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 Al droplets in the core flow; formation, dispersion and slag accumulation of aluminum oxide particles; and flow within cracks and other defects within the propellant.

Rocflu Development (Haselbacher)

Rocflu has progressed in two areas over the past year. The first is that *Rocflu* continues to mature as an increasing number of researchers apply it to a growing number of physical problems and that bug fixes and extensions are introduced as a result. There are currently two users of *Rocflu* outside of CSAR: One at the University of Colorado at Boulder who simulates supersonic multiphase jet flow through a gaseous medium, and another at the Geology department at UIUC investigating blast waves resulting from volcanic eruptions. *Rocflu* was extended for coupled runs in *Rocstar* to help diagnose time-step restrictions and is now capable of running with mixed unstructured grids inside *Rocstar*. This is helpful because structured-like arrays of hexahedral cells can be used to represent nozzles and bores of rockets, while geometrically complicated regions like the star grain, stress-relieve grooves, igniter, and submerged nozzles can be represented by tetrahedra. The flexibility afforded by unstructured grids significantly reduces the time required to generate a grid for a complicated geometry like the RSRM.

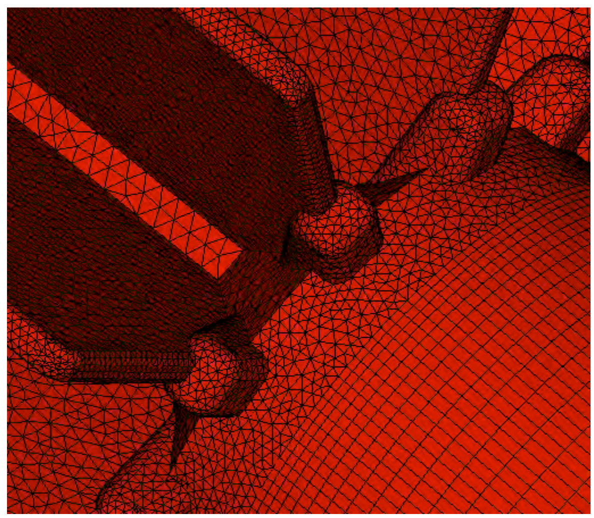

Fig. 3.4.1: *Rocflu* unstructured grid of RSRM star-grain stress relief notches

The second major area of progress is the outcome of the continuing development of *Rocflu*. The main advances over the past year are the incorporation of the second-order spatial discretization of the inviscid and viscous fluxes, and the development and integration of the multi-physics modules *Rocspecies*, *Rocpart*, *Rocsmoke*, and *Rocturb*. The second-order discretization is based on a novel explicit stencil-construction algorithm in which stencils are judged by their capability to compute gradients in a numerically robust fashion. The *Rocspecies* module employs a positivity-preserving spatial discretization, thereby ensuring that species mass fractions do not become negative. In the context of the multiphysics capability of *Rocflu*, the development of the *Rocspecies* module was particularly helpful because the subsequent integration of *Rocsmoke* was achieved very rapidly thanks to extensive reuse of *Rocspecies* routines. To track particles, a flexible and efficient new algorithm was developed in the Fluids group which is particularly suited to unstructured grids. The algorithm has undergone initial testing and is currently being further improved.

The development of *Rocflu* during the coming year will focus on two main areas. The first is the continued support for computations with *Rocstar* with particular emphasis on the use of adaptive grids. The second area of focus is the continued development of *Rocflu* by extending and improving its capabilities. The extension of capabilities will concentrate on the following topics:

- Variable material properties: To enable simulations with temperature dependent properties such as the ratio of specific heats (likely to have a big impact on rocket simulations) as well as sensitizing mixture properties such as the viscosity and conductivity to the relevant properties of its constituents.
- A higher-order scheme based on radial basis functions will be investigated. Radial basis functions are currently receiving much attention in the numerical analysis community for their favorable approximation properties. It should be possible to significantly reduce the numerical errors incurred by the spatial discretization by using radial basis functions in *Rocflu*.

Integrated Multiphase Flow Simulation (Najjar, Ferry, Haselbacher, Jiao, 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*) that encapsulates the complex interactions amongst the physical components, simplifies the consistent and conservative transfer of mass, momentum and energy. A breakup model based on critical Weber number has been added in *Rocpart*. A Conservative Random Ejection (CRE) model have been developed and implemented in *Rocpart* to properly simulate the random ejection of droplets from a surface element while maintaining a conservation constraint. Further, an aluminum combustion model accounting for aluminum oxide heat of vaporization properly does not allow the gas temperature to exceed the aluminum oxide boiling point. This capability has been fully integrated in *Rocstar* and tests are currently being performed.

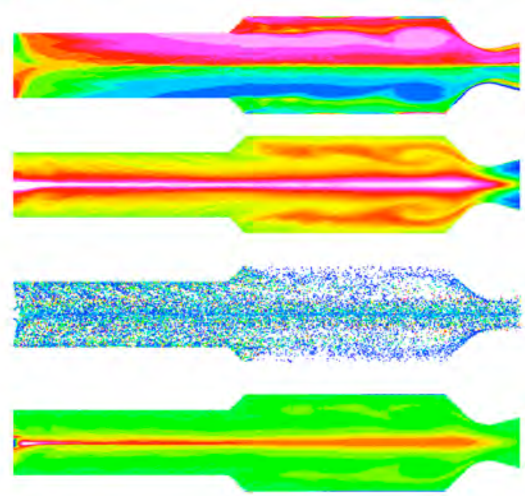

Fig. 3.4.2: *Rocflo* results for ONERA C1 with full-heat release and initial ejection particle diameter distribution based on skewed logarithmic distribution with mean 23μm and minimum and maximum values of 5μm and 230 μm:(a) spanwise vorticity (1/s), (b) temperature (K), (c) particle positions colored by particle diameter, (d) smoke concentration.

The multiphysics framework is assessed for the ONERA C1 configuration. Figure FM2 shows the particle location (colored by diameter with an initial particle diameter distribution based on a skewed logarithmic distribution obtained from agglomeration models by Jackson *et al.*), the mixture spanwise vorticity field, the mixture temperature, and the smoke concentration at one time instant. Highly unsteady flow consisting of large-scale vortices occurs in the rocket core chamber. The particle distributions are strongly affected by the flow field, and burn rapidly. Other test cases include the BATES motor geometry, in which 68,000 computational particles are tracked, representing 0.3 billion physical particles. Further, the fully-coupled simulations will be performed in *Rocstar*.

The results cited above were obtained using the *Rocflo* solver. Tracking Lagrangian particles on unstructured grids is a challenging task. Previous studies have presented a number of efficient algorithms; however, most of these algorithms do not treat boundary conditions naturally. A new algorithm based on ray tracing is developed which addresses 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*.

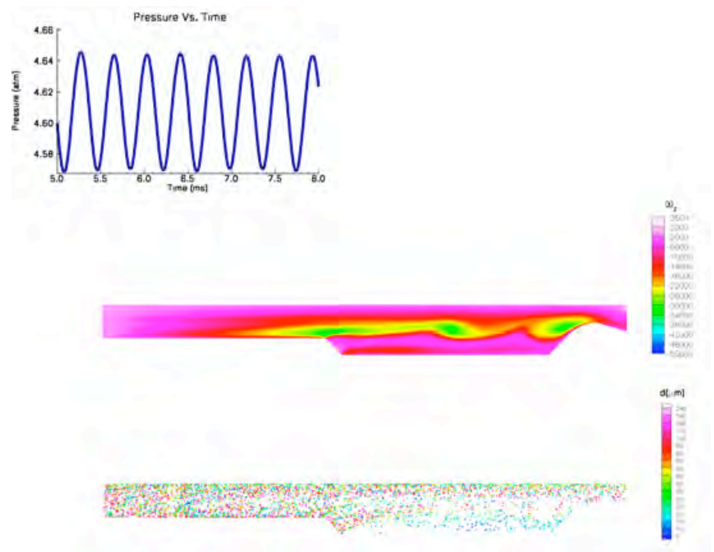

Fig. 3.4.3: *Rocflu* results for ONERA C1 with initial ejection particle diameter distribution based on skewed logarithmic distribution with mean 23μm and minimum and maximum values of 5μm and 230 μm:(top) head-end pressure vs time signal, (middle) spanwise vorticity (1/s), (bottom) particle positions colored by particle diameter.

Using the new algorithm, the full multiphysics capabilities have been integrated into Rocflu in serial. They are been evaluated for the ONERA C1 configuration. Figure 3.4.3 shows the temporal variation of the head-end pressure, the mixture spanwise vorticity field, and the particle location (colored by diameter size). It is observed the highly unsteady flow nature where large-scale vortices are forming and convecting in the rocket core chamber. An online movie can be viewed at: http://www.csar.uiuc.edu/F_viz/gallery/C1/c1_5msto8ms_comp.gif

The multiphase framework will be upgraded to include more sophisticated physical models, such as breakup models, radiation and species. Issues such as particle impingement on nozzle walls and trapping of particles in the bucket of a submerged nozzle are currently being pursued. Of great interest, is the development of turbulence-particle LES-based models for the stochastic evolution of the particle velocity field. The unstructured grid implementation will be expanded to run efficiently in parallel and will be integrated into *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.

Multi-Time-Scale Modeling (Moser, Najjar, and Haselbacher)

Detailed simulations of a solid-propellant rocket are hindered by the fact that there is an anomalously long time scale associated with the burn-back of the propellant, which is orders of magnitude larger than the fluids time scales. To simulate the entire burn of a solid rocket such as the RSRM, it will be necessary to address this time-scale disparity. The approach we are pursuing is to accelerate the burn-back time scale relative to fluid (and other) time scales. But in doing so, we must take care to not change the dynamics of the fast time scale phenomena.

In our approach, two-scale asymptotic analysis is used to develop equations for evolution on the fast and slow time scales. A modified set of equations and boundary conditions is then developed, in which the burn-back is accelerated, but which has the same fast and slow time-scale equations as the original. This approach has been formulated and is currently undergoing testing in simple flow situations. We anticipate accelerating the propellant burn-back by a factor of approximately 100, with little or no affect on the accuracy of the solutions.

Rocflo Enhancements (Wasistho and Blazek)

The active development of the structured grid solver *Rocflo* is largely completed. However a number of enhancements have been implemented. These include the porting of *Rocflo* to the *Rocstar* framework, grid dependent averaging, a better treatment of block edges and corners, and an enhancement of the utility tools. Validation efforts for multi-physics models in *Rocflo* are on-going, and a number of research efforts have been undertaken using *Rocflo* in the *Rocfluid* framework. One validation example is the C1x lab-scale rocket, for which literature data is available on the fundamental frequency of chamber pressure fluctuations (Figure 3.4.4)

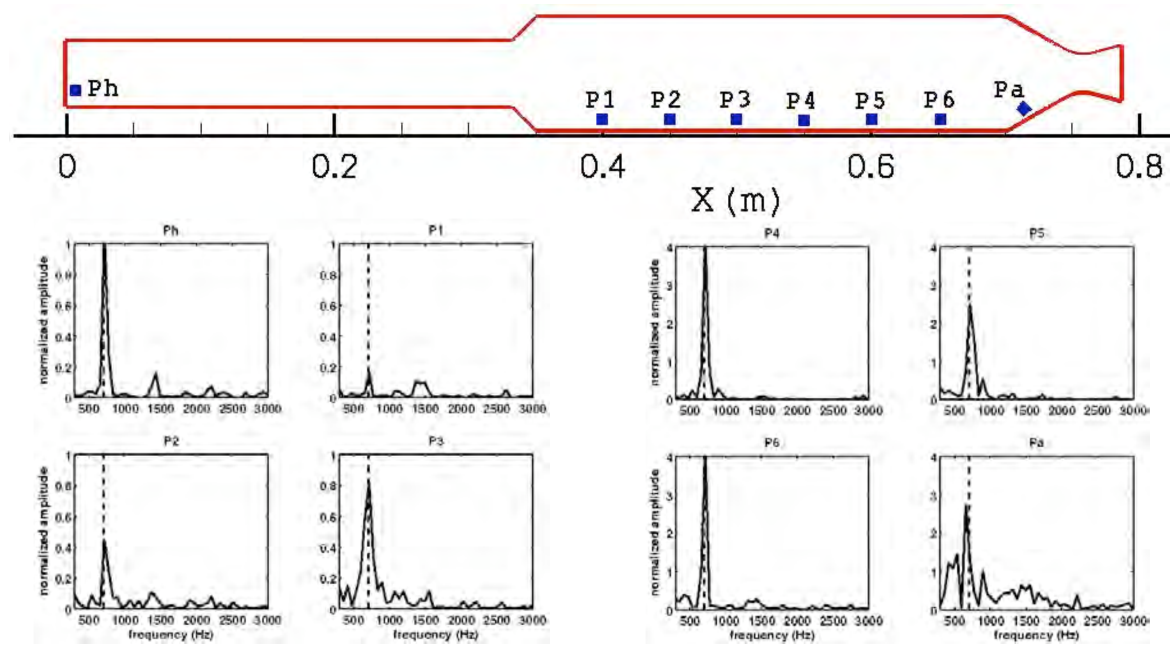

Fig 3.4.4: Pressure frequency spectra in C1x configuration from probes as indicated. Vertical dashed lines indicate experimental dominant frequency.

Large-Eddy Simulations of Wall and Shear-Layer Instabilities in a Cold Flow Motor Experiment (Najjar, Plourde [Collaborator from CRNS-ENSMA, Universite de Poitiers, France], Wasistho, and Balachandar)

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 a vortex shedding phenomenon in its wake while the main flow close to the injection wall supports a wall vortex shedding dynamics arising from the hydrodynamic instability. Computations are being performed with *Rocfluid*-MP with the LES turbulence module, *Rocturb*. A mesh resolution of over 3 million grid cells is used; while random turbulence fluctuations with an amplitude of 20% are injected to model the disturbances at the injection. Figure 3.4.5 presents contours of instantaneous total vorticity in this flow. The flow is highly unsteady with several large-scale vortices convecting through the domain. Further, near-wall structures are seen to evolve, similar to the Wall Vortex Shedding (WSP) phenomenon.

Detailed 3-D LES computations with 10 million grid points will be pursued 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.

Model Star-Grain Exit (Freund, Wasistho, and Topalian)

We have run *Rocflo* with a dynamic Smagorinski subgrid-scale LES turbulence model for the model star grain exit segment shown schematically in figure FM6. The flow from the star-grain slot is currently modeled as an inflow boundary conditions with a set profile with uniform mass flux of 150 kg/m^2s. This flows as a slot jet into the computational domain. The wall mass flux is 35kg/m^2s, consistent with burning propellant. The Reynolds number is 12500, based on v= 10 m/s, L= 0.02 m and the properties of air. Figure FM6 also shows a visualization of the vorticity magnitude. We see

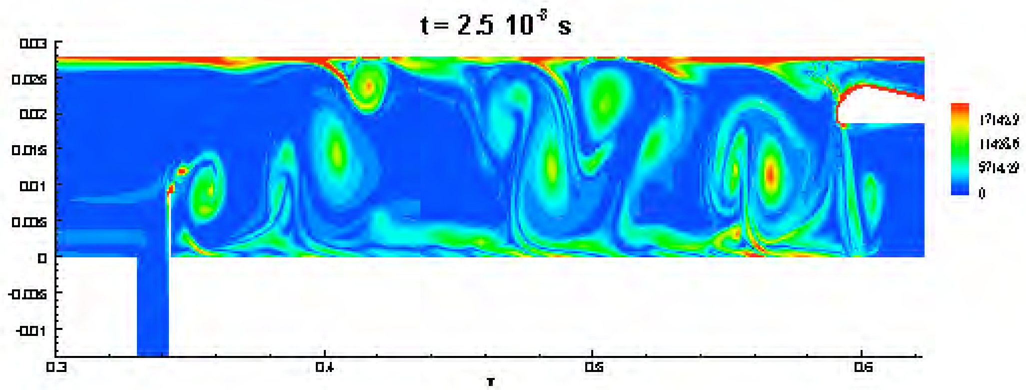

Fig. 3.4.5: Contours of instantaneous spanwise vorticity at xy and xz planes.

that the jet exiting the star-grain slot dominates the flow initially, but this is overwhelmed by the wall mass injection (from the burning propellant) further downstream. The transition between these two regimen is important for understanding of the overall flow dynamics and closing coarse-grain models for the star grain's influence on the rocket downstream. Notably, these simulations were completed on a "homemade" cluster of 16 dual-processor AMD linux workstations demonstrating the portability of the rocflo code.

Concurrently, we have developed a state-of-the-art non-dissipative but relative inflexible code against which to directly evaluate *Rocflo's* ability to do large-eddy simulation with the fidelity demanded by many scientific applications. In this code, a staggered mesh is used to improve the accuracy and conservation properties of the numerical discretizations and a recently proposed entropy constraint [Honin & Moin, in press JCP, 2004] is employed.

The first scientific objective for the coming year(s) is to evaluate the ability of the dissipative numerics in *Rocflo* against the more advanced but less flexible numerics of the special-purpose compressible flow solver that we have developed. At this point, there is no doubt that the LES models in *Rocflo* are correct, but the necessary resolution to match desired levels of fidelity is not well understood. Such an understanding is necessary for the more broad application of *Rocflo* and its LES model in scientific studies of rockets or other applications. To accomplish this the new code will be parallelized, which is straight forward for the algorithms used.

The second objective is to study the flow itself using *Rocflo*. We will run *Rocflo* to identify regions where the flow is dominated by the inflectional instabilities of the jet versus the turbulence

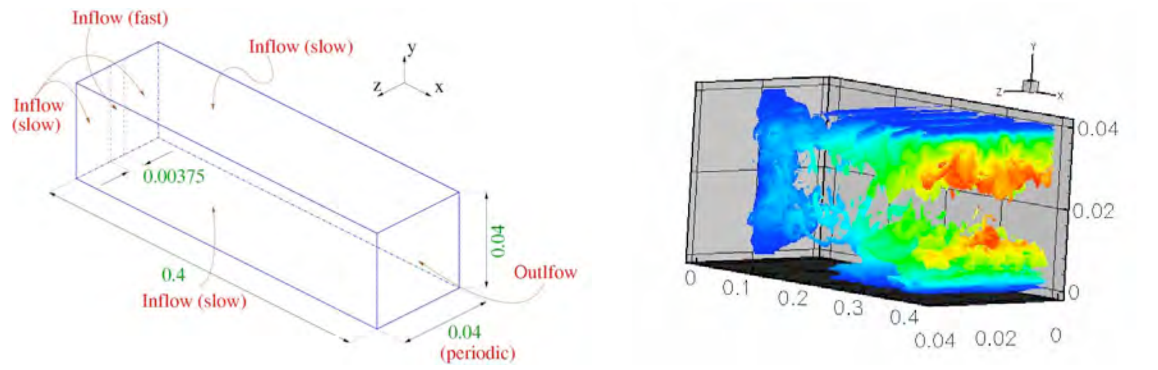

Fig. 3.4.6: Configuration for model star-grain exit (left) and contours of vorticity magnitude from *Rocflo* simulation

coming off the side walls. Scalings and parameterizations will be sought for the turbulence in this region. The dependence of the turbulence statistics on the parameters of the configuration will be needed for any coarse graining procedure applied to model the turbulence caused by the star grain's jet interacting with the wall.

Optimal LES Development (Moser, Wasistho, Zandonade, Vedula, Haselbacher, and Das)

There have been several important advances in the development of optimal LES, a new approach to the development of large eddy simulation models. First, theoretically based optimal models have been extended for use at arbitrary Reynolds number, by scaling some of the required empirical data, with good results, thus showing the consistency of the modeling approach. Second, dynamic approaches to provide statistical data not available *a priori* from theory have been implemented, and a number of refinements required for robust models have been identified and are being implemented. Third, a new approach for treating no-slip walls (as in the nozzle) has been shown to provide excellent results, thus pointing the way to a solution of the LES wall-modeling problem. Taken together these developments indicate that optimal LES models are sufficiently well developed for implementation in *Rocflo* and *Rocflu*, and an effort to pursue this implementation has begun.

As just one example of the developments, we discuss the dynamic optimal approach here in more detail. The optimal models require as input several multi-point velocity correlations. Of these, one (three-point third order correlations) cannot be determined theoretically. However, it and a several pf the other of the correlations (not all) can be computed dynamically from a running LES. When this is done, the resulting models can exhibit a number of problems because of the new dynamics introduced by the procedure. To produce robust accurate models, it was found that several constraints need to be adhered to: (i) for consistency, all correlations available dynamically should be determined dynamically; (ii) theoretically determined correlations should be constructed with dynamically determined coefficients (e.g dissipation rate); (iii) models should be constrained to have the correct energy dynamics (i.e. be dissipative); (iv) models should be formulated such that large-scale modes are represented with consistent accuracy (i.e. largely unaffected by the models). New models satisfying these constraints are being implemented and tested.

The continuing optimal LES work will proceed on two parallel tracks. First, model development and refinement will continue to be pursued. In particular, creation of a wall-model based on minimal empirical input will be pursued, and the dynamic approaches discussed above will continue to be refined. These efforts are designed to yield increasingly useful models for implementation in *Rocfluid* codes. Implementations of these models will be straight-forward given the general optimal LES infrastructure being built into these codes (see below).

The effort to implement optimal LES models in the *Rocfluid* codes will be pursued using a modular approach consistent with other physics modules integrated with the codes. The infrastructure to support a very general class of dynamic optimal models will be built, and the models as they are developed will be implemented in this infrastructure. First to be implemented will be the simplest theoretical models that rely to added empirical data (instead of dynamic correlations). The optimal models will be validated against standard turbulent test cases, and ultimately compared to standard models already implemented in *Rocfluid* for rocket cases.

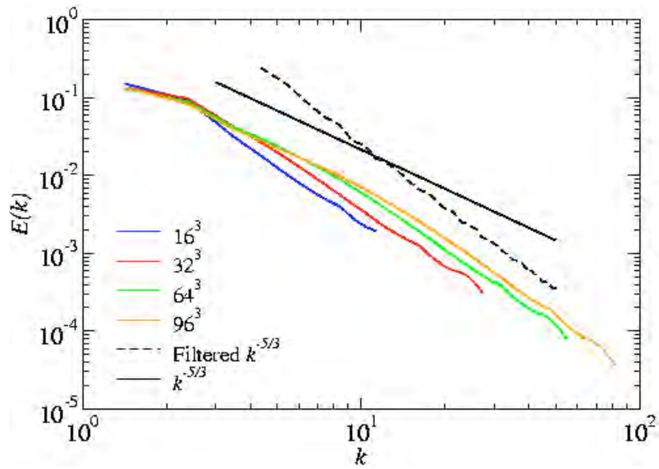

Fig. 3.4.7: Three-dimensional energy spectra of infinite Reynolds number isotropic turbulence simulated using theoretically based optimal LES with varying resolutions. Also shown are inertial-range slope valid for scales large compared to filter and filtered inertial range slope, valid near filter width.

Microscale Simulations of Multiphase Flow (Balachandar, Wakaba, and Zeng)

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 from inhibitors. In the downstream sections of the rocket, the flow is strongly turbulent. Despite these complications the traditional 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, so their use in multiphase rocket flow is unjustified. Nevertheless, they are commonly used because 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 develop improvements that can be incorporated in *Rocpart* and *Rocsmoke*.

Several 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. It is also apparent from figure 1b that added mass and Basset history effects do not improve the model. Freestream turbulence induced vortex shedding may be partly responsible for this behavior. A more productive approach may therefore be to include a stochastic component, to the standard drag law to capture particles' mean motion and dispersion behavior.

Over the next two years we plan to investigate: (i) freestream turbulence interaction with a freely moving particle; (ii) a finite-size particle moving in laminar and turbulent boundary layers (This of great relevance as it pertains to the question of wall impaction and scouring at the nozzle and submerged nozzle entrapment of particles); (iii) distribution of particles interacting with free turbulence, which will be the first ever detailed direct numerical simulations of multiphase flow turbulence; and (iv) the back effect of the particles on the carrier phase turbulence. Here the objective will be to encapsulate this back coupling in terms of simple models to be incorporated in *Rocturb* to account for the effect of particles on gas phase turbulence.

Research Plans

In addition to the follow on plans discussed above as part of current research and development, a number of research efforts will be pursued over the next year. These are discussed briefly here.

We plan to develop and implement a number of numerical enhancements to *Rocflu*, these include the ability to treat low-speed flows, the use of non-dissipative numerical schemes, and a more general treatment of boundaries (including their motion). These enhancements will allow *Rocflu* and associated physics modules to be used in a broader range of flows, in both the rocket context and more generally, and will help us pursue more rigorous validations (e.g. of turbulence models or multi-phase flow models).

Establishing confidence levels for codes like *Rocstar* is a very difficult task because of their complexity. Furthermore, it is crucial that the sensitivity of the results to the input parameters be established. The goal of this effort is to establish procedures for building confidence in and assessing the sensitivity of MP codes, through rigorous verification and validation testing.

A number of multi-phase flow phenomena of great interest in the rocket industry will be investigated using the *Rocfluid* codes. These include:

- Characterization of gas-particle coupling in supersonic accelerating flow: This will include back-coupling to the gas, droplet break-up due to fluid mechanic stresses, and interaction with shocks.
- Characterization of droplet impingement on nozzle walls: In the simulations, we will "measure" the particle impingement rates and momentum and energy exchange on the surface.
- Characterization of particle slag accumulation in submerged nozzles: The trapping of particles in the nozzle "bucket" will be analyzed in the simulations.

Relevant rocket motor configurations such as C1, C1x, BATES and Thiokol test motors will be used for these studies.