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# Project Title: Modeling and Simulation of Fluid Mixing for Laser Experiments and Supernova


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# A Abstract

The three year plan for this project is to develop novel theories and advanced simulation methods leading to a systematic understanding of turbulent mixing. A primary focus is the comparison of simulation models (Direct Numerical Simulation (DNS), Large Eddy Simulations (LES), full two fluid simulations and subgrid averaged models) to experiments. The comprehension and reduction of experimental and simulation data are central goals of this proposal. We will model 2D and 3D perturbations of planar or circular interfaces. We will compare these tests with models derived from averaged equations (our own and those of others). As a second focus, we will develop physics based subgrid simulation models of diffusion across an interface, with physical but no numerical mass diffusion. We will conduct analytic studies of mix, in support of these objectives. Advanced issues, including multiple layers and reshock, will be considered.

# B Three Year Milestones (From Proposal)

1. Simulation modeling of laser experiments showing hydrodynamic instabilities:
   (a) Highly compressible computations of Richtmyer-Meshkov (RM) and Rayleigh-Taylor (RT) instabilities
   (b) Comparison of DNS and averaged equations to each other and to experiment
2. Development of advanced numerical tools:
   (a) Model of physical diffusion across a tracked interface
   (b) Validation and improvement of multiphase subgrid modules

# C Comparison of Proposed Work to Accomplishments

Significant progress has been achieved on all of the above four bullets. For overall summaries of this progress, see [1, 6, 8, 2, 5].

In addition to progress on the Milestones for this proposal, we have improved the fundamental capability of our numerical Front Tracking method. We are developing a new tracking algorithm which is conservative in its interface propagation; this method is also higher order convergent [12]. We have developed methods for the modeling of bubbly flow and for the simulation of dynamical phase boundaries [15, 16, 14]. We have inserted dynamic models for LES simulation of turbulent mixing into our simulation framework and we are in the process of verifying and validating these algorithms in the RT and RM context. We note also the wave interaction study [7] with the surprising conclusion that four interacting rarefactions produce a shock wave as a consequence of their interaction.

## C.1 Verification of Richtmyer-Meshkov Instability Simulations (Milestone 1a)

**Milestone 1a.** The Stony Brook student Thomas Masser completed his PhD at LANL under the supervision of John Grove, and he is now a LANL Post Doc. He compared numerical solutions for the identical RM problem, using the LANL code RAGE and the Stony Brook code FronTier. For many of solution variables, he found satisfactory agreement between RAGE and FronTier. However, for the temperature field, after reshock, there was a significant difference in the peak temperatures observed. Continuing this work we also found significant differences in the probability distribution function for the molecular level mixing (the species concentration field) of the two constituents.

Our analysis of causes for the discrepancies [10, 11] is that the problem as formulated is indeterminate, in that the transport terms (viscosity and mass diffusion) were both set to zero. In many cases, they are both small, which is why such a (very common) choice was made. But the Schmidt number and the Prandtl number, each the ratio of two transport coefficients, were thus not specified. The two codes impose numerically very different Schmidt numbers and Prandtl numbers, leading to the two different solutions. From the point of view of physics, the Schmidt number for gasses is near unity, as the two coefficients are comparable, but for liquids, the Schmidt number is very small as mass diffusion for a liquid is a much smaller quantity than viscosity. Correspondingly, the two codes are very different in their treatment of mass diffusion across an interface between two fluids. The discrepancy was also analyzed by John Grove, who identified a Prandtl number related weakness in the physical model used by RAGE (and most other CFD codes), in that the single temperature description of the mixed fluid cells produces excessive and numerically based levels of thermal diffusion. He produced a revision of RAGE to correct this difficiency.

In [9], we showed that the Richtmyer-Meshkov interface, after reshock, is a fractal, diverging proportional to $\Delta x^{-1}$, for numerical solutions not regularized by viscosity. The interface is thus a volume, not a surface effect. For this reason, mass diffusion (whether numerical or physical) through this interface is also a volume effect, and thus is persistent under mesh refinement. In other words, codes are capable of producing apparently converged solutions which depend on the Schmidt number of the simulation, and if the physical Schmidt number is not properly resolved, the solution of such simulations will be determined by a numerical Schmidt number. Thus, we have an explanation of how two different codes can produce appearantly converged solutions to the same problem but which are in disagreement with each other. Since this set of ideas is not conventional in its conclusions, a detailed study was conducted [11, 10].

## C.2 Validation of Rayleigh-Taylor Instability Simulations (Milestones 1a, 1b, 2a)

**Milestone 1a.** We conducted preshot simulations of laser driven Rayleigh-Taylor instabilities [17]. The purpose of the simulation was to assess preheat effects and to aid in the design of the experiments. Specifically we investigated the separate effects of radiation preheat and electron preheat, and aided in the design of experiments for which the preheat will not be significant. After the experiments are performed, we can assess the extent to which the simulations have been validated by the experiments.

**Milestone 1b.** We have achieved agreement between experiment and simulation (validation) for two classes of Rayleigh-Taylor mixing. Agreement was reported in regard to the overall growth rate of the mixing layer ($\alpha$), in the bubble width to height ratio, in the fluctuations of the bubble height, and for the miscible experiment, in the local mixing rate described by the parameter $\theta$ [9].

**Milestone 2a.** In order to simulate the miscible Rayleigh-Taylor instability, for layers of heavy and light gasses, we included physical mass diffusion in the front tracking code [13]. The physical diffusion was below the level normally allowed in an untracked simulation; in fact after some 1000 time steps, the width of the diffusion layer between the two fluids was less than two mesh blocks. After some 100 time steps, this same width was on the order of a half or less of a mesh block. Starting with the front tracking FronTier, which allows no diffusion at all across an interface, we added a subgrid model, which computed the desired mass flux across the interface using the known solution of the one dimensional diffusion equation. This mass flux was forced to cross the tracked interface, and thereby the correct physical mass diffusion was achieved.

As described Sec. C.3, dynamic closure SGS models will be tested to allow LES simulations and practical grid levels. These models will allow a re-examination of the above RT simulations, with a properly designed LES code. The FronTier code has an advantage here, in that it will allow high Schmidt number simulations to be described with no further resolution beyond that needed to resolve the viscous terms in the equation.

## C.3 Development and Validation of Subgrid Models (Milestone 2b)

**Milestone 2b.** In [3], we studied in detail the closure terms for averaged equations in comparison to the exact expressions for the two fluid simulation data that the closures were modeling. This was carried out for the validated Rayleigh-Taylor simulation data and for the circular Richtmyer-Meshkov simulation data described above.

There were several principal findings. First the agreement was excellent, with about 10% in the overall error in the comparison. Secondly, we determined that most of the parameters in the closure model were not sensitive, and could be varied over wide ranges with no effect on the model. For all of these parameters, we proposed the value 1, thereby eliminating them from the model. The single remaining parameter occurs in the closure for the interface velocity, and it is set in terms of the motion of the edges of the mixing zone. So this parameter can also be eliminated from the model, and the model is free of all adjustable parameters. The model moreover satisfies boundary conditions at the edges of the mixing zone, and is totally hyperbolic. Thirdly, we compared this closure to a closure by Saurel et al, and found ours was considerably more accurate, with 10% overall error in contrast to 20% to 50% errors for Saurel et al.

Extension of this closure model to three or more phases was developed [4].

In [9], we address the question of whether a subgrid model is needed for mass diffusion in the RT simulations referenced above. In [11, 10], we explored the DNS convergence limit carefully, and came to the conclusion that sub grid models will be essential for LES simulations. Accordingly, we have adopted dynamic closure SGS models, and we are in the process of testing them in a systematic verification study.

# D Cost Status

See attached budget pages.

# E Schedule Status

We are on or somewhat ahead of schedule for completion of the three year milestones from the original proposal. We have identified significant scientific issues related to these milestones, in the chaotic nature of the unregularized simulations modeling Richtmyer-Meshkov mixing after reshock and the dependence of the simulated solution on the Schmidt and Prandlt numbers (physical or numerical artificial Schmidt and Prandtl numbers) of the simulation. Specifically, the dependence of the temperature and species concentration fields on the details of the physical transport and on the numerical analogues of this physical transport has been explored. This is a deep question, closely related to the original proposal. It has led to the adoption of dynamic closure SGS models for LES simulations, whose use we will explore in the coming year.

# F Changes in Approach; Actual or Anticipated Problems

See above.

# G Changes of Key Personnel

Roman Samulyak has been added as a co-PI, replacing Yongmin Zhang.

# H Technology Transfer Activities

## H.1 Publications


[1] W. Bo, B. Cheng, J. Du, B. Fix, E. George, J. Glimm, J. Grove, X. Jia, H. Jin, H. Lee, Y. Li, X. Li, X. Liu, D. H. Sharp, L. Wu, and Yan Yu. Recent progress in the stochastic analysis of turbulent

mixing. *Contemporary Mathematics*, 429:33–44, 2007. Stony Brook University Preprint Number SUNYSB-AMS-05-18, Los Alamos National Laboratory LAUR Number LAUR-05-7102.

[2] W. Bo, B. Fix, J. Glimm, X. Li, X. Liu, R. Samulyak, and L. Wu. Frontier and applications to scientific and engineering problems. *Proceedings in Applied Mathematics and Mechanics*, 2007.

[3] W. Bo, H. Jin, D. Kim, X. Liu, H. Lee, N. Pestieau, Y. Yu, J. Glimm, and J. Grove. Multi phase closure models. *Computers & Mathematics with Applications*, 2007. In Press. Stony Brook University Preprint Number SUNYSB-AMS-07-02.

[4] B. Cheng, J. Glimm, D. H. Sharp, and Y. Yu. A multifluid mix model for the layered incompressible materials. In *Proceedings of the TMBW07 Conference*. 2008.

[5] B. Fix, J. Glimm, R. Kaufman, X. L. Li, and L. L. Wu. Frontier and application to fluid instability study, verification and validation of frontier code and application to fluid interfacial instabilities. *Proceedings of World Conference on Turbulence Mixing and Beyond*, 2008. Accepted for publication.

[6] J. Glimm, B. Fix, X.-L. Li, J.-J. Liu, X.-F. Liu, T.-S. Liu, R. Samulyak, and Z.-L. Xu. Front tracking under TSTT. *Proceedings of the IGPP-CalSpace Conference, Astronomical Society of the Pacific*, 359:15, 2007.

[7] J. Glimm, X. Ji, J. Li, X. Li, P. Zhang, T. Zhang, and Y. Zheng. Transonic shock formation in a rarefaction riemann problem for the 2-D compressible euler equations. *SIAM J. Appl. Math.*, 2007. Submitted, University at Stony Brook preprint number AMS-07-08.

[8] H. Jin and J. Glimm. Verification and validation for turbulent mixing. *Nonlinear Analysis*, 2008. In press. Stony Brook University Preprint SUNYSB-AMS-07-04.

[9] H. Lee, H. Jin, Y. Yu, and J. Glimm. On validation of turbulent mixing simulations of Rayleigh-Taylor mixing. *Phys. Fluids*, 20:1–8, 2008. Stony Brook University Preprint SUNYSB-AMS-07-03.

[10] H. Lim, Y. Yu, J. Glimm, X.-L. Li, and D. H. Sharp. Chaos, transport, and mesh convergence for fluid mixing. *Acta Mathematicae Applicatae Sinica*, 2007. Submitted. Stony Brook University Preprint SUNYSB-AMS-07-09 Los Alamos National Laboratory preprint number LA-UR-08-0068.

[11] H. Lim, Y. Yu, H. Jin, D. Kim, H. Lee, J. Glimm, X.-L. Li, and D. H. Sharp. Multi scale models for fluid mixing. *Special issue CMAME*, 2007. Accepted for publication. Stony Brook University Preprint SUNYSB-AMS-07-05.

[12] Jinjie Liu, Hyun-Kyun Lim, James Glimm, and Xiaolin Li. A conservative front tracking method in N-dimensions. *J. of Sci. Comp.*, 31:213–236, 2007. Stony Brook University preprint number SUNYSB-AMS-06-04.

[13] X. F. Liu, Y. H. Li, J. Glimm, and X. L. Li. A front tracking algorithm for limited mass diffusion. *J. of Comp. Phys.*, 222:644–653, 2007. Stony Brook University preprint number SUNYSB-AMS-06-01.

[14] T. Lu, R. Samulyak, and J. Glimm. Direct numerical simulation of bubbly flows and its applications. *Phys. Fluid Eng.*, 129:595–604, 2007.

[15] T. Lu, Z. L. Xu, R. Samulyak, J. Glimm, and X. M. Ji. Dynamic phase boundaries for compressible fluids. *SIAMJSC*, 30:895–815, 2008. SB Preprint Number: SUNYSB-AMS-06-07.

[16] Z. L. Xu, J. Glimm, Y. Zhang, and X. Liu. A multiscale front tracking method for compressible free surface flows. *Chemical Engineering Science Journal*, 62:3538–3548, 2007. SB Preprint Number: SUNYSB-AMS-06-09.

[17] Y. Zhang, P. Drake, and J. Glimm. Numerical evaluation of the impact of laser preheat on interface structure and instability. *Physics of Plasma*, 14:1–10, 2007. SB Preprint Number: SUNYSB-AMS-06-10.

### H.2 Internet Sites

Access to FronTier software for downloading:
http://frontier.ams.sunysb.edu/download/download.php
User manual:
http://www.ams.sunysb.edu/ linli/FronTier.html

### H.3 Networks and Collaborations Fostered

1. Simulation of splitter plate experiments with experimental initial conditions recorded: Oleg Schilling (LLNL), Malcolm Andrews (LANL)
2. Resolution of discrepancies between two simulation codes in the temperature values for a Richtmyer-Meshkov simulation, after reshock: John Grove (LANL), Thomas Masser (Stony Brook, LANL), David Sharp (LANL)
3. Subgrid models for mix in curvilinear coordinates: Baolian Cheng (LANL), David Sharp (LANL)
4. Models of preheat for ICF experiments: Paul Drake (U. Michigan)
5. Uncertainty qunatification studies, participation in the Stanford University PSAAP consortium
6. Turbulent mixing studies for immiscible two phase flow. Initial focus on spray breakup of turbulent jet. Later focus on two fluid mixing simulations in a uranium fuel reprocessing chemical mix and separation device, to provide data needed to validate subgrid averaged models: Valmor D'Almeda (ORNL)
7. Fluid interface studies, with a focus on design of a fluid target for use in high energy accelerators: BNL Accelerator modeling group

### H.4 Technologies

### H.5 Inventions

None.

### H.6 Other

**Databases.** We have made a data base of multimode Rayleigh-Taylor experiments. The list includes all physical parameters, both those recorded in the experiment and reported in the publications, and those inferred from other sources. Specifically all transport coefficients (mass diffusion, thermal conductivity, viscosity) for both fluids are reported and for immiscible experiments, the values of surface tension. The dispersion theory of the most unstable length is found and using this as well as the observed initial disturbance length, a dimensionless value for the transport coefficients is determined. The value for the mixing layer growth rate $\alpha$ is given when this is part of the experimental record.

**Software.** The front tracking package FronTier is available for distribution.

**Educational Aids.** This project has been integrated into the graduate education offered at Stony Brook. The program has partially supported four graduate students. Our students have communicated with national labs using the knowledge and tools developed under this grant to assist research projects of DOE interests. Among these projects are shock and gravity driven instabilities (Los Alamos), combustion engine and fluid mixing chemical separation device (Oak Ridge National Lab) and groud water precipitation (PNNL). One of these students (Thomas Masser) completed his Ph. D. thesis related research at Los Alamos National Lab and is now a Post Doc there. We sent two students (Xingtao Liu and Wurigen Bo) to ORNL for a summer research project; one of these will be supported at BNL for the coming year on studies of turbulent mixing (as related to target design for high energy accelerators). We nominated students for international workshops (Brian Fix) organized by US DOE and other Labs.

We have organized a series of graduate student seminars introducing software development techniques, post-processing packages and skills for large scale parallel computation. These tutorials and workshops have been vidoetaped as an educational tools for new and incoming students.

We have encourages graduate students to meet and interact with scientists at national laboratories such as attending the ITAPS bootcamp of the common geometry related user interface.