3.4 Fluid Dynamics

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Overview

The Fluid Dynamics Group works on system-scale solid rocket motor multiphase compressible core flow code development, as well as subscale model development relevant to the turbulent dynamics of the combustion interface. This includes research projects that will intersect with the integrated code some time in the future include work in injection, dispersion and combustion of aluminum droplets in the core flow; formation, dispersion and slag accumulation of aluminum oxide particles; and flow within cracks and other defects within the propellant.

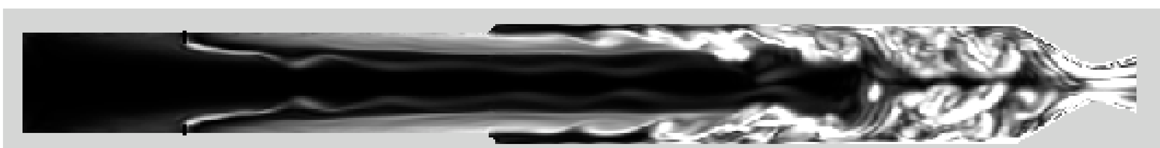

Fig. 3.4.1: *Rocflo* used to explore vorticity contours in C1x motor downstream of inhibitor

Rocflo and *Rocflu* Development

Rocflo (Wasistho, Balachandar, Moser, Wakaba)

Our structured grid fluids code, *Rocflo*, is considered mature and is undergoing only minimal further development. It has been integrated with the full set of *Rocfluid* multiphysics modules, including turbulence, discrete (Lagrangian) and continuum (Eulerian) particles, radiation, and the interaction engine governing mass, momentum and energy exchanges between various modules. *Rocflo* with all its physical modules is fully integrated into *Rocstar*. Example of multiphysics simulations using *Rocflo* can be seen in C1x simulations (AIAA 2005-4345), Figure 3.4.1 and Figure 3.4.2. While *Rocflu* is the primary code for use in realistic solid rocket geometries, *Rocflo* continues to be supported because of its utility and performance in simpler geometries and highly resolved LES simulations. Recent developments for *Rocflo* include the completion of a dual-timestepping (implicit) capability and the development of an advanced internal grid motion algorithm, capable of simulating fluid-structure interaction problems involving large deformations with minimal interference of external grid smoothing package, such as *Mesquite*. *Rocflo* internal grid-motion has been applied to flexible inhibitor simulations in the

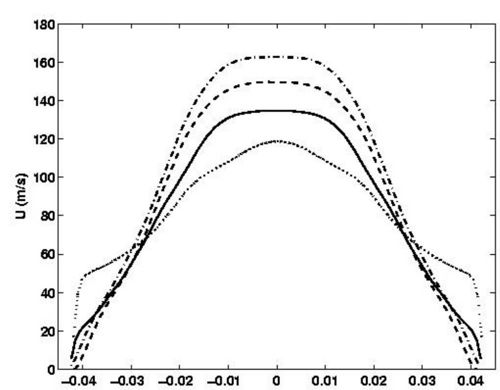

Fig. 3.4.2: Velocity profile at x = 0.65m location for clean SP case (solid), inhibitor SP case (dots), 10 *m*m MP case (dash), and 30 *m*m MP case (dashdot)

RSRM (Figure 3.4.3). *Rocflo* as part of *Rocstar* has also been used in numerous fluid-structure interaction simulations, such as shock panel, ACM rocket (M. Brandyberry), and wind past non-rigid building (D. Turner). Further enhancement of *Rocflo* will include incorporation of time-zooming (adding source terms) and *Mesquite* hex-smoothing, implementation of multi-grid method for a more efficient dual-timestepping, and implementation of new models in multi-physics modules.

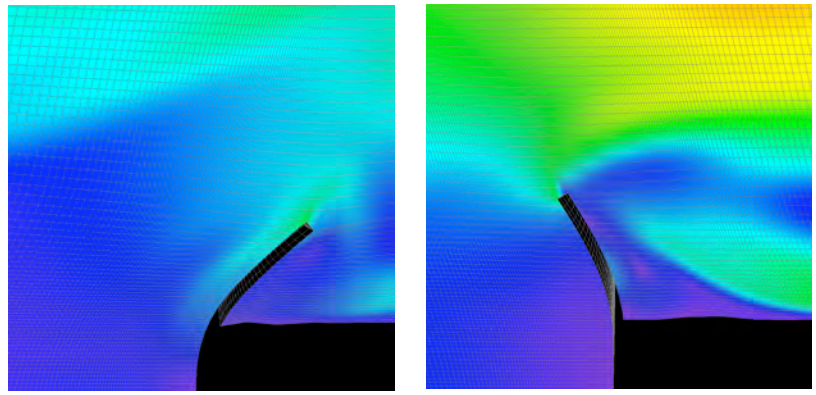

Fig. 3.4.3: Grid and velocity magnitude at 7ms (left) and at 17ms (right)

Rocflu (Haselbacher, Balachandar, Moser, Parmar, Zhao)

The unstructured grid flow solver, *Rocflu*, is nearing completion of its core capabilities. Continuing development is now mainly driven by the requirements specific problems, which may need extensions or additions to numerical techniques of physical models already implemented. Examples include:

- Development of a fully implicit Newton-Krylov solver based on PETSc (in collaboration with Heath Dewey).
- Development of non-inertial frame of reference for the simulation of the compressible flow over an isolated particle accelerated by drag and lift forces
- Incorporation of alternative spatial reconstruction schemes
- Implementation of new boundary conditions for jet flow resonance simulations.
- Incorporation of improved crack combustion model (in collaboration with B. Roe and L. Massa).
- Implementation of parallel particle-tracking (in collaboration with F. Najjar), completing the integration of *Rocpart* in *Rocflu*.
- Detailed verification and *substantial* improvements in the accuracy of the implementation of the Equilibrium Eulerian method.
- Incorporation of time-zooming (in collaboration with F. Najjar and L. Massa).
- Conversion from Charm to MPI for increased robustness and flexibility.
- Continuing development of an incompressible solver

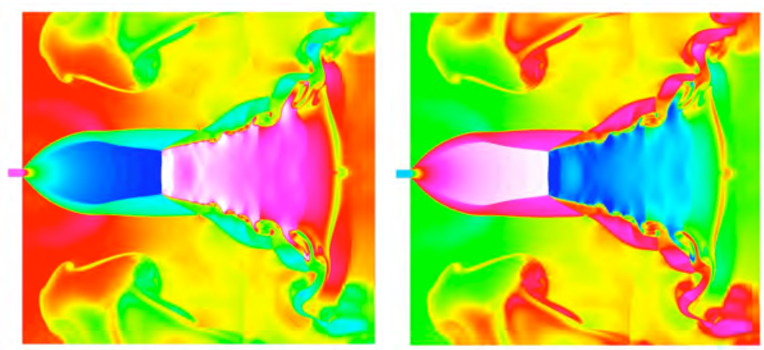

Fig. 3.4.4: *Rocflu* used for jet flow resonance studies

Verification and validation of *Rocflu* has continued For example, Results produced by *Rocflu* compared very well with experimental results for shock diffraction by cylinders and sharp corners. The growing maturity of *Rocflu* is reflected in its use in several other research projects:

- Multiphase flow in injector nozzles (Prof. O. Vasilyev, UC Boulder)
- Jet flow resonance (Prof. J. Freund, UIUC, AFOSR project; Figure 3.4.4)
- Compressible multiphase flow in the context of volcanic eruptions (Profs. S. Kieffer and S. Balachandar, UIUC)
- Assessment of added-mass forces acting on isolated spherical particles in compressible flows (Prof. Balachandar, UIUC)

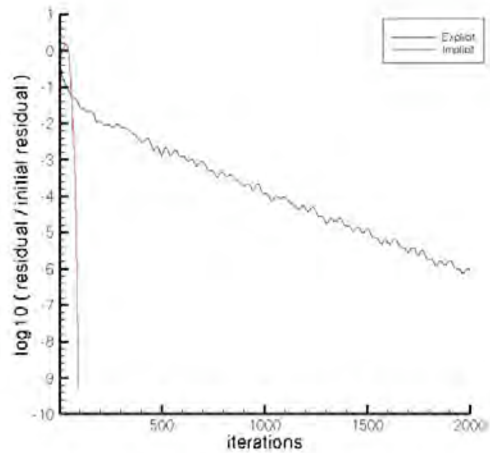

Fig. 3.4.5: *Rocflo* performance is good.

Finally, a number of performance improvements have been pursued (in collaboration with M. Campbell), in anticipation of performing large and long multi-physics computations. Single-processor performance was reduce by about 30%. A further 30-40% improvement in the overall run-time was achieved by A. Moody and C. Shereda of LLNL on the ALC cluster through more aggressive compiler optimization and more intrusive code tuning techniques. (These changes are currently being run on platforms other than ALC to assess platform-dependency.) Initial scalability studies on uP have demonstrated good performance on up to 480 processors.

Verification and Validation

Simulations are being performed using a high resolution, non-dissipative numerical scheme developed for this purpose. The method is based on a staggered grid formulation, which have been found to have many of the advantages exhibited for incompressible flows, even for the compressible flows of interest here. Efforts evaluating the *Rocstar* flow solvers using the test code have focused on a simplified geometric model of the star grain region of the propellant. This is a particularly challenging region to model because the turbulence changes character: inflection instabilities drive the turbulence in the jet flow that issues from the star grain slot but downstream the flow becomes driven by the wall conditions. Figure 3.4.6 shows (a) the streamwise velocity of the jet flow just downstream of the star grain, and (b) the streamwise vorticity magnitude at several downstream planes. In this

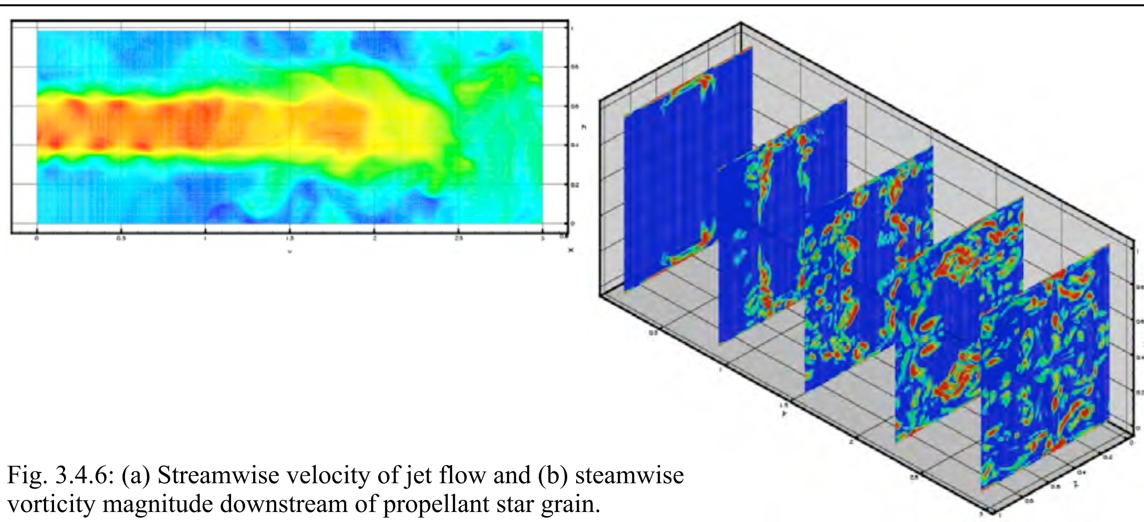

Fig. 3.4.6: (a) Streamwise velocity of jet flow and (b) steamwise vorticity magnitude downstream of propellant star grain.

demonstration, the vorticity features are barely resolved on the relatively coarse mesh selected, yet the algorithm is stable and the fluctuations are not dissipated by the numerics.

The main task will be further development of *Rocflu* as driven by problems specific problems, and to apply it to flow problems with *Rocstar*. Certain Rocflo enhancements will also be pursued as necessary, for example an incompressible capability is being considered.

Rocstar applications will include the BATES motors and the RSRM. Of particular interest will be RSRM simulations of the 4-segment booster at various burnout times to assess the effects of vortex shedding from the inhibitors on the acoustics of the chamber as well as on the droplet motion. In addition, special attention will be focused on quantifying the impact angles, diameter, momentum, temperature, and composition of droplets at the leading edge of the submerged nozzle, as well as the rate of accumulation of droplets in the bucket of the submerged nozzle. The resulting statistics will be of great use to the industry in developing greater understanding of the flow and improved impact and erosion models.

A second application focus will be on aeroelastic computations using the fully implicit solver currently being incorporated in *Rocflu*. This new capability will allow efficient computations of relatively low-frequency aeroelastic motions that would otherwise be inhibited by the stability limit of the explicit solver. Rocflu will then be extended to allow for a rotating coordinate systems in preparation for com-

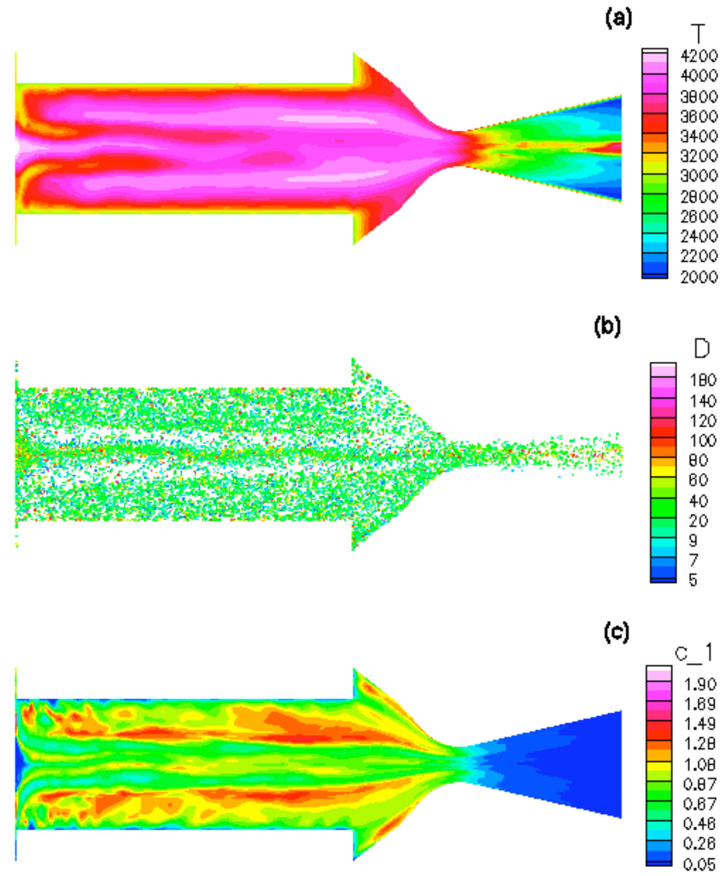

Fig. 3.4.7: Results for 15-lb BATES motor configuration for 15% aluminum propellant loading with full-heat release and initial ejection particle diameter distribution based on pdf distribution with mean 10mm and minimum and maximum values of 5mm and 150 mm:(a) temperature (K), (b) particle positions colored by particle diameter, (c) smoke concentration.

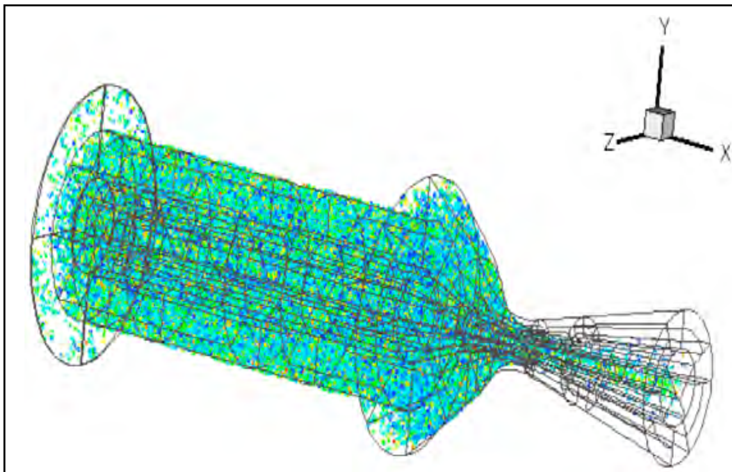

Fig. 3.4.8: Results from 3D multiphysics simulations of the 15-lb BATES motor for full-heat release with pdf-based initial distribution. Field contains 133,000 computational droplets representing 67 million real droplets.

puting the flow over a helicopter blade.

Because of the flexibility of *Rocflu's* data structure, it should be possible to seamlessly locally incorporate the structured high fidelity non-dissipative discretization used in the verification code directly into *Rocflu*. This will overcome the dissipation limitations of the current algorithm and greatly increase the range of scientific problems that it can tackle.

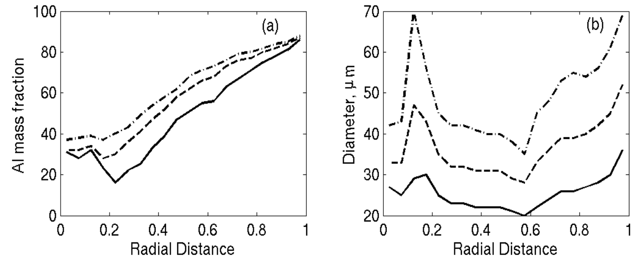

Fig. 3.4.9: Transverse distributions at the nozzle inlet (x=0.315m): (a) Aluminum composition, (b) Mass-mean diameter. Solid Line: 15% Al propellant loading, Dashed Line: 21%, Dashed-Dotted Line: 27%.

Multiphysics Framework and Multiphase Flow

Aluminum Particle Flows (Najjar and Balachandar)

To simulate the complex flow inside an aluminized solid propellant rocket motor, advanced physical models for the evolution of turbulence gas flow (*Rocflo*), burning aluminum Lagrangian particles (*Rocpart*), and aluminum-oxide smoke (*Rocsmoke*) as well as their interactions, are required. A separate module (*Rocinteract*) encapsulates the complex interactions amongst the physical components, and hence simplifies the consistent and conservative transfer of mass, momentum and energy. Recent developments in the multiphysics framework include: A breakup model for the Al droplets based on critical Weber number for *Rocpart,* a Conservative Random Ejection (CRE) to simulate the random ejection of droplets from a surface element while maintaining a conservation constraint, and, an aluminum combustion model based on aluminum oxide vapor energy formalism. The later permits the full heat release due to burning Lagrangian particles mechanism without artificially increasing the gas temperature beyond the aluminum oxide boiling point.

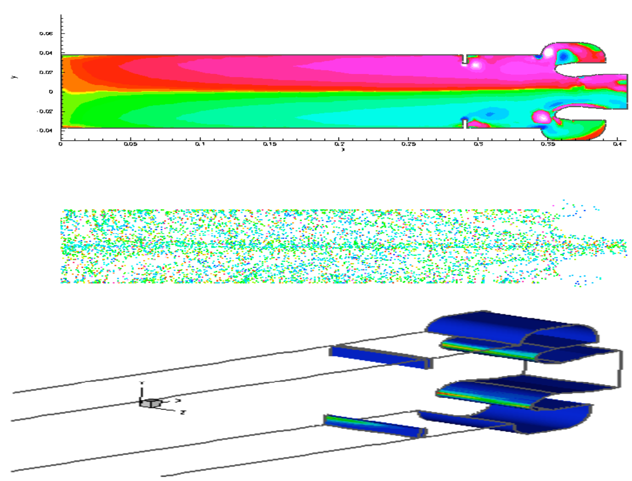

Fig. 3.4.10: Results for LP6 motor configuration (1/30-scale Ariane-V with 50% burnt propellant) using unstructured fluid solver, *Rocflu*, and initial injection droplet diameter distribution based on skewed logarithmic distribution with mean 23mm and minimum and maximum values of 5mm and 230 mm:(a) spanwise vorticity (1/s), (b) particle positions colored by particle diameter, (c) number of hits for droplets impinging on nozzle walls.

In addition to these multiphysics modeling improvements, the particle tracking algorithm in *Rocpart* has been greatly improved for use on unstructured grids, such as *Rocflu*. A new algorithm based on ray tracing is developed addressing these deficiencies while maintaining efficiency. The approach considers the intersections of the particle trajectory with the faces of the underlying grid. Together with a face-based data structure, the intersection point on a face directly indicates the cell into which a particle is moving. By focusing on intersections with faces, the algorithm deals with boundaries in a natural way. Further, efficient memory management using dynamic memory reallocation has been developed for *Rocpart*. This capability has been extended to run efficiently in parallel using MPI. The framework has been enhanced to handle droplet impingement on nozzle walls, while capabilities to track droplets being trapped in the bucket of a submerged nozzle are currently being pursued. This capability has been fully integrated into *Rocflu* and *Rocstar* and 3-D simulations for various configurations are currently being performed.

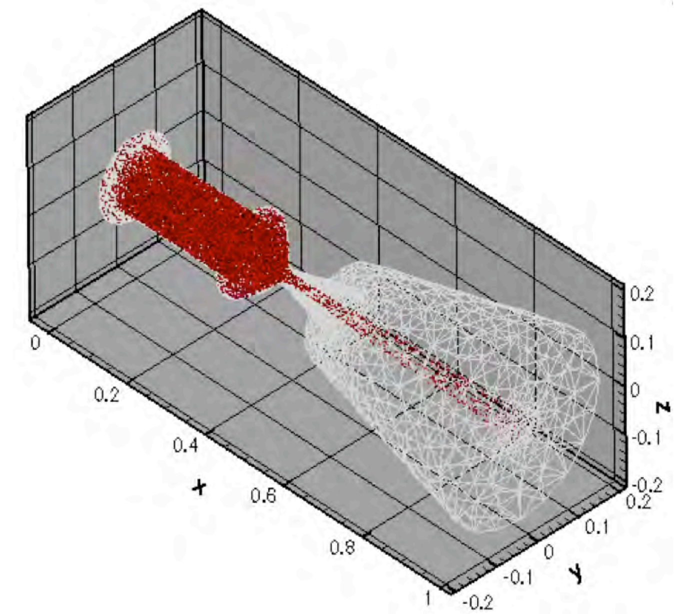

Fig. 3.4.11: Results for 15-lb BATES motor configuration using unstructured fluid solver, *Rocflu*: droplet locations at time instant using single droplet diameter distribution of 30mm at injection surface.

The multiphysics framework is assessed for the 15-lb AFRL BATES motor configuration. Several propellant loadings, including 15, 21 and 27%, have been investigated based on the BATES firing experiments. Example results are shown in Figures 3.4.7-11.

Future Plans The current multiphase framework will include more sophisticated physical models, such as breakup models, radiation and species. Issues such as particle impingement on nozzle walls, particle being trapped in the bucket of a submerged nozzle are currently being pursued. Of great interest is the development of turbulence-particle LES-based models in terms of stochastic equations for the particle velocity field. These issues are been actively studied.

This capability will be expanded to run efficiently in parallel and will be integrated in *Rocstar*. Currently, we are assessing the effects of superparticle loading on flow dynamics and particle evolution in the core rocket chamber. Further, we are in the process of expanding validation suites for MP problems.

In addition, a number of multiphase flow research topics will be pursued. These will include:

- Characterization of gas-particle coupling in supersonic accelerating flows, including shock-particle interaction.
- Characterization of droplet impingement on nozzle walls to provide input for nozzle ablation analsis.
- Characterization of particle slag accumulation in submerged nozzles.

Microscale Simulations of Multiphase Flow (Shotorban and Balachandar)

The flow within the rocket is characterized by a strong streamwise acceleration of the mean flow from the head end to the nozzle. There are also strong shear layers arising from the instability of the injection driven flow, viscous wall response to acoustic oscillations, and vortex shedding off inhibitors. In the downstream sections of the rocket, the flow is strongly turbulent. Despite these complications the tradition approach to tracking the injected Al droplets is to use a simple drag law, heat transfer coefficient and burn rate correlation. These correlations are typically developed under conditions of uniform flow and therefore their usage in the context of multiphase rocket flow is clearly outside their range of applicability. Nevertheless, their use is justified on the basis that there is nothing better available. The focus of the multiphase flow group is therefore to rigorously establish the limitations of the standard drag and lift laws and heat transfer coefficients and to suggest improvements that can be incorporated in *Rocpart* and *Rocsmoke* to accurately capture the complex multiphase physics relevant to rocket chamber.

Severals aspects of particle-flow interaction have been investigated by the group over the past year. Here we will highlight only those that pertain to particle-turbulence interaction. Our investigation shows that freestream turbulence has little systematic effect on time-averaged mean drag. The standard drag correlation by Schiller & Naumann, when applied based on instantaneous relative velocity, accurately captures the mean drag. It was observed that the standard drag correlation captures the instantaneous force fluctuation only when the particle is sufficiently smaller than the Kolmogorov scale. In contrast as the size of the particle increases the standard drag correlation fails to predict the actual time-history of the drag force. We believe freestream turbulence induced vortex shedding is partly responsible for such complex behavior. Inclusion of additional added-mass and history forces do not improve comparison. A more productive approach may be to include a stochastic component, with appropriate statistical properties, to the standard drag law in order to accurately capture particles' mean motion and dispersion behavior.

Project Plans:

Over the next two years we plan to consider the following activities:

- Extend our prior investigation of particle freestream turbulence interaction to the case of a freely moving particle.
- Investigate at the microscale the problem of a finite-sized particle moving through a boundary layer. Here we will consider the cases of particle motion through both a laminar shear layer and a turbulent boundary layer. This is an issue of great relevance as it pertains to the question of wall impaction and scouring at the nozzle and entrapment of particle in the submerged nozzle.
- We will consider the more complex problem of a distribution of particles interacting with free turbulence. These will be first-ever detailed direct numerical simulations of multiphase flow turbulence. The focus will be to investigate the wake-wake and particle-wake interaction on the forces experienced by the particle and the resulting effect on their motion.
- In the above cases considered we will pay particular attention to the back effect of the particles on carrier phase turbulence. Here the objective will be to encapsulate this back coupling in terms of simple models that could be incorporated in *Rocturb* to account for the effect of particles on gas phase turbulence.

Turbulence Simulation and Modeling (Moser, Balachandar, Venugopal, and Zandonade)

Large-eddy simulations of a solid rocket motor scale model are being performed in order to characterize the effects of turbulence on the sources of instabilities. The scale model is based on a cold gas experimental set-up reproducing the main geometric features of a segmented motor. The presence of inhibitors triggers vortex shedding in their wakes while the main flow close to the injection wall exhibits wall vortex shedding due to hydrodynamic instability. A mesh resolution of over 3 million grid cells is considered; while random turbulence fluctuations with an amplitude of 20% is injected over the mean value to maintain the three-dimensionality characteristics of the flow. In Figure 3.4.12, it is observed that the flow has reached a fully 3-D state with large-scale vortices breaking down into small sizes. Further, near-wall structures are seen to evolve similar to the Wall Vortex Shedding (WSP) phenomenon. It is also clear that the flow is fully turbulent (Figure 3.4.13).

Optimal LES is a new large eddy simulation approach under development at CSAR. The implementation of Optimal LES for use *Rocfluid* has now progressed to the testing phase. A number of modules required to implement the finite volume optimal LES approach have been implemented, tested (unit tests) and integrated into a stand-alone finite volume code in preparation for implementation in *Rocflu*. The modules have been designed for general use to allow integration into other codes as well.

The primary research concern for optimal LES has been the refinement of the dynamic approach required to provide statistical information that is not available from theory. It has been found that the errors introduced by the dynamic procedure can be catastrophic, producing a model that is unstable. The difficulty appears to be that the estimation procedure used to develop the models is particularly sensitive to the errors. To counteract this sensitivity, constraints have been developed to ensure that the resulting model has the required properties. The resulting model produces excellent results. Work is continuing to identify and correct the source of the excessive sensitivity that results in the need for these constraints. By removing the sensitivity, the model will be more general.

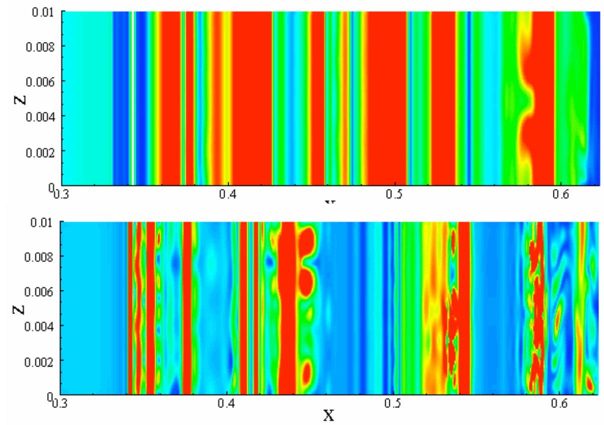

Fig. 3.4.12: Isocontours of vorticity in x-z plane at *t* = 13 ms (top) at 1 mm above injection wall, (bottom) in obstacle wake

Two novel models have been developed for the LES of particle-laden turbulent flows using a two-fluid approach. In the first model (LES-Equlibrium model), which is used in the large-eddy simulation (LES) of turbulence, a filtered Eulerian velocity field is defined and computed for the particle phase emloying the equilibrium approximation and then this field is utilized to solve the filtered particle concentration equation. In the other model (Two-Way-Equilibrium model), in order to take the effect of particle motion on the fluid phase (two-way coupling), the incompressibility property of a mixed velocity field defined based on the volume fractions of the particle and gas phases and their velocities, is used to solve the equations. To valildate the models, the equilibrium Eulerian formulation is utilized in the homogenous shear turbulence code. The accuracy of equilibrium approximation is assessed by comparison of the radial distribution function and other statistical quantities.

Two previously developed models to account for the effect of subgrid scales (SGS) on particles in LES have been modified and studied with more details. The proposed Langevin stochastic equation (Langevin model) has been modified for the inertial particles and assessed in the decaying isotropic turbulence. A good agreement between the model prediction and the exact (DNS) results is obsereved.

Fig. 3.4.13: Isosurface |w|=8500 s^{-1} of vorticity norm at *t* = 14 ms

<u>Future Plans</u> Detailed 3D LES computations of the inhibitor model problem with 4 million grid points will be pursued for various Mach numbers to gain further insight on the flow dynamics. Further comparison with experiments will be undertaken to substantiate the effects of turbulent on the instability mechanisms.

Research on filtering methods for Large-Eddy Simulation on unstructured grids in collaboration with Prof. Oleg Vasilyev will be continued. Issues such as filter-width specification, boundary stencils, and compact reconstruction methods will be addressed.

The continuing optimal LES work will proceed on two parallel tracks. First, model development and refinement will continue to be pursued. In particular, the refinement of the dynamical approach to eliminate excessive sensitivity to errors will continued, and it is anticipated that this will complete the development of OLES in the absence of strong inhomogeneities, such as walls, which is the primary requirement for the rocket flow. For walls, the development of the filtered-wall approach, and the theoretical representation of the required correlations are being pursued. The optimal LES implementation will be tested and completed by incorporating the results of the dynamic developments described above. The Optimal models will be validated against standard turbulent test cases, and ultimately compared to standard models already implemented in *Rocfluid* for rocket cases. We anticipate that the first optimal LES models will be ready for production use this year.

The LES-Equlibrium, Two-Way-Equilibrium, Langevin and ADM models will be implemented in *RocfluidMP* for the simulation of particle-laden turbulent flows which are encountered in various applications including solid-propollent rockets. The first two models need to be rigrously validated first in simple turbulent configurations.

Time Zooming (Moser, Haselbacher, and Najjar)

An improved formulation for time-zooming was developed based on experience with previous formulations. The new formulation explicitly distinguishes between burn-back and volume-filling time scales and, being cast in a finite-volume form, is more consistent with the *Rocflu* code. A dedicated test code was written based on the quasi-one-dimensional Euler equations to allow fast turn-around during testing of the new formulation. The new formulation with zooming factors of about 10-20 was shown to perform very well through comparisons with head-end pressures and chamber profiles between the zoomed and nominal computations. The new formulation was also implemented in the 3D *Rocflu* code and shown to reproduce nominal results while requiring only one tenth of the solution time. Even higher zooming rates are currently under investigation.

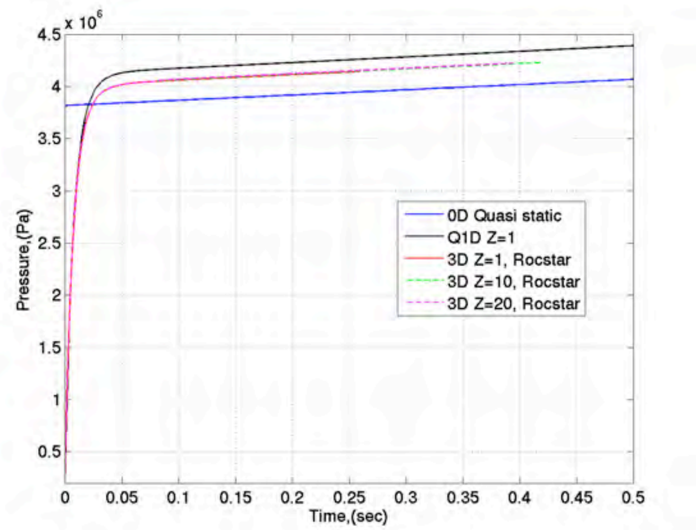

Fig. 3.4.14: Innovative CSAR-developed time zooming algorithms have been implemented in *Rocflu*

Future Plans The compound zooming formulation will continue to be developed, and tested in the quasi-one-dimensional test code, and will be moved into *Rocflu* when it is ready. This should be within the next several months. For the time-zooming approach to be useful for the coupled code, the formulation will need to be applied in solid mechanics and combustion, and a robust solution to the moving grid problem will be needed. Implementation and testing of time zooming in *Rocflu* will be completed, and tested on simple test rockets.