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Final Report

The Department of Energy

Applied Analysis and Computational Mathematics

Courant Mathematics and Computing Laboratory

Principal Investigators

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FINAL REPORT

This is the final report for the Courant Mathematics and Computing Laboratory (CMCL) research program for the years 1991 - 1993. Our research efforts encompass the formulation of physical problems in terms of mathematical models (both old and new), the mathematical analysis of such models, and their numerical resolution. This last step involves the development and implementation of efficient methods for large scale computation. Our analytic and numerical work often go hand in hand; new theoretical approaches often have numerical counterparts, while numerical experimentation often suggests avenues for analytical investigation.

The scientific research program of the CMCL was carried out by a combination of faculty members, one senior staff member, two full-time post-doctoral visitors, shorter term visitors, and ten graduate students.

The research carried out at the CMCL has had significant influence on the U. S. scientific community, and on the DOE scientific community in particular. Ideas, theories, numerical methods, algorithms and computer codes developed here have been accepted and widely used. There is close collaboration between members of the CMCL and the DOE National Laboratories: Marsha Berger is working with John Bell and Phil Colella at Livermore, and Jeff Saltzman at Los Alamos. Anne Greenbaum, formerly at Livermore, continues her collaboration with members of that laboratory. Peter Lax serves on the advisory committees for C Division at Los Alamos and the Center for Nonlinear Studies. Many of our former students are employed at DOE laboratories: our supported students often spend the summer at Los Alamos visiting the Center for Nonlinear Studies. In fact, not the least of our influence has been through students trained at the Courant Institute in areas of great interest to the DOE; many now occupy positions of responsibility at the DOE, in other government laboratories, and at leading research universities. We are confident that we can continue to play this role.

As the publication record shows, members of the CMCL collaborate actively with each other and the Courant Institute at large. A natural outcome of this is that members of our group whose original involvement lay in mathematical analysis develop an interest in computing. We have active scientific collaborations with several government laboratories other than those of the DOE: NASA Langley, NASA Ames and NIST, as well as industrial laboratories such as IBM Yorktown.

In the past, as well as in the present, DOE support has helped shape the research at the Courant Institute. It has made possible our emphasis on applied nonlinear analysis and scientific computing. As a consequence, major resources of the Courant Institute, in the form of faculty appointments, are in computational areas.

Marsha J. Berger

Adaptive Methods and Complex Geometry

Previous Accomplishments

Our research in the last three years has concentrated on three fronts: (i) we have continued to develop the basic adaptive methodology for compressible flows in the context of hyperbolic conservation laws, (ii) we have developed a strategy for simulating time-dependent flows around complex geometries using a Cartesian grid representation in two space dimensions, and (iii) we began a study of the suitability of local adaptive mesh refinement for massively parallel architectures such as the Connection Machine. I will describe these projects in turn.

The development of a (serial) three dimensional adaptive mesh refinement (henceforth AMR) algorithm for hyperbolic conservation laws has been completed. This work is in collaboration with John Bell and Michael Welcome, at Livermore National Laboratory, and Jeff Saltzman, of Los Alamos National Laboratory. To test the algorithm we conducted numerical experiments of the interaction of a shock and an ellipsoidal bubble of Freon (see figure 1). This is analogous to the laboratory experiments of Haas and Sturtevant. Our tests indicate that AMR reduced the computational cost by a factor of at least 20 over uniform fine grid computations of the same resolution. This work is described in [1].

Although most of the algorithm development was a straightforward extension of the two dimensional case, a new grid generation algorithm was developed. Our previous grid generation algorithm worked remarkably well at creating grids with efficiency ratings of approximately 50%, (i.e. at least half the points in the new fine grid needed to be refined), using no geometric information at all. If a fine grid was inefficient, it was simply bisected in the long direction and two new fine grids were produced. Unfortunately, when requesting efficiencies around 80%, this algorithm produced unacceptably many tiny grids. Since memory (to store the refined grids) and CPU time (to integrate them) is at a premium in three dimensions, we developed a better algorithm. The new procedure can be viewed as a “smart” bisection algorithm. Using techniques from computer vision and pattern recognition, such as a variation of the Marr-Hildreth operator and coordinate-based signatures, our new algorithm can obtain efficiencies around the 80% level, even if the feature is not aligned with a coordinate direction. This is described in [2].

In collaboration with Prof. Randy LeVeque at the University of Washington we have developed an algorithm for computing time dependent flows around complex geometries using a non-body-fitted Cartesian grid. This strategy fits in naturally with our previously developed AMR strategy of using locally uniform meshes. We retain the advantages (efficiency and accuracy) of uniform grids and are able to resolve fine scale flow features induced by complex geometries. We use our previously developed adaptive mesh refinement algorithm to achieve accuracy comparable to the body-fitted meshes, where grid points can be bunched in an a priori manner to improve the accuracy of the solution.

We have developed a rotated difference scheme for use at the irregular cells. This procedure is used at the edge of each control volume with an intersecting boundary surface as well as for the boundary segments. Essentially, the difference scheme uses an auxiliary coordinate system that is locally normal and tangential to the boundary. This “artificial” grid is obtained at each interface by creating a box extending a distance h away from the interface in the normal and tangential directions.

Solution values for the new box are obtained by conservatively averaging the states in the underlying Cartesian grid. By differencing over a box of size h rather than the irregular neighboring cell with (potentially orders of magnitude) less cell volume, we retain stability using a time step Δt based on the uniform grid cells.

Together with Jeff Saltzman from Los Alamos National Laboratory, we have developed a fully adaptive two dimensional local mesh refinement algorithm for the Euler equations on the CM-2. To our knowledge, this is the first time such an adaptive method has been implemented for structured meshes on a massively parallel machine. Again we use the AMR approach to adaptive mesh refinement; a collection of logically rectangular meshes makes up the coarse grid, refinements cover a subset of the domain and use smaller rectangular grid patches. (There is no complex geometry in this implementation). Many of the original design choices in AMR were based on considerations of vectorization. The question was whether this approach was still feasible, and even advantageous on a data parallel massively parallel architecture.

The main issues in adapting the algorithm for the CM-2 were partitioning the data to fill the machine (load balancing, rather simple on rectangular grids), and minimizing communication (which is the main issue for our hierarchical data structure). We have developed a data layout scheme which preserves locality between fine and coarse grids and minimizes global (router) communication. On two dimensional tests the performance of an 8K CM-2 was roughly equivalent to one head of a Cray Y-MP. This research is described in [3]. While this performance is not optimal, it would have been quite difficult to achieve without the use of locally uniform Cartesian grids.

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Anne Greenbaum

Iterative Methods for Solving Integral Equations

Previous Accomplishments

During the past year I worked with Anita Mayo of IBM in developing fast integral equation solvers for problems in magnetostatics [8,2]. In particular, we developed a 3-D code to compute the potential and electric field around a recording head. This code uses an integral equation formulation of Laplace's equation, with piecewise linear boundary elements. The dense linear systems that arise from this problem formulation are solved with any of several conjugate-gradient-like methods for nonsymmetric problems. The matrix-vector multiplications that are required at each step of the iteration are currently implemented using an ordinary dense matrix-vector multiply routine. However, Len Berman of IBM has recently developed a 3-D fast multipole code, which will replace the dense matrix-vector multiply routine, greatly reducing both the storage and operation count required for large problems. This should enable fast and accurate solution of large 3-D problems, which were previously unsolvable. Fig. 3 shows a typical triangulation of the surface of a U-shaped recording head, and Fig. 4 shows the number of GMRES iterations required to solve the integral equation for different values of the relative permeability a .

In addition, we extended this idea to evaluate volume integrals of potential theory [7]. This requires embedding the given irregular region in a cube, determining the value of the discrete Laplacian throughout the cube by solving an integral equation, and finally applying a fast Poisson solver on the cube. The evaluation of such volume integrals enables the rapid solution of more complicated equations than Laplace's equation; e.g., $\nabla \cdot a \nabla u = f$. It is also needed, for example, when applying the Biot Savart law to evaluate the magnetic field induced by a conducting wire.

I also worked on problems associated with the iterative solution of large systems of linear equations, such as those that arise from the integral equations described above. With Jane Cullum of IBM, I discovered a relationship between the size of the residual vectors generated by the QMR (quasi-minimal residual) algorithm and those generated by the BCG (biconjugate gradient) algorithm [1]. This relationship gives further understanding of the relative advantages and disadvantages of these two methods for solving nonsymmetric linear systems. Understanding and improving iterative techniques for solving highly non-normal matrices is another topic that has been addressed. For such problems, it is not the eigenvalues of the matrix that determine the convergence rate, but something else. My recent work with Z. Strakos of the Czech Academy of Sciences [2,6], L. Gurvits of Siemens Corp. [4], and L.N. Trefethen of Cornell [5] has focussed on these questions.

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Figure 2: U-shaped recording head.

Figure 3: No. of GMRES iterations required to solve integral equation.

Leslie Greengard

Fast Algorithms and Partial Differential Equations

Previous Accomplishments

Over the last several years, I have been involved in the continued development of efficient numerical algorithms as well as the application of these algorithms to problems of practical interest. Progress has been made in several areas.

Electrostatics of Composite Materials

A classical problem in electrostatics is the determination of the electrostatic field in a material consisting of a collection of dielectric inclusions embedded in a homogeneous background. A graduate student, Monique Moura, has completed her dissertation in this area. She and I have implemented a 2-D solver for such problems in both infinite domains and periodic lattices, based on an integral equation formulation and relying on the adaptive fast multipole method [1]. We have solved problems with one thousand inclusions (200,000 boundary points) on a scientific workstation in fifteen minutes.

M. Moura, *On the Numerical Calculation of Electrostatic Fields in Composite Media*, Ph.D. Thesis, New York University, 1993.

L. Greengard and M. Moura, *On the Numerical Evaluation of Electrostatic Fields in Composite Media*, in preparation.

Parabolic Partial Differential Equations

A graduate student, Patrick Lin, and I have developed a new method for solving the heat equation in unbounded domains. It relies on computing the *continuous* Fourier transform and a generalization of the algorithm of [2]. We have implemented explicit, unconditionally stable schemes for both fixed and moving boundary value problems in one space dimension. We are currently working on the extension to higher dimensional problems.

P. Lin, *On the Numerical Solution of the Heat Equation in Unbounded Domains*, Ph.D. Thesis, New York University, 1993.

L. Greengard and P. Lin, *On the Numerical Solution of the Heat Equation in Unbounded Domains*, in preparation.

Elliptic Partial Differential Equations

Two years ago, A. Greenbaum (Courant Institute), A. Mayo (IBM) and I constructed a fast algorithm for the solution of the biharmonic equation in two dimensions. It is based on a well-known integral equation formulation and a new fast summation algorithm. Last year we extended the method to be able to handle multiply connected domains.

A. Greenbaum, L. Greengard, and A. Mayo, *On the Numerical Solution of the Biharmonic Equation in the Plane*, *Physica D* **60**, 216-225 (1992).

Research has continued, in collaboration with A. McKenney (Courant Institute) and A. Mayo (IBM, T. J. Watson Research Center), on an integral equation-based fast solver for the Poisson equation and more general divergence form elliptic partial differential equations. We have a working code for the solution of the Poisson equation in interior or exterior, multiply connected domains

based on combining ideas of A. Mayo [3,4] with the fast multipole method. Asymptotically, this hybrid algorithm requires only about twice as much CPU time as a standard fast Poisson solver on a square despite the arbitrary geometry. The past year has been devoted to implementation details and modest algorithmic modifications, aimed at increasing the precision for a fixed amount of work.

In collaboration with L. Berman and A. Mayo (both at IBM, T. J. Watson Research Center), we have developed a fast solver for three dimensional potential problems in irregular regions based on an integral equation formulation and the fast multipole method (FMM). There are two principal difficulties which we have overcome in coupling the FMM with a complex surface triangulation. The first is that the FMM requires the computation of the multipole moments of the single and double layer source distributions. New quadrature formulas were developed for this purpose. The second is that the oct-tree data structure used to resolve the geometry must cope with triangular surface elements rather than point sources. Special care must be taken when such surface elements cut across box boundaries.

L. Berman, L. Greengard and A. Mayo, *A Fast Second Order Accurate Method for Solving Three Dimensional Potential Problems in Irregular Regions*, in preparation.

Lattice Sums and Particle Simulations

Lattice sums arise in many areas of applied physics, including the calculation of the thermal, electromagnetic, elastic and optical properties of crystals. They also arise in the solution of certain partial differential equations and in the imposition of periodic boundary conditions in a particle simulation. We have recently developed a new method for the evaluation of slowly convergent lattice sums based on renormalization ideas. Although developed specifically for circular and spherical harmonics, we believe this algorithm can be generalized and will be of broader interest.

L. Berman and L. Greengard, *A Renormalization Method for the Evaluation of Lattice Sums*, in preparation.

Published Papers Acknowledging Support from DOE

- A. Greenbaum, L. Greengard, and G. B. McFadden, *Laplace's Equation and the Dirichlet-Neumann Map in Multiply Connected Domains*, J. Comput. Phys. **105**, 267-278 (1993).
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Peter Lax

1. Generation and limiting behavior of oscillatory solutions of dispersive equations.

There are a variety of equations describing physical systems in which dissipative mechanisms are absent but which undergo dispersive processes. In the last 12 years an increasing number of researchers have investigated the limiting behavior of such systems when the dispersive term goes to zero. Experimental and theoretical investigations reveal oscillatory behavior in certain portions of space-time, smooth behavior in others. Of great interest is the mean (i.e. weak) convergence of these oscillatory solutions as the dispersive term tends to zero, and the laws governing the evolution of these mean quantities. Lax and Levermore have shown how to take advantage of the complete integrability of the Korteweg de Vries equation

$$u_t + uu_x + \epsilon^2 u_{xxx} = 0$$

to carry out this program for the limit $\epsilon \rightarrow 0$. Recent significant new developments have carried out analogous limiting procedures for other completely integrable systems.

Venakides, Deift and Oba have given a detailed analysis of the continuum limit $\Delta \rightarrow 0$ of the von Neumann shock problem for the Toda chain

$$\partial_t^2 X_k + \left[p \left(\frac{X_{i+1} - X_k}{\Delta} \right) - p \left(\frac{X_k - X_{k-1}}{\Delta} \right) \right] / \Delta = 0, \quad p = e^{-V},$$

i.e. the solution with initial data $X_k(0) = k\Delta$, $\partial_t X_k(0) = -a$ for $k > 0$, $X(t) = 0$, $a > 0$. They analyzed the supercritical case $a > 2$; subcritical motion was investigated by Kanvissis. Tom Hou and Peter Lax are investigating the continuum limit for very general initial data. Related investigations are carried out by Ken McLaughlin.

An expository article on these developments was prepared by Lax, Levermore and Venakides. The last section of this article scrutinizes numerical evidence gathered by Holian and Straub, Hou and Lax, Levermore and Liu, that strongly suggest that solutions of some nonlinear dispersive equations that are *not* completely integrable show a similar limiting behavior as the dispersive term tends to zero. In particular, vibrations of chains bound together by a force law $p(V)$ other than an exponential one appear to be strikingly similar to the vibrations of the Toda lattice. This seems to be a manifestation of an infinite dimensional analogue of the Kolmogorov-Arnold-Moser theorem; it would be highly desirable to find such an extension of the KAM theory. Perhaps Sergej Kuksin's recent extension of KAM theory to partial differential equations can be of some use.

Some aspects of the mean (weak) limits of oscillatory solutions discussed above are similar to those of mean fields obtained by ensemble averages of solutions of nonlinear equations. The crucial difficulty in both theories is that the mean of a product of two field variables is *not* the product of the mean values of the individual variables:

$$\overline{uv} \neq \bar{u} \bar{v}.$$

On the other hand, the oscillations encountered in solutions of the completely integrable equations are far more regular than the fluctuations typical of turbulence. It would be desirable to find a dispersive system simple enough to be analyzed exactly, yet complicated enough to have solutions

that oscillate on many scales. Recent investigations of David McLaughlin and Greg Forest, and David Levermore, indicate that the focusing cubic Schroedinger equation is a good candidate.

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Michael Ward

Singular Perturbations and Scientific Computing

Previous Accomplishments

Two topics of ongoing research are:

1. The asymptotic and numerical analysis of slow internal layer motion for various phase separation models, notably the Allen-Cahn (alias Ginzburg-Landau) and the Cahn-Hilliard models. The analysis of exponentially slow shock layer motion for a class of viscous shock problems.
2. The study of various problems with strong localized inhomogeneities that lead to infinite order logarithmic expansions. Numerical methods to sum these infinite logarithmic expansions.

1: Internal layers, Metastability and Coarsening

Consider a binary mixture where u is the dimensionless concentration of one of the species and $V(u)$ is a double-well potential with wells of equal depth. The phase separation model proposed by Cahn and Hilliard [3] (the Cahn-Hilliard equation) is

$$u_t = - \left[Q(u) + \epsilon^2 u_{xx} \right]_{xx}, \quad u_x(\pm 1, t) = 0, \quad u_{xxx}(\pm 1, t) = 0, \quad Q(u) = -V'(u), \quad (\text{Model A}),$$

Notice that mass is conserved. The phase separation process of diffusion against concentration gradients separates u into the two preferred phases separated by $O(\epsilon)$ phase boundaries or internal layers. The coarsening process involves the gradual migration and annihilation of phase boundaries.

Another phase separation model, which is related to Model A, is the Allen-Cahn equation

$$u_t = \epsilon^2 u_{xx} + Q(u), \quad -1 < x < 1, \quad t \geq 0, \quad (\text{Model B}).$$

Again $Q(u)$ arises from a double-well potential with wells of equal depth. The multi-dimensional analogue of Model B was proposed in Allen and Cahn [2] as a model for antiphase boundary motion in crystalline solids.

Another phase separation model, this one perhaps more closely related to Model A, is the following non-local mass-conserving Allen-Cahn equation:

$$u_t = \epsilon^2 u_{xx} + Q(u) - \sigma, \quad -1 < x < 1, \quad t \geq 0, \quad \sigma = \sigma(t) \\ u_x(1, t) = 0, \quad u_x(-1, t) = 0, \quad \int_{-1}^1 u \, dx = m, \quad (\text{Model C})$$

Here m is constant. The multi-dimensional version of this model was studied in Rubinstein and Sternberg [8].

The qualitative features of the dynamics for the simplest model, Model B, are as follows. Starting from two-phase initial data, a pattern of internal layers is formed on an $O(1)$ time scale. This is the process of phase separation. Through a sequence of layer collapse events, the original fine-grained mixture undergoes an exponentially slow coarsening process leading eventually to a stable equilibrium solution. A major step in quantifying this process was made by Carr and Pego [4] and Fusco and Hale [6]. For the Neumann problem, they gave a rigorous derivation of the equations of motion for the internal layer trajectories. Although some analytical and numerical results have been given for Models A and C (see [1] and [5]), the internal layer dynamics associated with these models are not nearly as well understood. Some of the questions which we have tried to address include:

1. Give a hybrid asymptotic-numerical description of the coarsening process for any one of these models. This would show the exponentially slow relaxation of an initial pattern to a stable equilibrium solution.
2. Study the constrained internal layer dynamics for Model A and Model C. In particular, what are the new laws of internal layer evolution?
3. Formulate full numerical methods to study the slow internal layer motion over exponentially long time scales. Previous computations of Elliot and French [5] and McKinney (described in [1]) for the Cahn-Hilliard model show only the very initial stages of the coarsening process. There are three main difficulties associated with undertaking a full numerical study using the original u variable: the equilibrium problem is exponentially ill-conditioned, the weak internal layer interactions may be below discretization errors (or even worse, below roundoff errors), the long time scale is determined only by resolving the weak layer interactions.
4. Identify other classes of problems with slow internal layer motion that share similar features with the phase separation models.

We now summarize some of our results.

In [3*], previous work for the Neumann problem for the Allen-Cahn equation (Model B) has been extended. In particular,

1. Equations of motion for the internal layer trajectories have been derived under various types of boundary conditions. The results show that the equilibrium solution for a one-layer pattern can be stable under Dirichlet boundary conditions.
2. Slow internal layer dynamics under a periodic nonlinearity $Q(u)$ has been studied. The results describe the effect of the internal layer motion of having *many*, rather than simply two, preferred phases.
3. We have formulated and applied a hybrid asymptotic-numerical method to study the coarsening process for small ϵ . The results quantify how an initial metastable pattern tends, after a series of layer collapse events, to a stable equilibrium solution.

In [4*], we studied some aspects of slow internal layer motion for the non-local Allen-Cahn equation (Model C). We also applied a nonlinear WKB-type change of variables to the unconstrained Allen-Cahn equation (Model B). The advantages of this transformation are mainly from a numerical perspective. Specifically, the exponentially weak layer interactions are magnified, the exponentially long time scale becomes transparent, and the exponential ill-conditioning associated with the steady problem is overcome. The results in [4*] include,

1. An asymptotic derivation of a nonlinear differential algebraic system describing the slow, constrained, internal layer evolution for Model C.
2. Using the WKB transformed version of Model B, we give a very simple alternative method to derive the internal layer dynamics which does not require exponential asymptotics.
3. Exponentially sensitive internal layer solutions are shown to be *easily* computable in terms of the WKB transformed problem.
4. The WKB transformed Allen-Cahn equation hinted at the fact that there may be some similarities between it and the initial boundary value problem for Burgers equation.

In [5*], motivated by the numerical study of [7], we analyze exponentially slow shock layer motion for a class of scalar viscous shock problems. Specifically, we consider

$$\begin{aligned} u_t + [f(u)]_x &= \epsilon u_{xx}, & 0 < x < 1, & \quad t > 0, \quad \epsilon \ll 1 \\ u(x, 0) &= u_0(x), & u(0, t) &= \alpha_+ > 0, \quad u(1, t) = -\alpha_- < 0, \end{aligned}$$

where the convex flux function satisfies $f(\alpha_+) = f(-\alpha_-)$. Our results include,

1. An asymptotic construction of the equilibrium solution and an asymptotic estimate for the principal eigenvalue associated with linearizations about the equilibrium solution.
2. An asymptotic derivation of a nonlinear ODE describing the exponentially slow evolution of the shock layer trajectory to its equilibrium location.
3. An examination of the relationship between the slow shock layer motion and the slow internal layer motion associated with the phase separation models.
4. A full numerical solution, using the WKB transformed problem, of the slow shock layer motion using a second order method in space and time. The numerical and asymptotic results agree to within 1-2% on time scales of order $10^7 - 10^8$.
5. We also obtain analogous results (equilibrium profiles, eigenvalue estimates, shock layer trajectories etc.) allowing for certain modifications of the boundary operator for u . In particular, we show that very minor changes in the boundary operator can de-stabilize the equilibrium solution.
6. For Burgers equation the asymptotic ODE for the shock layer trajectory and the asymptotic eigenvalue estimate are proven by using some exact solutions.

Further work on the viscous shock problem and its relationship to some classical linear singular perturbations having exponentially small eigenvalues is contained in [7*].

Some work in progress ([8*]) is to use the WKB transformed Allen-Cahn equation to provide accurate full numerical simulations of the coarsening process. We use fourth order finite differences in space and the DAE software DDASSL, developed by Petzold and co-workers, for the time integration. This strategy is very advantageous in that the WKB transformed problem arises as an evolution equation coupled to a non-evolutionary 'constraint' involving only spatial derivatives. Finally we have some work in progress describing the slow internal layer motion for the Cahn-Hilliard model [9*].

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2: Summing Logarithmic Expansions for Singularly Perturbed Problems

2.1 Linear and Nonlinear Eigenvalue Problems: Consider the nonlinear eigenvalue problem

$$\Delta u + \lambda F(u) = 0, \quad x \in D; \quad \partial_n u + b u = 0, \quad x \in \partial D, \quad D \subset R^m, \quad m = 2, 3. \quad (2.1)$$

When $F(u) = \exp[u/(1 + \beta u)]$, (2.1) is the simplest model in steady state thermal explosion theory for the dimensionless temperature u of a self-heating material. It is well-known that (2.1) can have multiple solutions for some range of λ . In previous work we have investigated the sensitivity of the critical value of λ signifying a thermal explosion (e. g. a jump from a low norm to a high norm solution for u) to various classes of perturbations. This critical value λ_c is a simple fold point in the bifurcation diagram of $\|u\|$ versus λ . In [2] we considered two classes of singular perturbations of (2.1): a) the effect of deleting a small subdomain D_ϵ of 'radius' ϵ from D and imposing a boundary condition on the surface of the resulting hole; b) the effect of replacing b in the boundary condition by a different value $\epsilon^{-1}k$ on a small part of ∂D . A physical application of a) is to determine the effect of a small cooling rod on the thermal stability of a tubular reactor while b) has applications to the modeling of building construction on a waste disposal site. In both cases, for $\epsilon \rightarrow 0$ singular perturbation techniques were used to construct expansions for $\lambda_c(\epsilon)$ in terms of some characteristic properties of the perturbation.

In some related work for problems of the class a) it was shown in [1*] that for a cooling rod in a two-dimensional domain, the expansion of $\lambda_c(\epsilon)$ begins with an infinite series in powers of $(-1/\log[\epsilon d])$. Here d is a certain constant associated with the perturbing subdomain. A hybrid asymptotic-numerical method was formulated to sum this infinite order logarithmic expansion. For various geometries, the sum of the logarithmic expansion for $\lambda_c(\epsilon)$ was found to compare very favorably, even for moderately small ϵ , with results obtained from a full numerical solution of the perturbed problem. Some related work on summing infinite order logarithmic expansions for linear eigenvalue problems was given in [1*]. In [2*] we extended the hybrid method to treat cubic fold points and we applied the results to chemical reactor theory.

2.2 Other Applications of Summing Logarithmic Expansions: It is well-known through the pioneering work of Cole, Kaplun, Lagerstrom and others in the 1950's that the asymptotic expansion for the drag coefficient C_D of a circular cylindrical body in a low Reynolds number flow begins with $C_D \sim 4\pi\epsilon^{-1}S(\epsilon)$. Here ϵ is the Reynolds number and S is an infinite logarithmic series in powers of $1/\log \epsilon$ (see [1] Chap. 8 and the references therein). For arbitrary cylindrical bodies, Kaplun showed that C_D is determined by replacing ϵ by ϵd where d is a constant associated with the shape of the cylinder (with $d = 1$ for a circular cylinder). This result is known as Kaplun's equivalence theorem. Although this result is qualitatively very interesting, its use is severely limited by the fact that it is only possible analytically to determine the first two terms in this expansion when $d = 1$. However, since the terms in $S(\epsilon)$ decrease only very slowly due to the logarithmic nature of the series, such a drastically truncated form is in very poor agreement with experimental and full numerical results for C_D unless ϵ is very small. Thus, for the last 30 years this problem has been a paradigm for problems where the method of matched asymptotic expansions fails to be of much practical use. To our knowledge, the summation of $S(\epsilon)$ is still a classical unsolved problem.

Our observation is that the form of the series for S pertaining to an arbitrary cylinder is exactly the same as that for the singularly perturbed eigenvalue problems described above. Thus in [10*] we

are currently trying to adapt the hybrid asymptotic-numerical method used in [1*] in order to sum S for various cross-sectional shapes of the cylinder.

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- [8*] L. G. Reyna, M. J. Ward, *An Accurate Numerical Study of Slow Internal Layer Motion for the Allen-Cahn Equation*.
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- [10*] M. J. Ward, J. B. Keller, *Summing The Logarithmic Expansion for the Drag Coefficient in a Low Reynolds Number Flow*

Zhouping Xin

Nonlinear Conservation Laws and the Boltzmann Equation

Previous Accomplishments

During the academic year 1992-1993, with partial support from DOE grant DE-FG-02-88ER-25053, Zhouping Xin has obtained the following results:

1. Relaxing Schemes

With Dr. Shi Jin, we introduce a class of numerical schemes for arbitrary systems of conservation laws in several space variables. The basic idea is to use the local relaxation approximation. For any given system of conservation laws, we can construct a corresponding linear hyperbolic system with a carefully designed stiff source term that approximates the original system of conservation laws with a small dissipative correction, which we call the relaxing system. The main advantage of numerically solving the relaxing system over the original conservation laws lies in its special structures of the linear characteristic fields and the localized source terms. The linear hyperbolic structure enables one to avoid the time consuming Riemann solvers which are commonly used by the standard high resolution methods for nonlinear hyperbolic systems. The characteristic speeds (frozen speeds) can be chosen to enforce the entropy conditions. Even though proper implicit time discretizations must be used to overcome the stability constraints brought on by the stiff source terms, solving nonlinear systems of algebraic equations can be avoided due to the special relaxation process. A second order Runge-Kutta type time discretization coupled with the standard higher order Godunov schemes can be used to solve this relaxing system effectively. These schemes will be called the relaxing schemes. The main feature of the relaxing schemes we proposed are their simplicity and generality. No hyperbolicity is required for the original systems of conservation laws. General systems in higher dimensions can be treated likewise where the constant linear characteristic fields for the relaxing systems allow one to apply the standard upwind schemes without the field-by-field decomposition and operator splittings[3]. One can indeed design highly efficient and well vectorized algorithms. Using the discrete analogy of the Chapman-Enskog expansion applied to the relaxing schemes, we also derive their leading order approximations in the limit of small relaxation time. The resulting schemes are called the relaxed schemes which are consistent and stable discretizations of the original conservation laws. They are shown to be total variation diminishing for scalar conservation laws and produce as good results as the relaxing schemes for small relaxation time. Numerical experiments for 1-D and 2-D gas dynamics problems are carried out. Our second order schemes seem to produce very promising results that are comparable to those produced by other high resolution methods. Figure 1 shows the density profile for the double Mach reflection problem computed use the relaxing schemes. Our test problem involves a planar Mach 10 shock incident on an oblique surface which forms a 30° angle to the direction of propagation of the shock. Ahead of the shock is the undisturbed air with a density of 1.4 and a pressure of 1.

2. Boundary Layers for the Broadwell Equations

With Jian-Guo Liu, we investigate the boundary layer behavior of solutions to the one dimensional Broadwell model of the nonlinear Boltzmann equation. We consider both the analogues of Maxwell's diffusive and reflexive and diffusive boundary conditions. The natural boundary conditions for the model Euler equations are obtained by matching the fluid solutions with the boundary

layer solutions for the Broadwell equations. It is shown that the boundary layers can be classified as either compressive or expansive according to the rate of change of the associated characteristic speed near the boundary. We found that even for such a simple model, there are boundary layers due to purely kinetic effects and which cannot be detected by the corresponding Navier-Stokes system. More importantly, we find by numerical experiments and matched asymptotic analysis that a compressive boundary layer is not always stable and it may detach from the solid boundary and move into the interior of the gas as a shock layer. It is shown that the expansive layers are always nonlinearly stable, while the compressive boundary layers are stable before the detachment from the solid boundary, so that the boundary effects are confined to the boundary with a distance of the order of the mean free path. A rigorous estimate for the distance between the kinetic solution and the fluid dynamic solutions in terms of the mean free path in L^∞ -norm is obtained provided that the interior fluid flow is smooth. Thus the validity of the fluid-dynamical approximations is verified in this case. The rate of convergence is optimal. One of the main difficulties in our analysis is the stiffness across the boundary. These results are obtained by using numerical methods, matched asymptotic analysis, and a delicate energy method which makes full use of the geometrical structures of boundary layers for the Broadwell equations. These studies should shed light on the boundary layer behavior of the general nonlinear Boltzmann equations.

3. Stability of Strong Detonation Waves

With Tan and Tesei, we investigate the stability of the strong detonation waves for a simple combustion model [1] which consists of a conservation law governing a lumped variable, partially representing the temperature, velocity and the pressure, coupled with the reaction equation for the chemical binding energy $qz(x, t)$ with the reaction rate k being infinity. The combustion process is viewed as the liberating of the binding energy. The jump discontinuous solutions of this model can be classified as either strong detonation waves, Chapman-Jouget detonation waves, or weak detonation waves. We show that the strong detonation waves are “physically” admissible in the sense that they are nonlinearly stable under both viscous perturbations and initial perturbations. More precisely, corresponding to the inviscid model with infinite reaction rate, we consider a more “physical” model

(Majda's model[2]) which has small but nonzero dissipations and the rate of reaction is assumed to be finite. Then our first result shows that the strong detonation waves are strong limits of the solutions to the "physical" model as both viscosity goes to zero and the rate of reaction goes to infinity but with their product being constant. Detailed asymptotic behaviors of the "physical" solutions around the strong detonation waves are obtained. It is also shown that the traveling wave solutions to the "physical" model associated a strong detonation wave is a large time asymptotic attractor for the Cauchy problem of the "physical" model with fixed viscosity and rate of reaction. The proof of these results are based on a weighted energy estimate and matched asymptotic analysis.

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- [1] The Relaxing Schemes for Systems of Conservation Laws in Arbitrary Space Dimensions (with Shi Jin), submitted to Comm. Pure Appl. Math. (1993).
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Robin Young

Systems of Conservation Laws with Large Data

Overview

I am studying nonlinear systems of inviscid hyperbolic conservation laws in one space dimension, that is equations of the form

$$(\varphi(u))_t + (f(u))_x = 0.$$

Here $u \in R^n$ is the state space, and the vector functions φ and f represent the conserved quantities and fluxes, respectively. The best known nonlinear feature of these systems is the formation and subsequent decay of shock waves, see [Lax]. Conservation laws include the equations of gas dynamics, and the nonlinear effects also occur in nozzle flow and related areas. My main interest lies in solutions for which the Cauchy data is of small oscillation, but large total variation. This includes the important case of periodic data.

My approach to the study of these systems is via elementary wave interactions. These are crucial in Glimm's scheme (see [G]), which remains the only rigorous means for obtaining existence results for more than two equations. My starting point is an estimate which identifies exactly the second order terms in an interaction. These second order terms are manifested as nonlinear changes of strength of incident waves, and waves which are generated as a result of the interaction, see [Y].

There are two conflicting phenomena that occur in solutions of systems of three or more equations : these are the generation of new waves in the third family when two waves of different families interact, and the tendency of waves in a single family to decay due to shock formation and expansion of rarefactions. The generation of new waves is not seen in systems of two equations. In this case, the families decouple and the Glimm-Lax decay theory applies, see [GL]. In larger systems, when the total variation of the initial data is small, waves in different families separate quickly, and decay takes over as the dominant effect for large time, see [Liu]. When the initial total variation is large, interactions between different families persist, and a resonance pattern may occur. In this situation there is a delicate interplay between the two phenomena, and large time behavior is not yet understood. The method of weakly nonlinear geometric optics is a formal tool for studying solutions via a simplified system of equations, and predicts new behavior, including the blowup of solutions in finite time, and inhibition of shock formation.

Previous Accomplishments

There are certain coefficients which arise naturally from the conservation law, and which determine the strength of wave interactions and rates of decay in each family, to leading order. These are given by the Hessians of φ and f , evaluated at the origin, and are thus an indication of the degree of nonlinearity of the system. Under suitable normalization, some of these coefficients can be made to vanish. This simplifies the effects of elementary wave interactions, and helps in the geometric interpretation of the results of interactions. I am writing a survey paper in which these coefficients are defined and given a geometric interpretation. In particular those coefficients which determine the generation of new waves and decay in a single family are isolated. Their occurrence in elementary interactions and the equations of geometric optics is indicated.

Together with Blake Temple, I have been studying the general Cauchy problem for data with small oscillation and large (finite) total variation. The problem of existence of global solutions for all time is reduced to an algebraic problem of bounding certain Glimm functionals measuring the total variation and interaction potentials. These are modified versions of Glimm's original nonlinear functionals, adjusted to account for the second order terms occurring in wave interactions via the method of reorderings introduced earlier. The functionals have been shown to be bounded assuming that two of the three interaction coefficients vanish, yielding an existence theorem. At present we are looking for a bound when one of these coefficients vanish. This includes the important case of gas dynamics.

In order to understand how the behavior of the solution is affected by the various coefficients, I have implemented Glimm's scheme numerically. In this implementation, instead of approximating the solution of the Riemann problem as is usually done, we work directly with the waves that occur in the scheme. This has the advantage of speed, in that one does not have to solve Riemann problems, although its relative performance in other areas is not yet known.

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