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FINAL REPORT

Multiscale Stochastic Simulation and Modeling

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1 Findings and Significance

We emphasize results from recent years.

Acceleration driven instabilities of fluid mixing layers include the classical cases of Rayleigh-Taylor (RT) instability, driven by a steady acceleration and Richtmyer-Meshkov (RM) instability, driven by an impulsive acceleration. References to this subject, which has attracted a high level of interest over many decades, include [12, 128]; more recent references can be traced from the series [32] and earlier volumes in this series.

Our program starts with high resolution methods of numerical simulation of two (or more) distinct fluids, continues with analytic analysis of these solutions, and the derivation of averaged equations. A striking achievement has been the systematic agreement we obtained between simulation and experiment by using a high resolution numerical method and improved physical modeling, with surface tension. Our study is accompanied by analysis using stochastic modeling and averaged equations for the multiphase problem. We have quantified the error and uncertainty using statistical modeling methods.

1.1 Advanced Numerical Methods

The front tracking method provides the high resolution we require. It has been our major tool for large scale computation. This method has was proved in comparison [43] to be superior to other interface methods such as the level set method and the volume of fluid method.

1.1.1 Local Grid Based Tracking

In grid free tracking, the tracked front is a triangulated surface, propagating freely through a rectangular volume filling mesh. In grid based tracking, the front is regularized, or reconstructed, at each time step. After propagation, the points of intersection of the front with all grid cell edges are determined. Assuming at most one such intersection for each grid cell edge, the complete interface is reconstructed in a simple manner from these intersections.

Grid based tracking is very robust. (It is similar to the level set in this sense, the presentation of the interface in both methods being derived from computer science graphics routines). However, grid based tracking is inaccurate, as is the level set method. Grid based tracking, the level set, and untracked simulations, which also determine an interface from grid based information, all have a form of interface smoothing which resembles surface tension.

Local grid based tracking [43] combines the two tracking algorithms, preserving the advantages of each. This algorithm relies on the more accurate grid free tracking unless there is a bifurcation. The algorithm is robust as the problems with the grid free propagation occur only with bifurcations of the interface. When a bifurcation occurs, a small box is constructed around it. Grid based propagation is used inside the box. The grid free surface triangulation near the box has to be rejoined to the reconstructed grid inside the box in a construction which also has a grid based flavor. The result is favorable: the accuracy of grid free tracking and the robustness of grid based tracking are both preserved.

We carried out a systematic study [43] of this new algorithm in comparison to other interface methods (level sets, volume of fluids), and found that locally grid based front tracking is the best of all methods tested.

1.1.2 Improved Physical Models

Front Tracking offers a very convenient framework to support surface based physics. Normal vectors and curvature tensors are supported by the code. Surface tension forces a pressure jump at the interface proportional to the surface curvature. In the front tracking algorithm, it introduces a modification to the Riemann solver, used in the normal propagation of the front.

To compute with physical mass diffusion, we first eliminate numerical mass diffusion, with the use of Front Tracking. The second step is to add limited amounts of mass diffusion back into the calculation, on the basis of prescribed values for the physical mass diffusion constant. Our algorithm computes the required diffusion per time step with the use of the analytic solution of the diffusion equation.

1.1.3 FronTier-Lite

We have extracted the purely geometrical (physics independent) parts of the front tracking code. This code is modular and can be called as an external library in other codes. It is released for public distribution. We have built a user-friendly interface for the interaction of the front tracking library with other scientific code with the dynamic interface as part of its scientific description. This library package can be accessed through the internet at the site:

`http://www.ams.sunysb.edu/FTdownload`

1.1.4 Simulation of Rayleigh-Taylor Instability

A signal success of our program has been the simulation of 3D Rayleigh-Taylor instability with results in agreement with experiment. Our improved front tracking method was combined with improved accuracy of physical

Experiment Simulation	Comment	α
Five experiments	Immiscible [124, 129]	0.060–0.073
FronTier	Immiscible [55]	0.062
TVD	Ideal Untracked [53]	0.035
FronTier	Ideal	0.09

Table 1: Mixing rates compared: FronTier simulation compared to experiment and contrasted to untracked (TVD) and ideal fluid FronTier simulations.

modeling for this purpose [55]. We compare simulation and experiment in terms of the growth rate of the bubble side of the mixing layer, defined by the dimensionless constant α in the equation

$$h = \alpha A g t^2 \tag{1}$$

for the bubble (light fluid) penetration h in terms of the Atwood number A, gravity g and time t. The values of $\alpha = \alpha_b$ are given in Table 1. Other statistical measures of the mixing rate (such as the bubble width) were also recorded and also agree with experiment.

1.2 Applied Mathematical Modeling

We derived the two-phase flow equations by averaging the microscopic dynamics. Let the function X_k be the phase indicator for material k ($k = 1, 2$); *i.e.*, $X_k(t, \mathbf{x})$ equals 1 if position $\mathbf{x}$ is in fluid k at time t, zero otherwise. We average the advection law [42] for X_k,

$$\frac{\partial X_k}{\partial t} + v_{\rm int} \cdot \nabla X_k = 0\ . \tag{2}$$

Here $v_{\rm int}$ is the microphysical velocity evaluated at the interface (the velocity component normal to the boundary ∂X_k is continuous so that $v_{\rm int}\dot{\nabla} X_k$ is well defined). We also average the microscopic conservation equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0 \ , \tag{3}$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \rho \mathbf{v}\mathbf{v} = -\nabla p + \rho g \ , \tag{4}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \rho \mathbf{v} E = -\nabla \cdot p \mathbf{v} + \rho \mathbf{v} g \ . \tag{5}$$

Here the dependent variables $\mathbf{v}$, ρ, p, g, and E denote, respectively, the velocity, density, pressure, gravity and total energy with $E = e + \mathbf{v}^2/2$ and e the internal energy.

We denoted the ensemble average $\langle \cdot \rangle$. The average $\langle X_k \rangle$ of the indicator function X_k is denoted β_k. The quantities ρ_k and p_k are, respectively, phase averages of the density ρ and pressure p while the quantities v_k and E_k are phase mass-weighted averages of the fluid z-velocity v_z and total energy E:

$$\rho_k = \frac{\langle X_k \rho \rangle}{\langle X_k \rangle} \ , \quad p_k = \frac{\langle X_k p \rangle}{\langle X_k \rangle} \ , \quad v_k = \frac{\langle X_k \rho v_z \rangle}{\langle X_k \rho \rangle} \ , \quad E_k = \frac{\langle X_k \rho E \rangle}{\langle X_k \rho \rangle} \ . \tag{6}$$

Applying the ensemble average to Eqs. (2)-(5), we obtain the one-dimensional two-pressure two-phase flow averaged equations. We follow [42, 15, 19, 125] to obtain

$$\frac{\partial \beta_k}{\partial t} + \langle \mathbf{v} \cdot \nabla X_k \rangle = 0 \ , \tag{7}$$

$$\frac{\partial \beta_k \rho_k}{\partial t} + \frac{\partial \beta_k \rho_k v_k}{\partial z} = 0 \ , \tag{8}$$

$$\frac{\partial \beta_k \rho_k v_k}{\partial t} + \frac{\partial \beta_k \rho_k v_k^2}{\partial z} + \frac{\partial (\beta_k p_k)}{\partial z} = \left\langle p \frac{\partial X_k}{\partial z} \right\rangle + \beta_k \rho_k g \ , \tag{9}$$

$$\frac{\partial \beta_k \rho_k E_k}{\partial t} + \frac{\partial [\beta_k v_k (\rho_k E_k + p_k)]}{\partial z} = \langle p \mathbf{v} \cdot \nabla X_k \rangle + \beta_k \rho_k v_k g \ . \tag{10}$$

In [79] the interface velocity v^*, where $v^* \partial \beta_k / \partial z =< v \cdot X_k >$, has been derived exactly from (7) and (8) independently of any closure assumption.

Theorem The interface quantity v^* has the exact formula

$$v^* = \frac{\beta_1 \left[\frac{\partial v_1}{\partial z} + \frac{D_1\rho_1}{\rho_1 Dt}\right] v_2 + \beta_2 \left[\frac{\partial v_2}{\partial z} + \frac{D_2\rho_2}{\rho_2 Dt}\right] v_1}{\beta_1 \left[\frac{\partial v_1}{\partial z} + \frac{D_1\rho_1}{\rho_1 Dt}\right] + \beta_2 \left[\frac{\partial v_2}{\partial z} + \frac{D_2\rho_2}{\rho_2 Dt}\right]} \equiv \mu_1^v v_2 + \mu_2^v v_1 \ , \qquad (11)$$

$$\mu_k^v = \frac{\beta_k}{\beta_k + d_k^v \beta_{k'}} \ , \quad d_k^v(z,t) = \left[\frac{\partial v_{k'}}{\partial z} + \frac{D_{k'}\rho_k{}'}{\rho_{k'} Dt}\right] / \left[\frac{\partial v_k}{\partial z} + \frac{D_k\rho_k}{\rho_k Dt}\right] \ . \qquad (12)$$

The factor $d_k^v(z,t)$ in (12) is a ratio of logarithmic rates of volume creation for the two phases. A closure condition of spatial homogeneity assumes

$$d_k^v(t) = \left[\int_{Z_k}^{Z_{k'}} \frac{\partial v_{k'}}{\partial z} + \frac{D_{k'\rho_k{}'}}{\rho_{k'} Dt}\, dz\right] / \left[\int_{Z_k}^{Z_{k'}} \frac{\partial v_k}{\partial z} + \frac{D_k\rho_k}{\rho_k Dt}\, dz\right] \ . \qquad (13)$$

The identity (13) states that the relative extent of volume creation for the two fluid species is independent of the spatial location in the mixing zone. In the incompressible case, this is seen clearly from the closed form solution

$$d_k^v(t) = \left|\frac{V_{k'}}{V_k}\right| \ . \qquad (14)$$

The p^* closure is presented in [79] following related ideas. Closed form incompressible solutions are given in [104], with extensions to an arbitrary number n of fluid layers in [26].

1.3 Stochastic Methods to Quantify Uncertainty

The need for computer assisted decision making is driven by two related factors. The first is the importance of complex scientific/technical decisions, such as those related to global warming, for which controlled experiments are not feasible. The second is the need for rapid or timely decisions, using incomplete information, such as in shortening the time to market of a product design cycle, mandating a reduction of the role of the human in the loop.

The central issue considered here is an accurate assessment of errors in numerical simulations [77]. Uncertainty quantification (UQ) can be viewed as the process of adding error bars to a simulation prediction. The error bars refer to all sources of uncertainty in the prediction, including data, physics and numerical modeling error. The requirement for UQ comes from the increasing use of simulation model based predictions to guide decision making. In this sense, the need for UQ is a natural consequence of simulation's attainment of a status parallel to that of experiment and theory. Our approach to uncertainty quantification uses a Bayesian framework. Specifically the Bayesian likelihood is (up to normalization) a probability, which specifies the probability of occurrence of an error of any given size. Our approach is to use solution error models as defining one contribution to this likelihood. We provide a scientific basis for the probabilities associated with numerical solution errors.

We have studied UQ for petroleum reservoir modeling [78, 113] and for shock physics simulations [119, 63, 64], with a focus on statistical analysis of errors in numerical solutions.

For chaotic interfacial mixing, the central UQ problem is to define the solution errors for chaotic flow regimes, since the chaotic simulations do not converge in a pointwise sense, but rather add new complexity with each new level of mesh refinement. See, for example Fig. 1. The solution is to look for convergence in averaged quantities, *i.e.*, the statistical moments, and the averages which define them.

The fine scale raw data is averaged, producing coarser data, which is subject to the normal tests of convergence and order of convergence studies, and which may satisfy its own averaged equations. Thus the problem is very much akin to turbulence modeling, which achieves repeatability only by

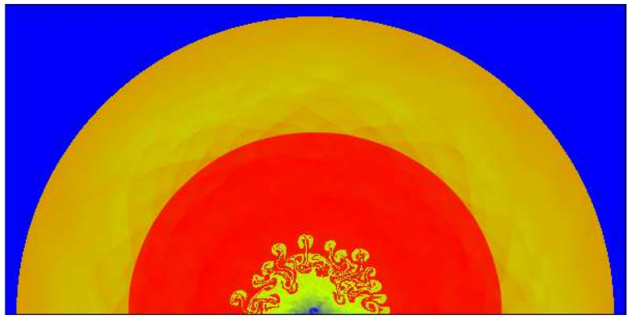

Figure 1: Density plot for a spherical implosion simulation with a perturbed interface. The outer orange-blue boundary is the edge of the computational domain. The red-orange circular boundary is an outgoing reflected shock and the chaotic inner interface is the object of study. The grid size is 800×1600.

use of averaged quantities or statistical descriptions of fluctuating quantities. Intrinsic variation, of importance in this study, is analyzed as statistical fluctuations, and these converge not pointwise, but in their statistical character, *i.e.* their means, variance and possible higher moments. See [138, 47]. The main conclusion of [138] is that convergence is very spotty, and depends on how it is defined. Different behavior is observed in the singly and doubly shocked material, in the single and the mixed phase material, and in the region near the origin, where circular waves give rise to transient singular pressures at the origin. In some cases, ensemble averages, spatial averages, and extremely fine meshes are needed to observe convergence, which may be as low as half order or marginal in Δx.

1.4 Publications Resulting from DOE Support

The publications (listed in the references section), supported from the completed grant were:

- 1991: [6, 33, 51, 58, 57, 62, 90, 97, 105, 109, 111]

- 1992: [16, 34, 36, 50, 52, 91, 94, 95, 139]
- 1993: [11, 17, 37, 39, 59, 96, 98, 115, 134]
- 1994: [5]
- 1995: [3, 28, 29, 60, 135]
- 1996: [10, 14, 13, 18, 61, 69, 99, 100, 121, 122, 130];
- 1997: [8, 30, 31, 84, 101, 106, 117]
- 1998: [4, 67, 82, 103, 102, 107, 142]
- 1999: [22, 38, 70, 104, 108, 110, 133]
- 2000: [68, 71, 75, 114]
- 2001: [21, 23, 66, 74, 76, 79, 89, 118, 83, 132];
- 2002: [24, 25, 72, 40, 41, 56, 65, 87, 86, 113, 73, 85, 9];
- 2003: [1, 2, 20, 45, 46, 54, 77, 80, 88, 92, 113, 35, 120, 126, 131, 143];
- 2004: [47, 48, 63, 119, 81, 78, 93, 116];
- 2005: [26, 53, 64, 27, 112];
- In press and submitted: [7, 43, 44, 49, 55, 137, 138, 123, 127, 136, 138, 137, 140, 141].

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