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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 (both Direct Numerical Simulation 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 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 and Rayleigh-Taylor 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, 5, 6, 7].

In addition to progress on the Milestones for this proposal, we have improved the fundamental capability of our numerical Front Tracking method. Comparison of this code with other interface techniques was documented in [3]. In this comparison, Front Tracking was the most accurate of the methods surveyed. We are developing a new tracking algorithm which is conservative in its interface propagation; this method is also higher order convergent [11, 12]. We have also developed methods for the modeling of bubbly flow and for the simulation of dynamical phase boundaries .

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

Milestone 1a. A circular convergent one layer Richtmyer-Meshkov problem was considered in [18]. The problem, especially after reshock, is highly chaotic, and fails to converge in a pointwise sense. We reformulated the notion of convergence and with this new formulation, convergence was in fact observed.

There were two main ideas in the new notion of convergence. The first, and most important, was to consider convergence in a statistical sense, so that average quantities were observed to converge. The problem has an approximate circular symmetry and averages over this variable in the range of 5 degrees to 45 degrees were sufficient in most cases. A few of the variables were too noisy, and a further ensemble average was needed.

The second main idea was to introduce wave filters, to isolate the dominate waves (incoming and outgoing shock, edges of the mixing zone), and to determine their location as a function of time in the simulation. Convergence of these locations was established, with averaging as above. Between the dominant waves, the solution is relatively smooth, and the errors were found be be convergent.

Recently, the Stony Brook student Thomas Masser went to LANL to work with John Grove, and he considered the identical problem, to be solved using the LANL code RAGE. For most of the solution and solution variables, he found satisfactory agreement between RAGE and the Stony Brook code

FronTier. However for the temperature field, after reshock, there was a significant difference in the peak temperatures observed.

Our analysis (to be confirmed with further study) 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, the ratio of these two transport coefficients, was thus not specified. Our view is that the two code impose by default very different Schmidt 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.

In [10], we showed that the Richtmyer-Meshkov interface, after reshock, is a fractal, diverging proportional to Δx^{-1}. It 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, it is capable of producing a converged solution which depends on the Schmidt number of the simulation, and if the physical Schmidt number is not properly resolved, the converged solution of such simulations will be determined by a numerical Schmidt number. In other words, we have an explanation of how two different codes can produce converged solutions to the same problem which are in disagreement. Since this set of ideas is not conventional in its conclusions, further study is required.

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

Milestone 1a. We conducted preshot simulations of laser driven Rayleigh-Taylor instabilities [19]. 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. For all of the experiments of Read and of Smeeton and Youngs with immiscible fluids and with no surfactants, and with sufficient data recorded, we modeled the surface tension with dimensionless values equal to that predicted by dispersion theory and basically in agreement with that given by direct observation of the of the initial length scale taken from the experiments. The simulations were enhanced by some improvements in the Front Tracking code itself, as well [4]. For the air-helium miscible fluid splitter plate experiments of Pra... and Andrews, we similarly obtained agreement between simulation and experiment [13]. 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 [10].

Milestone 2a. In order to simulate the miscible Rayleigh-Taylor instability, for layers of heavy and light gasses, we includeed physical mass difussion in the front tracking code [14]. 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.

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

Milestone 2b. We refined the formulation of our previously proposed subgrid mix model [8, 9]. A principle accomplishment was to resolve a question relating to the entropy variable. For the averaged equations, entropy is not conserved, even when the flow (before averaging) is isentropic. In fact, this property is not a flaw in the model, as the averaging itself is not entropy conserving. To replace this property, we derived an entropy inequality for the averaged equations.

In [2], we studied in detail the closure terms in comparison to DNS simulation data for the exact expressions that the closures were modeling. This was carried out for the vlaidated 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.

In [10], we address the question of whether a subgrid model is needed for mass diffusion in the DNS simulations referenced above. We examined this from several points of view, and reached the tentative conclusion that there is no need to augment the DNS simulations with a mass diffusion subgrid model, in the sense that doing so would not change the simulations appreciably. For example we evaluated the coefficient of a Smagorinsky type mass diffusion term and found that it was considerably smaller than the physical mass diffusion already present in the simulation.

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 fractal nature of the Richtmyer-Meshkov mixing after reshock and a conjectured dependence of the simulated solution on the Schmidt number (physical or numerical artificial Schmidt number) of the simulation. Specifically, the dependence of the temperature field on the details of the physical transport and on the numerical analogues of this physical transport will be explored. This is a deep question, closely related to the original proposal and one we hope to address in the remainder of the proposal period.

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. 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 Y. 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, H. Jin, D. Kim, X. Liu, H. Lee, N. Pestieau, Y. Yu, J. Glimm, and J. W. Grove. Compressible multi species multiphase flow models. *Phys. Rev. E*, 2007. Submitted. Stony Brook University Preprint Number SUNYSB-AMS-07-02, Los Alamos National Laboratory LAUR Number LAUR-07-1964.

[3] Jian Du, Brian Fix, James Glimm, Xicheng Jia, Xiaolin Li, Yunhua Li, and Lingling Wu. A simple package for front tracking. *J. Comp. Phys.*, 213:613–628, 2006. Stony Brook University preprint SUNYSB-AMS-05-02.

[4] E. George, J. Glimm, X. L. Li, Y. H. Li, and X. F. Liu. The influence of scale-breaking phenomena on turbulent mixing rates. *Phys. Rev. E*, 73:016304–1–016304–5, 2006.

[5] 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.

[6] J. Glimm and X. L. Li. Recent progress in turbulent mixing. In M. Legrand and M. Vandenboomgarde, editors, *Proceedings of the 10th International Workshop on the Physics of Compressible Turbulent Mixing, 17-21 July, Paris France*, 2006. Stony Brook University Preprint SUNYSB-AMS-06-13, In Press.

[7] H. Jin and J. Glimm. Verification and validation for turbulent mixing. *Journal of Nonlinear Analysis*, 2007. Submitted. Stony Brook University Preprint number SUNYSB-AMS-07-XX.

[8] H. Jin, J. Glimm, and D. H. Sharp. Compressible two-pressure two-phase flow models. *Phys. Lett. A*, 353:469–474, 2006.

[9] H. Jin, J. Glimm, and D. H. Sharp. Entropy of averaging for compressible two-pressure two-phase models. *Phys. Lett. A*, 360:114–121, 2006. Stony Brook University Preprint number SUNYSB-AMS-06-08 and Los Alamos National Laboratory.

[10] H. Lee, H. Jin, Y. Yu, and J. Glimm. On the validation of turbulent mixing simulations for rayleigh-taylor instability. *Phys. Fluids*, 2007. Submitted. University at Stony Brook Preprint Number SB-AMS-07-03.

[11] J.-J. Liu, J. Glimm, and X.-L. Li. A conservative front tracking method. In F. Asakura, H. Aiso, S. Kawashima, Matsumura A, S. Nishibata, and K. Nishihara, editors, *Hyperbolic Problems: Theory, Numerics, and Applications*, pages 57–62. Yokohama Publishers, Osaka, Japan, 2006.

[12] Jinjie Liu, Hyun-Kyung Lim, James Glimm, and Xiaolin Li. A conservative front tracking method in n-dimensions. *J. of Sci. Comp.*, 2006. In Press. Stony Brook University preprint number SUNYSB-AMS-06-04.

[13] X. F. Liu, E. George, W. Bo, and J. Glimm. Turbulent mixing with physical mass diffusion. *Phys. Rev. E*, 73:056301–1–056301–8, 2006.

[14] 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.

[15] T. Lu, R. Samulyak, and J. Glimm. Direct numerical simulation of bubbly flows and its applications. *Phys. Fluid Eng.*, 2007. In press.

[16] Z. L. Xu, M. Kim, W. Oh, J. Glimm, R. Samulyak, X. L. Li, and C. Tzanos. Discrete bubble modeling of unsteady cavitating flow. *International Journal for Multiscale Computational Engineering*, 2006. Accepted. SB Preprint Number: SUNYSB-AMS-05-08.

[17] Z. L. Xu, T. Lu, R. Samulyak, J. Glimm, and X. M. Ji. Dynamic phase boundaries for compressible fluids. *Siam J. on Scientific Computing*, 2006. Submitted. SB Preprint Number: SUNYSB-AMS-06-07.

[18] Y. Yu, M. Zhao, T. Lee, N. Pestieau, W. Bo, J. Glimm, and J. W. Grove. Uncertainty quantification for chaotic computational fluid dynamics. *J. Comp. Phys.*, 217:200–216, 2006. Stony Brook Preprint number SB-AMS-05-16 and LANL preprint number LA-UR-05-6212.

[19] Y. Zhang, P. Drake, J. Glimm, and P. Lavergne. Numerical measurement of impact of laser preheat on interface structure and instability. *Physics of Plasma*, 2007. In Press, 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), Peter Adams (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. Simulations of laser shocked gaps with off-hugoniot (preheat) initial data: Richard Holmes (LANL), Jonathan Workman (LANL), Jim Fink (LANL)

H.4 Technologies

H.5 Inventions

None.

H.6 Other

Databases. We have made a data base of all 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 now available for distribution.

Educational Aids.

This project has been incorperated with graduate education. The program has partially supported several graduate student, including four American students. These 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 (Oak Ridge National Lab) and groud water precipitation (PNNL). We have recommended one of these students (Thomas Masser) to conduct the Ph. D. thesis related research at Los Alamos National Lab, sent two students (Xingtao Liu and Wurigen Bo) to ORNL for summer research project, and 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 labs such as attending the ITAPS bootcamp of the common geometry related user interface.