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**MULTISCALE THEORIES AND
DUAL USE APPLICATIONS**

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PUBICATIONS AND TECHNICAL REPORTS

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REPORT OF INVENTIONS

No inventions were produced by the researchers during the twelve month period of this report.

BRIEF OUTLINE OF RESEARCH FINDINGS

During the last three years the major emphasis of our work was on theory and computation of fluid interfaces and stochastic flow problems. The interfaces may become unstable and this is a case of interest in much of our work. Since the instabilities lead to chaotic flow regimes for which a stochastic description is appropriate, these two topics for our work are in fact closely linked. Our point of view was explained in [24, 25].

Two Phase Flow and Fluid Instabilities.

Significant improvements in the stochastic modeling of unstable fluid mixing were achieved. A two-phase flow model for a planar constant acceleration mixing layer, described in the last report, was improved and extended to govern mixing under an arbitrary external acceleration [23, 20, 21, 22]. The physical assumptions underlying the new two-phase closures were identified and their consequences traced to physical features of the resulting two-phase flow. Analytical solutions for incompressible fluids were derived for arbitrary trajectories of the edges of the mixing layer. Thus these trajectories are necessary input to the two-phase flow model, which then predicts the variation of all dependent variables—the volume fraction, velocities, and pressures—along the mixing layer. Currently, the only available experimental data consists of volume fraction profiles measured at low density ratio, which indicate a linear variation in the volume fraction, in agreement with our model prediction.

The two edge trajectories are crucial components of a complete description of an evolving mixing layer, and remain poorly understood quantities. A potential breakthrough in this problem is the identification of an approximately universal property of mixing zone evolution under a smooth acceleration. The hypothesis of stationary mixing layer center of mass (COM) was applied to the case of constant acceleration [21, 22], leading to a prediction of the expansion ratio of the mixing layer (the ratio of the growth rates of the edges) as a function of density ratio, in good agreement with experimental data [41, 37] and improving on the predictions of other groups [12, 1]. This prediction in fact applies to self-similar mixing defined by a single

arbitrary length scale, not just to the t^2 behavior characteristic of constant acceleration mixing. Thus it is expected to be valid for smoothly varying acceleration profiles of the type considered in the experiments of Dimonte and Schneider [11], which give rise to approximately self-similar behavior. The stationary COM hypothesis, in flows where it is valid, effectively cuts the important edge trajectory problem in half by providing an explicit coupling between the two edges.

A more thorough study of the stationary COM hypothesis is reported in [7], where an explicit expression for the expansion ratio prediction described above is derived; the previous result was numerical. Further results described in this paper concern the close connection between the stationary COM and a weak notion of self-similarity. Specifically, it is shown that a COM stationary flow is exactly self-similar, within a first order perturbation expansion in powers of the deviation from exact self-similarity.

In conjunction with the theoretical work described above is a major effort to validate its predictions using highly resolved simulations of planar Rayleigh-Taylor (constant acceleration) and Richtmyer-Meshkov (impulsive) instability. Recent results, not yet published, demonstrate that accurate resolution of spike front evolution in two dimensions require far more mesh refinement than has been used in previous studies of this kind [12, 42, 2, 6]. Other aspects of the numerical solutions, such as loss of memory of initial data and convergence of average properties under ensemble averaging, are being studied.

An algorithm for the numerical solution of the one-dimensional compressible two phase flow equations, described in [7], was developed and is currently being used to understand the incompressible limit of the compressible flow. A modified version of this algorithm is being installed in the hydrodynamics code *FronTier* to simulate stochastic fluid mixing in multiple space dimensions. A version of the two phase flow equations that describe mixing in cylindrical and spherical geometry is being analyzed theoretically and numerically.

Elastic-Plastic Deformations. Our current work on elastic-plastic flow is based on a new formulation of the governing equations and a new approach to their computational modeling. This work has as its goal the improved numerical simulation of high strain-rate and large deformation flow problems, such as occur in penetration mechanics, tool cutting, punching, and other metal forming processes. The principle components of our approach are (a) a fully conservative, Eulerian formulation [35, 36, 18] with (b) material models based on a hyperelastic strain energy [13, 34], (c) Front Tracking [39, 30, 29], (d) improved physical modeling for rate-dependent plasticity [40], and (e) special modeling to allow tracking of shear bands [19]. This circle of ideas was discussed recently in [34], which emphasizes the physical principles underlying models of plastic flow of metals, the nature and validity of approximations involved, and the mathematical structure of the flow equations.

Recent and continuing work has focussed on the development of *FronTier-Solid*, a two-dimensional Front Tracking algorithm for solid mechanics, designed using the ideas just mentioned. A preliminary version of this code, described in [30, 29], was based on an approximate 2D Riemann solver constructed in a directionally unsplit manner to resolve the complex elastic-plastic wave structure. The Front Tracking method provides sharp resolution of interfaces in multi-material problems while eliminating spurious numerical diffusion and the need for mixed material cell constitutive models. Example problems, such as an impact problem, were presented as a test of the algorithm.

The *FronTier-Solid* code is currently undergoing further development and improvement. The focus of recent further development of this numerical algorithm has been constructing an exact Riemann solver at the material interface. We have taken advantage of the slip allowed at the interface to simplify the solver considerably. Shear waves can be treated linearly, and some of the boundary conditions at the interface can be solved explicitly. The resulting algorithm is closely modeled after the Godunov algorithm for gas dynamics and is therefore more efficient than previous Riemann solvers. This exact solver will increase the overall accuracy and reliability of the front tracking algorithm.

Currently, our code is used for two purposes. The first is to study impact and penetration problems, and the second is to study material microstructure. In the latter case, we are investigating Rayleigh-Taylor instability in metal plates accelerated by a high pressure gradient, following earlier ARO supported work of our collaborators.

The paper "Instability of Accelerated Elastic Metal Plates," by B. Plohr and D. Sharp, was completed and accepted for publication in *Zeitschrift für angewandte Mathematik und Physik*. When subjected to rapid acceleration, a metal plate that is not perfectly flat displays a type of Rayleigh-Taylor instability, which is affected by shear strength. The initial stage of this instability was investigated, assuming that the deviation from flatness is small and the pressure producing the acceleration is moderate. Under these assumptions,

the plate can be modeled as elastic and incompressible, and the linearized form of the governing are valid. A linear initial/boundary-value problem was derived to model the flow and obtain analytical formulae for the solutions. Solutions exhibit vorticity inside the plate, an important feature caused by shear strength that was omitted in previous solutions. The theoretical relationship between the acceleration and the critical perturbation wave length, beyond which the flow is unstable, agrees quantitatively with results of numerical simulations and a recent experiment.

Front Tracking Algorithm Development We have achieved major progress with technology transfer and proof of principle for Front Tracking. Grove is leading an effort to combine the Front Tracking code FrontTier with RAGE, an important developing code at Los Alamos National Laboratory. Since production codes developed at National Laboratories are a major source of codes for use by ARL and other Army facilities, this development brings Front Tracking much closer to use by Army scientists. Major progress was achieved in extending the front tracking code to three dimensions [15]. See also [14, 3]. Current work is to handle the interaction of material surfaces. Since other workers have had trouble with this algorithm, we explained in more detail the methods used in two dimensional interactions and the key factors contributing to our success [26].

Flow In Porous Media. The renormalization, or scale up methods introduced flow above were applied to flow in porous media. We showed [16] that renormalization of nonlinear flow requires typically a renormalization of the hyperbolic terms, rather than the dispersive terms in the flow equations. Key variables identified as influencing the renormalization included the mobility ratio, and the length scales, strength, and anisotropy of the geological heterogeneity. We also studied single mode instability growth [28].

Theory of conservation laws. A long standing problem in the theory of conservation laws was settled [5, 4] by proving the existence of radially symmetric solutions in an infinite domain for compressible gas dynamics. The proof was based on compensated compactness. The difficulty, successfully overcome in this work, is the possible presence of infinitely many waves (due to reflections and wave interactions) incoming from $r = \infty$.

Resin Transfer Molding New models for the transport of microbubbles were proposed for the Resin Transfer Molding (RTM) process for the manufacture of composite materials [8, 9, 10, 38], based on analogies to porous media equations.

Hamilton-Jacobi Equations In many applications (for instance etching and deposition processes) the motion of material boundaries is described by a Hamilton-Jacobi equation. The stability or bifurcation of sharp features, edges and corners, in such boundaries is of great interest. Their evolution is described by a reduced Hamilton-Jacobi equation with boundary conditions at infinity, a Riemann solution. Based on the theoretical study [17] of multi-dimensional Riemann problems reported, we developed a three dimensional Front Tracking algorithm for this problem [27].

The actual construction of such Riemann solutions, can be extremely difficult. A simple picture for the construction the Riemann solutions of Hamilton-Jacobi equations is that data is propagated inward from infinity in the hyperbolic region until the characteristics terminate upon reaching a domain where characteristics are not defined, the parabolic set of the equation. A theoretical analysis [32, 33, 31] shows that this picture is too simple. The characteristics may run into a generalized periodic orbit, composed of multiple one-sided sonic shock waves, completely in the interior of the hyperbolic region. On the inner (sonic) edge of these shocks, hyperbolic characteristics leave to define a portion of the hyperbolic set not directly "visible" via characteristics from infinity.

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