ANNUAL PROGRESS REPORT

January 1993

The Modeling of Complex Continua:
Fundamental Obstacles and Grand Challenges

Grant #DE-FG02-90ER25084

Applied Mathematics Subprogram
Office of Basic Energy Research
Department of Energy

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.
## Contents

1 Scientific Results
   1.1 Discontinuities and Adaptive Computation .......................... 1
   1.2 Chaotic Flows .................................................................... 3
   1.3 Dispersion of Flow in Porous Media ................................... 8
   1.4 Nonlinear Waves and Nonlinear Materials ............................ 12

2 Publications ........................................................................ 15
1 Scientific Results

Our research program has emphasized innovative computation and theory. The computation and theory support and enhance each other. Our approach depends upon abstracting mathematical concepts and computational methods from individual applications to a wide range of problems involving complex continua. The generic difficulties in the modeling of continua that guide this abstraction are

- multiple length and time scales, often involving sharply defined internal layers or boundaries [14,15],
- microstructures such as bubbles [24], droplets, vortices and crystal defects,
- chaotic or random phenomena described by a statistical formulation [15,16].

The merit of this scientific approach is discussed in [13,14].

1.1 Discontinuities and Adaptive Computation

Our main results are (a) parallelization, (b) three dimensional tracked computations (in progress) and (c) complex wave interactions well resolved on a coarse grid.

A. Parallelization. The parallelization of the purely hyperbolic component of the two-dimensional front tracking code has been fully implemented on the INTEL iPSC/860 hypercube, enabling the parallel computation of gas dynamics problems. This parallelization was achieved by domain decomposition [6,7,8,9]. The spatial domain is divided into a union of disjoint rectangular subdomains, with the accompanying division of the tracked physical discontinuity curves among the subdomains. An extended boundary region of \( n \) (typically 2) mesh blocks in each direction surrounds each subdomain providing, overlap into neighboring subdomains. Thus, the boundary region for mesh block \( i, j \) lies entirely in the eight mesh blocks surrounding it (neglecting the slight complication of physical boundaries). In Figure 1, we show a typical interface for a complex fluid mixing process, decomposed into 16 subdomains, with the overlapping boundaries displayed as well.

The tracking algorithm progresses iteratively as:

1. Each subdomain updates those boundary regions of neighboring subdomains that lie inside its own area. (A subdomain never updates its own boundary region, which lies entirely within neighboring subdomains.)
Figure 1: A typical interface at late time on a two-dimensional 320 x 300 mesh is decomposed into 16 subinterfaces. The narrow vertical strips shown here are the overlapping border domains shared by neighboring processors.
2. The discontinuities are propagated and solution obtained for the next time step solely within each subdomain, using boundary data from its boundary region, which is stored in local memory.

This scatter–gather type of algorithm is most efficient if all subdomains are equally busy during step 2. This requires a sub-domain assignment algorithm which will produce subdomains, not of equal measure in spatial volume, but of equal measure in propagation/solution update work. At present, a rather simple sub-domain assignment is in place. Current gas dynamics calculations have shown the parallelized code to be running at an efficiency of approximately 90%. The scientific power can be seen from the observation that the full parameter study [4] from which Figure 1 is extracted would have taken an estimated 17 years to complete on a SUN Sparcstation 1.

B. Three Dimensional Computations. Of critical physical interest is the ability to do computations in three spatial dimensions. We are well advanced in this development for the front tracking code. Algorithms for triangulating surfaces in three dimensions and for re-gridding dynamical points of the surfaces have been implemented. A preliminary algorithm for generating volume filling grids which match moderately complicated surfaces was constructed but further work in this area is required. Additionally, data structures and code changes to handle arbitrary (spatial) dimensionality have been implemented into the front tracking code to support calculations in 1-, 2- and 3-dimensions.

C. Complex Wave Interactions. Reported in [17] is a study of the impulsive acceleration using a random interface by a planar shock wave. Here the full power of front tracking allows a high level of resolution for the shock–contact diffraction patterns on a relatively coarse grid. In Figure 2, we show the passage of a shock wave through a random interface, with three levels of graphical enlargement. Note that the detail of wave interaction resolved with front tracking in one or two grid blocks might take close to one hundred grid blocks for comparable resolution by other methods. The success of the unique capability indicated in Figure 2 depends upon an explicit use in the solution algorithm of analytic knowledge derived from shock polars.

1.2 Chaotic Flows

Our results provide a growing body of knowledge for the Rayleigh-Taylor mixing layer, with agreement among theory, experiment and direct simulation for nearly incompressible flows. From computation, we discovered surprising new phenomena for compressible flows, in the form of a substantially increased growth rate of the mixing layer, and a loss of the universality which characterized the
Figure 2: The passage of a shock wave through a random interface separating two gases of differing densities. The computation is shown together with two levels of graphical enlargement. In the finest enlargement, one can see complex wave diffraction patterns resolved down to the level of a single mesh block, displaying a unique capability of front tracking. The long time behavior of this solution (not shown here) exhibits interface instability similar to that of Figure 1.
The mixing process is characterized by a penetration height $h(t)$, which measures the distance of the most advanced bubble from the position of the unperturbed interface. This height obeys a scaling law $h = \alpha Ag t^2$. The Atwood number $A$ is a buoyancy renormalization of the gravity $g$, and reflects a dimensionless density jump across the interface. The incompressible experiments of Read and Youngs found the growth constant, $\alpha$, to be a universal value $\alpha = 0.06$. We found agreement with this experimental growth rate in our nearly incompressible computations [19] and [20], but for even moderately compressible fluids, the mixing rate $\alpha$ may exceed twice the incompressible value. In addition, some loss of universality was observed through dependence of the growth rate on details of specification of the ensemble of initial conditions [3,4]. The dependence of the growth rate $\alpha$ on dimensionless compressibility, $M^2$, is shown in Figure 3.

In [24,26,33], a statistical, chaotic theory of the Rayleigh-Taylor mixing layer is given in terms of a renormalization group fixed point model. The renormalization group approach is used since the chaotic mixing layer involves dynamically changing length scales. The model is validated by comparing the predicted growth rate of the mixing layer with experiments and numerical computations [30]. The three main ingredients of this fixed point analysis are

1. a superposition hypothesis to specify the bubble – bubble interaction dynamics,
2. a theory of single bubble dynamics,

3. a statistical model to incorporate the above solutions to the one and two body problems for the bubble dynamics.

The superposition hypothesis was given in [19] and [20]. It describes the motion of the outer envelope in the Rayleigh-Taylor mixing layer as a superposition of individual bubble velocities and an envelope velocity. The superposition theory explains the phenomenon that the velocity of a more advanced bubble in a multi-bubble system exceeds the velocity of a bubble of the same size in a periodic or single bubble system. This theory also explains the fact that a less advanced bubble in a multi-bubble system changes its direction of movement at the end of its period of interaction with a more advanced neighboring bubble. The superposition hypothesis has the virtue of containing no free parameters. The predictions of the superposition hypothesis were confirmed, to within the accuracy of the experiments, for the incompressible case by analysis of the experiments of Read. Comparison with numerical computations for compressible fluids shows agreement with the superposition hypothesis for small compressibility values, but reveals disagreement for larger values of compressibility, outside the range covered by experiments. An explanation for the disagreement and a possible basis for modification of the superposition hypothesis is given in terms of density stratification of the fluids. Disagreement is also noted in cases where bubble splitting occurs, presumably due to omission of high frequency bubble splitting modes in the envelope description. Unexplained disagreement for computations at small Atwood number is also noted.

The superposition theory depends critically on a good description of the single (periodic) bubble dynamics. An extension of a previous theory for the growth of a single bubble with periodic boundary conditions, from a three parameter ODE to a four parameter ODE, was presented to remove an earlier ansatz which lacked physical basis. Two of the four parameters of the new theory are determined explicitly. The remaining two must be determined through numerical simulation of the single bubble problem. Such a determination, over a limited range of the independent variables (Atwood number $A$ and dimensionless compressibility $M^2$), was presented [20].

The statistical model on which the renormalization group fixed point is based describes an ensemble of bubbles of the same radius, whose heights are defined by a uniform probability measure restricted to a bounded interval. The statistical dynamics of flow with bubble merger is developed by treating pairwise interactions between adjacent bubbles drawn randomly from the ensemble. The dynamics of each pairwise merger is given by the superposition hypothesis [19]. Before merger, each bubble moves with a velocity given as the sum of a scaled single-bubble velocity, as treated
in [20], and an envelope velocity. At the end of a merger, the bubble of greater height doubles in size and the lower bubble is removed from the statistical ensemble. Differential equations are then obtained for the common radius, average height and variance of height of the ensemble of bubbles as a function of time. The variance of height is shown to have a natural interval in scaled variables. Its lower limit is a trivial fixed point corresponding to an (unstable) interface consisting of bubbles of identical height. Its upper endpoint is defined by instantaneous merger for bubble pairs of extreme separation. By studying the behavior of the rate of change of variance with time at these two endpoints, the existence of a non-trivial fixed point is shown.

An extensive body of experiment and computation predicts a constant acceleration for the leading edge of this mixing region, consistent with the conclusions of the fixed point predicted by this theory. The upper and lower limits placed on the value of the fixed point in this theory, are shown to yield upper and lower limits for this constant acceleration that are in full agreement with experiments and computations on incompressible and nearly incompressible systems. Further studies of the theory, including prediction of transient behavior, dependence on density ratio and compressibility, assumptions on uniform bubble radius, and extension to three dimensions remain to be carried out.

We are now studying the interior of the mixing zone itself, using computational data from well resolved direct simulation. Statistical analysis of fluctuating quantities reveals structure which is more complex than simple diffusion [3,4]. In particular, steady acceleration (Rayleigh–Taylor unstable) induced mixing of a randomly perturbed interface shows non-monotone density contours and interior structure in second order correlations of fluctuating quantities. This is consistent with theories of turbulent boundary layers, which show at least three distinct regions within the mixing layer. In a statistical study, moments of the fluctuating portion (i.e., with mean values subtracted) of the velocity and density fields, such as the Reynolds stress tensor, were tested for scaling behavior. The purpose of this study was to determine whether universality and scaling indicative of a renormalization group fixed point would hold. The conclusion was that this behavior holds only in a very limited domain of the problem parameter space. Specifically, scaling of the moments of the fluctuating fluid quantities holds only when two following conditions are both satisfied: when the analysis is restricted to the region of the flow near the edge of the mixing zone and when the flow parameters are nearly incompressible [3,4]. This fact suggests that the renormalization group fixed point is not a generic property within the space of RT problem parameters.
1.3 Dispersion of Flow in Porous Media

A substantial new theory of the proposers for anomalous dispersion has attained a fairly definitive state. This theory gives consistent answers in low order perturbation theory, and in renormalized perturbation theory, both in the Lagrangian and Eulerian pictures. It provides a conceptual framework which explains the scale dependence of macrodispersion both qualitatively and quantitatively. It has been checked numerically and seems to be valid for moderately large strengths of heterogeneity. It is consistent with observed field data. This theory was motivated by applications to petroleum reservoir engineering and to environmental remediation and restoration.

We formulated [10,25] a statistical model for the permeability field in a porous medium which accounts for spatial correlation via a two-point correlation function of the form

\[ \langle \xi(\vec{x})\xi(\vec{y}) \rangle = O(|\vec{x} - \vec{y}|^{-\beta}), \quad \beta > 0. \]

The model was applied to the effective mixing (fluid entrainment) zone that develops in tracer flow. At the level of lowest order perturbation theory, the model predicts a zone width which, in the long distance regime, grows as

\[ l(t) = O(t^\alpha), \quad \alpha = \max \{1/2, 1 - \beta/2\}. \]

From this formula, three qualitatively distinct regimes can be identified [23]. For \( \beta > 1 \), the dispersion is Fickian, and the macrodispersion integral of §1.2.2.A is finite. This case is called infrared finite. For \( 0 < \beta < 1 \), the dispersion is anomalous but infrared super-renormalizable, in the sense that the divergent contributions to the diffusion term in the perturbation expansion are finite in number and strongest at lowest order. This is the case which appears to be consistent with field data, when considered over multiple length scales. Finally, we consider the case \( \beta < 0 \), excluded above, which requires proper reformulation in Fourier space to achieve a positive definite distribution. This case corresponds to trends, and is infrared nonrenormalizable. Scaling laws derived in this case are either identically infinite, restricted to intermediate or transient length scales, or intrinsically dependent on long distance cutoffs. This tricotomy and its qualitative implications appear to be new.

One practical use of this scaling analysis will be in conditional simulation, in which incomplete geological data serve to restrict the ensemble from which the random geologies are drawn. See [22]. A second practical use of the scaling analysis will be to guide the acquisition of data by emphasizing the value of data containing multiple length scales.
In order to account for the important case of large heterogeneity strengths, Zhang [32] extended the second order scaling theory to the level of Corrsin's hypothesis, i.e., renormalized perturbation theory truncated at second order. At this level, an exact determination of scaling behavior was obtained for both the Lagrangian and Eulerian pictures, and agreement with the above scaling laws was obtained. These results are in contrast to the case of turbulence modeling, for which scaling laws in these various approximations do not coincide.

We have given [10,11,12,21,28] numerical verification of this theoretical result, and confirmed the prediction of the critical value $\beta_{cr} = 1$ above which the growth is Fickian and below which the growth is non-Fickian.

Typical computational solutions for passive transport through a random media are shown in Figure 4. The four plots represent calculations through permeability realizations constructed with self-similar exponents of, from left to right, $\beta = 0.5$, $\beta = 0.75$, $\beta = 1.0$ (upper), and $\beta = 1.25$ (lower). The colors indicate strength of the random permeability field, red indicating regions of high permeability, and blue low. Superimposed on each plot are the mixing fronts (dark lines) computed at several time values. The plots are shown with the correct relative spatial scaling.

Pure scaling theories are too simple to describe realistic geology. We therefore allow the scaling exponent $\beta$, which characterizes the geology, to depend on $r$, and obtain a much more flexible and general theory. Zhang [31] has produced an extension of the theoretical analysis, characterizing macrodispersivity scaling for a permeability field two-point correlation function with a distance dependent power law

$$\langle \xi(\vec{x})\xi(\vec{y}) \rangle = O(r^{-\beta(r)}), \quad \beta(r) > 0 \quad r \equiv |\vec{x} - \vec{y}|,$$

Again, the model has been applied theoretically to the growth of the effective mixing zone in tracer flow. An interesting result of this analysis concerns the fluid mixing behavior over a finite range of length scales, over which $\beta(r)$ is slowly varying. Zhang has shown that the behavior over such a range of length scales is determined by two competing effects, the decay of the integrated behavior of $\beta(r)$ from all shorter length scales, and the decay behavior over the indicated length range. Our numerical experience suggests that transient (i.e., nonconstant $\beta$) deviations from pure scaling behavior will be important in practical applications.

Zhang and Glimm [34] have obtained the exact inertial range (independent of cutoff parameters) scaling exponent for the case of laminar shear flow (independent layers). The analysis shows that this cutoff independent scaling rate is infinite for infrared nonrenormalizable heterogeneity correlation laws, implying a growth rate for $l(t)$ which is faster than a power law. A one–parameter family of
Figure 4: (Color plate, following page) Four computational solutions for passive transport through random media characterized from left to right by self-similar exponents of $\beta = 0.5$, $\beta = 0.75$, $\beta = 1.0$ (upper), and $\beta = 1.25$ (lower). Color indicates relative strength of permeability, with red high, and blue low. Superimposed on each plot are the mixing fronts (dark lines) computed at several time values.
cutoff dependent scaling laws is also obtained from the analysis.

The numerical generation of permeability field realizations for this work has relied significantly on the 128-processor INTEL iPSC/860 hypercube at Oak Ridge National Laboratory and a 32-processor INTEL iPSC/860 hypercube at Stony Brook.

The increasing use of reliability analysis to guide decision making in environmental remediation efforts and in reservoir engineering has prompted [5] a careful look at the joint probability distributions between porosity and permeability that are assumed in the reliability analysis models. It is demonstrated that an uncritical choice of the porosity-permeability joint probability distribution density can lead to unphysical results and incorrect predictions. Our work also contains an analysis of reliability predictions based upon experimentally determined joint probability distributions.

Work on the transition from laminar to slug flow in Hele-Shaw cell stream-tube flow is continuing. A theory had been previously developed [18] in terms of a dimensionless order parameter to characterize the variation in flow pattern from laminar to a chaotic regime of random (in time) pinch-off. It was found necessary to upgrade the numerical calculations with the inclusion of physical surface tension effects and a more accurate velocity field. Both upgrades have been completed, with the velocity and pressure fields being calculated using Raviart–Thomas mixed finite elements, resulting in a numerically divergence-free velocity field. The numerical simulations are currently being rerun to confirm the predictions of the theory.

1.4 Nonlinear Waves and Nonlinear Materials

Isaacson et al. [27] have produced a very important unifying framework for the fundamental waves occurring in general systems of \( n \) conservation laws. By using a local change of coordinates, the Rankine-Hugoniot relation is shown to take the form \( R \cdot F = 0 \), where \( R \) measures the strength of the discontinuity. The trivial solution set \( R = 0 \) can be eliminated, thereby obtaining a smooth manifold \( W \) of dimension \( n + 1 \), defined by \( F = 0 \), that is the closure of the set of shock points. The manifold \( W \) is termed the fundamental wave manifold. Significantly, both rarefaction and shock waves are represented within \( W \), in accordance with the heuristic idea that shocks of infinitesimal strength are infinitesimal rarefaction fans. The rarefaction points form an \( n \)-dimensional submanifold \( C \) of \( W \), the characteristic manifold. The geometry of \( C \) reflects the behavior of wave speeds for the conservation laws; for instance, the natural projection of \( C \) onto state space has a fold at a point where wave speeds coincide. The familiar rarefaction curves in state space for the system of conservation laws are projections of a single family of curves in \( C \) forming a one-dimensional foliation of \( C \). Correspondingly, the manifold \( W \) is foliated by two families of curves, called shock curves, that
project onto the classical shock curves in state space. The wave manifold framework sheds light on two fundamental problems in the theory of conservation laws. The first is the physical admissibility of shock waves, as determined by properties of dynamical systems that are parameterized by the points of $\mathcal{W}$. The second problem is the bifurcation of wave curves, which corresponds to loss of transversality between one-dimensional foliations and the boundary of the region of admissible waves.

The wave manifold $\mathcal{W}$ contains both admissible and inadmissible shock waves. The most fundamental notion of admissibility presently known is the viscous profile criterion, which states that the shock wave must be the limit, as the viscosity tends to zero, of traveling waves for an associated viscous conservation law. This viscous conservation law gives rise to a dynamical system with critical points corresponding to the states on the left and right of the shock wave. In Refs. [1,2], some of the mathematical issues associated with loss of admissibility are studied. Of particular interest is the demonstration that Hopf bifurcation can be the mechanism which leads to loss of admissibility. Similarly, homoclinic orbits are associated with a loss of admissibility. In Figure 5 we see that the connecting orbit bifurcates when crossing the Hopf bifurcation locus, so that one end is connected to the limit cycle emerging from the Hopf bifurcation. The connection between the end states of the shock wave is thus broken, implying the inadmissibility of this shock wave.

The transitional waves are the most curious of the novel shock waves discovered in the recent renewal of interest in Riemann problems. These waves have dynamical system orbits which connect saddle points to saddle points, and thus they appear to be inherently unstable. However, they have been essential to obtain a satisfactory existence and uniqueness theory for solutions of Riemann problems. Stability analysis has been used in the search for a more satisfactory basis for accepting these waves as physically meaningful. In Ref. [35] nonlinear stability was established on a numerical level for these shock waves.

In our study of nonlinear materials, a new and fully conservative formulation of plasticity was discovered [29]. The equations describing elastoplastic flow form a quasilinear system, but it was not known how to write this system in conservative form. Such a conservative form is necessary for treating discontinuous solutions, such as arise in Riemann problems. The interest in conservative formulations has been sparked by the importance of conservative numerical schemes in the effective computational modeling of fluid flow. Indeed, for the closely related system of gas dynamics, experience has shown that it is valuable to use numerical schemes that obey discretized conservation principles. Based on the importance of the conservation formulation for computations, we expect the conservative formulation of plasticity to be fundamental.
Figure 5: Shown here is a two dimensional slice of the wave manifold $\mathcal{W}$ for a representative $2 \times 2$ system of conservation laws with an elliptic region. The figure shows the influence of Hopf bifurcation on the admissibility of shock waves, when the viscous admissibility criterion is taken into account. The connecting orbit, oriented from $U_-$ to $U_+,$ represents a traveling wave between these two states, i.e., a viscous-admissible shock wave. The figure shows a “bubble” region in which the connection between $U_-$ and $U_+$ is prevented by the occurrence of a limit cycle, which starts at the Hopf manifold. The limit cycle ends in the homoclinic loop, beyond which the connection from $U_-$ to $U_+$ is established. The five phase diagrams, with associated singular points $U_-$ and $U_+,$ show orbits in the three open regions to the right of the characteristic manifold, and at two transitional boundary points. Only the shock waves in the shaded region are admissible.
2 Publications


