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13. ABSTRACT (Maximum 200 words) The principal directions of the research reported were fluid interface instabilities, multiphase flow, solid dynamics, flow in porous media, uncertainty quantification and photonics. Our Front Tracking code, FrontTier, has been extended to three dimensions, and is now functioning robustly for the simulation of three-dimensional complex fluid mixing flows. We have made a major effort in the study of multiphase flow, including a proposed model of averaged multiphase flow equations which seem to avoid most of the well known pitfalls for such equations. Validation studies for the Front Tracking code, FrontTier Solid have been performed. Photonics, a new project for this work, is conducted in collaboration with C. Bowden of Redstone Arsenal, and a group of his collaborators. We have developed a parallelized FDTD code to allow simulations in complex 3D geometries for photonic crystals and other photonic devices.				
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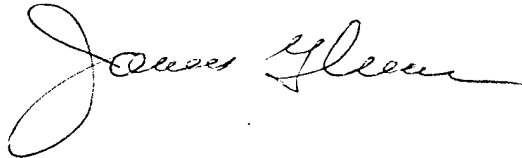
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Contents

A	Report Outline	1
B	LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER ARO SPONSORSHIP DURING THIS REPORTING PERIOD, INCLUDING JOURNAL REFERENCES	2
	B.1 Peer Reviewed Publications	3
	B.2 Technical Reports	5
	B.3 Manuscripts Submitted for Publication	6
	B.4 Conference Proceedings	7
C	SUMMARY OF MOST IMPORTANT RESULTS	8
D	Bibliography	10

A Report Outline

1. ARO PROPOSAL NUMBER: 38338-MA
2. PERIOD COVERED BY REPORT: 1 July 1998 – 30 June 2001
3. TITLE OF PROPOSAL: Turbulent Mixing and Solid Impact: Studies in Multiscale Modeling
4. CONTRACT OR GRANT NUMBER: DAAG55-98-10313
5. NAME OF INSTITUTION: State University of New York at Stony Brook
6. AUTHORS OF REPORT: James Glimm and Bradley Plohr
7. APPINDICES, ILLUSTRATIONS, and TABLES: None
8. PROBLEM SOLVED:
 - Theory and simulation were developed to agree with experimental data for acceleration driven turbulent mixing. New multiphase flow models were formulated.
 - A new solid mechanics code was developed, and is partially validated. This code is based on new principles, namely full conservation for an Eulerian formulation with Front Tracking to prevent mixed cells and mass diffusion across interfaces.

- A new FDTD electromagnetics code was developed for optics applications, with nonlinear and dispersive media capabilities.
- Models for solution error for numerical simulation were developed and applied to engineering problems.

9. SUMMARY OF MOST IMPORTANT RESULTS: See below.

10. TECHNOLOGY TRANSFER: Our photonics work is conducted as a collaboration with C. Bowden of Redstone Arsenal. We interact with Tim Wright of ARL. J. Glimm is chair of the External Advisory Board of the Weapons and Materials Science Directorate of ARL and a member of the Technical Advisory Board of ARL. He was also a member of the External Review Committee for the Dynamical Experimentation Division of Los Alamos National Laboratory.

Discussions with E. Schmidt of ARL concerned the use of FronTier-MHD for armor-antiarmor applications.

This simulation code FronTier is in use at Los Alamos National Laboratory, both for fluid and for solid deformation modeling. It is used in fluid modeling in collaboration with staff of Livermore National Laboratory and Brookhaven National Laboratory.

Work on uncertainty quantification is in use at Los Alamos National Laboratory and in collaboration with British Petroleum and with Chevron. The research on porous media involves collaboration with personnel at Petrobras.

11. SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT AND DEGREES AWARDED WHILE EMPLOYED ON PROJECT:

(a) Senior Personnel: B. Plohr

(b) Postdoctoral Personnel: W. Lee, J. Pinezich, D. Yu

(c) Students: C. Ju, A. Lin, J.-Y. Nam, N. Stojic, Y. Zhou

(d) Ph. D. Degrees Awarded (Students Supported by this Grant): A. Lin

12. REPORT OF INVENTIONS (BY TITLE ONLY): No inventions were produced by the researchers.

13. COPIES OF TECHNICAL REPORTS: Sent Previously

B LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER ARO SPONSORSHIP DURING THIS REPORTING PERIOD, INCLUDING JOURNAL REFERENCES

B.1 Peer Reviewed Publications

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- [22] N. STOJIC, J. GLIMM, Y. DENG, AND J. HAUS, *Transverse magnetic modes in two-dimensional triangular photonic crystals*, tech. rep., BNL, 2000.

B.2 Technical Reports

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B.4 Conference Proceedings

- [1] J. WALTER, J. GLIMM, J. GROVE, H.-C. HWANG, X. LIN, B. J. PLOHR, D. H. SHARP, AND D. YU, *Eulerian front tracking for solid dynamics*, in Proceedings of the 15th US Army Symposium on Solid Mechanics, K. Iyer and S. chin Chou, eds., Myrtle Beach, SC, 1999, Battelle Memorial Institute, Battelle Press (www.battelle.org/bookstore), pp. 343–366. published on CD-ROM (ISBN 1-57477-083-7).

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C SUMMARY OF MOST IMPORTANT RESULTS

Introduction. The principal directions of our research were fluid interface instabilities, multiphase flow, solid dynamics, flow in porous media, uncertainty quantification, and photonics. All of this work has involved developments in theory, modeling, and computation.

Additional Army-related activities of the project PI, James Glimm, include: chair of the External Advisory Board for the Weapons and Material Science Directorate of the ARL; a member of the Technical Advisory Board of ARL; member of the Technical Advisory Board of the Dynamic Testing Division of Los Alamos National Laboratory; and scientific interaction with Tim Wright of ARL and Chuck Bowden of Redstone Arsenal.

Front Tracking Algorithm Development and Interface Instability. Our Front Tracking code, FronTier, has been extended to three dimensions, and is now functioning robustly for the simulation of three-dimensional complex fluid mixing flows [15]. Rapid progress has been achieved in the evolution of the Front Tracking algorithm. The interface description is simpler, robust, and thus suitable for application usage, which is now occurring.

Definitive results have been obtained for the simulation of Rayleigh-Taylor flows, with agreement between simulation and experiment [6, 14]. The importance of the agreement obtained by FronTier between experiment and simulation is emphasized by the widespread disagreement between most codes and experiment for this problem. Instabilities in axisymmetric implosions and explosions were simulated [20, 19].

Application to the evolution of a mercury jet, used for design of a target in a high energy accelerator, is given in [27].

Multiphase Flow. We have made a major effort in the study of multiphase flow. This study includes direct numerical simulation (DNS) of the microscale of complex fluid mixtures [6, 14] based on the Front Tracking algorithm. It includes a proposed model of averaged multiphase flow equations which seem to avoid most of the well known pitfalls for such equations [6]. These equations are well-posed mathematically and are free from physical assumptions and limitations on thermodynamical equilibration processes associated with mixed material thermodynamics. The equations have an analytic solution, in closed form, for one-dimensional incompressible flow. We have developed predictions for the motion of the edges of the mixing zone, which are the main input into the multiphase flow equations [8]. These equations are being installed as a flow simulation option for our Front Tracking code FronTier. Reduced equations based on a diffusive mixing model were derived in [11].

Elastic-Plastic Flow. Validation studies for the Front Tracking code FronTier-Solid have been performed [42]. Front Tracking is advantageous relative to traditional Lagrangian codes because the fixed Eulerian computational mesh is not subject to mesh distortion; and it is advantageous relative to standard Eulerian codes because the tracking eliminates spurious numerical diffusion at interfaces and the need for artificial mixed-material computational cells. FronTier-Solid is a two-dimensional solid dynamics code based on a fully conservative formulation of the governing equations for large-strain deformation, a hyperelastic equation of state that allows for large volumetric change, and a rate-dependent plasticity model for high strain rates. The code features conservative finite differencing, a Riemann solver that accounts for the nonlinearity of longitudinal waves, and an implicit method for integrating the plastic source term. An overview of the FronTier Solid code with applications to high-

velocity impact and shock-accelerated interface problems is presented in [42]. See also [42], where further validation studies are performed.

Research of the graduate student supported by this grant concerns Richtmyer-Meshkov instability, which is a shock-driven, interfacial instability. The novel feature of this work is that the materials separated by the interface are elastic solids, not fluids. The current focus of effort is on linearized solutions, which will serve as a validation standard for nonlinear simulations. The unperturbed solution will be obtained using the Riemann solver that is part of the FronTier Solid code. The corresponding linearized equations will be solved numerically using an extension of the Evolve code framework for one-dimensional evolutionary problems (which was used in the three-phase flow simulations described below). The main result will be the prediction of the growth rate of the perturbation amplitude.

Flow in Porous Media. We study probability based models for numerical solution error associated with the upscaled equations. The error models will be used in a risk management strategy, related to our program on uncertainty quantification (described below).

In other work [36, 37], we established that for immiscible three-phase flow, potentially three-quarters of the oil recovered through a WAG process can be caused by a non-Buckley-Leverett “transitional” shock wave, with a significant increase in total oil recovery compared to other WAG recovery wave paths. This non-classical kind of wave, recently the focus of much mathematical research, is common in three-phase flow. We showed how transitional waves arise in WAG flow and how they can be calculated by semi-analytic methods, which are helpful in the design of effective WAG recovery strategies. We showed that capillary effects enlarge the region of instability for three phase flow [4] while hysteresis has the potential to regularize it [38].

Hyperbolic Conservation Law Theory. A quasi Riemann problem is a Riemann problem for a viscously perturbed hyperbolic conservation law [5]. Quasi Riemann solutions are investigated in cases of saddle-saddle connections for which the structure of the Riemann solution shows unusual behavior, such as nonuniqueness of solutions. The quasi Riemann solutions are needed to resolve this nonuniqueness. They provide a better picture of the long but not infinite time asymptotics. They provide a better and understandable picture of the dependence of the solutions on initial conditions and parameters.

In [39] we investigated solutions of Riemann problems for systems of two conservation laws. We used an approach in which Riemann solutions are organized into strata of successively higher codimension. The codimension-zero stratum consists of Riemann solutions that are structurally stable: the number and types of waves in a solution are preserved under small perturbations of the flux function and initial data. Codimension-one Riemann solutions, which constitute most of the boundary of the codimension-zero stratum, violate structural stability in a minimal way. At the codimension-one stratum, either the qualitative structure of Riemann solutions changes or solutions fail to be parameterized smoothly by the flux function and the initial data. In this paper, an overview of the phenomena associated with codimension-one Riemann solutions is given. A complete list is formulated for the different kinds of codimension-one solutions, classified according to their geometric properties, their roles in solving Riemann problems, and their relationships to wave curves.

The topic of [43] is the influence of the choice of viscosity matrix on the structure of solutions of the Riemann problem. The models investigated have homogeneous quadratic

flux functions and constant viscosity matrices. Such models arise in the study of three-phase flow in petroleum reservoirs. As is important in applications like this one, the viscosity matrix is not restricted to be a multiple of the identity matrix. We derived a necessary and sufficient condition for the presence of transitional shock waves. Using this condition we constructed a full description of the regions in the wave manifold that correspond to transitional shock waves. Moreover, we found the boundaries in the space of model parameters that separate models with differing numbers of transitional regions and thereby classified quadratic models according to the structure of Riemann solutions.

Uncertainty Quantification. The purpose of this project is to assess and quantify the uncertainty of predictions made with simulation codes. As the codes are being used to make operational decisions, and as the degree of experimental testing is diminished, the verification and validation (V&V) of simulation codes becomes of increasing importance. Quantification of uncertainty is a key component of the whole V&V effort. In this study, we found that the interplay between the forward and inverse problems, with Bayesian analysis to include the added information of experiments was important. Also the study of probabilistic error models for solution errors is important. Following this lead, we have begun a study of solution errors [24, 22]. Application to LANL programmatic problems are given in [1].

Photonics. This is a new project, conducted in collaboration with C. Bowden of Redstone Arsenal, and a group of his collaborators. We have developed a parallelized FDTD code to allow simulations in complex 3D geometries for photonic crystals and other photonic devices [40]. We will build on our prior experience in parallel software development, in construction of low cost parallel hardware, and in geometrically adaptive mesh methods for complex interfaces.

Our program is specially designed to study finite photonic devices with three-dimensionally heterogeneous dielectrics. The changes in the dielectric function occur on the scale of the electromagnetic wavelength and the contrast between the dielectric constants is large. We consider applications to finite devices for frequency doublers and high quality cavities for VCSEL lasers. The code will be used to simulate application specific device geometries to resolve design issues. We will work with experimental groups to model the devices and optimize the parameter values. We will develop computational tools capable of handling the complicated geometry of real-world applications.

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