mean rotation have been found. Constants in the expressions obtained are *specified* by the theory as integrals of functions of the longitudinal correlation.

Future plans in this area are primarily related to the theoretical predictions that have been found over this past semi-annual period. Additional theoretical work is required but most of our endeavours, in this area, will focus on numerical validation of the theory using data-bases of homogeneous compressible flows. Validation will be sought in some of the simpler flows in which experimental data exist. Codes are being modified to test the model and compare it flows such as the mixing layer and the wall bounded flow for which widely differing behavior has been seen. Inspection of the model indicates that it will be able to catch both these behaviors. Our next step, theoretically, will be extending this methodology to flows in which temperature effects are more important.

The 2DMFI Rapid-Pressure Covariance

A variable coefficient rapid-pressure model, referred to in the last annual report, has been completed. The 2DMFI model insures that the modeled equations are frame invariant when the flow is horizontally divergence-free as is required by the Navier Stokes equations. This situation occurs in bounded rotating flows (Taylor-Proudman theorem), in flows two-dimensionalized by stable stratification or small aspect ratio effects (in shallow water flows or vertically confined flows). This is a an issue thought to be of substantial importance in the Reynolds stress computation of any complex flow and particularly those in which rotation, buoyancy or curvature effects are important.

The 2DMFI model is a representation for the rapid pressure covariance that has variable coefficients. The functional dependence of these coefficients is set to insure that the representation is consistent with the differing asymptotic states the turbulence can achieve. The model has been tested in a number of homogeneous flows: it performs quite well and quite robustly.

Future plans in this area are primarily related to the investigation of the 2DMFI's model incorporation into algebraic stress type formulations.

The Round Jet / Plane Jet Anomaly

The inability of a turbulence model to predict the spread rates of both the round and plane jet has never been satisfactorily understood or fully resolved mathematically. A proper turbulence model, constructed in a tensorially consistent way, should not have these problems. The objective of our work is to resolve this anomaly, or at least ascertain that it is not due to a tensorially inconsistent formulation.

In work done with B. Younis it appears that a resolution of the round jet - plane jet spread rate anomaly has been achieved. Physical intuition had suggested that a tensorially correct turbulence transport model may resolve this issue. Reynolds stress computations with a more fundamental model for the turbulent transport appear to have verified this conjecture.

This is work currently in progress the details of which will be more fully developed during this next semi-annual period.

Energy Transfer in Rotating Turbulence

The effects of rotation in substantially modifying the spectral cascade of energy are well known. These effects have never been mathematically understood to the point that a successful parameterization of the effects of rotation have been incorporated in Reynolds stress closure setting.

In work done with A. Mahalov and Y. Zhou an EDQNM analysis of the Poincare transformed Navier-Stokes equations is being undertaken.

Subsequent to the EDQMN analysis it is expected that suitable arguments about the triadic interactions will lead to the scaling analyses sought. From which point the cascades dependence on rotation may be able to be parameterized in a way suitable for Reynolds stress closures.

SUTANU SARKAR

Computation of Sound Generated by Turbulent Flows

Noise generated by turbulent flows is a problem of current interest in aerospace, automotive and naval technology. A hybrid simulation scheme is being developed for noise prediction. In this scheme, the unsteady motion associated with the flow is simulated by large-scale computation and then used to obtain the compact source in an acoustic analogy for the far-field noise. The ability of such a hybrid scheme to predict the acoustic power and frequency spectrum in simple turbulent flows is the subject of ongoing investigation.

The specific problem of sound generated by unforced, isotropic turbulence is being considered with the hybrid method. Direct numerical simulation (DNS) of the flow is performed by a scheme that uses spectral collocation for the space discretization and a third-order, Runge-Kutta scheme for the time advancement. The Lighthill acoustic analogy is used to obtain an integral representation of the instantaneous acoustic pressure and thereby an expression for the acoustic power spectrum. The two-point, two-time covariance that appears in this expression for the power spectrum is directly computed from the DNS data. The results indicate that the frequency at which the power spectrum peaks can be parameterized by the energy-containing scales of motion.

Future efforts in collaboration with Gordon Erlebacher will extend the hybrid simulation scheme to forced isotropic turbulence and sheared turbulence. The ability of large-eddy simulations to provide a sufficiently good approximation of the acoustic source will also be evaluated.

PATRICIA L. SHAH

Boundary Layer-Structure Interaction

Boundary layer-structure interaction is an important component responsible for the generation of aircraft noise. Turbulent boundary layer flow over the fuselage generates sound. The "quadrupole" sources in the boundary layer generate sound, which is transmitted into the cabin and radiated to the sides. Another important source of sound is generated by the non-acoustic components of the boundary layer pressure field scattered at structural irregularities of the fuselage structures. This work is being done with Michael S. Howe.

The boundary layer-structure interactions responsible for the generation of sound were modeled analytically. The model included many of the characteristics of this interaction so that the sound

and structural excitation could be calculated. The model consisted of a line vortex moving adjacent to an elastic plate under the influence of "images". The elastic plate has a concentrated line discontinuity in mechanical properties.

The results from the idealized analysis will be used to validate a numerical simulation of the interaction. The numerical modeling is expected to begin in October 1994.

SIVA THANGAM

Two r-RNG Based Equation Models: Validation

Turbulent separated flows involving shear layers are of common occurrence in physical systems of considerable importance to aerospace applications. The primary effort of the present study is focussed towards the development and validation of efficient two-equation turbulence models based on the recursion renormalization group theory that have the capability to accurately predict turbulent flows of practical importance. In addition, the study will include a formal analysis and development of pressure-dilatation and dilatational-dissipation for compressible turbulent flows.

The limitations in computer capacity and speed often preclude the direct solution of the equations of motion for complex flows of relevance to technical applications. The current practice for high Reynolds number flows of practical interest involves some type of modeling for the turbulent stresses. In this context, the development of two-equation turbulence models that have wide range of predictive capability for separated flows was undertaken from analytical and computational point of view. This is a collaborative work involving Drs. Ye Zhou, R. Ristorcelli and M.Y. Hussaini of ICASE, Dr. George Vahala of William & Mary and Dr. T.B. Gatski of NASA. The work is currently in its third phase during which a recursion renormalization group theory (r-RNG) based anisotropic two-equation model for incompressible turbulent flows which includes the effects of both local and nonlocal interactions was extensively utilized to analyze separated flows as well as plane wakes. The model itself was developed during the earlier phase and validated for the benchmark test case of separated flow past a backward-facing step. During this phase the emphasis was on the development of recursion-rng based near wall representation and flow parameter dependent model coefficients. During this phase, preliminary investigations on the development of pressure-dilatation and dilatational-dissipation for kinetic energy in the equations of motion for compressible turbulent flows have been developed. The expression was obtained based on a perturbation analysis and is found to as an added mass term which can be either positive or negative depending on the local production/dissipation balance. As such the representation gives has different behavior in the shear layers of a wall-bounded flow in comparison to the mixing layer.

During the next phase, the model (which includes the near wall effects as well as flow parameter dependent coefficients for the higher order terms) will be applied to a wide range external and internal flows and validated. In addition, the effort on the development of pressure-dilatation and dilatational-dissipation for compressible turbulent flows will be continued. The modeled form of equations of motion will be implemented in a generalized finite-volume algorithm and applied for shear layers and plane wakes.

L. TING

Structural/Acoustic Interaction Problem

The structural/acoustic interaction problem is essential for the prediction and control of panel fatigue and the transmission of external acoustic waves through panels of an airframe into the interior. Numerical and experimental investigations were carried out for the case where the airframe and the medium are at rest. Studies are being carried out for the case where the airframe is moving at a constant velocity, subsonic or supersonic. We are initiating the analysis for the interaction problem when the airframe is moving at an unsteady velocity, for example, accelerating to or decelerating from a supersonic speed.

In collaboration with Drs. A. Frendi and L. Maestrello of NASA we are developing numerical programs to study the structural/acoustic interaction problem simulating the experiments conducted at NASA. A numerical program for the medium and the panel both at rest was described in ICASE Report No. 93-18. An updated version of this report with additional examples is accepted for publication in the Journal of Sound and Vibration. The numerical program is being extended to allow for the medium to move at a constant subsonic or supersonic speed relative to the panel at rest.

In collaboration with Drs. F. Bauer of Courant Institute, New York University and L. Maestrello of NASA we are carrying out our theoretical investigation on the interaction problem when the airframe is moving at an unsteady velocity. This problem is much more complex because the explicit solution for the wave propagation can only be obtained in the coordinate system $\bar{\mathbf{x}}$ with the medium at rest while numerical solution of the panel oscillation will be much simpler in the coordinate system $\mathbf{x}$ moving with the panel. To study the acoustic field in $\mathbf{x}$, we consider an initial value problem for an acoustic field induced by an unsteady source distribution, $\bar{q}(t, \bar{\mathbf{x}})$ with $\bar{q} \equiv 0$ for $t \leq 0$, in the coordinate system $\bar{\mathbf{x}}$ with the medium at rest. In the coordinate system $\mathbf{x}$, the medium is moving with a uniform unsteady velocity $U(t)\hat{i}$, and signals issued from a point S in the domain of dependence $\mathcal{D}$ of an observation point P at time t , can arrive at point P at time t more than once corresponding to different retarded times, $\tau \in [0, t]$. The number of times of arrival is called the multiplicity of the point S . We are developing rules to define the domain of dependence $\mathcal{D}$ for a given $U(t)\hat{i}$ and partition $\mathcal{D}$ into subdomains of multiplicity one.

Our next step is to prepare a paper describing our theoretical investigations on wave propagation in a medium moving at unsteady velocity. Meanwhile, we are extending our numerical program for structural/acoustic interaction to account for source distribution or the jet noise moving at constant subsonic or supersonic speed relative to the panel. The numerical results can then be compared with the experimental investigations in progress at NASA.

NICK VERHAAGEN

Vortical Flows over Double-Delta Wings

The objective of the research is to provide an experimental data base for the purpose of understanding the behavior of the vortical flow over double-delta wings and for validating Computational Fluid Dynamics (CFD) methods. The data will help to improve the aerodynamic characteristics

of wings to be employed for high-speed and highly-maneuverable aircraft. The research is made in the frame of a cooperative research program between ICASE, NASA LaRC, the Naval Air Warfare Center (NAWC) and the Delft University of Technology (TUD).

Data has been processed and analyzed of an experimental research conducted on a 76/64-degrees double-delta wing at the Basic Aerodynamics Research Tunnel (BART) of NASA LaRC. Flow visualization tests have provided insight into the effects of angle of attack and Reynolds number on the vortex-dominated flow both on and off the surface of a double-delta wing. Upper surface pressure recordings from pressure tabs and pressure sensitive paint (PSP) have provided data on the pressures induced by the vortices. Surveys of the vortex flowfield carried out at an angle of attack of 10 degrees provided data on the distribution of the pressure and velocities in the vortices. The experimental data was compared with numerical solutions of compressible thin-layer Navier-Stokes equations computed at NAWC.

Results of the experimental and numerical research will be published and presented at the AIAA 33rd Aerospace Sciences Meeting, to be held at Reno, Nevada in January 1995. To further validate CFD solutions, balance measurements as well as vortex flow surveys at angles of attack other than 10 degrees will be needed. No date has been set yet for these tests.

R. V. WILSON

Simulation of Complex, Three-Dimensional Turbulent Jets

Three-dimensional, turbulent jets issuing from elliptic or rectangular nozzles exhibit many complex phenomena including strong azimuthal instabilities, switching of major and minor axes, and increased entrainment rates leading to increased mixing. The objective of the present work is to perform numerical simulations of these flows in order to understand such phenomena.

The study will include Large Eddy and Direct Numerical Simulations of rectangular jets issuing from nozzles and orifices and circular jets with vorticity generating tabs. Three-dimensional simulations of planar mixing layers were performed and results indicate that the computed coherent structures are dependent on whether the flow is forced at the inflow plane with 2-D or 3-D forcing functions.

Simulations of the above mentioned 3-D jets will be performed and compared to available experiments and the Reynolds-Stress computations of Demuren.

P.K. YEUNG

Lagrangian Study of Incompressible Mixing

The transport of passive scalars in turbulence is strongly related to the disorderly motion and deformation of material fluid elements. We study the process of turbulent mixing using a Lagrangian approach. This work is performed in collaboration with S. Girimaji.

Based on the values of passive scalars and their Eulerian spatial gradients following a collection of fluid particles, we have calculated the Lagrangian scalar derivative (with respect to initial particle coordinates). Although the Eulerian scalar field decays, we find that the Lagrangian derivative can become large because any two initially close together fluid particles tend to move apart rapidly from

each other. We have also calculated conditional dissipation following fluid particles and related it to material element deformation characteristics. An *enhanced diffusion* model of mixing proposed recently by Girimaji appears to perform well at early stages of mixing, but requires modification at later times.

In further work, we plan to study the Lagrangian statistics of passive scalars following fluid particles and particle pairs. This will provide direct information on the role that the motion of material elements plays in turbulent scalar transport.

Lagrangian Statistics in Compressible Turbulence

Compressible turbulence is an important subject in the study of high-speed flows occurring in aerospace applications. In the past few years direct numerical simulations have led to significant advances in basic understanding in the dynamics of compressible turbulence. However, little information on the mechanisms of compressibility effects on fluid particle motion and turbulent mixing is known. Compressible mixing is, in particular, important in high-speed combustion.

To obtain Lagrangian statistics for compressible turbulence, the particle-tracking algorithm of Yeung & Pope has been adapted to a compressible direct numerical simulation code provided by Gordon Erlebacher. A fourth-order cubic-spline interpolation scheme is used to calculate the velocities of fluid particles, whose positions are advanced in time using a low-storage third-order Runge Kutta scheme. As a numerical test, fluid particles are followed in a frozen compressible flow field. As for incompressible flow, the r.m.s. particle displacement initially increases linearly with time, and the square root of time at times large compared to an integral time scale. However, special care is needed to interpret the effects of compressibility on other Lagrangian statistics such as the velocity autocorrelation function. For instance, in contrast to incompressible flow, one-point Eulerian and Lagrangian mean quantities are not equivalent even in homogeneous turbulence.

Besides continuing work on Lagrangian statistics, we have begun the search for a suitable numerical forcing scheme to produce statistically stationary isotropic compressible turbulence. We will test and *extend* the (incompressible) method of Eswaran & Pope, which is already incorporated in the compressible code. Future plans also include the addition of passive scalars to study compressible turbulent mixing.

YE ZHOU

On the Lighthill Relationship and Sound Generation from Isotropic Turbulence

In 1952, Lighthill developed a theory for determining the sound generated by a turbulent motion of a fluid. With some statistical assumptions, Proudman applied this theory to estimate the acoustic power of isotropic turbulence. Recently, Lighthill established a simple relationship that relates the fourth-order retarded time and space covariance of his stress tensor to the corresponding second-order covariance and the turbulent flatness factor, without making statistical assumptions for a homogeneous turbulence. Lilley revisited Proudman's work and applied the Lighthill relationship to directly evaluate the radiated acoustic power from isotropic turbulence. After choosing the time separation dependence in the two-point velocity time and space covariance based on the insights gained from direct numerical simulations, Lilley concluded that the Proudman constant is determined by the turbulent flatness factor and the second-order spatial velocity covariance, $f(r)$.

In order to estimate the Proudman constant at high Reynolds numbers, we analyzed a unique data set of measurements in a large wind tunnel and atmospheric surface layer that covers a range of the Taylor microscale based Reynolds number $2.0 \times 10^3 \leq R_\lambda \leq 12.7 \times 10^3$. Our measurements demonstrate that the Lighthill relationship is a good approximation, providing additional support to Lilley's approach. The flatness factor is found between 2.7 – 3.3 and the second order spatial velocity covariance is obtained. Based on these experimental data, the Proudman constant is estimated to be 0.68 – 3.68

The measured values for $f(r)$ at very high Reynolds numbers offer a unique opportunity to compute the values of constants appearing in a new two equation and Reynolds averaged compressible turbulence closure. Specifically, a pseudo-sound constitutive relationship for the pressure dilation and dilatational covariances in compressible turbulence has been developed by J.R. Ristorcelli and myself. The constants in the expressions have a precise and definite physical significance being related to the microscale length scale and to various integrals of the longitudinal correlation.

Scale Disparity and Spectral Transfer in Anisotropic Numerical Turbulence

Underlying the high Reynolds number Kolmogorov similarity theory of 1941 is the implication that interactions among motions at different length scales are statistically dominated by interactions which scale on a single local length scale r , so long as r is much smaller than the integral scale l . If this is the case, then (a) net energy transfer from motions surrounding scale $r \ll l$ is not directly influenced by integral-scale motions, and (b) the local structure of the motions at scales $r \ll l$ is isotropic.

To study the effect of cancellations within long-range interactions on local isotropy at the small scales, we use a single scale disparity parameter “ s ” to re-analyze the spectral transfer in previous direct numerical simulations in which the small scales were found to become anisotropic in response to coherent anisotropic forcing at the large scales. We find that the marginally distant interactions in the simulation do not cancel out under summation and that the development of small-scale is indeed a direct consequence of the distant triadic group. Although a reduction of anisotropy at later times occurs as a result of the isotropizing influences of more local energy-cascading triadic interactions, the local-to-nonlocal triadic group persists as an anisotropizing influence at later times. We find that, whereas long-range interactions, in general, contribute little to net energy transfer into or out of a high wavenumber shell k , the degree of anisotropy of component energy transfer within the shell increases with increasing scale separation s . These results suggest that the anisotropizing influences of long range interactions should persist to higher Reynolds numbers .

The energy transfer process in compressible turbulence and in multiscale mixing at different Schmidt numbers is of practical importance and will be analyzed next.

APPLIED COMPUTER SCIENCE

DAVID C. BANKS

Visualizing Vortices in an Unsteady Flow

Direct Numerical Simulation (DNS) of an unsteady flow can produce hundreds of gigabytes of data. We wish to extract the important flow features from the data and compress their representation enough to fit in workstation memory. This enables the scientist to interactively examine time-varying data using a local machine. This work is being done in collaboration with Bart Singer.

We used a modified vortex-line to extract vortex skeletons from an unsteady shear flow, calculated over 231 time steps. By representing the cross-sections of the tubes as truncated Fourier series, we were able to compress the representation of the flow substantially.

We plan to enhance the surface representation of the vortex tubes by using dynamic texture-maps and dynamic displacement-maps along the tubes. These techniques require high-end graphics hardware and/or supercomputing capability.

Interactive, Immersive Visualization of Time-varying Data

It can be difficult to comprehend the development of 3D data. The problem is made worse by viewing the data on a 2D computer screen, controlling it by a 2D mouse. We wish to give the scientist an immersive view of 3D data by using stereoscopic display, 3D tracking, and real-time scene updates.

We developed an interactive, immersive system to view time-varying data. The hardware tools include SGI graphics workstations with texture boards, stereo glasses, and 3D head and hand tracking. The software tools include libraries from the Electronic Visualization Laboratory, the University of Alberta, and the San Diego Supercomputer Center. The system has been used to investigate the onset of turbulence in a shear flow over a flat plate. It was also demonstrated at the ACM SIGGRAPH conference in Orlando.

We plan to use the system to examine other unsteady flows and to investigate the geometry of a fluttering airfoil. This work has been done in collaboration with Michael Kelley.

SHAHID BOKHARI

Performance Issues in Parallel Computing

This research focusses on the impact of communication overhead on the performance of parallel computing systems. Communication is a key issue in parallel computing and considerable effort is required to minimize the impact of communication overhead in a parallel algorithm. Some of the problems that have been addressed in the past include the issues of mapping algorithms to processors, load balancing, and partitioning.

Recent research has addressed the Complete Exchange communication pattern, which requires each processor in a system to send a unique message to every other processor. The multiphase approach to achieving this pattern looks at a family of algorithms and chooses the best for a given

machine size (number of processors) and message length. This approach has been found very useful on hypercubes. Variants of this approach have also been developed for two-dimensional meshes.

Contention for network links can degrade a parallel computation's performance to the extent that communication algorithms are frequently designed to avoid, entirely, all contention. However the price paid for contention-freedom is under-utilization of network links. We are interested in understanding contention and its severity on the Intel Paragon, and in developing communication algorithms that accept limited contention to achieve higher performance. This work was performed with David Nicol.

Our approach has been to experimentally measure the effect of contention on the Paragon, looking for the relationship between performance on *link contention*—the maximal number of communications sharing a given link, and *path contention*—the total interference on a path that a long message may encounter. We have determined that a link may handle as many as three concurrent messages with somewhat limited effect on performance, and take advantage of that with new algorithms for the complete-exchange operation that guarantee limited link contention, and in doing so provide higher performance than contention-free complete-exchange algorithms.

Our future plans are to develop analytic models of the cost of message-passing under contention, and to use these models to understand the tradeoffs between accepting and avoiding contention, on additional communication primitives.

XIAO-CHUAN CAI

Optimal Domain Decomposition Algorithms for the Full Potential Equation

We are studying the Newton-Krylov-Schwarz (NKS) algorithm for solving the full potential equation on parallel machines, in collaboration with David Keyes. NKS is a domain decomposition-based preconditioned iterative method, and is designed for the implicit solution of nonlinear partial differential equations, especially on distributed memory parallel computers. During my visit, we implemented a version of the NKS algorithm, which consists of three basic components: an inexact finite difference Newton solver, a restarted Krylov solver, and a two-level overlapping additive Schwarz preconditioner. The full potential equation is discretized by a bilinear finite element method and has been solved on two types of parallel machines, namely a cluster of Sun workstations at ICASE and an IBM-SP1 at Argonne. Our focus is on the interplay of the three components. We have found that even a small coarse grid solution can considerably speed up the convergence at least in the subsonic case. We plan to study the transonic case as well.

We began to study another aspect of the overlapping Schwarz domain decomposition algorithm in collaboration with M. Driss Tidriri, namely its interaction with the underlying discretization schemes. A number of MUSCL-type finite volume schemes are being considered, such as those of Van Leer and Roe. Our goal is to develop an optimal two-level MUSCL-Schwarz algorithm, which can be used for the parallel implicit solution of aerodynamic problems.

GIANFRANCO CIARDO

Advances in the Description and Solution of Stochastic Petri Nets (SPNs)

SPNs are often used in the performance and dependability arena. The resulting stochastic process is either solved numerically, if a continuous or a discrete time Markov chain (CTMC or DTMC), or studied using discrete-event simulation, when analytically intractable. We have recently been involved in the definition of more general classes of SPNs for which an analytical solution is still feasible, albeit using more sophisticated algorithms. However, no single computer tool currently implements all of these results in a coherent framework.

We have started the definition of a strictly-typed input language for SPS, a new "Stochastic Process Solver." The main feature of SPS is the ability to manage multiple models in a cooperative fashion. This is essential to allow fixed-point solution schemes based on the concept of "dependency graph," targeted to the approximate solution of very large modeling problems. Another important feature is the ability to explicitly specify CTMCs, DTMCs, independent semi-Markov processes (ISMPs), and semi-Markov processes (SMPs), and use them to describe the timing behavior of higher-level models. For example, the firing time of a transition in a SPN can be set to the time to absorption of a previously defined DTMC. Hence, we can specify SPNs whose underlying process is a generalized semi-Markov process (GSMP), or, in many cases, a semi-regenerative process, a SMP, ISMP, CTMC, or DTMC. In all but the GSMP case, numerical solution algorithms exist and will be implemented, in addition to discrete-event simulation.

The implementation of the parser for the input language will begin soon. For the solution algorithms, some code will be reused from SPNP, a tool implemented by the author, while new code will have to be written for the new algorithms. The ability to model the same system using a continuous-time, discrete-time, or hybrid model will prove invaluable in gaining insight into the efficiency and appropriateness of the different modeling approaches existing today for discrete-event systems.

THOMAS W. CROCKETT

Visualization and Graphics for Parallel Applications

The objective of this work is to develop algorithms and methodologies for generating live visual feedback from parallel scientific and engineering computations. By applying the power of the parallel machines to the graphical rendering process, we can reduce the size of the output data stream and provide important feedback for debugging and execution monitoring. With appropriate interfaces, we can extend this work to provide interactive steering of parallel applications and to support computationally-intensive data exploration and visualization operations on large datasets.

Our approach has four main components. We are (1) developing parallel polygon rendering algorithms, (2) incorporating them into a prototype parallel graphics library, (3) demonstrating the library on parallel applications of interest to NASA, and (4) developing interactive interfaces to the applications. Recent work has focussed on improving the performance and functionality of our prototype parallel graphics library, known as PGL. The PGL renderer was enhanced to allow image partitioning by interleaved scanlines, which provides improved static load balancing. We also

added supersampled anti-aliasing for generating high-quality images, and a point primitive to better support the particle-based DSMC simulations which we are using as test applications. Performance of the renderer on the Intel Paragon was re-examined when the message-coprocessors were enabled in late June. Results show a factor of 2.5 improvement with short message buffers due to reduced latencies. Work also began on a workstation-based user interface for PGL applications. This interface will initially provide interactive control of the graphical parameters, and will eventually be extended to support visualization and application-specific parameters.

Future work will proceed on all four fronts. Algorithmic issues remain relating to scalability, load-balancing, and image display. Performance will be assessed analytically, as well as with actual applications. PGL will be ported to the IBM SP2, and its performance characteristics on that platform will be examined. We will apply PGL to additional applications, including a parallel isosurface code developed at Sandia National Lab. Work will proceed on the interactive interface to improve its usability and extend its functionality. Producing an interface which can be easily extended to support application-specific requirements is a significant research goal in this work.

CHITA R. DAS

Parallel Simulation of Adaptive Routing Algorithms for Network Architectures

Wormhole switching has become the switching mechanism of choice for current multiprocessors due to its high performance and low buffer space requirement. This switching mechanism along with adaptive routing of messages can utilize the network resources most effectively and hence can provide maximum attainable performance. In view of this, design and analysis of adaptive routing algorithms for various network architectures has been an active area of research. The objective of such studies is to design low-cost, deadlock and livelock free partially and fully adaptive routing algorithms. These algorithms are studied via extensive simulation. Simulation of these algorithms are done at the flit level and so the simulation time is unacceptably large specifically for large networks. One possible approach to reduce the simulation cost is to parallelize the simulation experiment.

We are currently formalizing various research issues to parallelize adaptive routing algorithm simulation. Problems that are addressed here are :

- partitioning of the network to map on to the parallel machine,
- selection of window size for synchronization of events,
- synchronization mechanism among processes, and
- performance prediction and analysis.

This work will be conducted in collaboration with David Nicol.

We plan to analyze the above issues in detail, and implement the simulator on available parallel machines such as IBM SP1/SP2 and nCUBE.

PAUL A. FISHWICK

A Modeling Tool for Performability

Most of my time has been devoted to team discussions on the problem of how to build a modeling language – or a visual formalism – which yields both performance and reliability statistics. The combination of performance and reliability is termed *performability*. While the formation and design of such an integrated tool was the primary objective of our meetings, many discussions also centered around the more general problem of combining Monte Carlo simulation, continuous simulation and analytic methods within a unified framework.

We agreed that the user (engineer or scientist) of our modeling system should not be concerned with low level details concerning the *solution methodology*. Instead, the user should have a view of the physical system that maps best to the structure of the system. Moreover, the user should have tools for organizing system knowledge. The team agreed that the object oriented paradigm provides a solid starting point with regard to overall system design. With that in mind, we are looking at existing examples of programs supporting reliability and performance modeling, as well as object-oriented modeling programs. For performance, several programs have been discussed such as BoNes, SimPack, RESQ and OmSim. For reliability or dependability, we have reviewed the salient attributes of REST, RESQ and the many variants of HARP (such as SHARPE).

The plan is to first create a preliminary design of a good performability language. Once these design aspects have been discussed, we will collaborate to build an object-oriented language that supports performability from the engineer's perspective. The tool will be available under an X windows environment, and we are studying software packages to help us to construct a graphical user interface (GUI). One such tool is Tcl/Tk. I plan to review the features of Tcl/Tk to see if it supports the construction of graph-based models using arbitrary icons for each graph node. Our ultimate goal is to have a graphical front end which is portable and allows for object-oriented design and modification. The front end will allow for models to be simulated and tested, possibly using existing base programs for reliability and performance.

MATTHEW HAINES

Runtime Support for Task and Data Parallelism

Integrating task and data parallelism requires sophisticated runtime support to handle issues of communication and synchronization among parallel tasks in an application, each of which may execute in a data parallel manner. Additionally, mapping these tasks onto a limited set of physical resources may require sharing resources among several tasks, which may or may not be related. Our objective is to design and implement a thread-based runtime system that can provide an efficient solution to the problems of integrating task and data parallelism. This work is being done in collaboration with Piyush Mehrotra, and students David Cronk and Bryan Hess.

We have divided the runtime project into two layers, a lower layer for supporting language-independent, lightweight threads capable of communication in a distributed memory environment (Chant), and a higher layer for providing the support required by the Opus language (Opus Runtime). We have designed and implemented Chant atop POSIX pthreads and MPI, and are currently

running on the Intel Paragon and a network of workstations. In addition to supporting Opus Runtime, we are using Chant to determine the benefits of combining threads with data parallel compilers and scientific applications. Specifically, we are using Chant to explore the utility of threads in a data parallel compiler (in collaboration with Thomas Fahringer, University of Vienna), and in parallel PDE computations (Nikos Chrisochoides, Syracuse University).

We plan to continue development of these two layers of the runtime system, integrating them at some point in the near future. We also plan to use the Chant layer as a vehicle for studying issues related to load balancing, irregular scientific problems, and thread-based performance prediction and evaluation.

ULF HANEBUTTE

Performance Evaluation of Large Scale Direct Numerical Simulation Application on the IBM SP-1

The focus of the study was to determine the feasibility of using the IBM SP-1 for laminar-to-turbulent boundary-layer transition computations. We did a comprehensive performance evaluation of a direct numerical simulation (DNS) code. Using the IBM SP-1 located at Argonne National Laboratory, we are able to establish the required experience base. This work was done in collaboration with Ron Joslin from NASA and M. Zubair from Old Dominion University and IBM.

The spatial evolution of disturbances within boundary-layer flow is computed by solving the three-dimensional nonlinear Navier-Stokes equations with high-order finite-difference methods, spectral methods, and a three-stage Runge-Kutta method for time advancement. Mappings and inverse mappings of the computational domain allow all numerical calculations to be local (performed independently on each computational node). Global communication costs result from this domain-mapping procedure; however, the communication cost is minimized compared with the cost of parallel algorithm solvers on a distributed data set.

The performance of a Navier-Stokes simulation code on the IBM SP-1 was compared with Cray Y/MP for a test case which was used by Joslin and Streett (1994) to study the role of stationary crossflow-vortex instabilities in the laminar transition to turbulence on swept wings. The performance results indicate that with as few as 8 nodes, the SP-1 would yield results in less time than the Y/MP. The DNS code on the IBM SP-1 ideally achieved 55 MFLOPS per processor, which translates to 7 GFLOPS using 128 nodes with 16 Gbytes of available memory. In practice, communication cost and idle time led to 40-50% efficiency. In comparison, the serial DNS code achieved 240 MFLOPS on a single processor of a Cray Y/MP which was limited to 256 Mbytes. The mapping and inverse mapping procedure can be easily implemented on many real-world computer codes to modify a serial code for use on parallel computers.

In the future, we would like to perform large scale simulations on the IBM SP-2, which is currently being installed at Langley Research Center.

HARRY JORDAN

Parallel Data Movement Metrics

The way in which data moves among parallel processors has an important effect on their performance. Some programs inherently make heavier demands on data movement than others, and some can be transformed to decrease their demands. This research is aimed at quantifying this effect with program metrics and verifying the metrics through experimentation.

Simple metrics which depend on the dynamic requirements for data movement have been based on ideas similar to the working set in virtual memory or the cache footprint. We have compared the predictions from these metrics with the performance of test codes on the KSR-1 cache-only multiprocessor with semi-quantitative agreement between metric predictions and actual performance. A detailed, architecture dependent model has also been developed which gives accurate predictions of performance.

We intend to discover whether specific architecture models can be decoupled from specific programs by using the correct set of program metrics as parameters to a machine model. If so, such metrics could be used to predict performance and guide program restructuring for parallel machines.

Uncertainty in Time-of-Flight Design

Time-of-flight (ToF) digital circuits use no flip-flops or other latching elements to implement high speed computer circuits. The technique was developed in connection with optical computing, where the assumption that circuit delays can be accurately controlled is justified. The method is related to the wave pipelining technique used in VLSI design. We are extending these design techniques to account for the influence of delay uncertainty.

The need to synchronize feedback loops leads to a variant of the minimal feedback edge set problem. We adapt Lempel and Cederbaum's algorithm to place a minimal set of synchronizing gates to solve this problem. We formulate a constrained minimization problem based on the influence of specific devices on timing uncertainty and on constraints which uncertainty must satisfy for correct circuit operation.

We are developing an algorithm to solve the constrained minimization problem for the minimum clock period at which the circuit can be operated. We will also investigate using time multiplexing with the highly pipelined designs that arise from this design method.

MICHAEL KELLEY

Virtual Reality Visualization of Fluid Experiments

Fluid experiments are capable of producing terabytes of data. The scientist must sift through this large amount of data to find relevant pieces of information. A three-dimensional computer visualization of the experimental data allows the researcher to explore his time-varying dataset in an environment that closely relates to the original experimental conditions. Mathematica and FAST are two visualization systems that allow the user to create such visualizations, but users are still limited to the flat monitor and mouse to view and interact with the visualizations.

The use of virtual reality as a tool to aid the scientist has become a popular research topic. In order to evaluate the usefulness of virtual reality as a tool for scientists, we have created an experimental virtual reality visualization system. Successful design of our system relied on three goals: the use of inexpensive hardware, ease of use for the scientist, and reusability of code. This work is being done in collaboration with David Banks, Bart Singer, and Tom Crockett.

Our first version of the system was tailored to work with the CAVE, a 1990's version of Star Trek's "holodeck" created at the Electronic Visualization Laboratory, University of Illinois at Chicago. This version was shown at SIGGRAPH '94 to conference attendees. The CAVE allows the user to view and interact with the visualization in a large three-dimensional environment. Since the CAVE is an expensive piece of hardware, a second version was created that could be used at ICASE without the CAVE.

In order to build and evaluate a system, a scientist with experimental data was needed. Bart Singer provided us with simulation data of vortices developing over a flat plate. Using this dataset, a program was created that allowed Dr. Singer to view and interact with his data in a three dimensional environment. A "through the window" paradigm, where the monitor is thought of as a window into a virtual environment, was used for viewing. LCD stereo shutter glasses provide the user with cues about the depth relation between objects, and a Polhemus Fastrak provides six degree-of-freedom input. Since the user's head position and orientation are tracked, the correct perspective projection is computed based on the viewpoint. This improves the realism of the display, as the user can now look around objects. With a second tracker for the hand, the translation and rotation of objects in the virtual environment becomes easier.

Once the first version of the visualization system was completed, the scientist was permitted to use the program. Since the researcher could view a significant interval of the time-varying data, vortex formations and dissipations could be followed. Interesting and unusual vortex formations were viewed by the specialist, which might otherwise have remained hidden among two-dimensional data plots.

The application consists of several distinct libraries in the hope that the useful elements may be re-combined for other applications. A file format was created that can accept multi-dimensional datasets. The library that passes this file format can also display the datasets in three-dimensions. Another library handles the input and output devices, so any programmer that might want to interface with the stereo display and the Polhemus Fastrak could do so without having to write the code from scratch.

There are many additions that could be made in order to produce a visualization system with which a scientist could do significant research. The current system could be extended to accept other datasets, so other researchers could evaluate and use the system. New tools for interacting with the dataset could also be added. Interfacing with supercomputers, such as the IBM SP2, would allow the use of a compute process that could handle real-time data interpolation. Porting the application to more expensive hardware, such as a BOOM or a head-mounted display, would increase the user's sense of immersion within the visualization system.

DAVID E. KEYES

Parallel Algorithms for CFD Applications

The focus of our research has been on parallel algorithms that can bridge between physical applications and parallel computer architectures, while making substantial reuse of algorithms designed for conventional computers. The adaptation and incorporation of a particular family of algorithms into real engineering codes has been undertaken. One part of the effort has shown the competitiveness of the algorithms in overall convergence rate with the best serial methods. The other part has shown the parallelizability of the compute-intensive kernel of the algorithms. Taken together, these efforts show that the algorithms, dubbed "NKS" for "Newton-Krylov-Schwarz", may be ready for implementation in many practical codes.

Four representative steady flow models have been pursued: full potential, Euler, Navier-Stokes, and the shallow water equations, which are a variant of the Euler equations for incompressible flow. The first three of these models are in daily use in the aerospace industry, the last in weather and climate modeling. Our implementation focus has shifted towards networks of workstations, because of industrial and academic interest. The full potential problem (studied with X.-C. Cai) is the most elementary, and the furthest along. Portable parallel implementations using a full Newton method in standard or matrix-free form have been completed for simple geometry. In addition, we are working with the TRANAIR group at Boeing to incorporate a two-level Schwarz method into that workhorse full potential code. The Euler problem (studied with M. D. Tidriri) has been parallelized in the inner (linear) kernel; it remains to parallelize the Newton part. The unstructured Navier-Stokes problem (studied with W. K. Anderson) is in the Newton-Krylov stage only. Here, it is competitive with the multigrid code currently most CPU-efficient on conventional computers, while being free of the hierarchical sequence of grids required by multigrid. This sequence is inconvenient to generate in the unstructured case, especially in three dimensions, and unstructured grids are favored for three-dimensional full aircraft computations. In contrast, three-dimensional Newton-Krylov results were straightforward to obtain once the boundary conditions were made fully implicit. In iteration count (comparing Newton-GMRES cycles with multigrid V-cycles), the Newton-GMRES method is far superior, but its cycles are more expensive, leading to an overall CPU time ratio of 1.5 for subsonic Navier-Stokes. By making recourse to coarser grids in the NKS method in the form of grid-sequencing only, this CPU disadvantage can be removed. The shallow water problem (studied with J. C. Levin) is the only method that is not fully implicit. We use the semi-implicit/semi-Lagrangian formulation in order to suppress gravity waves, but maintain symmetry in the implicit part. The implicit phase has been parallelized so far, and the entire application runs on an Ethernet network of workstations.

We intend to continue to increase the geometric complexity, dimensionality, and portability of our implicit solvers until computational aerodynamicists and geophysicists find them sufficiently attractive to incorporate in parallel production codes.

Communication Modeling in Cluster Computing

I. Stoica, F. Sultan and I have recently introduced a uniform framework for analyzing and predicting communication performance of parallel algorithms in real parallel processing environments. We include under "parallel processing environments" systems supporting computing on both traditional dedicated tightly coupled parallel computers and clusters of loosely coupled workstations.

However, "multitasking," that is, the simultaneous execution of "randomly" interfering parallel jobs, is excluded.

The communication system is modeled as a directed communication graph in which terminal nodes represent the application processes that initiate the sending and receiving of the information and in which internal nodes, called communication blocks (*CBs*), reflect the layered structure of the underlying communication architecture. The direction of graph edges specifies the flow of the information carried through messages. Each *CB* is characterized by a two-parameter hyperbolic function of the message size that represents the service time needed for processing the message. The parameters are evaluated in the limits of very large and very small messages. Rules are given for reducing a communication graph consisting of many *CBs* to an equivalent two-parameter form, while maintaining a good approximation for the service time, which is exact in both large and small limits. The model has been validated on a dedicated Ethernet network of workstations by experiments with communication subprograms arising in scientific applications, for which a tight fit of the model predictions with actual measurements of the communication and synchronization time between end processes is demonstrated. The model has been used to evaluate the performance of two simple parallel scientific applications from partial differential equations: domain decomposition and time-parallel multigrid. In limits for which direct comparisons can be made, we have also shown the compatibility of the hyperbolic model (to within a factor of 3/4) with the recently proposed LogP model of the Berkeley group. The hyperbolic model will allow us to determine whether the bottlenecks in applications codes we port to workstations in the future are in the actual communication or in synchronization caused by load imbalance and other factors, and will become a standard part of the process for improving parallel performance in distributed environments.

LARRY LEEMIS

The ICASE Modeling Project (IMP)

A range of performance and reliability modeling tools such as RESQ, SPNP, BONES and SHARPE have been developed. Integrating these tools into a single integrated modeling language would increase accessibility of them all, since each can only be applied to certain types of models.

A preliminary architecture for an Integrated Modeling and Analysis System to be developed at ICASE in the future was discussed. Preliminary design criteria were discussed and agreed upon. These criteria include ease of use, automated tool selection, hierarchical system description, consistency checks if several tools can be applied to a single model, and inclusion of discrete-event simulation code.

My part of the future work on this model might include work on: a discrete-event simulation output analysis package, variate generation routines, automated implementation of variance reduction techniques, confidence interval estimation of reliabilities from large samples of binary data, and inclusion of sampling information on system components.

SCOTT T. LEUTENEGGER

Data Base Support for Subset Retrieval and Visualization of Scientific Data

The focus of this project was to design and implement a prototype database to facilitate retrieval of subsets of large scientific data sets. The data subsets are anticipated to be used as inputs to other codes, such as for visualization or MDO.

Currently many scientist store and retrieve data sets as files. When the scientist is interested in a subset of the data they read in the entire data set and strip out the portion of interest. This is not practical when data sets are large. Our approach is to provide database support to retrieve only those pages from disk that contain the desired data. Typical CFD data sets are two or three dimensional, thus we provide a multi-attribute indexing technique.

There are several multi-attribute indexing techniques proposed in the database literature and no conclusive study had been done comparing them. A substantial portion of our time was spent conducting a comparison study of the three most accepted multi-attribute indexing techniques: gridfiles, R-trees, and R^* -trees. Our initial system used the Exodus system, an academic object oriented database system from the University of Wisconsin, as a database engine. Implementation work by student Adrian Filipi-Martin showed the gridfile to be the best for our purposes.

The overhead of the Exodus system, plus lack of control over logging, necessitated the development of our own database system. Our system currently consists of a catalog which keeps track of various meta data associated with a data set and a gridfile holding the data for each data set. Our database system is significantly faster for both loading and querying the database than our earlier system using Exodus. Our prototype currently supports loading and querying of three dimensional single block of a block structured CFD grid. We have been interacting with NASA scientist Mark Sanetrik who has supplied us with a data set. The coordinate system of the data is an O-grid where the third coordinate is time.

In collaboration with David Nicol we have begun addressing unstructured CFD grids by developing a bulk loading algorithm. We have developed and implemented a rectilinear partitioning algorithm and compared the computation time of our algorithm with a recently proposed dynamic programming algorithm. Our algorithm is three to four orders of magnitude faster for small data sets. Our algorithm has not yet been incorporated into the prototype.

We will continue development of the prototype by first incorporating our bulk load algorithm and comparing it with the conventional load technique of inserting one tuple at a time. Incorporation of the bulk load algorithm will allow the prototype to store the data portion of unstructured grids. Work needs to be done to determine the best way to store the grid structure. Extension of the prototype to multiple block structured grids and other formats is dependent on future funding.

KWAN-LIU MA

The Design of a Parallel Volume Rendering Library

Interactive visual monitoring of large-scale three-dimensional CFD simulations running on massively parallel computers like the Intel Paragon helps researchers keep track of how the flow phenomena develop and how computations progress. In a parallel and distributed computing environment,

the traditional postprocessing approach becomes inadequate due to the amount of data that must be stored and transferred. The ultimate goal of this research is to develop a parallel volume visualization library. An application simulation can then make use of this library to render images of the simulated phenomena in-place at each processing node without moving the data to a dedicated computer for postprocessing.

The library is partially based on a parallel volume rendering algorithm developed previously (ICASE Report 93-59). A few key design considerations include data distribution, library interface and image compositing. The library only works for structured and regular volume data. This restriction does not make the library less useful since a majority of parallel CFD simulations use a structured and regular grid. An unsteady three-dimensional compressible flow simulation has been used for testing the library. Tests had been performed for up to 64 nodes on the Intel Paragon. As a result, the original PVM3 implementation has been ported to NX, the Paragon's native communication library, to achieve better performance.

To make this library more flexible, easy to use and efficient, we will continue improving the design, implementation and in particular, interface of this library. For further tuning, performance evaluation will be performed on an Intel Paragon with larger number of processors (512-1024). Later, we plan to use MPI (Message Passing Interface) so that it is portable to other machines such as the IBM SP2. It is important to make it available to more users so the design and improvements will be done appropriately.

PIYUSH MEHROTRA

Evaluation and Extension of HPF

The stated goal of High Performance Fortran (HPF) was to "address the problems of writing data parallel programs where the distribution of data affects performance." We have been using data parallel codes of interest to NASA to evaluate the effectiveness of the language features of HPF. This work is being done in collaboration with John Van Rosendale, Dave Middleton, Kyle Winn, H. Zima.

We have been studying the expressiveness of HPF for the following data parallel codes: a single grid version of ISAAC, TLNS3D a multi-block code, and DSMC a Monte Carlo code. Based on this evaluation we have proposed a set of extensions for HPF. These include: processor views (for matrix algorithms), distribution to subsets of processors (for multigrid and block-structured algorithms), general block distributions (for load balancing, e.g., in PIC and DSMC codes), indirect distributions (for unstructured grids), and user defined distributions and alignments (for unstructured grids and other complex applications). We have been attempting to use Applied Parallel Research's and Portland Group Inc.'s HPF compilers and University of Vienna's Vienna Fortran Compiler to evaluate the performance of the HPF code. However, we have not had a lot of success since the first two do not support most of the optimizations and the last is an academic project and hence cannot handle large codes.

We plan to continue our evaluation, in particular studying the performance of these HPF codes as the compilers become more sophisticated.

Integration of Task and Data Parallelism

Multidisciplinary optimization codes exhibit both task and data parallelism: the individual discipline codes can be internally data parallel while being executed concurrently with each other. We have designed a set of language extensions, called Opus, for exploiting both levels of parallelism. The objective is to provide a high-level programming environment for implementing such codes in a plug-compatible manner on a network of parallel and distributed machines. This work is being done in collaboration with Matthew Haines, Bryan Hess, John Van Rosendale, and H. Zima.

Opus consists of language constructs to create and manage data parallel tasks. These tasks interact with each other using Shared Data Abstractions (SDAs) which encapsulate data and provide exclusive access via the methods invoked by these tasks. We have been evaluating the design of the language based on preliminary implementations of MDO codes. We have also designed the Opus Runtime system which provides the protocols necessary to support SDAs including the redistribution of method arguments. In order to validate our design, we have built a C++ prototype of the runtime system targeted to a network of Sun workstations and the Intel Paragon.

We plan to continue evaluating the language design, modifying it as necessary. We are implementing the Opus Runtime system on top of Chant, the thread based portable language independent system that we are developing. We also plan to build a source-to-source translator so that Opus programs can be directly transformed to target the runtime system.

PORTS: An Interface for a Portable Runtime System

A number of research groups, including one at ICASE, are actively pursuing methodologies to support the integration of task and data parallelism. Recently, we have formed an informal consortium, called the PORTS group, in an attempt to design a interface for a thread-based, portable runtime system that will support inter-operable task and data parallelism. The participating institutions include: Argonne National Labs, Caltech, Indiana University, University of Colorado, University of Oregon, University of Maryland, University of Vienna, and IBM. Matthew Haines and Piyush Mehrotra are representing ICASE in this effort.

The goal of the group is to define a common interface (a set of routines and their arguments) for thread-based runtime systems executing on a variety of architectural platforms, including a heterogeneous network of workstations and massively parallel machines. This interface would provide a standard target for parallelizing compilers supporting both task and data parallelism, and allow for code sharing among the various research groups.

The group has met a total of four times, starting with the first meeting at Supercomputing 93. At this point, the group has divided the proposed interface into three parts: context management, thread management, and communication support. We are currently in agreement on the interface for the thread management portion, and are in the process of developing a library of routines to implement the accepted interface. The context management and communication support portions of the interface are still under consideration. We plan to continue with these meetings until a consensus can be reached on the entire interface.

DAVID NICOL

Parallel Simulation of Message Passing Codes

As massively parallel computers become increasingly available, users' interest in the scalability of their parallel codes is growing. However, such computers are in high demand, and access to them is restricted. We are developing a system called LAPSE (Large Application Parallel Simulation Environment) that allows one to use a small number of parallel processors to simulate the behavior of a message-passing code running on a large number of processors of a "target" machine. With LAPSE, a user could performance tune a code for massive parallelism before actually using large numbers of processors. This work was performed with Phillip Dickens and Philip Heidelberger.

The approach taken in LAPSE is to actually run the application using a separate process (called a Virtual Processor, or VP) for each simulated physical processor. The VPs are multitasked onto the available physical nodes. Application message-passing calls are trapped by LAPSE and redirected to the appropriate VP. In addition, the number of instructions executed by the application between message passing calls is determined and passed to a timing simulator. The timing simulator, which is also parallelized, models delays in the target machine's interconnection network, as well as certain message-passing overheads and delays in the target machine's operating system. In previously reported work we implemented LAPSE on the Intel Paragon. Since then we have implemented LAPSE using the **nx-lib** software libraries, public domain software, which provide Paragon functionality on networks of workstations. The integration of LAPSE provides these libraries with timing accuracy, a feature formerly lacking.

Our future plans are to broaden the number the applications run under LAPSE, for the purposes of both validating LAPSE timing predictions and understanding LAPSE execution speeds. We are performance tuning the **nx-lib** implementation.

Accepting Contention on the Intel Paragon

Contention for network links can degrade a parallel computation's performance to the extent that communication algorithms are frequently designed to avoid, entirely, all contention. However the price paid for contention-freedom is under-utilization of network links. We are interested in understanding contention and its severity on the Intel Paragon, and in developing communication algorithms that accept limited contention to achieve higher performance. This work was performed with Shahid Bokhari.

Our approach has been to experimentally measure the effect of contention on the Paragon, looking for the relationship between performance on *link contention*—the maximal number of communications sharing a given link, and *path contention*—the total interference on a path that a long message may encounter. We have determined that a link may handle as many as three concurrent messages with somewhat limited effect on performance, and take advantage of that with new algorithms for the complete-exchange operation that guarantee limited link contention, and in doing so provide higher performance than contention-free complete-exchange algorithms.

Our future plans are to develop analytic models of the cost of message-passing under contention, and to use these models to understand the tradeoffs between accepting and avoiding contention, on additional communication primitives.

Partitioning of Regular Graphs

k-ary n-cubes are a class of graph that underlie many parallel communication topologies. The graph structure becomes important when considering how one partitions a parallel computation to be run on a k-ary n-cube network. By understanding the graph structure we are better able to address partitioning issues. This work was performed with Weizhen Mao.

Our approach is to mathematically determine the minimum number of edges one must cut to create a subgraph of m nodes, and/or lower bounds on this number. Using these results we have classified partitions that are optimal with respect to the "bottleneck" metric (maximum sum of computation and communication costs, taken over all processors), and have shown how these results may be used in a branch-and-bound partitioning algorithm.

Our future plans are to develop and study partitioning algorithms based upon these results.

Integrated Modeling Project

System designers use a bewildering array of tools to study different aspects of the systems they design. The models used are different, and the analytic techniques used are different. Principles for integrating these disparate approaches are clearly needed. This work was performed with Kishor Trivedi, Arun Somani, Larry Leemis, Gianfranco Ciardo, Paul Fishwick, and Chita Das.

Our approach is to attempt integration using object-oriented techniques, in the context of the C++ language. We seek to develop classes and methods for those classes that abstract the essential features of models, and permit the automated transformation of a model specified using these classes into the input language of an existing tool. By using C++ and existing analytic capabilities we hope to focus attention on the essential modeling issues, rather than be detracted with language and compiler design issues.

Our future plans are to develop classes and methods for supporting the tools SPNP, SHARPE, and Assure (developed under NASA sponsorship).

ALEX POTHEN

Spectral Algorithms for Partitioning and Ordering

Our work concerns the solution of linear systems of equations from unstructured mesh computations on parallel and serial computers. In parallel computing, one is required to partition the mesh into submeshes and then map the submeshes to processors. The desired goals are that the work associated with each processor be balanced, and that the communication costs of the solution algorithm (necessitated by the submesh boundaries) be low. In earlier work we had developed a spectral partitioning algorithm employing an eigenvector of the Laplacian matrix of the mesh to solve the partitioning problem. Extensive experiments show that recursive spectral bisection is capable of providing high quality partitions, and has been used in the solution of fluid flow problems (among others) on the iPSC/860 and the Thinking Machines CM-2. In recent work we have applied the spectral method to compute orderings for direct methods and to solve envelope-reduction problems from structural analysis.

Spectral Nested Dissection and Envelope-Reduction

My Ph. D. student Lie Wang and I have developed a nested dissection ordering algorithm (SND) for solving linear systems of equations by direct methods in parallel. SND outperforms other ordering algorithms by a wide margin on the Intel Paragon for many large problems from diverse application areas such as fluid flow, structural analysis, circuit simulation, and financial modeling. We have extended a mathematical programming formulation of the partitioning problem due to Franz Rendl and Henry Wolkowicz to explain the success of the spectral partitioning algorithm; this was published in the Proceedings of the Seventh Domain Decomposition conference.

Stephen Barnard, Horst Simon, and I have also applied the spectral method to compute orderings for reducing the envelope-size (profile) of sparse matrices. This work has applications in computing incomplete-factorization-preconditioners, and in frontal methods for structural analysis. The spectral method is capable of reducing the envelope-size by a factor of two over other algorithms for many problems, leading to a four-fold savings in the computational work. Alan George and I have provided a *raison d'être* for the spectral envelope-reduction algorithm by formulating the problem as a quadratic assignment problem, and then showing that the spectral algorithm finds an approximate solution. This technique also can be used to prove tight lower bounds for the related 2-sum problem, that shows the spectral orderings are nearly optimal for this problem. Two papers have been completed and submitted to archival journals in addition to conference presentations and papers in proceedings.

In future work we will consider extending the partitioning algorithm to convective, anisotropic, and heterogeneous problems, where there are preferred directions for partitioning the problem. The application of profile-reducing orderings to incomplete factorization preconditioners will be studied; our preliminary results are very encouraging. We are developing techniques to speed up the spectral algorithm, and also considering its application to dynamic load balancing problems for adaptive, unstructured mesh computations.

XIAN-HE SUN

Incorporating the PDD Algorithm into the CDNS Simulation Package

The Parallel Diagonal Dominant (PDD) algorithm (see ICASE report 93-6) is a newly proposed tridiagonal solver. Both analytic and experimental results suggest that the PDD algorithm is an efficient parallel solver for tridiagonal systems. Despite its high potential, the performance of the algorithm on CFD applications remained unknown. In a three dimensional CFD simulation, the initial data distribution and run-time data movement would influence the performance significantly. Also, communication and load balance issues would be much more involved.

During the summer of 1994, the PDD algorithm has been incorporated into the CDNS (Compressible Directed Navier-Stokes Simulation) code (more precisely the 3-D kernel of the CDNS code), developed at ICASE, NASA Langley. Experimental results show that the new, incorporated CDNS code is more scalable than the original version. For instance, on a 4 by 4 mesh, where the X- and Y- directions were parallelized by 4 processors respectively and the Z-direction was solved locally, these two versions gave essentially the same performance on the NASA-Langley Intel Paragon machine. On a 16 by 4 mesh, where 16 processors were used for the X-direction, the new version

reduced the execution time by more than 20 percent and increased the achieved speed in the direction from 600 MFLOPS to 800 MFLOPS. The measured results show the applicability of the PDD algorithm in CFD applications. Equally important, the measured results match our predicted performance well. They confirm that the performance of parallel algorithms can be predicted over a range of machine size, and an appropriate algorithm can be selected for optimal performance.

The algorithm incorporation is preliminary. Limited by the three months visit, the PDD algorithm is used only along the direction and only for periodic boundary conditions. Many works remain to be done. Since the CDNS code is only one of many CFD applications relying on solving tridiagonal systems and since the PDD algorithm is only one of the scalable algorithms designed in recent years, the current result seems to be the first step in developing efficient, scalable simulation software for CFD applications.

MOULAY DRISS TIDRIRI

Newton-Krylov-Schwarz algorithms in CFD

We are investigating the Newton-Krylov-Schwarz algorithm (NKS) algorithm for compressible Euler problems, in collaboration with David Keyes. Transition to a full Newton method (CFL number approaching infinity) is precluded by explicit boundary conditions. To overcome this, we have replaced the explicit boundary conditions in a compressible Euler code with fully implicit conditions. We have developed two treatments of the boundary conditions: in the first, the numerical boundary conditions are treated using characteristics variables, while the second is based on the solution of the boundary Riemann problem. In the future we are planning to exploit the parallelism inherent in this approach. The application of mixed-discretization domain-decomposed preconditioners to 3D Navier-Stokes will also be considered.

Coupling Navier-Stokes with Boltzmann

Computing flows around maneuvering vehicles at high altitudes involves different regimes, characterized by the Knudsen number. At altitudes of 70 km or below, the Knudsen number is very small, and the flows are described by the Navier-Stokes equations. It is well known that Navier-Stokes equations cease to be valid for higher altitudes corresponding to Knudsen numbers larger than 10^{-3} . At this level, slip effects can be observed in the boundary layer and the gas is rarefied in the wake. Such effects can lead to significant changes in the aerodynamic coefficients of the vehicle. A standard solution is to use analytical slip boundary conditions; however, the constants involved are hard to identify and their validity is questionable. On the other hand, a direct simulation of the kinetic problem is too expensive. In our earlier work we have proposed to use locally a kinetic model in the boundary layer coupled to a global Navier-Stokes solver. The coupled problem was solved by a time-marching algorithm we had introduced in previous work. At that time the model used to solve Boltzmann equation was simply the hard sphere model and for Navier-Stokes the viscosity was assumed to be constant. We have continued our investigation into such coupling and developed more sophisticated physical models for both the viscosity and internal energy. We highlighted the convergence of the method and obtained excellent agreement of the results with those obtained by a direct kinetic simulation. However, our strategy can be applied in some cases where the direct

simulation is not possible. The coupling strategy allowed also the treatment of experimental situations in transitional regimes. The results obtained are coherent with the experimental results and lead to the determination of a realistic accommodation coefficient at the body.

LINDA F. WILSON

Performance Issues in Distributed Object-Oriented Simulation Tools

In distributed simulation, a single simulation program is distributed among multiple processors in an effort to reduce the overall execution time. Because of sequencing constraints among the events under simulation, it is difficult to distribute the simulation efficiently across multiple processors. We are examining the related issues of automated load balancing, object migration, and communication/synchronization in an effort to improve the performance of distributed object-oriented simulation tools. This work is being performed in collaboration with David Nicol.

The SPEEDES simulation package, developed by Jeff Steinman at the Jet Propulsion Laboratory, provides a general-purpose framework for object-oriented simulation on distributed systems. In order to examine a variety of large simulation projects, we have started porting the SPEEDES package to the Intel Paragon.

Once the port of SPEEDES is complete, we plan to study the performance of the air traffic control simulation from MITRE's CONDOR project on the Intel Paragon. In particular, we will examine methods to efficiently accomplish automated load balancing and object migration. We anticipate that new methods for synchronization and communication will be developed during this study.

REPORTS AND ABSTRACTS

Gaster, Michael, Chester E. Grosch, and Thomas L. Jackson: *The velocity field created by a shallow bump in a boundary layer*. ICASE Report No. 94-21, April 4, 1994, 23 pages. Submitted to Physics of Fluids.

We report the results of measurements of the disturbance velocity field generated in a boundary layer by a shallow three-dimensional bump oscillating at a very low frequency on the surface of a flat plate. Profiles of the mean velocity, the disturbance velocity at the fundamental frequency and at the first harmonic are presented. These profiles were measured both upstream and downstream of the oscillating bump. Measurements of the disturbance velocity were also made at various spanwise and downstream locations at a fixed distance from the boundary of one displacement thickness. Finally, the spanwise spectrum of the disturbances at three locations downstream of the bump are presented.

Banks, David C., and Bart A. Singer: *Vortex tubes in turbulent flows: identification, representation, reconstruction*. ICASE Report No. 94-22, April 5, 1994, 16 pages. Submitted to the October Meeting of Visualization '94.

In many cases the structure of a fluid flow is well-characterized by its vortices, especially for the purpose of visualization. In this paper we present a new algorithm for identifying vortices in complex flows. The algorithm produces a skeleton line along the center of a vortex by using a two-step predictor-corrector scheme. The vorticity vector field serves as the predictor and the pressure gradient (in the perpendicular plane) serves as the corrector. We describe an economical description of the vortex tube's cross-section: a 5-term truncated Fourier series is generally sufficient, and it compresses the representation of the flow by a factor of 4000 or more. We reconstruct the vortex tubes as generalized cylinders, providing a polygonal mesh suitable for display on a graphics workstation. We show how the reconstructed geometry of vortex tubes can be enhanced to help visualize helical motion in a static image.

Hall, Philip: *A phase equation approach to boundary layer instability theory: Tollmien-Schlichting waves*. ICASE Report No. 94-23, April 5, 1994, 38 pages. Submitted to the Journal of Fluid Mechanics.

Our concern is with the evolution of large amplitude Tollmien-Schlichting waves in boundary layer flows. In fact, the disturbances we consider are of a comparable size to the unperturbed state. We shall describe two-dimensional disturbances which are locally periodic in time and space. This is achieved using a phase equation approach of the type discussed by Howard and Kopell (1977) in the context of reaction-diffusion equations. We shall consider both large and $O(1)$ Reynolds numbers flows though, in order to keep our asymptotics respectable, our finite Reynolds number calculation

will be carried out for the asymptotic suction flow. Our large Reynolds number analysis, though carried out for Blasius flow, is valid for any steady two-dimensional boundary layer. In both cases the phase equation approach shows that the wavenumber and frequency will develop shocks or other discontinuities as the disturbance evolves. As a special case we consider the evolution of constant frequency/wavenumber disturbances and show that their modulational instability is controlled by Burgers equation at finite Reynolds number and by a new integro-differential evolution equation at large Reynolds numbers. For the large Reynolds number case the evolution equation points to the development of a spatially localized singularity at a finite time. The three-dimensional generalizations of the evolution equations is also given for the case of weak spanwise modulations.

Powell, Kenneth G.: *An approximate Riemann solver for magnetohydrodynamics (that works in more than one dimension)*. ICASE Report No. 94-24, April 8, 1994, 15 pages. Submitted to Journal of Computational Physics.

An approximate Riemann solver is developed for the governing equations of ideal magnetohydrodynamics (MHD). The Riemann solver has an eight-wave structure, where seven of the waves are those used in previous work on upwind schemes for MHD, and the eighth wave is related to the divergence of the magnetic field. The structure of the eighth wave is not immediately obvious from the governing equations as they are usually written, but arises from a modification of the equations that is presented in this paper. The addition of the eighth wave allows multi-dimensional MHD problems to be solved without the use of staggered grids or a projection scheme, one or the other of which was necessary in previous work on upwind schemes for MHD. A test problem made up of a shock tube with rotated initial conditions is solved to show that the two-dimensional code yields answers consistent with the one-dimensional methods developed previously.

Haines, Matthew, David Cronk, and Piyush Mehrotra: *On the design of Chant: a talking threads package*. ICASE Report No. 94-25, April 7, 1994, 27 pages. Submitted to Supercomputing '94.

Lightweight threads are becoming increasingly useful in supporting parallelism and asynchronous control structures in applications and language implementations. However, lightweight thread packages traditionally support only shared memory synchronization and communication primitives, limiting their use in distributed memory environments. We introduce the design of a runtime interface, called Chant, that supports lightweight threads with the capability of communication using both point-to-point and remote service request primitives, built from standard message passing libraries. This is accomplished by extending the POSIX pthreads interface with global thread identifiers, global thread operations, and message passing primitives. This paper introduces the Chant interface and describes the runtime issues in providing an efficient, portable implementation of such an interface. In particular, we present performance results of the initial portion of our runtime system: point-to-point message passing among threads. We examine the issue of thread scheduling in the presence of polling for messages, and measure the overhead incurred when using this interface as opposed to using the underlying communication layer directly. We show that our design can

accommodate various polling methods, depending on the level of support present in the underlying thread system, and imposes little overhead in point-to-point message passing over the existing communication layer.

Haines, Matthew, Bryan Hess, Piyush Mehrotra, John Van Rosendale, and Hans Zima: *Runtime support for data parallel tasks*. ICASE Report No. 94-26, April 7, 1994, 22 pages. Submitted to Supercomputing '94.

We have recently introduced a set of Fortran language extensions that allow for integrated support of task and data parallelism, and provide for shared data abstractions, (SDAs) as a method for communication and synchronization among these tasks. In this paper we discuss the design and implementation issues of the runtime system necessary to support these extensions, and discuss the underlying requirements for such a system. To test the feasibility of this approach, we implement a prototype of the runtime system and use this to support an abstract multidisciplinary optimization (MDO) problem for aircraft design. We give initial results and discuss future plans.

Dickens, Phillip M., David M. Nicol, Paul F. Reynolds, Jr., and J.M. Duva: *Analysis of optimistic window-based synchronization*. ICASE Report No. 94-27, April 13, 1994, 23 pages. Submitted to ACM Transactions on Modeling and Computer Simulation.

This paper studies an analytic model of parallel discrete-event simulation, comparing the costs and benefits of extending optimistic processing to the YAWNS synchronization protocol. The basic model makes standard assumptions about workload and routing; we develop methods for computing performance as a function of the degree of optimism allowed, overhead costs of state-saving, rollback, and barrier synchronization, and LP aggregation. This allows an approximation-based analysis of the range of situations under which optimism is a beneficial extension to YAWNS. We find that limited optimism is beneficial if the processor load is sparse, but that aggregating LPs onto processors improves YAWNS relative performance.

Zhang, Hong: *A note on windowing for the waveform relaxation*. ICASE Report No. 94-28, April 13, 1994, 13 pages. Submitted to Applied and Numerical Mathematics.

The technique of windowing has been often used in the implementation of the waveform relaxations for solving ODEs or time dependent PDEs. Its efficiency depends upon problem stiffness and operator splitting. Using model problems, the estimates for window length and convergence rate are derived. The effectiveness of windowing is then investigated for non-stiff and stiff cases respectively. It concludes that for the former, windowing is highly recommended when a large discrepancy exists between the convergence rate on a time interval and the ones on its subintervals. For the latter, windowing does not provide any computational advantage if machine features are disregarded. The discussion is supported by experimental results.

Mavriplis, D.J.: *A three dimensional multigrid Reynolds-Averaged Navier-Stokes solver for unstructured meshes*. ICASE Report No. 94-29, May 3, 1994, 28 pages. Submitted to AIAA.

A three-dimensional unstructured mesh Reynolds averaged Navier-Stokes solver is described. Turbulence is simulated using a single field-equation model. Computational overheads are minimized through the use of a single edge-based data-structure, and efficient multigrid solution technique, and the use of multi-tasking on shared memory multi-processors. The accuracy and efficiency of the code are evaluated by computing two-dimensional flows in three-dimensions and comparing with results from a previously validated two-dimensional code which employs the same solution algorithm. The feasibility of computing three-dimensional turbulent flows on grids of several million points in less than two hours of wall clock time is demonstrated.

Webb, J.C., S.R. Otto, and G.M. Lilley: *On the nonlinear stability of viscous modes within the Rayleigh problem on an infinite flat plate*. ICASE Report No. 94-30, May 25, 1994, 41 pages. Submitted to the Journal of Fluid Mechanics.

The stability has been investigated of the unsteady flow past an infinite flat plate when it is moved impulsively from rest, in its own plane. For small times the instantaneous stability of the flow depends on the linearised equations of motion which reduce in this problem to the Orr-Sommerfeld equation. It is known that the flow for certain values of Reynolds number, frequency and wavenumber is unstable to Tollmien-Schlichting waves, as in the case of the Blasius boundary layer flow past a flat plate. With increase in time, the unstable waves only undergo growth for a finite time interval, and this growth rate is itself a function of time. The influence of finite amplitude effects is studied by solving the full Navier-Stokes equations. It is found that the stability characteristics are markedly changed both by the consideration of the time evolution of the flow, and by the introduction of finite amplitude effects.

Masad, Jamal A., and Yousef H. Zurigat: *Effect of pressure gradient on first mode of instability in high-speed boundary layers*. ICASE Report No. 94-31, April 19, 1994, 51 pages. Submitted to Physics of Fluids.

The effect of a pressure gradient on the first mode of instability of compressible subsonic and supersonic boundary layers is investigated using linear stability theory. Formulations are presented for nonsimilar boundary-layer mean flow and linear quasi-parallel stability problems that account for variable fluid properties. A pressure gradient is studied that generates potential-flow Mach number distributions at the edge of the boundary layer of the form $M_e = cx^n$, where c is a constant and x is the dimensionless streamwise distance. Variations are calculated for the maximum growth rates of three-dimensional first-mode waves with different edge Mach numbers and different levels of both adverse and favorable pressure gradients. A favorable pressure gradient is shown to have a stabilizing effect on first-mode waves. However, at high edge Mach numbers, a favorable pressure gradient becomes less effective in stabilizing first-mode waves. The frequencies and streamwise and

spanwise wave numbers that correspond to the maximum growth rates of first-mode waves decrease as the pressure gradient become more favorable at all Mach numbers when the Reynolds number $R = 1500$ and at $Me \geq 2$ when $R = 600$. Setting the Prandtl number to unity significantly increases the maximum growth rates of first- and second-mode waves at high Mach numbers compared with setting it to the realistic value of 0.72.

Wilson, R.V., and A.O. Demuren: *Numerical simulation of two-dimensional spatially-developing mixing layers*. ICASE Report No. 94-32, May 3, 1994, 44 pages. Submitted to Physics of Fluids.

Two-dimensional, incompressible, spatially developing mixing layer simulations are performed at $Re = 10^2$ and 10^4 with two classes of perturbations applied at the inlet boundary; (i) combinations of discrete modes from linear stability theory, and (ii) a broad spectrum of modes derived from experimentally measured velocity spectra. The effect of the type and strength of inlet perturbations on vortex dynamics and time-averaged properties are explored. Two-point spatial velocity and autocorrelations are used to estimate the size and lifetime of the resulting coherent structures and to explore possible feedback effects. The computed time-averaged properties such as mean velocity profiles, turbulent statistics, and spread rates show good agreement with experimentally measured values. It is shown that by forcing with a broad spectrum of modes derived from an experimental energy spectrum many experimentally observed phenomena can be reproduced by a 2-D simulation. The strength of the forcing merely affected the length required for the dominant coherent structures to become fully-developed. Thus intensities comparable to those of the background turbulence in many wind tunnel experiments produced the same results, given sufficient simulation length.

Gottlieb, David, and Chi-Wang Shu: *On the Gibbs Phenomenon IV: recovering exponential accuracy in a sub-interval from a Gegenbauer partial sum of a piecewise analytic function*. ICASE Report No. 94-33, May 3, 1994, 18 pages. Submitted to Mathematics of Computation.

We continue our investigation of overcoming Gibbs phenomenon, i.e., to obtain exponential accuracy at all points (including at the discontinuities themselves), from the knowledge of a spectral partial sum of a discontinuous but piecewise analytic function. We show that if we are given the first N Gegenbauer expansion coefficients, based on the Gegenbauer polynomials $C_k^\mu(x)$ with the weight function $(1 - x^2)^{\mu - \frac{1}{2}}$ for any constant $\mu \geq 0$, of an L_1 function $f(x)$, we can construct an *exponentially convergent* approximation to the point values of $f(x)$ in any sub-interval in which the function is analytic. The proof covers the cases of Chebyshev or Legendre partial sums, which are most common in applications.

Chapman, Barbara, Piyush Mehrotra, and Hans Zima: *Extending HPF for advance data parallel applications*. ICASE Report No. 94-34, May 12, 1994, 30 pages. Submitted to IEEE Parallel and Distributed Technology.

The stated goal of High Performance Fortran (HPF) was to "address the problems of writing data parallel programs where the distribution of data affects performance". After examining the current version of the language we are led to the conclusion that HPF has not fully achieved this goal. While the basic distribution functions offered by the language - regular block, cyclic, and block cyclic distributions - can support regular numerical algorithms, advanced applications such as particle-in-cell codes or unstructured mesh solvers cannot be expressed adequately. We believe that this is a major weakness of HPF, significantly reducing its chances of becoming accepted in the numerical community. The paper discusses the data distribution and alignment issues in detail, points out some flaws in the basic language, and outlines possible future paths of development. Furthermore, we briefly deal with the issue of task parallelism and its integration with the data parallel paradigm of HPF.

Malek, Alaeddin and Timothy N. Phillips: *Pseudospectral collocation methods for fourth order differential equations*. ICASE Report No. 94-35, May 16, 1994, 35 pages. Submitted to Mathematical Computation.

Collocation schemes are presented for solving linear fourth order differential equations in one and two dimensions. The variational formulation of the model fourth order problem is discretized by approximating the integrals by a Gaussian quadrature rule generalized to include the values of the derivative of the integrand at the boundary points. Collocation schemes are derived which are equivalent to this discrete variational problem. An efficient preconditioner based on a low-order finite difference approximation to the same differential operator is presented. The corresponding multi-domain problem is also considered and interface conditions are derived. Pseudospectral approximations which are C^1 continuous at the interfaces are used in each subdomain to approximate the solution. The approximations are also shown to be C^3 continuous at the interfaces asymptotically. A complete analysis of the collocation scheme for the multi-domain problem is provided. The extension of the method to the biharmonic equation in two dimensions is discussed and results are presented for a problem defined in a non-rectangular domain.

Hu, Fang Q.: *A fast numerical solution of scattering by a cylinder: spectral method for the boundary integral equations*. ICASE Report No. 94-36, May 16, 1994, 37 pages. Submitted to Journal of Acoustic Society of America.

It is known that the exact analytic solutions of wave scattering by a circular cylinder, when they exist, are not in a closed form but in a closed form but in infinite series which converges slowly for high frequency waves. In this paper, we present a fast numerical solution for the scattering problem in which the Boundary Integral Equations, reformulated from the Helmholtz equation, are solved

using a Fourier spectral method. It is shown that the special geometry considered here allows the implementation of the spectral method to be simple and very efficient. The present method differs from previous approaches in that the singularities of the integral kernels are removed and dealt with accurately. The proposed method preserves the spectral accuracy and is shown to have an exponential rate of convergence. Aspects of efficient implementation using FFT are discussed. Moreover, the boundary integral equations of combined single and double-layer representation are used in the present paper. This ensures the uniqueness of the numerical solution for the scattering problem at all frequencies. Although a strongly singular kernel is encountered for the Neumann boundary conditions, we show that the hypersingularity can be handled easily in the spectral method. Numerical examples that demonstrate the validity of the method are also presented.

Eidson, T.M., and G. Erlebacher: *Implementation of a fully-balanced periodic tridiagonal solver on a parallel distributed memory architecture*. ICASE Report No. 94-37, May 29, 1994, 49 pages. Submitted to Concurrency, Practice and Experience.

While parallel computers offer significant computational performance, it is generally necessary to evaluate several programming strategies. Two programming strategies for a fairly common problem—a periodic tridiagonal solver—are developed and evaluated. Simple model calculations as well as timing results are presented to evaluate the various strategies.

The particular tridiagonal solver evaluated is used in many computational fluid dynamic simulation codes. The feature that makes this algorithm unique is that these simulation codes usually require simultaneous solutions for multiple right-hand-sides(RHS) of the system of equations. Each RHS solutions is independent and thus can be computed in parallel. Thus a Gaussian-elimination-type algorithm can be used in a parallel computation and the more complicated approaches such as cyclic reduction are not required.

The two strategies are a transpose strategy and a distributed solver strategy. For the transpose strategy, the data is moved so that a subset of all the RHS problems is solved on each of the several processors. This usually requires significant data movement between processor memories across a network. The second strategy attempts to have the algorithm follow the data across processor boundaries in a chained manner. This usually requires significantly less data movement. An approach to accomplish this second strategy in a near-perfect load-balanced manner is developed. In addition, an algorithm will be shown to directly transform a sequential Gaussian-elimination-type algorithm into the parallel, chained, load-balanced algorithm.

Wiecek, Malgorzata M., and Hong Zhang: *A scalable parallel algorithm for multiple objective linear programs*. ICASE Report No. 94-38, June 6, 1994, 14 pages. To be submitted to Computational Optimization and Applications.

This paper presents an ADBASE-based parallel algorithm for solving multiple objective linear programs (MOLPs). Job balance, speedup and scalability are of primary interest in evaluating efficiency of the new algorithm. Implementation results on Intel iPSC/2 and Paragon multiprocessors

show that the algorithm significantly speeds up the process of solving MOLPs, which is understood as generating all or some efficient extreme points and unbounded efficient edges. The algorithm gives specially good results for large and very large problems. Motivation and justification for solving such large MOLPs are also included.

Mehrotra, Piyush, and Matthew Haines: *An overview of the Opus language and runtime system*. ICASE Report No. 94-39, May 24, 1994, 16 pages. Submitted to the Seventh Annual Workshop on Languages and Computers for Parallel Computing.

We have recently introduced a new language, called *Opus*, which provides a set of Fortran language extensions that allow for integrated support of task and data parallelism. It also provides shared data abstractions (SDAs) as a method for communication and synchronization among these tasks. In this paper, we first provide a brief description of the language features and then focus on both the language-dependent and language-independent parts of the runtime system that support the language. The language-independent portion of the runtime system supports lightweight threads across multiple address spaces, and is built upon existing lightweight thread and communication systems. The language-dependent portion of the runtime system supports conditional invocation of SDA methods and distributed SDA argument handling.

Smith, Ralph C.: *A Galerkin method for linear PDE systems in circular geometries with structural acoustic applications*. ICASE Report No. 94-40, May 26, 1994, 33 pages. Submitted to the SIAM Journal on Scientific Computing.

A Galerkin method for systems of PDE's in circular geometries is presented with motivating problems being drawn from structural, acoustic and structural acoustic applications. Depending upon the application under consideration, piecewise splines or Legendre polynomials are used when approximating the system dynamics with modifications included to incorporate the analytic solution decay near the coordinate singularity. This provides an efficient method which retains its accuracy throughout the circular domain without degradation at the singularity. Because the problems under consideration are linear or weakly nonlinear with constant or piecewise constant coefficients, transform methods for the problems are not investigated. While the specific method is developed for the 2-D wave equations on a circular domain and the equation of transverse motion for a thin circular plate, examples demonstrating the extension of the techniques to a fully coupled structural acoustic system are used to illustrate the flexibility of the method when approximating the dynamics of more complex systems.

Banks, H.T., and R.C. Smith: *Parameter estimation in a structural acoustic system with fully nonlinear coupling conditions*. ICASE Report No. 94-41, May 26, 1994, 41 pages. Submitted to Inverse Problems.

A methodology for estimating physical parameters in a class of structural acoustic systems is presented. The general model under consideration consists of an interior cavity which is separated from an exterior noise source by an enclosing elastic structure. Piezoceramic patches are bonded to or embedded in the structure; these can be used both as actuators and sensors in applications ranging from the control of interior noise levels to the determination of structural flaws through nondestructive evaluation techniques. The presence and excitation of patches, however, changes the geometry and material properties of the structure as well as involves unknown patch parameters, thus necessitating the development of parameter estimation techniques which are applicable in this coupled setting. In developing a framework for approximation, parameter estimation and implementation, strong consideration is given to the fact that the input operator is unbounded due to the discrete nature of the patches. Moreover, the model is weakly nonlinear as a result of the coupling mechanism between the structural vibrations and the interior acoustic dynamics. Within this context, an illustrating model is given, well-posedness and approximation results are discussed and an applicable parameter estimation methodology is presented. The scheme is then illustrated through several numerical examples with simulations modeling a variety of commonly used structural acoustic techniques for system excitation and data collection.

Banks, H.T., R.C. Smith, and Yun Wang: *Vibration suppression with approximate finite dimensional compensators for distributed systems: computational methods and experimental results*. ICASE Report No. 94-42, May 26, 1994, 16 pages. To Appear in the Proceedings for the Second International Conference on Intelligent Materials.

Based on a distributed parameter model for vibrations, an approximate finite dimensional dynamic compensator is designed to suppress vibrations (multiple modes with a broad band of frequencies) of a circular plate with Kelvin-Voigt damping and clamped boundary conditions. The control is realized via piezoceramic patches bonded to the plate and is calculated from information available from several pointwise observed state variables. Examples from computational studies as well as use in laboratory experiments are presented to demonstrate the effectiveness of this design.

Banks, H.T., D.E. Brown, Vern L. Metcalf, R.J. Silcox, R.C. Smith, and Yun Wang: *A PDE-based methodology for modeling, parameter estimation and feedback control in structural and structural acoustic systems*. ICASE Report No. 94-43, May 26, 1994, 11 pages. To Appear in the Proceedings of the 1994 North American Conference on Smart Structures and Materials.

A problem of continued interest concerns the control of vibrations in a flexible structure and the related problem of reducing structure-borne noise in structural acoustic systems. In both cases, piezoceramic patches bonded to the structures have been successfully used as control actuators.

Through the application of a controlling voltage, the patches can be used to reduce structural vibrations which in turn leads to methods for reducing structure-borne noise. A PDE-based methodology for modeling, estimating physical parameters, and implementing a feedback control scheme for problems of this type is discussed. While the illustrating example is a circular plate, the methodology is sufficiently general so as to be applicable in a variety of structural and structural acoustic systems.

Leutenegger, Scott, and Graham Horton: *On the utility of the multi-level algorithm for the solution of nearly completely decomposable Markov chains*. ICASE Report No. 94-44, June 1, 1994, 15 pages. Submitted to Second International Workshop on the Numerical Solution of Markov Chains.

Recently the Multi-Level algorithm was introduced as a general purpose solver for the solution of steady state Markov chains. In this paper we consider the performance of the Multi-Level algorithm for solving Nearly Completely Decomposable (NCD) Markov chains, for which special-purpose interactive aggregation/disaggregation algorithms such as the Koury-McAllister-Stewart (KMS) method have been developed that can exploit the decomposability of the Markov chain. We present experimental results indicating that the general-purpose Multi-Level algorithm is competitive, and can be significantly faster than the special-purpose KMS algorithm when Gauss-Seidel and Gaussian Elimination are used for solving the individual blocks.

Ma, Kwan-Liu, and Z.C. Zheng: *3D Visualization of unsteady 2D airplane wake vortices*. ICASE Report No. 94-45, June 10, 1994, 19 pages. To appear in the Proceedings of Visualization 1994.

Air flowing around the wing tips of an airplane forms horizontal tornado-like vortices that can be dangerous to following aircraft. The dynamics of such vortices, including ground and atmospheric effects, can be predicted by numerical simulation, allowing the safety and capacity of airports to be improved. In this paper, we introduce three-dimensional techniques for visualizing time-dependent, two-dimensional wake vortex computations, and the hazard strength of such vortices near the ground. We describe a vortex core tracing algorithm and a local tiling method to visualize the vortex evolution. The tiling method converts time-dependent, two-dimensional vortex cores into three-dimensional vortex tubes. Finally, a novel approach calculates the induced rolling moment on the following airplane at each grid point within a region near the vortex tubes and thus allows three-dimensional visualization of the hazard strength of the vortices. We also suggest ways of combining multiple visualization methods to present more information simultaneously.

Sarkar, Sutanu: *The stabilizing effect of compressibility in turbulent shear flow*. ICASE Report No. 94-46, June 20, 1994, 40 pages. Submitted to the Journal of Fluid Mechanics.

Direct numerical simulation of turbulent homogeneous shear flow is performed in order to clarify compressibility effects on the turbulence growth in the flow. The two Mach numbers relevant to homogeneous shear flow are the turbulent Mach number M_t and the gradient Mach number

M_g . Two series of simulations are performed where the initial values of M_g and M_t are increased separately. The growth rate of turbulent kinetic energy is observed to decrease in both series of simulations. This 'stabilizing' effect of compressibility on the turbulent energy growth rate is observed to be substantially larger in the DNS series where the initial value of M_g is changed. A systematic comparison of the different DNS cases shows that the compressibility effect of reduced turbulent energy growth rate is primarily due to the reduced level of turbulence production and not due to explicit dilatational effects. The reduced turbulence production is not a mean density effect since the mean density remains constant in compressible homogeneous shear flow. The stabilizing effect of compressibility on the turbulence growth is observed to increase with the gradient Mach number M_g in the homogeneous shear flow DNS. Estimates of M_g for the mixing layer and the boundary layer are obtained. These estimates show that the parameter M_g becomes much larger in the high-speed mixing layer relative to the high-speed boundary layer even though the mean flow Mach numbers are the same in the two flows. Therefore, the inhibition of turbulent energy production and consequent 'stabilizing' effect of compressibility on the turbulence (over and above that due to the mean density variation) is expected to be larger in the mixing layer relative to the boundary layer in agreement with experimental observations.

Coward, Adrian V., Demetrios T. Papageorgiou, and Yiorgos S. Smyrlis: *Nonlinear stability of oscillatory core-annular flow: a generalized Kuramoto-Sivashinsky equation with time periodic coefficients*. ICASE Report No. 94-47, July 1, 1994, 44 pages. Submitted to ZAMP.

In this paper the nonlinear stability of two-phase core-annular flow in a pipe is examined when the acting pressure gradient is modulated by time harmonic oscillations and viscosity stratification and interfacial tension is present. An exact solution of the Navier-Stokes equations is used as the background state to develop an asymptotic theory valid for thin annular layers, which leads to a novel nonlinear evolution describing the spatio-temporal evolution of the interface. The evolution equation is an extension of the equation found for constant pressure gradients and generalizes the Kuramoto-Sivashinsky equation with dispersive effects found by Papageorgiou, Maldarelli & Rumschitzki, Phys. Fluids A 2(3), 1990, pp.340-352, to a similar system with time periodic coefficients. The distinct regimes of slow and moderate flow are considered and the corresponding evolution is derived. Certain solutions are described analytically in the neighborhood of the first bifurcation point by use of multiple scales asymptotics. Extensive numerical experiments, using dynamical systems ideas, are carried out in order to evaluate the effect of the oscillatory pressure gradient on the solutions in the presence of a constant pressure gradient.

McGreevy, J.L., A. Bayliss, and L. Maestrello: *On the interaction of jet noise with a nearby structure*. ICASE Report No. 94-48, June 14, 1994, 29 pages. Submitted to AIAA Journal.

The model of the interaction of the noise from a spreading subsonic jet with a panel-stringer assembly is studied numerically in two dimensions. The radiation resulting from this flow/acoustic/structure coupling is computed and analyzed in both the time and frequency domains. The jet is

initially excited by a pulse-like source inserted into the flow field. The pulse triggers instabilities associated with the inviscid instability of the jet mean flow shear layer. These instabilities in turn generate sound which provides the primary loading for the panels. The resulting structural vibration and radiation depends strongly on their placement relative to the jet/nozzle configuration. Results are obtained for the panel responses as well as the transmitted and incident pressure. The effect of the panels is to act as a narrow filter, converting the relatively broad band forcing, heavily influenced by jet instabilities, into radiation concentrated in narrow spectral bands.

Crockett, Thomas W.: *Design considerations for parallel graphics libraries*. ICASE Report No. 94-49, June 14, 1994, 23 pages. To appear in 1994 Intel Supercomputer Users Group Conference.

Applications which run on parallel supercomputers are often characterized by massive datasets. Converting these vast collections of numbers to visual form has proven to be a powerful aid to comprehension. For a variety of reasons, it may be described to provide this visual feedback at runtime. One way to accomplish this is to exploit the available parallelism to perform graphics operations in place. In order to do this, we need appropriate parallel rendering algorithms and library interfaces. This paper provides a tutorial introduction to some of the issues which arise in designing parallel graphics libraries and their underlying rendering algorithms. The focus is on polygon rendering for distributed memory message-passing systems. We illustrate our discussion with examples from PGL, a parallel graphics library which has been developed on the Intel family of parallel systems.

Dickens, Phillip, Philip Heidelberger, and David Nicol: *Parallelized direct execution simulation of message-passing parallel programs*. ICASE Report No. 94-50, June 14, 1994, 27 pages. Submitted to IEEE Transactions on Parallel and Distributed Systems.

As massively parallel computers proliferate, there is growing interest in finding ways by which performance of massively parallel codes can be efficiently predicted. This problem arises in diverse contexts such as parallelizing compilers, parallel performance monitoring, and parallel algorithm development. In this paper we describe one solution where one directly executes the application code, but uses a discrete-event simulator to model details of the presumed parallel machine, such as operating system and communication network behavior. Because this approach is computationally expensive, we are interested in its own parallelization, specifically the parallelization of the discrete-event simulator. We describe methods suitable for parallelized direct execution simulation of message-passing parallel programs, and report on the performance of such a system, LAPSE (Large Application Parallel Simulation Environment), we have built on the Intel Paragon. On all codes measured to date, LAPSE predicts performance well, typically within 10% relative error. Depending on the nature of the application code, we have observed low slowdowns (relative to natively executing code) and high relative speedups using up to 64 processors.

Quirk, James J.: *A cartesian grid approach with hierarchical refinement for compressible flows*. ICASE Report No. 94-51, June 28, 1994, 23 pages. Submitted to European Community Computational Mechanics Symposium.

Many numerical studies of flows that involve complex geometries are limited by the difficulties in generating suitable grids. We present a Cartesian boundary scheme for two-dimensional, compressible flows which is unfettered by the need to generate a computational grid and so it may be used, routinely, even for the most awkward of geometries. In essence, an arbitrary-shaped body is allowed to blank out some region of a background Cartesian mesh and the resultant cut-cells are singled out for special treatment. This is done within a finite-volume framework and so, in principle, any explicit flux-based integration scheme can take advantage of this method for enforcing solid boundary conditions. For best effect, the present Cartesian boundary scheme has been combined with a sophisticated, local mesh refinement scheme, and a number of examples are shown in order to demonstrate the efficacy of the combined algorithm for simulations of shock interaction phenomena.

Arian, Eyal, and Shlomo Ta'asan: *Multigrid one shot methods for optimal design problems: infinite dimensional control*. ICASE Report No. 94-52, July 1, 1994, 25 pages. Submitted to the Journal of Computational Physics.

The multigrid one shot method for optimal control problems, governed by elliptic systems, is introduced for the infinite dimensional control space. In this case the control variable is a function whose discrete representation involves increasing number of variables with grid refinement. The minimization algorithm uses Lagrange multipliers to calculate sensitivity gradients. A preconditioned gradient descent algorithm is accelerated by a set of coarse grids. It optimizes for different scales in the representation of the control variable on different discretization levels. An analysis which reduces the problem to the boundary is introduced. It is used to approximate the two level asymptotic convergence rate, to determine the amplitude of the minimization step, and the choice of a high pass filter to be used when necessary. The effectiveness of the method is demonstrated on a series of test problems. The new method enables the solutions of optimal control problems at the same cost of solving the corresponding analysis problems just a few times.

Alexandrov, Natalia, and Dennis, J.E., Jr.: *Multilevel algorithms for nonlinear optimization*. ICASE Report No. 94-53, June 21, 1994, 21 pages. To appear in Proceedings of CODAC/ICAM Workshop on Optimal Design and Control, April 8-9, 1994, Blacksburg, VA.

Multidisciplinary design optimization (MDO) gives rise to nonlinear optimization problems characterized by a large number of constraints that naturally occur in blocks. We propose a class of multilevel optimization methods motivated by the structure and number of constraints and by the expense of the derivative computations for MDO. The algorithms are an extension to the nonlinear programming problem of the successful class of local Brown-Brent algorithms for

nonlinear equations. Our extensions allow the user to partition constraints into arbitrary blocks to fit the application, and they separately process each block and the objective function, restricted to certain subspaces. The methods use trust regions as a globalization strategy, and they have been shown to be globally convergent under reasonable assumptions. The multilevel algorithms can be applied to all classes of MDO formulations. Multilevel algorithms for solving nonlinear systems of equations are a special case of the multilevel optimization methods. In this case, they can be viewed as a trust-region globalization of the Brown-Brent class.

Bodin, François, Thierry Priol, Piyush Mehrotra, and Dennis Gannon: *Directions in parallel programming: HPF, shared virtual memory and object parallelism in pC++*. ICASE Report No. 94-54, June 22, 1994, 39 pages. To appear in the Proceedings of the Summer Institute on Parallel Computer Architectures, Languages and Algorithms, IEEE Press.

Fortran and C++ are the dominant programming languages used in scientific computation. Consequently, extensions to these languages are the most popular for programming massively parallel computers. We discuss two such approaches to parallel Fortran and one approach to C++. The High Performance Fortran Forum has designed HPF with the intent of supporting data parallelism on Fortran 90 applications. HPF works by asking the user to help the compiler distribute and align the data structures with the distributed memory modules in the system. Fortran-S takes a different approach in which the data distribution is managed by the operating system and the user provides annotations to indicate parallel control regions. In the case of C++, we look at pC++ which is based on a concurrent aggregate parallel model.

Horton, Graham: *Adaptive relaxation for the steady-state analysis of Markov chains*. ICASE Report No. 94-55, June 23, 1994, 14 pages. To be submitted to Numerical Solution of Markov Chains Conference.

We consider a variant of the well-known Gauss-Seidel method for the solution of Markov chains in steady state. Whereas the standard algorithm visits each state exactly once per iteration in a pre-determined order, the alternative approach uses a dynamic strategy. A set of states to be visited is maintained which can grow and shrink as the computation progresses. In this manner, we hope to concentrate the computational work in those areas of the chain in which maximum improvement in the solution can be achieved. We consider the adaptive approach both as a solver in its own right and as a relaxation method within the multi-level algorithm. Experimental results show significant computational savings in both cases.

Criminale, W.O, T.L. Jackson, D.G. Lasseigne: *Towards enhancing and delaying disturbances in free shear flows*. ICASE Report No. 94-56, June 24, 1994, 29 pages. Submitted to Journal of Fluid Mechanics.

The family of shear flows comprising the jet, wake, and the mixing layer are subjected to perturbations in an inviscid, incompressible fluid. By modeling the basic mean flows as parallel with piecewise linear variations for the velocities, complete and general solutions to the linearized equations of motion can be obtained in closed form as functions of all space variables and time when posed as an initial-value problem. The results show that there is a continuous as well as the discrete spectrum that is more familiar in stability theory and therefore there can be both algebraic and exponential growth of disturbances in time. These bases make it feasible to consider control of such flows. To this end, the possibility of enhancing the disturbances in the mixing layer and delaying the onset in the jet and wake is investigated. It is found that growth of perturbations can be delayed to a considerable degree for the jet and the wake but, by comparison, cannot be enhanced in the mixing layer. By using moving coordinates, a method for demonstrating the predominant early and long time behavior of disturbances in these flows is given for continuous velocity profiles. It is shown that the early time transients are always algebraic whereas the asymptotic limit is that of an exponential normal mode. Numerical treatment of the new governing equations confirm the conclusions reached by use of the piecewise linear basic models. Although not pursued here, feedback mechanisms designed for control of the flow could be devised using the results of this work.

Macaraeg, Michèle G., T.L. Jackson and M.Y. Hussaini: *Ignition dynamics of a Laminar diffusion flame in the field of a vortex embedded in a shear flow*. ICASE Report No. 94-57, June 28, 1994, 34 pages. Submitted to Combustion Science and Technology.

The role of streamwise-spanwise vorticity interactions that occur in turbulent shear flows on flame/vortex interactions is examined by means of asymptotic analysis and numerical simulation in the limit of small Mach number. An idealized model is employed to describe the interaction process. The model consists of a one-step, irreversible Arrhenius reaction between initially unmixed species occupying adjacent half-planes which are then allowed to mix and react in the presence of a streamwise vortex embedded in a shear flow. It is found that the interaction of the streamwise vortex with shear gives rise to small-scale velocity oscillations which increase in magnitude with shear strength. These oscillations give rise to regions of strong temperature gradients via viscous heating, which can lead to multiple ignition points and substantially decrease ignition times. The evolution in time of the temperature and mass-fraction fields is followed, and emphasis is placed on the ignition time and structure as a function of vortex and shear strength.

Stott, Jillian A.K., and Peter W. Duck: *The effects of viscosity on the stability of a trailing-line vortex in compressible flow*. ICASE Report No. 94-58, July 1, 1994, 21 pages. Submitted to Physics of Fluids.

We consider the effects of viscosity on the inviscid stability of the Batchelor (1964) vortex in a compressible flow. The problem is tackled asymptotically, in the limit of large (streamwise and azimuthal) wavenumbers, together with large Mach numbers. This problem, with viscous effects neglected, was discussed in Stott & Duck (1994). The authors found that the nature of the solution passes through different regimes as the Mach number increases, relative to the wavenumber. This structure persists when viscous effects are included in the analysis. In the present study, as in that mentioned above, the mode present in the incompressible case ceases to be unstable at high Mach numbers and a centre mode forms, whose stability characteristics are determined primarily by conditions close to the vortex axis. We find generally that viscosity has a stabilising influence on the flow, whilst in the case of centre modes, viscous effects become important at much larger Reynolds numbers than for the first class of disturbance.

Harten, Ami: *Multiresolution representation and numerical algorithms: A brief overview*. ICASE Report No. 94-59, July 29, 1994, 32 pages. Proceedings from the ICASE/LaRC Workshop on Parallel Numerical Algorithms.

In this paper we review recent developments in techniques to represent data in terms of its *local* scale components. These techniques enable us to obtain data compression by eliminating scale-coefficients which are sufficiently small. This capability for data compression can be used to reduce the cost of many numerical solution algorithms by either applying it to the numerical solution operator in order to get an approximate sparse representation, or by applying it to the numerical solution itself in order to reduce the number of quantities that need to be computed.

Propst, G.: *Discretized energy minimization in a wave guide with point sources*. ICASE Report No. 94-60, July 8, 1994, 25 pages. Submitted to Numerical Functional Analysis and Optimization.

An anti-noise problem on a finite time interval is solved by minimization of a quadratic functional on the Hilbert space of square integrable controls. To this end, the one-dimensional wave equation with point sources and pointwise reflecting boundary conditions is decomposed into a system for the two propagating components of waves. Wellposedness of this system is proved for a class of data that includes piecewise linear initial conditions and piecewise constant forcing functions. It is shown that for such data the optimal piecewise constant control is the solution of a sparse linear system. Methods for its computational treatment are presented as well as examples of their applicability. The convergence of discrete approximations to the general optimization problem is demonstrated by finite element methods.

Gottlieb, David, and Chi-Wang Shu: *On the Gibbs phenomenon V: recovering exponential accuracy from collocation point values of a piecewise analytic function.* ICASE Report No. 94-61, July 8, 1994, 18 pages. Submitted to Numerische Matematic.

The paper presents a method to recover exponential accuracy at all points (including at the discontinuities themselves), from the knowledge of an approximation to the *interpolation polynomial* (or trigonometrical polynomial). We show that if we are given the collocation point values (or an highly accurate approximation) at the Gauss or Gauss-Lobatto points, we can reconstruct an *uniform exponentially convergent* approximation to the function $f(x)$ in any sub-interval of analyticity. The proof covers the cases of Fourier, Chebyshev, Legendre, and more general Gegenbauer collocation methods.

Mavriplis, D., and V. Venkatakrishnan: *Agglomeration multigrid for turbulent viscous flow.* ICASE Report No. 94-62, July 11, 1994, 29 pages. Submitted to Computers in Fluids (Journal).

Agglomeration multigrid, which has been demonstrated as an efficient and automatic technique for the solution of the Euler equations on unstructured meshes, is extended to viscous turbulent flows. For diffusion terms, coarse grid discretizations are not possible, and more accurate grid transfer operators are required as well. A Galerkin coarse grid operator construction and an implicit prolongation operator are proposed. Their suitability is evaluated by examining their effect on the solution of Laplace's equation. The resulting strategy is employed to solve the Reynolds-averaged Navier-Stokes equations for aerodynamic flows. Convergence rates comparable to those obtained by a previously developed non-nested mesh multigrid approach are demonstrated, and suggestions for further improvements are given.

Hou, Steven L., and James C. Turner: *Finite element approximation of optimal control problems for the von Karman equations.* ICASE Report No. 94-63, July 11, 1994, 17 pages. To be submitted to Numerical PDE's.

This paper is concerned with optimal control problems for the von Kármán equations with distributed controls. We first show that optimal solutions exist. We then show that Lagrange multipliers may be used to enforce the constraints and derive an optimality system from which optimal states and controls may be deduced. Finally we define finite element approximations of solutions for the optimality system and derive error estimates for the approximations.

Zhou, Ye, P.K. Yeung, and James G. Brasseur: *Scale disparity and spectral transfer in anisotropic numerical turbulence.* ICASE Report No. 94-64, August 16, 1994, 40 pages. To be submitted to Physics of Fluids.

To study the effect of cancelations within long-range interactions on local isotropy at the small scales (Waleffe, *Phys. Fluids A*, 4, 1992), we calculate explicitly the degree of cancelation in

distant triadic interactions in the simulations of Yeung & Brasseur (*Phys. Fluids A*, **3**, 1991) and Yeung, Brasseur & Wang (to appear, *J. Fluid Mech.*) using the single scale disparity parameter " s " developed by Zhou (*Phys. Fluids A*, **5**, 1993). In the simulations, initially isotropic simulated turbulence was subjected to coherent anisotropic forcing at the large scales and the smallest scales were found to become anisotropic as a consequence of direct large-small scale couplings. We find that the marginally distant interactions in the simulation do not cancel out under summation and that the development of small-scale anisotropy is indeed a direct consequence of the distant triadic group, as argued by Yeung, et al. A reduction of anisotropy at later times occurs as a result of the isotropizing influences of more local energy-cascading triadic interactions. Nevertheless, the distant triadic group persists as an anisotropizing influence at later times. We find that, whereas long-range interactions, in general, contribute little to net energy transfer into or out of a high wavenumber shell k , the anisotropic transfer of component energy within the shell increases with increasing scale separation s . These results are consistent with results by Zhou, and Brasseur & Wei (*Phys. Fluids*, **6**, 1994), and suggest that the anisotropizing influences of long range interactions should persist to higher Reynolds numbers. The residual effect of the forced distant triadic group in this low-Reynolds number simulation is found to be forward cascading, on average.

Roe, Philip: *Linear bicharacteristic schemes without dissipation*. ICASE Report No. 94-65, July 14, 1994, 23 pages. To be submitted to SIAM Journal on Scientific Computing.

This paper is concerned with developing methods for the propagation of linear waves in several space dimensions. The methods are time-reversible, and hence free from numerical dissipation. They are based on bicharacteristic forms of the governing equations, and are made possible by adopting forms of staggered storage that depend on the precise equations under consideration. Analysis is presented for the equations of acoustics, electromagnetics, and elastodynamics.

Roe, Philip: *Local reduction of certain wave operators in one-dimensional form*. ICASE Report No. 94-66, July 14, 1994, 8 pages. To be submitted to Applied Mathematics Letters.

It is noted that certain common linear wave operators have the property that linear variation of the initial data gives rise to one-dimensional evolution in a plane defined by time and some direction in space. The analysis is given for operators arising in acoustics, electromagnetics, elastodynamics, and an abstract system.

Shu, Chi-Wang, and Peter S. Wong: *A note on the accuracy of spectral method applied to nonlinear conservation laws*. ICASE Report No. 94-67, July 15, 1994, 14 pages. Submitted to Journal of Scientific Computing.

Fourier spectral method can achieve exponential accuracy both on the approximation level and for solving partial differential equations if the solutions are analytic. For a linear partial

differential equation with a discontinuous solution, Fourier spectral method produces poor point-wise accuracy without post-processing, but still maintains exponential accuracy for all moments against analytic functions. In this note we assess the accuracy of Fourier spectral method applied to nonlinear conservation laws through a numerical case study. We find that the moments with respect to analytic functions are no longer very accurate. However the numerical solution does contain accurate information which can be extracted by a post-processing based on Gegenbauer polynomials.

Hesthaven, J. S., and D. Gottlieb: *A stable penalty method for the compressible Navier-Stokes equations. I. Open boundary conditions.* ICASE Report No. 94-68, July 26, 1994, 43 pages. Submitted to SISC.

The purpose of this paper is to present asymptotically stable open boundary conditions for the numerical approximation of the compressible Navier-Stokes equations in three spatial dimensions. The treatment uses the conservation form of the Navier-Stokes equations and utilizes linearization and localization at the boundaries based on these variables. The proposed boundary conditions are applied through a penalty procedure, thus ensuring correct behavior of the scheme as the Reynolds number tends to infinity. The versatility of this method is demonstrated for the problem of a compressible flow past a circular cylinder.

Booty, Michael, and Gregory Kriegsmann: *Microwave heating and joining of ceramic cylinders: a mathematical model.* ICASE Report No. 94-69, July 25, 1994, 16 pages. Submitted to Methods and Applications of Analysis.

A thin cylindrical ceramic sample is placed in a single mode microwave applicator in such a way that the electric field strength is allowed to vary along its axis. The sample can either be a single rod or two rods butted together. We present a simple mathematical model which describes the microwave heating process. It is built on the assumption that the Biot number of the material is small, and that the electric field is known and uniform throughout the cylinder's cross-section. The model takes the form of a non-linear parabolic equation of reaction-diffusion type, with a spatially varying reaction term that corresponds to the spatial variation of the electromagnetic field strength in the waveguide. The equation is analyzed and a solution is found which develops a hot spot near the center of the cylindrical sample and which then propagates outwards until it stabilizes. The propagation and stabilization phenomenon concentrates the microwave energy in a localized region about the center where elevated temperatures may be desirable.

Younis, Bassam A., Thomas B. Gatski, and Charles G. Speziale: *On the prediction of free turbulent jets with swirl using a quadratic pressure-strain*. ICASE Report No. 94-70, August 23, 1994, 26 pages. To be Submitted to ASME - Journal of Fluids Engineering.

Data from free turbulent jets both with and without swirl are used to assess the performance of the pressure-strain model of Speziale, Sarkar and Gatski which is quadratic in the Reynolds stresses. Comparative predictions are also obtained with the two versions of the Launder, Reece and Rodi model which are linear in the same terms. All models are used as part of a complete second-order closure based on the solution of differential transport equations for each non-zero component of $\overline{u_i u_j}$ together with an equation for the scalar energy dissipation rate. For non-swirling jets, the quadratic model underestimates the measured spreading rate of the plane jet but yields a better prediction for the axisymmetric case without resolving the plane jet/round jet anomaly. For the swirling axisymmetric jet, the same model accurately reproduces the effects of swirl on both the mean flow and the turbulence structure in sharp contrast with the linear models which yield results that are in serious error. The reasons for these differences are discussed.

Demuren, A.O.: *Modeling jets in cross flow*. ICASE Report No. 94-71, August 8, 1994, 36 pages. To be published in Handbook of Fluid Dynamics and Fluid Machinery.

Various approaches to the modeling of jets in cross flow are reviewed. These are grouped into four broad classes, namely: empirical models, integral models, perturbation models, and numerical models. Empirical models depend largely on the correlation of experimental data and are mostly useful for first-order estimates of global properties such as jet trajectory and velocity and temperature decay rates. Integral models are based on some ordinary-differential form of the conservation laws, but require substantial empirical calibration. They allow more details of the flow field to be obtained; simpler versions have to assume similarity of velocity and temperature profiles, but more sophisticated ones can actually calculate these profiles. Perturbation models require little empirical input, but the need for small parameters to ensure convergent expansions limits their application to either the near-field or the far-field. Therefore, they are mostly useful for the study of flow physics. Numerical models are based on conservation laws in partial-differential form. They require little empirical input and have the wide range of applicability. They also require the most computational resources. Although many qualitative and quantitative features of jets in cross flow have been predicted with numerical models, many issues affecting accuracy such as grid resolution and turbulence model are not completely resolved.

Nicol, David and Weizhen Mao: *On bottleneck partitioning k-ary n-cubes*. ICASE Report No. 94-72, August 19, 1994, 11 pages. To be submitted to Parallel Processing Letters.

Graph partitioning is a topic of extensive interest, with applications to parallel processing. In this context graph nodes typically represent computation, and edges represent communication. One seeks to distribute the workload by partitioning the graph so that every processor has approximately

the same workload, and the communication cost (measured as a function of edges exposed by the partition) is minimized. Measures of partition quality vary; in this paper we consider a processor's cost to be the sum of its computation and communication costs, and consider the cost of a partition to be the *bottleneck*, or maximal processor cost induced by the partition. For a general graph the problem of finding an optimal partitioning is intractable. In this paper we restrict our attention to the class of k -ary n -cube graphs with uniformly weighted nodes. Given mild restrictions on the node weight and number of processors, we identify partitions yielding the smallest bottleneck. We also demonstrate by example that some restrictions are necessary for the partitions we identify to be optimal. In particular, there exist cases where partitions that evenly partition nodes need not be optimal.

Kopriva, David A.: *Spectral solution of the viscous blunt body problem II: multidomain approximation*. ICASE Report No. 94-73, September 27, 1994, 28 pages. Submitted to AIAA Journal.

We present steady solutions of high speed viscous flows over blunt bodies using a multidomain Chebyshev spectral collocation method. The region within the shock layer is divided into subdomains so that internal layers can be well-resolved. In the interiors of the subdomains, the solution is approximated by Chebyshev collocation. At interfaces between subdomains, the advective terms are upwinded and the viscous terms are treated by a penalty method. The method is applied to five flows the Mach number range 5-25 and Reynolds number range 2,000 - 83,000, based on nose radius. Results are compared to experimental data and to a finite difference result.

Leutenegger, Scott T. and David M. Nicol: *Efficient bulk-loading of gridfiles*. ICASE Report No. 94-74, August 26, 1994, 25 pages. Submitted to IEEE Transaction on Knowledge and Data Engineering.

This paper considers the problem of bulk-loading large data sets for the gridfile multi-attribute indexing technique. We propose a rectilinear partitioning algorithm that heuristically seeks to minimize the size of the gridfile needed to ensure no bucket overflows. Empirical studies on both synthetic data sets and on data sets drawn from computational fluid dynamics applications demonstrate that our algorithm is very efficient, and is able to handle large data sets. In addition, we present an algorithm for bulk-loading data sets too large to fit in main memory. Utilizing a sort of the entire data set it creates a gridfile without incurring any overflows.

Quirk, James J. and Smadar Karni: *On the dynamics of a shock-bubble interaction*. ICASE Report No. 94-75, September 27, 1994, 37 pages. To be submitted to the Journal of Fluid.

We present a detailed numerical study of the interaction of a weak shock wave with an isolated cylindrical gas inhomogeneity. Such interactions have been studied experimentally in an attempt to elucidate the mechanism whereby shock waves propagating through random media enhance

mixing. Our study concentrates on the early phases of the interaction process which are dominated by repeated refractions and reflections of acoustic fronts at the bubble interface. Specifically, we have reproduced two of the experiments performed by Haas and Sturtevant.

Girimaji, Sharath S. and Charles G. Speziale: *A modified restricted Euler equation for turbulent flows with mean velocity gradients*. ICASE Report No. 94-76, September 26, 1994, 21 pages. Submitted to Physics of Fluids.

The restricted Euler equation captures many important features of the behavior of the velocity gradient tensor observed in direct numerical simulations (DNS) of isotropic turbulence. However, in slightly more complex flows the agreement is not good, especially in regions of low dissipation. In this paper, it is demonstrated that the Reynolds-averaged restricted Euler equation violates the balance of mean momentum for virtually all homogeneous turbulent flows with only two major exceptions: isotropic and homogeneously-sheared turbulence. A new model equation which overcomes this shortcoming and is more widely applicable is suggested. This model is derived from the Navier-Stokes equation with a restricted Euler type approximation made on the fluctuating velocity gradient field. Analytical solutions of the proposed modified restricted Euler equation appear to be difficult to obtain. Hence, a strategy for numerically calculating the velocity gradient tensor is developed. Preliminary calculations tend to indicate that the modified restricted Euler equation captures many important aspects of the behavior of the fluctuating velocity gradients in anisotropic homogeneous turbulence.

Alexandrov, Natalia and J.E. Dennis, Jr.: *Algorithms for bilevel optimization*. ICASE Report No. 94-77, September 26, 1994, 12 pages. Scheduled to appear in Proceedings of 5th AIAA/NASA/USAF/ISSMO Symposium on Multidisciplinary Analysis & Optimization.

General multilevel nonlinear optimization problems arise in design of complex systems and can be used as a means of regularization for multicriteria optimization problems. Here for clarity in displaying our ideas, we restrict ourselves to general bilevel optimization problems, and we present two solution approaches. Both approaches use a trust-region globalization strategy, and they can be easily extended to handle the general multilevel problem. We make no convexity assumptions, but we do assume that the problem has a nondegenerate feasible set. We consider necessary optimality conditions for the bilevel problem formulations and discuss results that can be extended to obtain multilevel optimization formulations with constraints at each level.

Stoica, Ion, Florin Sultan, and David Keyes: *A simple hyperbolic model for communication in parallel processing environments*. ICASE Report No. 94-78, September 27, 1994, 12 pages. To be submitted to Journal of Parallel and Distributed Computing.

We introduce a model for communication costs in parallel processing environments, called the "hyperbolic model," which generalizes two-parameter dedicated-link models in an analytically simple way. Dedicated interprocessor links parameterized by a latency and a transfer rate that are independent of load are assumed by many existing communication models; such models are unrealistic for workstation networks. The communication system is modeled as a directed communication graph in which terminal nodes represent the application processes that initiate the sending and receiving of the information and in which internal nodes, called communication blocks (*CBs*), reflect the layered structure of the underlying communication architecture. The direction of graph edges specifies the flow of the information carried through messages. Each *CB* is characterized by a two-parameter hyperbolic function of the message size that represents the service time needed for processing the message. The parameters are evaluated in the limits of very large and very small messages. Rules are given for reducing a communication graph consisting of many *CBs* to an equivalent two-parameter form, while maintaining an approximation for the service time that is exact in both large and small limits. The model is validated on a dedicated Ethernet network of workstations by experiments with communication subprograms arising in scientific applications, for which a tight fit of the model predictions with actual measurements of the communication and synchronization time between end processes is demonstrated. The model is then used to evaluate the performance of two simple parallel scientific applications from partial differential equations: domain decomposition and time-parallel multigrid. In an appropriate limit, we also show the compatibility of the hyperbolic model with the recently proposed LogP model.

Arbarbanel, Saul, Mark Carpenter, and David Gottlieb: *On the removal of boundary errors caused by Runge-Kutta integration of non-linear partial differential equations*. ICASE Report No. 94-79, September 27, 1994, 9 pages. To be submitted to the Journal of Computational Physics.

It has been previously shown that the temporal integration of hyperbolic partial differential equations may, because of boundary conditions, lead to deterioration of accuracy of the solution. A procedure for removal of this error in the linear case has been established previously.

In the present paper we consider hyperbolic p.d.e's (linear and non-linear) whose boundary treatment is done via the SAT-procedure. A methodology is present for recovery of the full order of accuracy, and has been applied to the case of a 4th order explicit finite difference scheme.

Hanebutte, Ulf R., Ronald D. Joslin, and Mohammad Zubair: *Scalability study of parallel spatial direct numerical simulation code on IBM parallel supercomputer*. ICASE Report No. 94-80, September 27, 1994, 20 pages. To be submitted to the Journal of Scientific Computing.

The implementation and the performance of a parallel spatial direct numerical simulation (PS-DNS) code are reported for the IBM SP1 supercomputer. The spatially evolving disturbances that

are associated with laminar-to-turbulent in three-dimensional boundary-layer flows are computed with the PS-DNS code. By remapping the distributed data structure during the course of the calculation, optimized serial library routines can be utilized that substantially increase the computational performance. Although the remapping incurs a high communication penalty, the parallel efficiency of the code remains above 40 percent for all performed calculations. By using appropriate compile options and optimized library routines, the serial code achieves 52-56 Mflops on a single node of the SP1 (45 percent of theoretical peak performance). The actual performance of the PS-DNS code on the SP1 is evaluated with a "real world" simulation that consists of 1.7 million grid points. One time step of this simulation is calculated on eight nodes of the SP1 in the same time as required by a Cray Y/MP for the same simulation. The scalability information provides estimated computational costs that match the actual costs relative to changes in the number of grid points.

ICASE COLLOQUIA

April 1, 1994 - September 30, 1994

Name/Affiliation/Title	Date
Vibha Dixit-Radiya, Ohio State University "Mapping on Wormhole-Routed Distributed-Memory Systems: A Temporal Communication Graph-Based Approach"	April 1
Christopher Kennedy, University of California, San Diego "The Numerical Simulation of Variable-Density Compressible Shear Layers"	April 4
Liang Chen, Georgia Institute of Technology "Conservation Principle of Parallel Simulations and its Applications on Performance Analysis"	April 8
Farrokh Mistree, Georgia Institute of Technology "Robust and Axiomatic Design of Engineering Systems: A Decision-Based Approach"	April 11
Thomas C. Corke, Illinois Institute of Technology "Cross-Flow Instability with Periodic Distributed Roughness"	April 12
Tim Harris, University of Edinburgh "The Use of Decoupling in Shared Memory Multiprocessors"	April 14
Daniel C. Haworth, General Motors NAO R&D Center "Numerical Simulation of Flame-Wall Interaction in Turbulent Premixed Combustion"	April 15
Graham Horton, University of Erlangen-Nuernberg "A Multi-Level Solver for Large Markov Chains"	April 18
Brian Totty, University of Illinois "Tunable Shared-Memory Abstractions for Distributed Data Structures"	April 22
Vadim Maslov, University of Maryland "Exact Array Dataflow Dependence Analysis: Why and How"	April 25
Christopher Hunter, Florida State University "The Dynamics of Collisionless Stellar Systems"	April 28
Yusheng Feng, The University of Texas at Austin "Parallel Domain Decomposition for HP Finite Element Methods"	April 29
Kemal Hanjalic, Michigan Technological University "On Modelling and Computation of Non-Equilibrium Wall Flows at Transitional and Higher Reynolds Numbers with a Second-Moment Closure Model"	May 2

Name/Affiliation/Title	Date
Sorin Costiner, The Weizmann Institute of Science, Israel "New Multigrid Techniques for Design, Optimization, and Computational Electromagnetism"	May 4
Linda F. Wilson, The University of Texas at Austin "Performance Analysis of Distributed Algorithms Based on Communication and Synchronization Patterns"	May 6
Mark Sussman, University of California, Los Angeles "A Level Set Approach for Computing Solutions to Incompressible Two-Phase Flow"	May 9
Richard Balling, Brigham Young University "A Critical Overview of Fundamental Approaches to Multidisciplinary Design Optimization"	May 19
Ayodeji Demuren, Old Dominion University "Analysis Modelling and Computations of Complex Turbulent Flows"	May 26
Leonidas Sakell, Air Force Office of Scientific Research "AFOSR Program in External Aerodynamics and Hypersonics"	June 3
Michael Booty, New Jersey Institute of Technology "The Modulation of a Subsonic Flame"	July 6
Laura Rodham, Nielsen Engineering & Research, Mountain View, CA "A Knowledge-Based System for Analyzing Technical Data"	July 8
Robert Rubinstein, ICOMP, NASA Lewis Research Center "Langevin Equations in Turbulence Theory and Modelling"	July 11
Michael Howe, Boston University "The Influence of Mean Shear on Sound Produced by Turbulent Flow over Slots and Louvres"	July 14
John D. McCalpin, University of Delaware "Recent Developments in the Mathematics of Large-Scale Ocean Circulation Modelling"	July 20
Philip Roe, University of Michigan "Two-Dimensional Upwinding"	July 27
Mark Hale, Georgia Institute of Technology "Using Agent Technologies in a Design Environment"	August 1
Ki D. Lee, University of Illinois, Urbana "Experience in Aerodynamic Design Optimization Using the Navier-Stokes Equations"	August 2

Name/Affiliation/Title	Date
August Verhoff, McDonnell Douglas Corporation “Complementing Numerical Fluid Dynamic Simulations with Classical Analytic Methods”	August 5
Lambertus Hesselink, Stanford University “Visualization of Vector and Tensor Datasets”	August 8
Bram van Leer, W.M. Keck Foundation Laboratory for Computational Fluid Dynamics, University of Michigan “Uses of Preconditioned Euler Equations”	August 10
David Sidilkover, Courant Institute, New York University “A New Genuinely Two-Dimensional Scheme for the Compressible Euler Equations”	August 11
Mark Short, University of Bristol, United Kingdom “Stability Detonation for Chain-Branching Reactions”	August 19
M. Ehtesham Hayder, ICOMP, NASA Lewis Research Center “Boundary Conditions for Jet Flow Computations”	August 22
Alain Dervieux, INRIA of Sophia-Antipolis “Multi-level Methods for Unstructured Meshes”	August 23
Nikos Chrisochoides, Syracuse University “Multi-Thread Load Balancing Approach for Parallel PDE Computations”	August 24
Hillel Tal-Ezer, Tel-Aviv University “K-Spectra and Non-Normal Matrices”	August 26
Eli Turkel, Tel-Aviv University “Preconditioning the Fluid Dynamics Equations – Part 3”	September 8
Antony Jameson, Princeton University “High Resolution Symmetric and Upstream Limited Difference Schemes for the Gas Dynamic”	September 9
Jim E. Jones “Accurate Computation of Fluid Velocities in Porous Media”	September 16
Jim Leathrum, Old Dominion University “Accelerated Panel Codes Using the Fast Multipole Method”	September 19
W.D. Lakin, University of Vermont “A Hybrid Asymptotic-Numerical Study of a Model for Intracranial Pressure Dynamics”	September 22

ICASE SUMMER ACTIVITIES

The summer program for 1994 included the following visitors:

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Abarbanel, Saul Tel-Aviv University, Israel	7/18 - 9/27	Applied & Numerical Mathematics
Appel, Justin Virginia Polytechnic Institute & State University	5/23 - 7/29	Applied & Numerical Mathematics
Banks, H. Thomas North Carolina State University	8/17 - 8/19 9/20 - 9/23	Applied & Numerical Mathematics
Bayliss, Alvin Northwestern University	6/14 - 6/16 7/11 - 7/15 7/31 - 8/04	Fluid Mechanics
Berger, Stanley A. University of California, Berkeley	7/05 - 8/12	Fluid Mechanics
Bokhari, Shahid Pakistan University of Engineering & Technology	6/10 - 9/02	Computer Science
Booty, Michael New Jersey Institute of Technology	6/13 - 7/08	Fluid Mechanics
Brown, Thomas M., III Vanderbilt University	5/23 - 7/28	Fluid Mechanics
Bryan, Kurt Rose-Hulman Institute of Technology	7/05 - 7/22	Applied & Numerical Mathematics
Burns, John Virginia Polytechnic Institute & State University	5/11 - 5/13 8/15 - 8/18	Applied & Numerical Mathematics
Cai, Wei University of North Carolina, Charlotte	8/15 - 8/26	Applied & Numerical Mathematics
Cai, Xiao-Chuan University of Kentucky	8/01 - 8/26	Computer Science

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Castanon, David A. Boston University	8/15 - 8/19	Fluid Mechanics
Chrisochoides, Nikos Syracuse University	6/27 - 7/22	Computer Science
Ciardo, Gianfranco College of William & Mary	6/27 - 7/29	Computer Science
Corke, Thomas Illinois Institute of Technology	7/25 - 8/05	Fluid Mechanics
Criminale, William University of Washington	6/06 - 7/15	Fluid Mechanics
Dando, Andrew University of Manchester, England	6/13 - 7/01	Fluid Mechanics
Das, Chita Pennsylvania State University	8/01 - 8/12	Computer Science
Deang, Jennifer Virginia Polytechnic Institute & State University	5/23 - 7/29	Applied & Numerical Mathematics
Duck, Peter University of Manchester, England	7/25 - 8/19	Fluid Mechanics
Fahringer, Thomas University of Vienna, Austria	7/16 - 10/14	Computer Science
Fischer, Paul Brown University	8/15 - 9/02	Applied & Numerical Mathematics
Fishwick, Paul University of Florida	7/11 - 7/15	Computer Science
Funaro, Daniele Universita de Pavia, Italy	8/15 - 9/02	Applied & Numerical Mathematics
Geer, James State University of New York	6/27 - 7/01 8/15 - 8/19	Fluid Mechanics
Gottlieb, David Brown University	5/23 - 5/26 7/18 - 7/29 8/08 - 8/19	Applied & Numerical Mathematics

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Grosch, Chester E. Old Dominion University	7/05 - 7/29	Fluid Mechanics
Gunzburger, Max Virginia Polytechnic Institute & State University	5/09 - 5/13 6/20 - 6/24 8/15 - 8/19	Applied & Numerical Mathematics
Hall, Philip University of Manchester, England	6/07 - 9/15	Fluid Mechanics
Hammerton, Paul University of Cambridge, United Kingdom	6/20 - 7/08	Fluid Mechanics
Harten, Amiram Tel-Aviv University, Israel	5/23 - 5/27	Applied & Numerical Mathematics
Holt, Maurice University of California, Berkeley	8/08 - 8/12	Applied & Numerical Mathematics
Horton, Graham Universtat Erlangen-Nuremberg, Federal Republic of Germany	8/01 - 8/26	Applied & Numerical Mathematics
Hou, Gene J-W Old Dominion University	5/23 - 6/03	Applied & Numerical Mathematics
Howe, Michael Boston University	7/05 - 7/15	Fluid Mechanics
Hu, Fang Old Dominion University	5/09 - 8/05	Fluid Mechanics
Jordan, Harry University of Colorado, Boulder	7/11 - 7/29	Computer Science
Kapila, Ashwani Rensselaer Polytechnic Institute	8/01 - 8/19	Fluid Mechanics
Karni, Smadar Courant Institute	8/22 - 8/26	Applied & Numerical Mathematics
Kelly, Michael A. San Diego Supercomputer Center	6/01 - 8/31	Computer Science

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Keyes, David Old Dominion University	5/31 - 6/24 8/03 - 8/26	Computer Science
Kopriva, David Florida State University	5/31 - 6/10 8/15 - 8/19	Applied & Numerical Mathematics
Kozusko, Frank Old Dominion University	5/16 - 7/15	Fluid Mechanics
Kreiss, Heinz-Otto University of California, Los Angeles	5/10 - 5/13	Applied & Numerical Mathematics
Lasseigne, D. Glenn Old Dominion University	5/16 - 7/08	Fluid Mechanics
Lee, Ki D. University of Illinois, Urbana - Champaign	8/01 - 8/12	Fluid Mechanics
Leemis, Larry College of William & Mary	7/05 - 7/29	Computer Science
Leonard, Anthony California Institute of Technology	9/15 - 9/21	Fluid Mechanics
Liandrat, Jacques Universite d'Aix-Marseille II, France	9/23 - 10/28	Applied & Numerical Mathematics
MacCormick, Robert Stanford University	7/25 - 8/05	Applied & Numerical Mathematics
Mahalov, Alex Arizona State University	6/06 - 7/01	Fluid Mechanics
Mesaros, Lisa University of Michigan, Ann Arbor	8/01 - 9/30	Applied & Numerical Mathematics
Mitter, Sanjoy Massachusetts Institute of Technology	8/15 - 8/19	Fluid Mechanics
Nicolaides, R.A. Carnegie-Mellon University	8/08 - 8/19	Applied & Numerical Mathematics
O'Hallaron, David Carnegie-Mellon University	8/01 - 8/05	Computer Science

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Otto, Stephen R. University of Birmingham United Kingdom	7/18 - 9/23	Fluid Mechanics
Papageorgiou, Demetrius New Jersey Institute of Technology	6/06 - 6/17	Fluid Mechanics
Parpia, Ijaz H. University of Texas	8/01 - 8/26	Applied & Numerical Mathematics
Patera, Anthony Massachusetts Institute of Technology	7/26 - 7/28	Fluid Mechanics
Pothen, Alex Old Dominion University	7/25 - 8/26	Computer Science
Protzel, Peter FORWISS, Germany	6/20 - 6/24	Applied & Numerical Mathematics
Radespiel, Rolf DLR, Institute for Design Aerodynamics, Germany	6/30 - 7/09	Applied & Numerical Mathematics
Roe, Philip University of Michigan, Ann Arbor	5/31 - 6/08 7/04 - 7/29	Applied & Numerical Mathematics
Sarkar, Sutanu University of California, San Diego	9/05 - 9/23	Fluid Mechanics
Shah, Patricia Slechta Boston University	8/08 - 8/26	Fluid Mechanics
Short, Mark University of Bristol, England	8/01 - 8/19	Fluid Mechanics
Shu, Chi-Wang Brown University	5/23 - 6/10 7/11 - 7/15 9/05 - 9/09	Applied & Numerical Mathematics
Sidilkover, David New York University	8/01 - 8/26	Applied & Numerical Mathematics
Smith, Ralph Iowa State University	6/06 - 6/10 6/27 - 7/22	Applied & Numerical Mathematics

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Somani, Arun K. University of Washington	7/11 - 7/22	Computer Science
Speziale, Charles G. Boston University	7/11 - 7/22	Fluid Mechanics
Sun, Xian-He Louisiana State University	5/16 - 8/12	Computer Science
Tai, Chang Hsian IBM T.J. Watson Center	7/31 - 8/16	Applied & Numerical Mathematics
Tal-Ezer, Hillel Tel-Aviv University, Israel	8/08 - 8/26	Applied & Numerical Mathematics
Tam, Christopher Florida State University	6/13 - 6/17 8/22 - 8/26	Applied & Numerical Mathematics
Thangam, Siva Stevens Institute of Technology	6/06 - 7/08	Fluid Mechanics
Ting, Lu New York University	6/06 - 6/10 7/25 - 8/05	Fluid Mechanics
Trivedi, Kishor Duke University	7/11 - 7/22	Computer Science
Turkel, Eli Tel-Aviv University, Israel	7/11 - 9/16	Applied & Numerical Mathematics
van Leer, Bram University of Michigan, Ann Arbor	7/25 - 9/02	Applied & Numerical Mathematics
Verhaagen, Nick Delft University of Technology The Netherlands	8/29 - 9/30	Fluid Mechanics
Verhoff, Gus McDonnell Douglas Aerospace	8/01 - 8/12	Fluid Mechanics
Whitaker, Nathaniel University of Massachusetts, Amherst	8/08 - 8/12	Applied & Numerical Mathematics
Wu, J.Z. University of Tennessee Space Institute	6/06 - 7/01	Fluid Mechanics

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Yeung, P.K. Georgia Institute of Technology	6/20 - 7/29	Fluid Mechanics
Younis, Bassam A. City University, England	6/06 - 7/29	Fluid Mechanics
Zubair, Mohammed IBM - T.J. Watson Research Center	7/05 - 7/15	Computer Science
Zurigat, Yousef H. University of Jordan	6/13 - 7/08	Fluid Mechanics

OTHER ACTIVITIES

On May 23-25, 1994, ICASE and NASA LaRC co-sponsored a Workshop on Parallel Numerical Algorithms at the Radisson Hotel in Hampton, VA. The objective of this Workshop was to update developers of high-performance applications codes based on partial differential equations or integral equations with the state-of-the-art in parallel algorithms and the parallel computational environment. There were 74 attendees. The proceedings of this workshop will be published.

ICASE STAFF

I. ADMINISTRATIVE

M. Yousuff Hussaini, Director. Ph.D., Mechanical Engineering, University of California, 1970.

Linda T. Johnson, Office and Financial Administrator

Etta M. Blair, Accounting Supervisor

Barbara A. Cardasis, Administrative Secretary

Shannon L. Keeter, Technical Publications Secretary

Rachel A. Lomas, Payroll and Accounting Clerk

Shelly D. Millen, Executive Secretary/Visitor Coordinator

Emily N. Todd, Conference Manager

Gwendolyn W. Wesson, Contract Accounting Clerk

Leon M. Clancy, System Manager

Sharon S. Paulson, Assistant System Manager

Avik Banerjee, System Operator

II. SCIENCE COUNCIL

Ivo Babuska, Professor, Institute for Physical Science & Technology, University of Maryland.

Geoffrey Fox, Director, Northeast Parallel Architectural Center, Syracuse University.

Ashwani Kapila, Professor, Department of Mathematics and Science, Rensselaer Polytechnic Institute.

James P. Kendall, Jet Propulsion Laboratory.

Heinz-Otto Kreiss, Professor, Department of Mathematics, University of California at Los Angeles.

Sanjoy Mitter, Professor of Electrical Engineering, Massachusetts Institute of Technology.

Steven A. Orszag, Professor, Program in Applied & Computational Mathematics, Princeton University.

Eli Reshotko, Department of Mechanical and Aerospace Engineering, Case Western Reserve University.

Ahmed Sameh, Department Head of Computer Science, University of Minnesota.

M. Y. Hussaini, Director, Institute for Computer Applications in Science and Engineering, NASA Langley Research Center.

III. SENIOR STAFF SCIENTISTS

Gordon Erlebacher - Ph.D., Plasma Physics, Columbia University, 1983. Computational Fluid Dynamics. (November 1989 to November 1994)

Thomas Jackson - Ph.D., Mathematics, Rensselaer Polytechnic Institute, 1985. Fluid Mechanics. (January 1994 to January 1997)

Dimitri Mavriplis - Ph.D., Mechanical and Aerospace Engineering, Princeton University, 1988. Grid Techniques for Computational Fluid Dynamics. (February 1987 to September 1995)

Piyush Mehrotra - Ph.D., Computer Science, University of Virginia, 1982. Programming Languages for Multiprocessor Systems. (January 1991 to September 1994)

Shlomo Ta'asan - Ph.D., Applied Mathematics, The Weizmann Institute of Science, 1985. Multigrid Methods for Partial Differential Equations. (July 1991 to August 1994)

John R. Van Rosendale - Ph.D., Computer Science, University of Illinois, 1980. Parallel Systems and Algorithms. (July 1989 to June 1994)

V. Venkatakrishnan - Ph.D., Mechanical and Aerospace Engineering, Princeton University, 1987. Applied & Numerical Mathematics. (June 1993 to June 1995)

IV. SCIENTIFIC STAFF

Natalia Alexandrov - Ph.D., Computational & Applied Mathematics, Rice University, 1993. Applied & Numerical Mathematics [Multidisciplinary Optimization]. (March 1994 to March 1996)

David Banks - Ph.D., Computer Science, University of North Carolina, 1993. Computer Science [Visualization]. (April 1993 to April 1995)

Phillip M. Dickens - Ph.D., Computer Science, University of Virginia, 1992. Computer Science [System Software]. (January 1993 to August 1995)

Sharath S. Girimaji - Ph.D., Mechanical and Aerospace Engineering, Cornell University, 1990. Fluid Mechanics [Turbulence and Combustion]. (July 1993 to July 1995)

Matthew D. Haines - Ph.D., Computer Science, Colorado State University, 1993. Computer Science [System Software]. (August 1993 to August 1995)

Ulf R. Hanebutte - Ph.D., Mechanical Engineering, Northwestern University, 1992. Computer Science [Parallel Numerical Algorithms]. (October 1992 to September 1994)

Leland M. Jameson - Ph.D., Applied Mathematics, Brown University, 1993. Applied & Numerical Mathematics. (October 1993 to October 1995)

Michael A. Kelley - B.S., Computer Science, University of California-San Diego, 1993. Computer Science. (June to August 1994)

Scott T. Leutenegger - Ph.D., Computer Science, University of Wisconsin-Madison, 1990. Computer Science [Performance Analysis]. (September 1992 to August 1994)

Kwan-Liu Ma - Ph.D., Computer Science, University of Utah, 1993. Computer Science [Visualization]. (May 1993 to May 1995)

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