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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 model 2D and 3D perturbations of planar or circular interfaces. We compare these tests with models derived from averaged equations (our own and those of others). As a second focus, we develop physics based subgrid simulation models of diffusion across an interface, with physical but no numerical mass diffusion. Multiple layers and reshock are considered here.

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

Progress has been achieved on all of these bullets over the three year grant period. For overall summaries of recent progress, see [1, 4, 7, 10, 11, 13].

In addition to progress on the milestones for this proposal, we have improved the fundamental capability of our numerical Front Tracking method. We have developed methods for the modeling of bubbly flow and for the simulation of dynamical phase boundaries [14]. We have inserted dynamic models for LES simulation of turbulent mixing into our simulation framework and we have verified these algorithms in the RM context. We are presently validating them in the RT context.

C.1 Hydrodynamic Instabilities (Milestones 1a, 1b)

A former Stony Brook student Thomas Masser, now a LANL Post Doc, discovered discrepancies between the LANL code RAGE and the Stony Brook code FronTier, for solutions of an identical RM instability problem. 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, 13] 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

$Re \approx$	liquid: $Sc = 10^3$, $Pr = 30$ c to f	m to f	gas: $Sc = 1$, $Pr = 1$ c to f	m to f
300	0.48	0.23	0.21	0.08
6000	0.33	0.28	0.40	0.32
$600K$	0.31	0.15	0.33	0.19

Table 1: Relative mesh errors for the chemical production rate (w) pdf, for an activation temperature $T_{AC} = 15,000K$ in the middle of the observed temperature range. Comparison is coarse mesh (c) to fine (f) and medium (m) to fine.

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 Δx^{-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 [13, 10, 12]. Extracting from that study, we show convergence for the chemical reaction rate pdf in Table 1.

Details with additional parameter values will be published separately.

Work on Rayleigh-Taylor validation, which was addressed in the previous progress report, is ongoing. 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 (α), 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 θ [9].

Dynamic closure SGS models were 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 allows high Schmidt number simulations to be described with no further resolution beyond that needed to resolve the viscous terms in the equation.

C.2 Development of Advanced Numerical Tools (Milestone 2a, 2b)

A major accomplish of the work on this project has been the devemopment of dynamic subgrid models for turbulent mixing. We use the dynamic subgrid models of the Stanford Turbulence Center, but very far from their normal domain of use. We use them for problems which have sharp gradients even at a grid level. In this way, we combine separate traditions of turbulence modeling from the capturing community and the turbulence community, and enhance this combination with our own sharp interface and steep gradient capabiities. The result is ideally suited for computation of reaction rates in turbulent mixing with an extremely small time scale, a property that (in the opinion of the project members) has not been achieved by any other group. Since many practical turbulent mixing computations, such as neutron yield in ICF capsules, depend on such numerical issues for their modeling, we believe that this capability will have value to a wide community.

In [2], 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 [3].

In [9], we address the question of whether a subgrid model is needed for mass diffusion in the RT simulations referenced above. In [13, 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 have tested them in a systematic verification study.

D Cost Status

To be reported on SF 269 Financial Status Report.

E Schedule Status

We have completed most 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 demonstrated. 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. Using these models, we have achieved convergence for microphysical variables (such as temperature, species concentration and chemical reaction rates) for LES simulations of RM mixing, including high Schmidt number cases.

F Changes in Approach; Actual or Anticipated Problems

See above.

G Changes of Key Personnel

None

H Technology Transfer Activities

H.1 Publications

[1] W. Bo, B. Fix, J. Glimm, X. L. Li, X. T. Liu, R. Samulyak, and L. L. Wu. Frontier and applications to scientific and engineering problems. *Proceedings of International Congress of Industrial and Applied*

Mathematics, 2008. Accepted for publication.

[2] 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*, 56:1291–1302, 2008. Stony Brook University Preprint Number SUNYSB-AMS-07-02.

[3] B. Cheng, J. Glimm, D. H. Sharp, and Y. Yu. A multifluid mix model for the layered incompressible materials. *Physica Scripta*, 2008. Proceedings of World Conference on Turbulence Mixing and Beyond, Accepted for publication.

[4] 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. *Physica Scripta*, 2008. Proceedings of World Conference on Turbulence Mixing and Beyond, Accepted for publication.

[5] 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.*, 69:720–742, 2008. University at Stony Brook preprint number AMS-07-08.

[6] G. Iaccarino, R. Pecnik, J. Glimm, and D. H. Sharp. Towards a qmu approach for predicting the operability limits of air-breathing hypersonic vehicles. *CMAME*. Submitted for publication.

[7] H. Jin and J. Glimm. Verification and validation for turbulent mixing. *Nonlinear Analysis*, 69:874–879, 2008. Stony Brook University Preprint SUNYSB-AMS-07-04.

[8] K. S. Kang, J. W. Davenport, J. Glimm, D. E. Keyes, and M. McGuigan. Linear augmented slater type orbital method for free standing clusters. *J. Comp. Chem.*, 30:1185–1193, 2009.

[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*, 24:355–368, 2008. Stony Brook University Preprint SUNYSB-AMS-07-09 Los Alamos National Laboratory preprint number LA-UR-08-0068.

[11] H. Lim, Y. Yu, J. Glimm, X. L. Li, and D. H. Sharp. Subgrid models in turbulent mixing. *ASTRONUM proceedings*, 2008. Stony Brook Preprint SUNYSB-AMS-09-01 and Los Alamos National Laboratory Preprint LA-UR 08-05999; Submitted for Publication.

[12] H. Lim, Y. Yu, J. Glimm, X. L. Li, and D. H. Sharp. Subgrid models for mass and thermal diffusion in turbulent mixing. *Phys. Fluids*, 2009. Stony Brook Preprint SUNYSB-AMS-08-07 and Los Alamos National Laboratory Preprint LA-UR 08-07725; Submitted for Publication.

[13] 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. *Compu. Methods Appl. Mech. Engrg.*, 197:3435–3444, 2008. Stony Brook University Preprint SUNYSB-AMS-07-05.

[14] 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.

[15] R. Samulyak, J. Du, J. Glimm, and Z. Xu. A numerical algorithm for MHD of free surface flows at low magnetic reynolds numbers. *J. Comput. Phys.*, 226:1532–1546, 2007.

[16] R. Samulyak, T. Lu, P. Parks, J. Glimm, and X. Li. Simulation of pellet ablation for tokamak fuelling with itaps front tracking. *Journal of Physics: Conf. Series*, 125:012081, 2008.

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.

8. A student (Brian Fix) will spend a summer at LANL.

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 α 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 was supported at BNL for studies of turbulent mixing (as related to target design for high energy accelerators). A student, Brian Fix, will spend next summer at LANL.

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.