# REPORT DOCUMENTATION PAGE

AFRL-SR-AR-TR-06-0137

| 1. REPORT DATE (DD-MM-YYYY) | 2. REPORT TYPE | 3. DATES COVERED (From - To) |
|---|---|---|
| 10-March 2006 | Final Performance Report | 1 Sep 2002 – 31 Oct 2005 |

| 4. TITLE AND SUBTITLE | 5a. CONTRACT NUMBER |
|---|---|
| Les of Multi-Phase flows in Complex Domains | |
| | 5b. GRANT NUMBER |
| | F49620-02-1-0431 |
| | 5c. PROGRAM ELEMENT NUMBER |

| 6. AUTHOR(S) | 5d. PROJECT NUMBER |
|---|---|
| Suresh Menon | |
| | 5e. TASK NUMBER |
| | 5f. WORK UNIT NUMBER |

| 7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) | 8. PERFORMING ORGANIZATION REPORT NUMBER |
|---|---|
| Georgia Tech Research Corporation<br>Georgia Institute of Technology<br>Atlanta, GA 30332-0420 | |

| 9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) | 10. SPONSOR/MONITOR'S ACRONYM(S) |
|---|---|
| The Air Force Office of Scientific Research<br>875 N. Randolph Street, Suite 325, Room 3112<br>Arlington, VA 22203-1768<br>Dr. Fariba Fahroo | AFOSR/NM |
| | 11. SPONSOR/MONITOR'S REPORT NUMBER(S) |

**12. DISTRIBUTION / AVAILABILITY STATEMENT**

Distribution A: Approved for Public Release; Distribution Unlimited

Distribution A

**13. SUPPLEMENTARY NOTES**

**14. ABSTRACT**

One Agent Defeat scenario of primary interest to the US Air Force involves; the explosion of a warhead in ground-fixed target structures and storage facilities. Since, improper deployment can have potentially hazardous consequences, numerical studies can understand the dynamics of this process. Simulation of this process requires a multi physics code capable of treating both shocks a turbulence in complex geometries as well as single and multiphase chemistry. Smooth flow solvers can simulate turbulent flows, t These codes usually have significant difficulty in treating discontinuities such as shock waves without introducing unphysical oscillations into the flow.

# 20060601078

**15. SUBJECT TERMS**

| 16. SECURITY CLASSIFICATION OF: | | | 17. LIMITATION OF ABSTRACT | 18. NUMBER OF | 19a. NAME OF RESPONSIBLE PERS( |
|---|---|---|---|---|---|
| a. REPORT | b. ABSTRACT | c. THIS PAGE | UL | | Suresh Menon |
| Unclassified | Unclassified | Unclassified | | | 19b. TELEPHONE NUMBER (include ar |
| | | | | | 404-894-9126 |

# SIMULATION OF SHOCK-SHEAR INTERACTIONS IN COMPLEX DOMAINS

F49620-02-1-0431

Suresh Menon and Bruce Fryxell
Computational Combustion Laboratory
School of Aerospace Engineering
Georgia Institute of Technology

**Abstract**

One Agent Defeat scenario of primary interest to the US Air Force involves the explosion of a warhead in ground-fixed target structures and storage facilities. Since, improper deployment can have potentially hazardous consequences, numerical studies can help understand the dynamics of this process. Simulation of this process requires a multi-physics code capable of treating both shocks and turbulence in complex geometries as well as single and multiphase chemisty. Smooth flow solvers can simulate turbulent flows, but these codes usually have significant difficulty in treating discontinuities such as shock waves without introducing unphysical oscillations into the flow. Shock capturing methods do a good job at treating shocks and contact discontinuities, but the dissipation in these methods can provide an incorrect treatment of the turbulent features in the flow. In this project, we have developed a hybrid code, which combines a high-order smooth-flow solver with a high-resolution shock-capturing method. The shock-capturing method is used only near discontinuities, while the smooth-flow solver is used to treat the remainder of the flow. The hybrid method is capable of producing solutions that are more accurate than could be obtained with either method by itself.

The baseline code is LESLIE3D[1,2,3,4], a well-established DNS/LES solver developed for scalar mixing and combustion applications. The code contains a smooth-flow Navier-Stokes solver that is second-order accurate in time and fourth order in space. It employs a localized dynamics model for the subgrid closure of the unresolved momentum and energy fluxes that has been shown to be highly robust and stable in all types of flows. There are no adjustable constants or coefficients in this model, since the coefficients adapt automatically to the problem of interest. The code has the ability to deal with multiphase (gas-liquid-solid) flows using a combined Eulerian-Lagrangian approach, in which the gas phase is treated on a fixed Eulerian grid, while the liquid and solid particles are tracked in a grid-free Lagrangian manner. The code has been extensively verified and validated against a wide variety of experimental and canonical flows.

Although LESLIE3D works very well for smooth flows, it cannot accurately handle strong shocks and contact discontinuities, which produce unphysical oscillations in the flow. A major accomplishment under this grant has been to incorporate a high-resolution shock-capturing method into the code. The scheme we use for shock capturing is the Piecewise-Parabolic Method (PPM) of Colella and Woodward[5]. This method has been widely used, particularly for astrophysics calculations, where strong shocks appear on a regular basis. The implementation used here is based on the PROMETHEUS code[6], which is also the basis of the hydrodynamic solver in the FLASH code[7], developed at the

University of Chicago as part of the DOE ASCI Alliance Program. The code has been used by many groups throughout the world and has been extensively validated[8,9].

PPM is a high-order extension of Godunov's method[10]. The algorithm was designed specifically to produce accurate solutions of flows with sharp discontinuities through the use of nonlinearity and "smart" dissipation algorithms. It also performs very well in smooth flows. Godunov's approach is to calculate the fluxes in the gas dynamic equations by solving Riemann's problem at each zone interface. This produces an upwind-centered flux and also introduces nonlinearity into the difference equations. This nonlinearity permits the method to calculate narrow discontinuities without generating spurious oscillations. Godunov's method assumes a piecewise-constant profile of each variable. This limits the accuracy of the scheme to first order.

A formalism for extending Godunov's method to higher order was developed with the MUSCL scheme[11], in which second-order accuracy in both space and time is achieved by representing the flow variables as piecewise-linear instead of piecewise-constant functions. Another major advance of MUSCL was the incorporation of monotonicity constraints instead of artificial viscosity to eliminate oscillations in the flow. PPM takes the next logical step by representing the flow variables as piecewise-parabolic functions. This corresponds to switching to Simpson's rule for numerical integration.

The problem of a point explosion in a confined domain was performed as an initial test of the accuracy and robustness of the shock-capturing method for agent defeat simulations. The calculation tests the ability of the code to capture both strong and weak shocks accurately and its ability to compute complex shock reflections and interactions. The initial setup consists of a cubical box 25 m wide containing air at room temperature. An explosion is initiated off-center in the box by raising the pressure at a single grid point by a factor of $10^6$. Figure 1 shows the results of a 2D 600 x 600 simulation at four different times. The boundaries were treated as slip walls. The explosion was initiated at a point 1/3 of the way across the box from the left and bottom walls. As the simulation evolves, the reflections of the blast wave off the walls of the box and the resulting shock interactions result in a very complex pattern of waves. The shock strength rapidly decays, and by the end of the simulation, the maximum overpressure is less than 1%
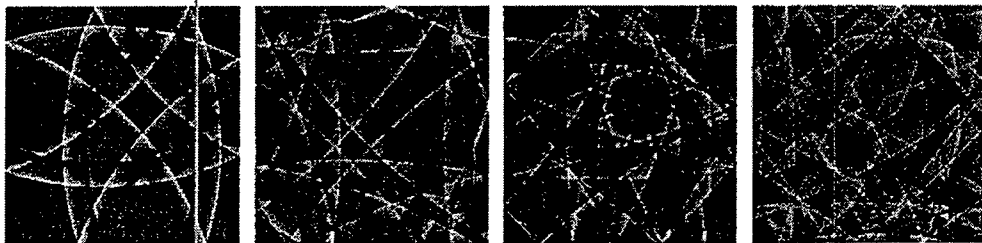


Figure 1. Time sequence of the pressure distribution resulting from a point explosion in a box. The simulation was performed with PPM in two dimensions using a 300 x 300 grid.

A three-dimensional simulation of the problem, performed on a 192 x 192 x 192 grid is shown in Figure 2. For this simulation, a small hole was inserted into one wall to allow some of the explosion energy to escape.
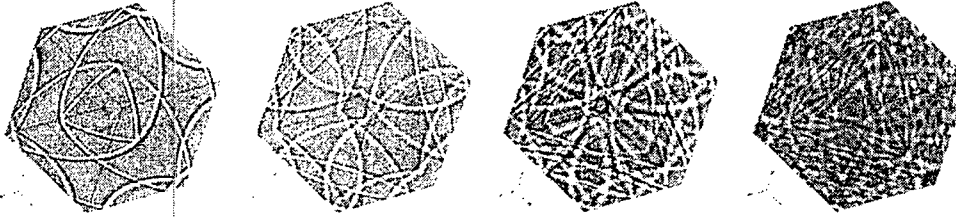
Figure 2. Time sequence of the pressure distribution resulting from a point explosion in a box. The simulation was performed with PPM in three dimensions using a $192^3$ grid.

In this study, we have developed a new hybrid method, which uses PPM only near discontinuities and calculates the remainder of the flow using the smooth-flow solver. We define a smoothness parameter given by

$$S_i = \frac{|Q_{i+1} - 2Q_i + Q_{i-1}|}{|Q_{i+1} - Q_i| + |Q_i - Q_{i-1}|}$$

where $Q_i$ is any variable of interest. This is similar to the refinement criterion for adaptive mesh refinement proposed by Löhner[12]. Typically, we use both pressure and density. To avoid detecting numerical noise, the smoothness parameter is set to 0 if either the numerator or denominator is less than some small value, typically 0.05. For multidimensional simulations, we take the maximum of the smoothness parameter for each coordinate direction, ignoring cross derivatives. If the smoothness parameter is greater than 0.35 at a grid point, we use the PPM fluxes to update the conserved quantities at that point. Where the smoothness parameter is less than 0.35, the fluxes from the smooth-flow solver are used. In order to minimize any numerical noise that might be generated when switching between the two methods, we take the average of the two fluxes at any grid point bordering a point in which the PPM fluxes are needed.

We illustrate the hybrid method by simulating Richtmyer-Meshkov instability. The left side of the grid contains hydrogen, while the right side of the grid consists of helium. A sinusoidal interface is placed between the two fluids, with a second higher-order perturbation with 1/5 the wavelength and 1/10 the amplitude superimposed on the large-scale sinusoidal perturbation. A planar shock with an overpressure of 300 is placed just to the left of the interface. The results of a two dimensional simulation on a 1024 x 256 grid are shown in Figure 3 and the 3D simulation using a 480x120x120 grid is shown in Fig. 4. The instability shows the characteristic bubble and spike morphology. The shock is located just to the right of the left boundary. A diamond-shaped pattern of contact discontinuities, which are subject to Kelvin-Helmholtz instabilities, develops between the shock and the interface, and a series of Kelvin-Helmholtz instabilities forms along the interface. The top frame in Fig. 3 shows the magnitude of the density gradient obtained with PPM, the middle frame shows the results of the hybrid method, and the bottom frame shows where each flux was used. The dark gray regions were calculated with the PPM fluxes, the light gray regions used the fluxes from the smooth-flow solver, and the average of the two fluxes was used in the black regions. PPM and the hybrid method give virtually identical results.

The hybrid method is also being used for LES of turbulence. The simulation shown here is of a planar shock propagating through isotropic turbulence. The initial conditions were taken from a DNS simulation of Mahesh, Lele and Moin[13], who used a 6th order method on a 231 x 81 x 81 grid. Our simulation was performed with the hybrid method on a 62 x 32 x 32 grid. The average turbulent kinetic energy as a function of distance is shown in Figure 5. The plot on the left shows the results obtained using the smooth-flow solver by itself and using PPM by itself. The diamonds represent the results of the DNS simulation. The smooth-flow solver (solid line) produces a shock that is too wide and overestimates the amount of post-shock turbulence. PPM underestimates the peak of the post-shock turbulence. The plot on the right shows the result of the hybrid method. This result matches the results of the DNS very well.

The final simulation presented here is a 1D multi-phase detonation. The detonation is ignited in a mixture of $2H_2 + O_2 + 3Ar$, originally at 26 kPa. The particles are 15 $\mu$m Al particles with a mass loading of 20 g/m$^3$. A 7-step, 7-species H2-O2 mechanism is used. Al combustion is by a 3-step reaction mechanism. Pressure traces at two points downstream from the ignition point are shown in Figure 6. The Al particles absorb some of the reaction energy, heating up until they start evaporating. The heat exchange between the particles and the gas acts as an energy loss to the gas, thus generating pressure losses in the post-shock region. As a consequence, the propagation velocity of the detonation is slower when the particles are included.
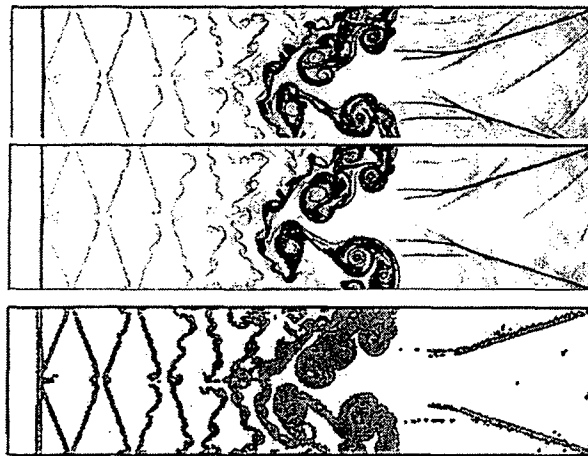


Figure 3. Two-dimensional simulation of a R-M instability on a 1024 x 256 grid.

Figure 4. Temperature iso-surfaces from a three-dimensional simulation of a Richtmyer-Meshkov instability computed using the hybrid method on a 480 x 120 x 120 grid.

The final simulation presented here is of a one-dimensional multi-phase detonation. The detonation is ignited in a mixture of $2H_2 + O_2 + 3Ar$, originally at 26 kPa. The particles used in the simulation were 15 μm Al particles with a mass loading of 20 $g/m^3$. The chemistry of the gaseous phase is treated with a 7-step, 7-species mechanism. Once the Al particles evaporate, they are allowed to react with the gaseous phase using a 3-step reaction mechanism. Pressure traces at two points downstream from the ignition point are shown in Figure 6 for detonations both with and without the Al particles. The Al particles absorb some of the reaction energy, heating up until they start evaporating. The heat exchange between the particles and the gas acts as an energy loss to the gas, thus generating pressure loss in the post-shock region. As a consequence, the propagation velocity of the detonation is slower when the particles are included.
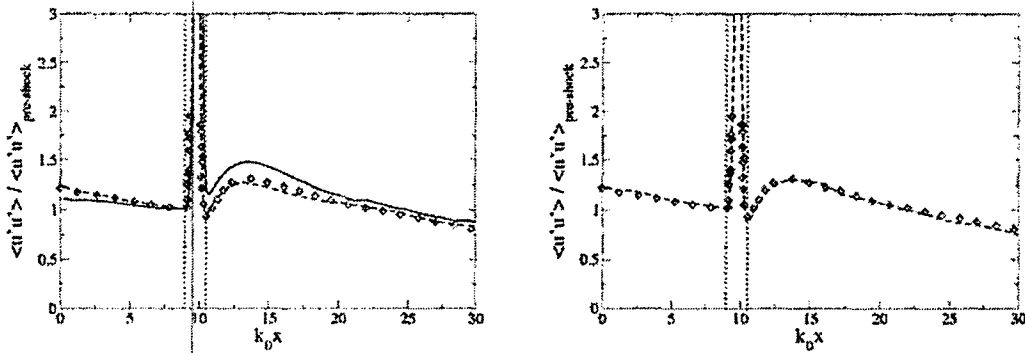


Figure 5. Turbulent kinetic energy obtained from an LES simulation of the propagation of a planar shock through isotropic turbulence. The plot on the left shows the results obtained with the smooth-flow solver (solid line) and with PPM (dashed line). The diamonds are the results obtained from a DNS simulation.
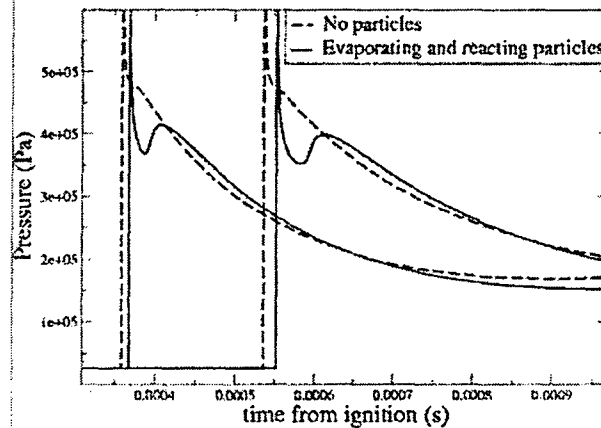


Figure 6. Pressure profiles 0.7 m and 1.4 m downstream from the ignition point for detonations both with and without evaporating and reacting Al particles.

**References**

1. S. Menon, Computational and Modeling Constraints for Large-Eddy Simulations of Turbulent Combustion, International Journal of Engine Research, 2000, 1: 209-227.

2. W.-W. Kim and S. Menon, Numerical Modeling of Turbulent Premixed Flames in the Thin-Gas Turbine Combuster, Combustion Sci and Technology, 1999, 143: 25-62.

3. W.-W. Kim and S. Menon, Numerical Modeling of Fuel-Air Mixing in a Dry Low-Reaction-Zones Regime, Combustion Science and Technology, 1999, 60: 113-150.

4. C. Stone and S. Menon, Parallel Simulations of Swirling Turbulent Flames, Journal of Supercomputing, 2003, 22: 7-28.

5. P. Colella and P. Woodward, The Piecewise-Parabolic Method (PPM) for Gas Dynamical Simulations, Journal of Computational Physics, 1984, 54: 174-201.

6. B. Fryxell, E. Müller, and D. Arnett, Hydrodynamics and Nuclear Burning, Max-Planck-Institute für Astrophysik Report 449, 1989.

7. B. Fryxell, K. Olson, P. Ricker, F.X. Timmes, M. Zingale, D.Q. Lamb, P. MacNeice, R. Rosner, J.W. Truran, and H. Tufo, FLASH: An Adaptive Mesh Hydrodynamics Code for Modeling Astrophysical Thermonuclear Flashes, Astrophysical Journal (Supplement), 2000, 131: 273-334.

8. P. Woodward and P. Colella, The Numerical Simulation of Two-Dimensional Fluid Flow with Strong Shocks, Journal of Computational Physics, 1984, 54: 115-173.

9. A. Calder, B. Fryxell, T. Plewa, R. Rosner, L. Dursi, V. Weirs, T. Dupont, H. Robey, J. Kane, B. Remington, R. Drake, G. Dimonte, M. Zingale, F. Timmes, K. Olson, P. Ricker, P. MacNeice, and H. Tufo, On Validating an Astrophysical Simulation Code, Astrophysical Journal (Supplement), 2002, 143: 201-229.

10. S. Godunov, A Finite Difference Method for the Computation of Discontinuous Solutions of the Equations of Fluid Dynamics, Mat. Sb., 1959, 47: 357-393.

11. B. van Leer, Towards the Ultimate Conservative Difference Scheme V. A Second Order Sequel to Godunov's Method, Journal of Comp. Physics, 1979, 32: 101-136.

12. R. Löhner, Computational Methods in Applied Mech Engineering, 1987, 61: 323.

13. K. Mahesh, S. Lele, and P. Moin, The Influence of Entropy Fluctuations on the Interaction of Turbulence With a Shock Wave, Journal of Fluid Mechanics, 1997, 334: 225-247.

## Personnel Supported During Duration of Grant
Jason Hackl — Graduate Student, Georgia Institute of Technology, Atlanta
Bruce Fryxell — Senior Research Scientist, Georgia Institute of Technology, Atlanta
Suresh Menon — Professor, Georgia Institute of Technology, Atlanta

## Publications
B. Fryxell, S. Menon, F. Genin, and J. Hackl, A Hybrid Method for Large Eddy Simulations With Strong Shocks, AIAA Journal, to be submitted.

Fryxell, B. and Menon, S.,"Hybrid Simulations of Richtmyer-Meshkov Instability," AIAA-2005-0314, 43rd AIAA Aerospace Sciences Meeting, Reno, NV, January, 2005.

Menon, S., Fryxell, B. and Genin, F., "Parallel Simulations of Detonation in Multi-Phase Turbulent Reacting Mixtures," 2005 DOD HPC Users Group Conf., June 28, 2005.

Genin, F., Fryxell, F, and Menon, S., "Simulation of Detonation Propagation in Turbulent Gas-Solid Reactive Mixtures,"AIAA-2005-3967, 42nd AIAA/ASME/ASEE Joint Propulsion Conference, July 11-14, 2005.

Genin, F., Fryxell, B. and Menon, S., "Hybrid Large-Eddy Simulation of Detonation in Reactive Mixtures," to be presented at the 20th International Conference on Detonations, Explosions and Shock Waves, Montreal CA, August 1-4, 2004.

## Invited Talks
Bruce Fryxell, Calculation of Turbulent Flows with Strong Shocks, Los Alamos National Laboratory, May 25, 2005

## AFRL Point of Contact
Douglas Nance, AFRL/MNAC, Eglin AFB, FL, Phone 850-882-8302 x 3208. Regular bi-monthly meeting at Georgia Institute of Technology.

## Transitions
The LESLIE3D and LESLIE-PPM codes have been delivered to AFRL/MNAC for their in-house classified studies of the Agent Defeat problems. Successful application of these codes to practical problems has been demonstrated at Eglin AFB.

## New Discoveries