DOE/ER/03077-168

COURANT MATHEMATICS AND COMPUTING LABORATORY

NEW YORK UNIVERSITY

PROGRESS REPORT NO. 56

October 1, 1979 to September 30, 1980

Prepared for
Applied Mathematics Research Program
Office of Basic Energy Sciences
U. S. Department of Energy
Under Contract DE-AC02-76ER03077

October 1, 1980

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DISCLAIMER

COURANT MATHEMATICS AND COMPUTING LABORATORY

The Courant Mathematics and Computing Laboratory forms one of the divisions of the Courant Institute of Mathematical Sciences, a world renowned center devoted to research and training in the mathematical sciences.

The Laboratory was established in 1952 when the AEC Physical Research Division placed a UNIVAC I at the Courant Institute. Since then the Laboratory has successively managed an IBM 704, a 7090, a 7094, and currently a CDC 6600 and a VAX 11/780. The Laboratory has pioneered in techniques leading to time sharing and remote utilization of computers.

The expertise of the Laboratory lies in the development and analysis of mathematical models and efficient computing methods for the rapid solution of technological problems of interest to DOE. The primary focus of this energy related research involves the detailed calculation on large computers of complicated fluid flows in which reactions and heat conduction may be taking place. These flows are governed by partial differential equations, usually in three dimensions plus time, which require new mathematical and new programming techniques.

The research program of the Laboratory encompasses two broad categories: (a) analytical and numerical methods, which include applied analysis, computational mathematics, and numerical methods for partial differential equations, and (b) advanced computer concepts, which include software engineering, distributed systems, and high performance systems.

The training of personnel to apply advanced mathematical and computer methods constitutes a concomitant to these research functions. Over the years we have trained and graduated several hundred Ph.D. students who now populate technical fields throughout the country.

Contents

I. ANALYTICAL AND NUMERICAL METHODS

A. Applied Analysis

1. Mathematical Problems in Geophysics

During this year we have made considerable progress in studying the one-dimensional inverse problem of exploration geophysics.

This work falls into two parts: (a) understanding and evaluating existing numerical techniques used in oil exploration; (b) development and testing of new techniques.

Part (a) has led to an understanding of the role of the integral equations of inverse scattering theory and related discrete (Toeplitz) systems which resulted in a report which is now in press. (See Sect. V, publication no. 5.)

A general conclusion from this aspect of our work was (i) that these integral equations are indeed closely related to the so-called inverse impulse-response problems of exploration geophysics, (ii) that they are not readily adaptable for nonideal data such as arise in practice.

Part (b) has resulted in the development of a scheme which is a direct numerical integration of the original differential equations with a simultaneous calculation of the unknown coefficient. This method, developed by Dr. Kenneth Bube, appears to be readily adaptable to non-impulse-response data.

We plan to publish papers describing the analysis and numerical experiments we have performed using the integral equations and also the new method outlined above.

R. Burridge

2. On the Notion of Hyperbolicity

This work shows that a system of nonlinear partial differential equations has a positive conserved quantity only if the equation is hyperbolic, i.e., if it has no complex characteristics.

The averaged equations describing the motion of two compressible fluids which are allowed to slide past each other constitute a system which has complex characteristics. The theory of the initial value problem for this system has been studied numerically but not theoretically. In some of the engineering literature it is asserted that the conservation of total energy provides an a priori bound. (See Sect. V, publication no. 28.) This, however, is not right, for kinetic energy is only conditionally positive, i.e., only when $\rho > 0$. To show tha ρ always stays positive for solutions of the averaged two-fluid equations requires yet another a priori inequality which so far is missing.

This work sheds light on the puzzling appearance of complex characteristics in the equation of two-phase flow, and shows the need for further theoretical (and numerical) study on the suitability of these equations.

Multifluids and multiphase flow appear in many problems of interest to DOE, in particular, in studying the excursions of a nuclear reactor undergoing large perturbations.

P. D. Lax

3. Reacting Flow Computations

Numerical methods are being tested and developed for the solution of detailed mathematical models of combustion in this project. Two parallel studies are being performed. The first deals with the computation of ignition and propagation of one-dimensional deflagration waves (flames). This problem focuses attention on the treatment of the important reaction and diffusion terms in the governing conservation equations. The second study involves the solution of the equations of one-dimensional inviscid compressible gas dynamics. This focuses on methods for the convective terms in the governing equations.

Results have been obtained for the ozone flame system of equations using the unconditionally stable explicit method of Saul'yev for the diffusion terms. We have developed a stiffly stable noniterative method for the reaction terms and have applied an adaptive grid method which increases resolution within the flame zone. The results indicate that explicit methods can offer the potential for increases in computational efficiency and accuracy.

In the second study computations have been made with an explicit method which is based on concepts from the kinetic theory of gases. The flow variables are computed using the Boltzmann equation with an operator splitting approach and the method is unconditionally stable. The results indicate that this method can offer significant advantages over standard finite difference methods for compressible gas dynamics problems.

Advanced computer codes are becoming available for the solution of combustion problems. In some cases, these are versions of previously existing fluid dynamics codes which were modified to include combustion effects. However, further research into specialized numerical methods for the energy and chemical species conservation equations has been necessitated by the fact that these energy release effects play a dominant role in many combustion applications.

In this study, we address this need and the additional difficulties which are met in the numerical solution of mathematical models of internal combustion engine phenomena. This includes an analysis of the problems associated with the solution of a large number of stiff coupled chemical species equations, and of fulfilling the requirement that the flow field be resolved accurately within the relatively thin energy release zone.

Our approach is to study numerical methods as applied to relatively simple model systems, each of which focuses on individual aspects of the overall task. We anticipate that the component projects will be united and that the combination will allow computations to be made of coupled fluid dynamics and combustion equations, with complete chemical kinetic mechanisms, for the study of multidimensional internal combustion engine phenomena.

Detailed mathematical models of combustion phenomena yield information about the local and instantaneous events which occur within a combustion device. This information is helpful in the design of clean and efficient energy consuming units such as internal combustion engines and furnaces. Numerical techniques are being developed in this study to permit efficient and accurate computations of multidimensional internal combustion engine phenomena.

R. D. Reitz

B. Computational Mathematics

1. Finite Element Capacitance Matrix Methods

This work, which is a continuation of a major research effort, aims at the extension of the use of fast Poisson solvers to an important family of elliptic problems on arbitrary bounded regions. Such methods and related software can be used profitably as subprograms when solving, for example, fluid dynamics problems.

Recently, this effort has been focused on developing methods which exploit attractive features of both the finite-difference and finite-element methods. A first such project has been completed and the numerical experiments show that these new methods offer considerable advantages in comparison with the finite-difference capacitance matrix methods previously employed.

Only the Neumann problem for Laplace's equation was investigated so far and implemented in detail. Several central theoretical questions on the fast convergence of methods of this kind have been settled in recent months, most notably the proper design of rapidly convergent iterative finite-element capacitance matrix methods for Dirichlet problems. These results are likely to provide a very adequate theory for the entire family of methods and are also expected to serve as a most valuable design tool for methods for higher order elliptic problems.

O. Widlund

2. A Model Problem on Substructures

A topic of much current interest among computational engineering scientists, numerical analysts working on sparse matrix problems, and some computer scientists interested in new computer architectures is the use of substructures. A simple problem of such a kind, a discrete Laplace's equation defined on the union of rectangles, has been analyzed. A new preconditioned conjugate gradient method to solve for the mesh variables common to the different rectangles has been designed

and shown to converge rapidly. Once the values of those variables are known with enough accuracy, the entire problem can be solved straightforwardly.

O. Widlund

3. Numerical Methods for Stationary Discrete Stokes Equations

The use of two different conjugate gradient-like methods to solve the large sparse, symmetric, indefinite linear systems of equations that arise when Stokes' equation is discretized has been studied numerically. Test problems were provided by a Lagrangian polygon approximation method due to C. Peskin. The use of incomplete Cholesky factorizations and conjugate gradient methods was successful, in particular, when the approximate solution of the pressure field was attempted prior to that of the velocity field.

For the same problem, it was also shown that a large family of symmetric permutations can be found a priori which all assure the success of a LDLT factorization without pivoting. For such problems existing software for pivoting for sparsity can be employed. The choice of pivot sequence requires information only of the graph of a principal submatrix.

O. Widlund

4. Combustion

The two step combustion model has been programmed for an alternating direction explicit method for solution of the hydrodynamic equations. The method of Glimm is used at shock and combustion fronts while a Lax-Wendroff method is used in the smooth part of the flow. Since it is hoped to apply this model to the internal combustion chamber dynamics, correct modeling of mixing processes is important. With regard to this point, the method must allow vortical motions to be correctly predicted. In this regard work has started on methodology for implementing fast Poisson and Poisson-like solvers. The work has proceeded on small DEC-like computing machines rather than large scale computers. The goal is to achieve a computational algorithm that has a parallel structure which may be solved on a parallel machine.

S. Z. Burstein

5. Methods for Nonlinear Minimax and Ll Optimization Problems

The nonlinear minimax problem is that of finding a point in n dimensions which minimizes the maximum of m continuously differentiable functions. These problems are unconstrained optimization problems in which the objective functions are not everywhere differentiable. They are however well known to be equivalent to constrained optimization problems with differentiable objective functions and constraints. Indeed, if the functions were linear, the problems would be equivalent to linear programming problems. Nonetheless these equivalent problems have special features which are ignored if they are solved by general purpose methods for constrained optinization. The purpose of this work is to provide efficient algorithms based on the best methods for

constrained optimization but taking advantage of the special structure of the problems.

Work on these problems has been continued. Working algorithms developed in the investigator's Ph.D. thesis have been tested on further problems and seem very promising. Various fine details of the algorithms have undergone further study.

Both problems have many applications in data fitting since they can be viewed as minimizing the L^∞ and the L1 norms respectively of nonlinear functions. Special applications of the minimax problem include the design of circuits, and of transformers for power lines.

M. Overton

6. A Method for Minimizing a Sum of Euclidean Norms

This problem has a long history, dating back to Fermat in the 17th century who proposed the problem of finding a point in the plane which minimized the sum of the distances from it to each of three fixed points. This special case was solved geometrically, but the analysis of the problem generalized to a weighted sum of distances from one point to n other points was not successful until comparatively recently. The problem can be further generalized to that of minimizing a sum of m Euclidean norms of linear vector functions of n variables. Although a number of methods have been proposed for solving this problem none of them are very satisfactory since they are unable to deal with the essential nondifferentiabilities in the problem. Unlike the minimax and L1 problems, it is not apparently possible to find useful equivalent differentiable constrained optimization formulations. Therefore, the approach must be to handle the discontinuities directly. Nonetheless, the problem is closely related to the L1 problem which is in fact a special case when the vectors whose norms are to be summed are actually scalars. Therefore, the algorithm to be designed will have many features in common with the L1 algorithm.

Initial work has recently been done on this problem. The mathematical characterization of the solution to this problem has been investigated and a preliminary method for its solution has been designed. This is a difficult problem and many details of the algorithm have yet to be worked out.

This problem has an enormous number of applications, including the single facility and multifacility location problems, which are of great interest to energy planners. Another quite different but important application is in solving the minimal surface problem.

M. Overton

7. Two-Stage Iterative Methods for Systems of Linear Equations

Often one wishes to solve the linear system of equations $(M - N)x = b$ by an iterative method, where at each step of this "outer" iteration it is necessary to solve the linear system $Mz = r$, the vector r being the current residual. Frequently, it is also desirable to

solve the systems Mz = r by an "inner" iterative procedure. We have analyzed how the rate of convergence of the outer iteration depends on the accuracy required for each inner iteration, when the second-order Richardson method is used for the outer iteration. In particular, we give a condition relating the Euclidean norm of the inner iteration to that of the outer iteration which is sufficient for convergence of the outer iteration. The results are applicable both in the case that M and N are symmetric and in the case that M is symmetric and N is skew-symmetric.

Theoretical analysis has been done analyzing how the rate of convergence of a method for solving a system of linear equations depends on the accuracy required at each step of the computation. A computer program has been implemented showing that the algorithm is just as efficient as predicted by the theory.

There are many applications where very large systems must be solved and the two-stage iterative technique is the only feasible method for an efficient solution. These applications include the many systems arising from the discretization of partial differential equations.

M. Overton

C. Numerical Methods for PDE's

1. MHD Equilibrium and Stability

We have developed a computational method to analyze equilibrium and stability problems in magnetohydrodynamics. Our ideas have been implemented in several general purpose codes which at this stage are sophisticated enough to provide a very useful tool in the design of future experiments.

Our main effort has been on a thorough study of equilibrium and stability β limits for current-free stellarators. This question has become extremely important since the new experimental results obtained by the Wendelstein VII-a experiment at Garching.

We have extended our vacuum code so that we need only to prescribe a winding law for current carrying conductors in the vacuum region to compute an equilibrium. This is a step closer to the real experiment and allows us to use the code to examine which configurations are more desirable and how we should produce them.

We have also studied nonlinear effects on ballooning modes in tokamaks. We have found evidence of nonlinear saturation and island formation. These results may provide some insight into results of current experiments, such as the ISX-B Tokamak at Oak Ridge Laboratory.

We have also begun a cooperative effort with H. Grad and A. Bayliss to develop a code to study 3-D diffusion problems.

O. Betancourt

2. Magnetohydrodynamic Theory

The purpose of this research is to gain understanding of the stability of conducting fluids and plasmas in magnetic fields. In particular, attention has been given to "ballooning", or pressure-driven instabilities, and tearing modes, which involve magnetic field line reconnection. Both analytic and numerical approaches are taken. Nonlinear, three-dimensional equations of motion, based on orderings in parameters such as toroidal aspect ratio, have been derived and solved numerically. Other analytic work includes the study of tearing modes with resistivity models appropriate to realistic plasmas. The research results can be applied to understanding plasma physics experiments performed for DOE on tokamaks and stellarators, and may also be used to predict the effects of substantially raising the plasma pressure in such devices, as would be necessary for commercially viable fusion reactors.

During the past year, the high beta tokamak equations were expanded to higher order. Computational studies of the tearing mode with finite pressure, "ballooning" effects, began. A study was made of the stability of stellarators to pressure-driven MHD modes.

H. R. Strauss

3. A Random Choice Finite-Difference Scheme for Hyperbolic Conservation Laws

In this scheme we modify the random choice method of Glimm by replacing the exact solution of the Riemann problem with an approximate finite difference approximation. Our modification resolves discontinuities as well as Glimm's scheme, but is computationally more efficient and is easier to extend to more general situations.

In the course of analyzing our method we estimate the probability of gross error by the random choice method; this estimate is a great improvement on the (alarmingly) high previous estimates.

Glimm's random choice method is a semi-analytical technique for calculating discontinuous solutions of hyperbolic systems of conservation laws. The main advantages of the method for numerical calculations are the sharp resolution of discontinuities and absence of over and undershoots. Chorin has pointed out that these features were decisive for calculations of combustion problems, and has made significant use of the method for these problems.

A drawback of the method is the need to solve exactly many Riemann problems. This is a time consuming procedure and furthermore stands in the way of extending the method to situations where exact solutions are not available. Our goal is to show how to replace the exact solution of the Riemann problem by an approximate one while retaining the advantages of Glimm's method.

Many Department of Energy projects are concerned with the calculation of flows with shock waves, apart from weapon design and

weapon effects, these include the flows in combustion and the propagation of detonation waves.

P. D. Lax

4. Numerical Techniques for Multiphase Fluid Flows

We have devised new numerical procedures for studying multiphase fluid flow problems. These problems are usually characterized by the occurrence of shock fronts at which physical quantities are discontinuous. Such discontinuities cause considerable difficulty for standard numerical methods. The new techniques give high resolution at shock fronts with no numerical diffusion, and even highly-fingered unstable shocks can be studied.

We have used the random sampling method with good results provided that the spatial grids are aligned with the fluid flow direction, which usually requires a change of coordinates. A shock tracking scheme gives excellent results even in problems with very high fluid mobility ratios. Applications of these methods have been made to secondary and tertiary oil recovery and to gas dynamics.

A closely associated problem is the development of efficient accurate equation solvers for elliptic boundary value problems where the elliptic equation has coefficients which are discontinuous along a curve. Such a solver has been developed using finite element techniques.

A large variety of physical processes can be described as multiphase flows. Examples are the secondary recovery of residual oil from reservoirs by the injection of brine or other fluids and the extraction of uranium by chemical leaching. These flows typically involve one or more interfaces separating different media or phases. At such interfaces physical quantities may be discontinuous, for example, pressures, densities, or velocities. These discontinuities cause serious difficulty for the mathematical modeling of such processes.

The usual finite difference methods of numerical analysis assume that the relevant state variables are continuous over the region of interest. Historically, the normal approach to these problems has been to add to the equations an extra diffusion term which has the effect of smearing out any discontinuities. The state variables are then continuous and so the classical techniques apply. While many physical processes do involve diffusion, frequently the amount of physical diffusion is far smaller than would be described by the diffusion term necessary for the finite difference methods. For example, in many oil reservoir computations the physical diffusion is too small to be seen even on a 100 by 100 spatial grid.

The Uniform Sampling Method of Glimm and Chorin is capable of giving very high resolution of discontinuities with no diffusion. In a series of papers we have demonstrated the usefulness of the method in the context of secondary oil recovery and of gas dynamics. This method was first applied to such problems by Concus and Proskurowski. As has

been pointed out by A. Majda, the Uniform Sampling Method in higher dimensions introduces an effective numerical dispersion if the spatial grid is not aligned with the fluid flow. Thus a crucial aspect of our sampling procedures has been to first choose a suitably oriented grid by using a coordinate transformation.

Shock tracking schemes associate extra degrees of freedom with discontinuity fronts as well as with the fluid volume. These shock points may be propagated very accurately by moving them along characteristics. In our shock tracking method sufficient geometrical information is retained to fully resolve the shock even on a subgrid level. These methods have proven very successful when applied to typical oil reservoir simulation problems.

Ellipic partial differential equations describe the pressure distribution in incompressible fluids. In multiphase fluid flows the coefficients of these equations are likely to be discontinuous across shock fronts. In some of our applications the coefficients of the pressure equation were discontinuous by factors of up to 100. Thus it is essential to have accurate elliptic solvers for such problems. In particular, for shock tracking schemes the fluid velocities are required exactly on the shock fronts. We have recently developed an elliptic solver well suited to such problems. It utilizes linear finite elements, piecewise continuous on triangles. The grid is chosen to be as close to rectangular as possible except near the discontinuity curves where grid points are placed on the curve in such a way that no triangle is intersected by the curve. The algorithm used allows even highly fingered curves to be fitted very closely by triangle edges, but with the triangle nodes retaining a simple one to one correspondence with points of a regular rectangular mesh.

An associated aspect of this work is the use of advanced tools for software development. We have used a high-level efficient programming language, C, which has the capability of calling FORTRAN subroutines if desired. This has speeded up program development and maintenance enormously. Equally important has been the software development environment and powerful utility programs of the UNIX operating system. Final production codes can be translated into FORTRAN.

O. McBryan

5. Numerical Methods in Fluid Dynamics

a. A two layered shallow water model has been formulated for the atmosphere, in order to study the rare occurrence of unusually high winds on the downstream (lee) side of mountains (at Colorado Springs, Boulder, etc.). When the Lax-Wendroff scheme is used with a von Neumann-Richtmyer artificial viscosity term restricted to apply only in "compression" regions, it is found that for certain wind speeds spurious disturbances arise from a point on the upstream side of the mountain with one stationary characteristic. At this point the basic scheme is not dissipative. It is possible to avoid this defect in three different ways: (i) eliminate the restriction on the use of the pseudo-viscosity term, (ii) use a hybrid scheme, and (iii) use a filtering method. The three methods yield the same solution and thus

provide us with a means to satisfactorily forecast the occurrence of strong winds on the lee side of mountain ranges.

b. In progress is the study with Alvin Bayliss and Michael Ghil of how to introduce "nonreflecting" boundary conditions at artificially introduced boundaries. In particular, we are examining the primitive equations of meteorology in order to determine how best to introduce a "top" to the atmosphere at a finite height.

c. Also in progress is the study of how best to introduce incomplete and inaccurate observations of atmospheric data (e.g. from satellites) into a numerical forecasting procedure so as to produce better predictions. This work is being done with M. Ghil, K. Bube, S. Cohn, and J. Tavantzis.

These problems are unconventional, but important in developing general techniques for treating fluid dynamical flows in engineering applications.

E. Isaacson

6. Quantum Many-Body Systems

Our work is directed at exploration of computational methods in quantum many-body problems. The scientific problems are drawn from low temperature physics (properties of helium fluids and crystals), from nuclear physics (properties of neutron and nuclear matter), and from chemistry (properties of large molecules). We have succeeded in producing methods and results which are computationally and physically more nearly exact than has been done before.

The calculations are formulated explicitly as many-body simulations and are in turn of two types. In variational calculations, trial functions which approximate either ground state wave functions or density matrices are formulated and used in variational principles. The resulting many dimensional integrations are carried out by Monte Carlo mehods. Exact methods use integral equation formulations equivalent to the Schrodinger or Bloch equations; these integral equations are solved by different Monte Carlo methods.

This research is important for fundamental understanding of quantum fluids and crystals including effects of superfluidity. There are physical and chemical systems that exhibit quantum mechanical effects on a bulk level. For example, the behavior of liquid helium at low temperatures is a direct consequence of quantum effects. Superconductivity of electricity is another example that directly relates to energy technology. Quantum many-body investigtions impact significantly upon chemistry through the study of atomic forces and methodologically upon problems in astrophysics, in nuclear physics, and in the theory of electrons in solids.

Our survey of existing two-body potentials for helium using the GFMC code was completed. The HFDHE2 potential proposed by Aziz et al. gives an excellent description of condensed helium when three-body potentials are neglected. Analysis has begun on the triplet

correlation function in condensed helium. The testing of the Schwinger variational method for the Bloch Equation was completed and was found satisfactory except for the estimation of the kinetic energy. The GFMC method was applied to model three-body fermion systems.

Monte Carlo calculations explicitly employing triplet correlations in the variational wave function for the ground state of ^{4}He were carried out. A significant lowering of energy was obtained, accounting for 75% of the discrepancy between previous Jastrow variational calculations and the known exact numerical results. The density dependence of the energy was improved and the pair correlation function sharpened leading to much better agreement with the exact ground state.

Using the HFDHE2 potential between helium atoms and a new graphite-helium interaction, variational calculations of helium films were undertaken. Previous purely two-dimensional calculations give a good representation of our new results for submonolayer coverages. At higher densities multilayer structure is observed consistent with experimental observation.

Variational wavefunctions for fluid ^{3}He have been improved by the inclusion of symmetric triplet correlations and backflow orbitals in the Slater determinant. These -- especially the latter -- lower the ground state energy by about 0.6 K to -1.6 K at $\rho\sigma^3 = 0.277$, the experimental equilibrium. We have begun to experiment with a naive version of GFMC for this problem. This method has the disadvantage that the accuracy falls off with computing time as $(\log T)^{-1/2}$ rather than the usual $T^{-1/2}$. At intermediate times an estimate of the ground state energy can be made; our preliminary result is -2.2 ± 0.3 K, much closer to experiment.

Work continues on a more robust algorihm for this problem.

M. H. Kalos et al.

7. Modeling of Alloys

This research deals primarily with the properties of matter that is not in thermodynamic equilibrium. In solid systems we are principally concerned with the development of grains in alloys quenched from the melt. This is of great importance since the metallurgical properties are determined in large part by the imperfections that develop. Two kinds of phenomena seem to be involved. One is classical nucleation and growth in which clusters form and grow at the expense of smaller clusters and isolated atoms. Another is "spinodal decomposition" in which random composition is unstable against the formation of macroscopic zones of different compositions. In the liquid vapor system, nucleation -- usually with the help of impurity nuclei -- is responsible for the formation of rain and aerosol droplets.

Our primarly tool of investigation is computer simulation of atomic models with some form of dynamics that drives the system toward equilibrium. Of necessity, the thermodynamics of these systems must be investigated when they are not adequately known. For alloy systems, we

use Kawasaki kinetics in which adjacent atoms are exchanged when such a change is energetically favorable. For fluid systems, specific atomic force laws are used along with molecular dynamics as an algorithm.

In FY 1980, we have investigated, via Monte Carlo computations, the phase diagram of an ordering binary alloy -- equivalent to an Ising spin system -- on an fcc lattice with nearest and next-nearest neighbor pair interactions:

$$H = J \sum_{nn} \sigma_i\sigma_j - \alpha J \sum_{nnn} \sigma_i\sigma_j, \quad \sigma_i = \pm 1, \; J > 0.$$

Our studies indicate that this system undergoes a first order transition, i.e., there is a discontinuity in the energy and order parameters as a function of temperature, for values $-1 \lesssim \alpha \lesssim 0.25$. For larger values of $|\alpha|$, the transition appears to be continuous without any metastable states.

We have carried out novel computer simulations of the time evolution of an ordering model binary alloy following quenching from a disordered state at a high temperature. The results are interpreted using ideas of Lifshitz and of Cahn and Allen; the ordering process is described by a kinetic equation for the motion of the walls separating domains with different orderings. The characteristic length increases as $t^{1/2}$, and the structure function scales as $k^{1/2}t$.

The time scaling for the structure function of segregating alloy that was discovered last year has been found to apply to all our simulation data for quenches in the coexistence regime. In addition, recent experimental data on Au-Pt and Al-Zn alloys as well as light scattering in binary liquid mixtures were shown to exhibit the same regularity.

M. H. Kalos

8. Polymer Systems

We study the behavior of individual polymers and of systems of polymeric molecules by setting up simplified models of chain molecules. We use models that have enough of the features of real polymers to prevent their mathematical solution by purely analytical methods, but not so many that they apply to only a few special systems. We expect that the properties found will be broadly characteristic, and we are particularly interested in the limit of very long chains.

The major tool of our investigation is computer modeling, and we use three classes of algorithms: Monte Carlo methods for the equilibrium properties of polymer ensembles, Monte Carlo methods for the solution of certain stochastic dynamical models, and molecular dynamics for the investigation of strictly atomic models. These models are complementary. In particular, the first furnishes an economical algorithm for providing sets of initial conditions for the second two.

As always, we are interested in technical questions as well as getting numerical results. Currently, we are investigating the properties of a method called reptation in which chain molecules move at random in a snakelike fashion.

Better theoretical understanding of conformational and dynamic effects in polymers is needed in their use as structural materials and in studies of biological macromolecules.

During 1980 we carried out additional simulations and analyses to elucidate the nature of the transition to a collapsed phase in dilute polymer solutions. We used new, more efficient Monte Carlo methods to investigate the response of long chains to stretching forces and the scaling properties of the distribution function of the end-to-end vector in the good and poor solvent regimes.

We began the study of time dependent properties of polymer solutions.

A new exact and efficient Green's function method for the Monte Carlo integration of the Smoluchowski equation was discovered.

M. H. Kalos

9. Quantum Chemistry

Recently, a new program was initiated to simulate a many-fermion system by a Monte Carlo variational method. This research will aid the development of compact and accurate correlation functions for many electron atomic and molecular systems. The principal advantage of the method is that the inter electronic distance, r_{ij}, may be included directly in the wave function without adding significant computational complexity. In addition, other quantities of physical and theoretical interest such as electron correlation functions and representations of coulomb and fermi "holes" are very easily obtained.

In FY 1980 the Monte Carlo evaluation of electronic energies was carried out. Results were obtained for He, H_2, and Li_2. Those for Li_2 were particularly noteworthy in that an accurate energy (well below the Hartree-Foch limit) was obtained using a rather simple correlation function inaccessible to conventional quantum chemistry methods.

M. H. Kalos

10. Chemical Kinetics

This research deals with the computer simulation of the individual collisions of atoms and molecules that result in chemical reactions. One approach to this problem that will be used is to numerically solve the classical equations of motion for the reaction of interest. Initially, the types of reactions studied will be collisions between atoms and molecules in the gas phase. We will be particularly interested in reactions that are believed to occur in combustion systems.

The considerable interest in the elementary reactions that occur in combusting systems stems from the desire to understand and be able to model these systems on the molecular level. The rate constants of the component reactions are often not accessible to experimental measurement, so a computer calculation can be of great assistance in giving estimates of unknown rate constants. Other types of information available from a trajectory calculation are differential cross sections of the scattered product, vibrational-rotational distributions of the products, the activation energy to reaction, and whether vibrational enhancement of the reaction rate occurs.

The detailed understanding of macroscopic chemical reactions, for example, those in combustion systems, requires elucidation of the reaction mechanisms at the microscopic level. Through these calculations predictions have been made both on systems accessible to experiment and on important intermediate step reactions that as yet cannot be observed.

During FY 1980, the reactions

$$C(^1D) + D_2 \rightarrow CD + D$$

and

$$C(^1D) + HS \rightarrow \begin{matrix} CH + D \\ CD + H \end{matrix}$$

were investigated at a collision energy of 2.88 k cal/mole. Both mass effects and properties of collision complexes were studied in great detail.

A preliminary, one-dimensional study of vibrational enhancement in the reaction $O(^3P) + H_2$ was completed. The three-dimensional trajectory code is being modified to introduce importance sampling into the Monte Carlo evaluation of the rate integral.

Work has started on an investigation of the ion molecule exchange reaction

$$H_3^+ + D \rightarrow H_2D^+ + H \ .$$

The reaction involves several potential energy surfaces with charge exchange as well as reaction occurring. We are particularly interested in the affect of reactant vibrational energy on product vibrational and translational distributions.

Future emphasis will be on simulating reactions in quantum many body systems by Green's function Monte Carlo. Preliminary work on the algorithm should begin in FY 1981.

P. A. Whitlock

II. ADVANCED COMPUTER CONCEPTS

A. Software Engineering

1. PUMA Operating System (POS-II)

Work on the second version of the PUMA Operating System (POS-II) is now almost completed. POS-II is a major new version of the POS-I operating system which is being used to run jobs on the PUMA.

POS-I was the initial operating system written to allow jobs to run on the PUMA. It was written as one large program to run on the PDP-11 and simulate requests and commands of the NOS operating system. It enables many programs which execute under NOS on the 6600 to execute on the PUMA and has been in use for over a year. However, it does not support enough of the requests of NOS to allow program compilation and development.

To allow more varied use of the PUMA, a new operating system, POS-II, was developed. This operating system is composed of multiple tasks which are analogous to the PP programs on a 6600 running NOS. These tasks are synchronized by the RSX11-M operating system running on the PDP-11. Because of the flexibility afforded by this approach, these tasks are able to implement a much larger number of operating system requests. Specifically, enough of the NOS system requests are supported to allow the FORTRAN compiler and loader and miscellaneous system utilities such as COPY and UPDATE to execute. Also, all of the control statements which POS-II supports will be executed by the same central program which provides that function under NOS, thus assuring compatibility at the control statement level in addition to the system request level.

In addition, because of the flexibility of the RSX11-M operating system, multiple jobs can be run concurrently on the PUMA although minimal scheduling will be provided initially.

Most of the code required for POS-II has been written and debugged. We now are able to run multiple copies of a batch job which compiles, links, and executes a benchmark program simultaneously.

Most of the remaining work involves adding support for some system calls whose need we did not anticipate and adding a rudimentary accounting system. In addition, we plan to develop utilities to allow easy use of the system by its users and to allow use of the PUMA by users on the VAX by use of DECnet.

J. T. Schwartz

2. Architecture and Software of Large-Scale Parallel Computer Systems

The Courant Institute has recently undertaken a substantial research effort in the area of large parallel computer systems. We are studying a number of scientific application codes, converting them to parallel programs and investigating the effect of alternative architectures and programming styles on their performance. We have

also studied a number of more fundamental algorithms and their relation to parallel architectures, particularly the processor interconnection networks. Much of our work focused on the use of the "perfect shuffle" network as a processor interconnection network.

Our involvement with the project has been in assisting in the development of the parallel simulator and emulator and in preparing designs for a small-scale parallel processor array. A parallel simulator is currently operational and being used to debug and evaluate some small scientific applications. A microprogram which will enable the PUMA to emulate an array of parallel processors is currently being prepared; this emulator will make use of the PUMA writeable control store, which was recently completed. The effort of designing a small parallel processor array, to test our hypotheses for hardware and software design, has just started, so only the most preliminary of designs have been prepared.

R. Grishman

3. Data Flow Analysis Techniques for Program Test Data Selection

We have developed a family of software test data selection criteria incorporating data flow analysis techniques. Whereas these techniques are commonly used in compiler optimization, program test data selection criteria have generally relied solely on the program's control flow. In general, a progam is considered adequately tested provided a set of test data has been developed which fulfills the stated criterion and such that each input in the set has yielded the correct output.

We are currently comparing the cost and effectiveness of test data selection criteria based solely on the program's control flow and our newly defined criteria. Since our criteria properly subsume these standardly used criteria, we are interested in trying to characterize the types of errors our criteria are able to reveal which are not exposed by the usual criteria. In addition we are considering the cost in terms of additional tests needed to fulfill our criteria.

E. Weyuker

B. Distributed Systems

1. Distributed Systems and Resource Sharing

This activity focuses on the implications of a geographically dispersed, multicomputer environment on communities of scientific users. The role of the small computer in large scale computational modeling is also being studied.

The approach being taken is essentially experimental and consists of: (a) providing a variety of computer facilities to the CMCL community of users; (b) acquiring and devising means to easily enable communication among the various hardware and software elements comprising the collections of facilities; (c) discovering and

implementing access methods that reduce the impact on the user of the complexity inherent in multicomputer environments.

A network consisting of the VAX-11/780 and four PDP-11 computers has been configured. The PDP-11 systems provide paths to the ARPANET, the on-site CDC-6600, and the locally developed PUMA computers which are CDC-6600 emulators. Thus program development, analysis of results, and job execution may be separately assigned to the various systems by the user.

The implementation of the second version of the PUMA operating system (POS) is near completion. Although POS can run independently, the design assumes that it will exist in a multicomputer environment and that the user will distribute his task over more than one system. Thus the full range of operating system facilities need not be available on the PUMA itself.

A 300 megabyte disk storage unit has been connected to the PUMA PDP-11 satellite. In addition to providing on-line storage for PUMA use, this disk is used for staging data to the VAX-11/780 through the communication network.

Early analysis and planning for an advanced system interconnection method has been started.

E. Franceschini and M. Goldstein

2. Systems Programing and User Services: CDC-6600

a. Software Maintenance

Software maintenance took the form of installation of corrective code provided by software suppliers, trouble shooting system failure, diagnosing and correcting program errors, and designing and implementing modifications for improved system performance. The major systems and programs maintained were:

NOS Operating System
Remote Entry System
Telecommunications control software
Indiana Univesity permanent file management system
Graphics subroutine packages and utilities
NYU library of subroutines and utility programs
DAP cross-assembler for Honeywell series 16 minicomputers
Compilers for various languages, e.g., FORTRAN, BASIC, ALGOL, SNOBOL, LISP.

b. User Services

Expert help is available to provide education, advice, and aid in diagnosing computational problems.

System bulletins are issued to provide users with important information in a timely manner.

A library of user supplied programs is maintained to facilitate interuser exchange.

Documentation of programs and subrouties available at the Laboratory is kept in machine readable form for ease of maintenance.

E. Franceschini and M. Goldstein

3. Systems Programming and User Services: VAX-11/780

a. Software Maintenance

Software maintenance consisted of installation of corrective code supplied by Digital Equipment Corporation (DEC) and installation of a completely new version of VMS, DEC's VAX operating system, along with several DEC product offerings. Study and experimentation were devoted to configuring the VMS operating system parameters to provide efficient service and resource utilization. In particular, a "field test" version of DEC's network support product, DECnet, was installed and currently is being evaluated. In addition, locally-developed products, such as a powerful electronic mail system and an adequate disk backup facility were written and made operational. (These developments are mentioned here because they represent direct extensions to or replacements of standard operating system facilities.) A commercially available version of the C Programming Language was installed; initial testing and modification made it rapidly operational.

b. Software Development

Continuing effort has improve the VAX-to-ELF (ARPANET) interface, and a new, higher-speed, more reliable interface is being implemented.

The LBL version of the "Software Tools" was installed with several substantial improvements.

Preliminary design of an enhanced accounting and accounts management system for VMS was begun.

c. User Services

Users of the VAX were provided with advice, direct assistance, and limited informal education. Timely operational and systems bulletins were delivered to users via the mail system mentioned above. Direct cooperation was encouraged among users in the areas of program- and data-sharing, interchange of experience and expertise, and cooperation in the use of resources. VAX/VMS operating system facilities and the locally-developed mail system support well such cooperation.

E. Franceschini and M. Goldstein

C. High Performance Systems

1. Studies of Large Scale Parallel Computation

We have continued our studies of highly parallel architectures and associated software systems. Our software considerations have begun to be influenced significantly by study of an interesting architectural proposal made by Burroughs Corporation to the NASA Ames Laboratory, which envisages a machine more like our 'paracomputer' than our 'ultracomputer' model of parallelism. Shuffle-based ultracomputer algorithms supporting important paracomputer primitives have been found by our group, and we are beginning to shape a view of some of the architectural details of an ultracomputer/paracomputer. A series of software simulations of parallel variants of several important scientific applications, taken from the normal CIMS job stream, has begun.

These studies, if successful, will prepare for the construction of super-large computers attaining floating instruction rates measured in the tens of billions of instructions per second.

J. T. Schwartz

2. Computer Systems Design Automation

Over the past several years we have developed a powerful set of tools for the specification, simulation, automatic wiring, and testing of large digital systems. In order to exercise these tools and to augment the computing power of our laboratory, we designed a moderately-large-scale scientific computer system, the PUMA. This processor is code compatible with the Control Data 6600 central processor, and executes at 40-80% of the speed of the 6600, depending on the code being run. In addition to the prototype, two processors have been completed to date; one is currently running production, while the other is being used for operating system and hardware development.

The main addition to the PUMA is a writeable control unit, which was designed, constructed, and tested this year. Concomitant improvements in the microprogram assembler and other PUMA utility software have also recently been completed. This new control unit will facilitate use of the PUMA by Brookhaven National Laboratories with their emulated peripheral processors. It will also enable us to use the PUMA as an emulator for parallel processor arrays, as part of our research into the architecture and software of highly parallel systems.

R. Grishman

III. RELATIONSHIP TO OTHER PROJECTS

A. DOE Laboratories and Contractors, Government Agencies, Industry, Universities, and International Entities

O. Betancourt

Close collaboration continues with the Wisconsin stellarator group headed by J. L. Shohet. This includes collaboration on the design of a future stellarator at Wisconsin. We also continue, and in the near future will expand, collaboration with ORNL to study 3-D problems. We have just begun developing contacts with Japanese scientists, specifically Wakatani and Uo in Kyoto and Nagao in Sendai. In October 1980 we participated in the Japan-USA Stellarator Workshop. Fruitful dialogue continues with German scientists at Garching, including Nuhremberg and Wobig.

R. Burridge

Extensive interaction with the oil industry and with Bell Telephone Company.

S. Z. Burstein

Consultation continues with P. Crowley and W. Nah of LLL.

E. Franceschini and M. Goldstein

Our consideration of the user impact of distributed systems is closedly related to research in command languages for distributed systems at LBL. The work on advanced interconnection methods is allied to work being undertaken by DARPA. We are working with the Naval Laboratories Committee on Computer Networks (NALCON) in certain specific aspects of the interconnection protocol effort.

R. Grishman

Close contact with BNL in the development of an emulator for CDC 6600 peripheral processors, to be used in conjunction with the PUMA. This emulator will permit the use of unmodified Control Data operating systems on the PUMA. A PUMA just delivered to BNL will be coupled to the peripheral processors being built there.

M. H. Kalos

Kalos' team maintains contacts with B. Alder and D. Ceperly, LLL; J. Cahn, I. Sanchez and P. H. Verdier, NBS; L. Campbell, IASL; J. T. Muckerman and P. Kroger, BNL. Innumerable exchanges

take place with industry and with academic institutions both here and abroad.

P. D. Lax

Active in the following: Advisory Committee, ICASE, NASA-Langley Research Center, Hampton, Va.; Visiting Committee for Mathematics, Harvard University; T-Division Advisory Committee, LASL; Computer Science Department Committee, Stanford University; ORNL Committee; Advanced Code Review Group, NRC; National Science Board member. The work "On the Notion of Hyperbolicity" would be of interest to researchers in two-phase flow as applied to reactor accidents; such work is sponsored by DOE and NRC at LASL, BNL, Idaho Laboratory, and EPRI. The work with A. Harten on hyperbolic conservation laws is relevant to the combustion research conducted by A. Chorin at LBL, P. Colella at LLL, researchers at LASL, and NASA researchers at AMES and Langley.

O. McBryan

Much of the research on multiphase flows has been done jointly with J. Glimm and E. Isaacson, Rockefeller University, and D. Marchesin, Pontificia Universidade Catolica do Rio de Janeiro. Currently, we are working closely with D. Sharp, Theoretical Physics Division, LASL. Close ties exist with several oil corporations, for example, Exxon and Chevron, that are interested in the more applied aspects of the work. Contact with various university research groups working on similar problems, for example, at the University of Chicago, Univesity of California, Berkeley, and Rice University.

M. Overton

Collaboration with W. Murray, systems Optimization Laboratory, and G. Golub, Computer Science Department, both at Stanford University.

R. D. Reitz

Information exchanges with DISC Engine group, the cooperative effort between government laboratories and General Motors Corp. Collaboration is anticipated with the DOE supported team headed by F. V. Bracco at Princeton, which carries out experimental and theoretical studies of multidimensional internal combustion engine modeling.

J. T. Schwartz

Our parallel architectural concepts were presented during the past year in lectures given at LLL and at LASL, and have served to heighten awareness of the possible applications of parallel computing there. Lectures on our work were delivered during June at NASA Goddard, and

found to be of active interest by their picture processing and simulation groups. Active contact has also been maintained with the FMP group at Burroughs Corporation, and the large Systems Architecture group at IBM Research. Presentations of our work were made at MIT, at Rutgers Univesity, at the University of Manitoba in Canada, and at a NASA Langley organized Symposium on Large Scale Computation.

H. R. Strauss

The MHD theory research is closely related to DOE projects in controlled fusion and is carried out in part in collaboration with workers at the Plasma Physics Laboratory at Princeton, at the MFD Division at the Courant Institute, and at the Fusion Research Center at the Univesity of Texas, Austin.

O. Widlund

In the DOE community, contacts are maintained with the numerical analysis group at Stanford University, in particular Gene Golub; at Berkeley with A. Chorin, O. Hald, and P. Concus; at the Univesity of Texas, Austin, with D. M. Young; at ORNL with D. Scott and P. Gaffney; at LASL with B. L. Buzbee. The capacitance matrix methods we have developed are used by industry. Contacts are maintained with J. Cooley, J. Cullum, and R. Willoughby, IBM Laboratory at Yorktown Heights. Exchanges continue with H. Kreiss, Cal. Tech.; I. Babuska, D. P. O'Leary, and B. Kellog, University of Maryland; Computer Science Departments in Stockholm and Uppsala Universities, Sweden; R. Glowmiski and B. Mercier, INRIA, Paris. Collaboration continues with W. Proskurowski, University of Southern California.

B. Courant Institute and New York University

The Laboratory has many ties with other research groups within the Courant Institute and New York University. The interrelationships take the form of reciprocal theoretical support, sharing of computational expertise and resources, and the training of personnel to apply advanced mathematical and computer methods. Within this purview the Laboratory has lent support to the following projects and researchers:

1. Courant Institute

Stochastic Aspects of Atmospheric Behavior	M. Ghil
Shock Formation in Gas Pipelines	D. Marchesin and P. J. Paes-Leme
Flow Patterns Around Heart Valves	C.S. Peskin, D.M. McQueen and A. Wolfe
Regulation of Ovulation Number in Mammals	C.S.Peskin, H.M. Lacker and J. Percus
Renal Control Mechanisms	C.S. Peskin and E. Kourou
Combinatorial Geometry	R. Pollack
Application of Ray Theory to Ship Waves	L. Ting

2. New York University

Employing Vaporized Fuel for the Enhancement of the Hydrocarbon Efficiency	A. Agnone
Theoretical Computation of Nucleic Acid Conformations by Classical Potential Energy Methods	S. Broyde
Non-Additive Contributions to Preferred Orientations of Water Molecules	E. Campbell
Bed Expansion and Heat Transfer Modeling and Correlation Studies in a Pressurized Coal Fired Fluidized Bed	G. Miller
The Development of Accurate and Compact Correlation Functions for Many Electron, Atomic, and Molcular Systems	J. W. Moskowitz
Organic Chemistry in Interstellar Clouds	Y. E. Rhodes
Linguistic String Project	N. Sager
Model of the World Economy	D. B. Szyld
Theoretical Studies of Carcinogens	C. Underwood

C. Resource Sharing: CDC 6600 Computer System

The Laboratory maintains and operates a CDC 6600 computer system. Excess time on the 6600 is made available to other DOE contractors and government agencies.

During FY 1980, time available on the 6600 was allocated as follows:

Courant Institute/DOE	82.1%
DOE Research Divisions	3.5
NYU/Federal Government Affiliations	3.2
Other Universities/Federal Government	4.8
Federal Government Agencies	6.4
	100.0

About 35 non-DOE Federal agency contractors were allocated 1600 hours of computer time as follows:

Defense Nuclear Agency (DNA)	11.0%
Environmental Protection Agency (EPA)	5.2
National Aero. Space Admin. (NASA)	8.2
National Cancer Institute (NCI)	13.7
National Institute of Health (NIH)	5.7
National Science Foundation (NSF)	19.8
Office of Naval Research (ONR)	17.0
All Others	19.4
	100.0

IV. SEMINARS

During FY 1980, CMCL sponsored a series of seminars in Numerical Analysis and in Computer Science. The topics and speakers follow:

Numerical Analysis Seminars

"Adaptive Zoning of the Computational Mesh"
J. Brackbill
CIMS
Oct. 5, 1979

"On the Coupling of Boundary Integral and Element Methods"
C. Johnson
Chalmers Institute of Technology, Göteborg, Sweden
Oct. 12, 1979

"Application of a Multigrid Alternating Direction Method to Transonic Flow Calculations"
A. Jameson
CIMS
Oct. 19, 1979

"Implicit Versus Explicit Schemes for Meteorology"
E. Isaacson
CIMS
Oct. 26, 1979

"Boundary Conditions for Elliptic Problems in Exterior Domains"
A. Bayliss and E. Turkel
ICASE and CIMS
Nov. 2, 1979

"Radiation Boundary Condition for Seismology and Unsteady Transonic Flow"
A. Majda
University of California, Berkeley, and CIMS
Nov. 9, 1979

"Reactive Systems with and Without Diffusion"
A. Chorin
University of California, Berkeley
Nov. 16, 1979

"Reliable Error Estimates and Adaptive Procedures in the Finite Element Method"
I. Babuska
University of Maryland
Nov. 30, 1979

"The Finite Element Method with Mesh Refinement for Unbounded Domains"
C. Goldstein
Brookhaven National Laboratory
Dec. 7, 1979

"Difference Methods for Initial-Boundary-Value Problems and Computation of Flow Around Bodies"
Yu Lan Chu
Chinese Academy of Sciences
Dec. 14, 1979

"Large Unsymmetric Sparse Eigenvalue Problems"
F. Chatelin
Grenoble University
Feb. 15, 1980

"A Random Choice Finite-Difference Scheme for Hyperbolic Conservation Laws"
A. Harten
Tel Aviv University
Feb. 22, 1980

"Fractional Step Methods for Multidimensional Two-Phase Flow"
B. Stewart
Brookhaven National Laboratory
Feb. 29, 1980

"Structure and Instability on the New Minimal Fourier Transform Algorithms"
E. Feig
CUNY
March 7, 1980

"Computing the Shape of a Slender Stream of Fluid"
J. Strikwerda
ICASE
March 14, 1980

"The Infinite Element Method"
Ying Lung-An
Peking University and CIMS
March 21, 1980

"Point Cyclic Reduction Methods"
E. Detyna
University of Reading, England
April 11, 1980

"Equidistributing Meshes with Constraints"
J. Kautsky
Flinders University of South Australia
April 18, 1980

"Sparse Matrix Calculations and Their Application to a Model of the World Economy"
D. B. Szyld
CIMS
April 25, 1980

"Curve Fitting by Cornu Spirals"
J. Stoer
University of Wurzwig and National Bureau of Standards
May 2, 1980

"Computable Error Bounds for Linear Systems"
G. Golub
Stanford University
May 9, 1980

"Optimization Algorithms Based on Rational Approximation"
J. Nocedal
University of Mexico and CIMS
May 16, 1980

Computer Science Seminars

"Minimax and L_1 Approximation Problems and Relations with Mathematical Programming"
M. Overton
CIMS
Oct. 5, 1979

"Problems of Industrial Robots"
J. Meyer
T. J. Watson Research Center IBM
Oct. 11, 1979

"Computing in China: A Report of a Year at Qunghua University, Peking, China"
E. Chi
CUNY
Oct. 19, 1979

"Practical Simplification"
D. C. Oppen
Stanford University
Nov. 2, 1979

"Choosing an Efficient Storage Structure"
F. Tompa
University of Waterloo
Nov. 9, 1979

"Bounds on the Performance of Communication Protocols"
N. Pippenger
T. J. Watson Research, Center, IBM
Nov. 30, 1979

"An Abstract Theory of Machines"
S. Amoroso
Fort Monmouth, N. J.
Dec. 7, 1979

"On Specifying Verifiers"
V. Pratt
MIT
Dec. 14, 1979

"Algorithmic Information Theory and Foundations of Probability Theory"
L. Levin
MTI
Feb. 8, 1980

"Three Directions of General Computational Complexity Theory"
L. Levin
MIT
Feb. 8, 1980

"Asymptotic Analysis of the Gatlinburg Seating Problems"
B. Aspvall
Stanford University
Feb. 12, 1980

"Sensitivity Analysis of Combinatorial Optimization"
D. Fusfield
University of California, Berkeley
Feb. 22, 1980

"Statistical Analysis Using Partitioned Data Bases"
M. Blattner
National Science Foundation
Feb. 25, 1980

"Applications of a Cellular Decomposition Algorithm to Logic Mathematics and Computer Graphs"
D. Arnon
University of Wisconsin
Feb. 27, 1980

"On Reliability in Loosely Coupled Systems"
S. Smoliar
General Research Corporation
March 4, 1980

"Generalized Network Flows with an Application to Multiprocessor Scheduling"
C. Martel
University of California, Berkeley
March 7, 1980

"Isomorphism for Graphs Embeddable on the Projective Plane"
D. Lichtenstein
University of California, Berkeley
March 10, 1980

"Finite Reversal Multicounter Machines"
Tat-Hung Chan
Cornell University
March 12, 1980

"Alternating Multihead Finite Automata"
K. N. King
University of California, Berkeley
March 14, 1980

"Program Verification and user Defined Data Types: New Developments in the Cornell Program Verifier"
R. Constable
Cornell University
March 14,19,21, 1980 (Parts 1,2,3)

"Network Reliability Analysis"
R. Van Slyke
Network Analysis Corporation
March 24, 1980

"Optimum Coalesced Hashing"
J. Vitter
Stanford University
March 25, 1980

"Algorithm Analysis to Reduce Interconnection Complexity
on Limited Interconnection Networks and VLSI Architecture"
R. Kuhn
University of Illinois at Urbana-Champaign
March 24, 1980

"Preserving Functional Dependencies"
P. Honeyman
Princeton University
April 7, 1980

"A Subexponential Algorithm for Cubic Graph Isomorphism"
M. Furst
Cornell University
April 10, 1980

"Knowledge Insensitive Theorem Proving and Learning"
D. Cohen
Carnegie-Mellon
April 11, 1980

"Organization and Retrieval from Long-Term Episodic Memory"
J. Kolodner
Yale University
April 14, 1980

"Logic as a Computer Language"
R. Kowalski
Imperial College, London
April 17, 1980

"Abstraction and Efficiency: The Interaction of Language and
Analysis"
M. Shaw
Carnegie-Mellon
April 17, 1980

"Expression Procedures and Program Derivation"
W. Scherlis
Stanford University
May 1, 1980

"The Russell Language: A Novel Treatment of Data Types"
A. Demers
Cornell University
May 16, 1980

"The Semantics of the Universal Instance Database Model"
E. Scione
Princeton University
May 20, 1980

"Programming by Transformation"
J. Darlington
London University
May 19, 23, 1980 - Parts 1, 2

V. PUBLICATIONS

1. F. Bauer, O. Betancourt, and P. R. Garabedian.
   Nonlinear Magnetohydrodynamic Stability.
   Physics of Fluids. To appear.

2. F. Bauer, O. Betancourt, and P. R. Garabedian.
   Numerical Studies of New Stellarator Concepts.
   Jour. Comp. Phys. 35:341-355, May 1980.

3. F. Bauer, O. Betancourt, P. R. Garabedian et al.
   Recent Progress in Torsatron/Stellarator Research in the USA.
   IAEA 8th International Conference on Plasma Physics and Controlled Nuclear Fusion Research, Brussels, July 1980.

4. O. Betancourt.
   MHD Equilibrium and Stability for an $\ell = 2,3$ Stellarator.
   Proceedings of International Conference on Plasma Physics, Nagoya, Japan, April 1980.

5. R. Burridge.
   The Gelfand-Levitan, Marchenko, and Gopinath-Sondhi Integral Equations of Inverse Scattering Theory Viewed in the Context of Inverse Impulse-Response Problems.
   Wave Motion, Oct. 1980. In press.

6. E. Franceschini.
   Experiences with Teleconferencing and Electronic Mail.
   Proceedings of U.S. DOE AESOP XXI Conference, Cincinnati, Ohio, May 1980.

7. E. Franceschini.
   Performance of the VAX-11 Computer for Typical DOE Computational Models.
   In preparation.

8. P. R. Garabedian.
   Magnetic Flux Surfaces in a Stellarator Field.
   Jour. d'Anal. Math. 36:44-49 (1979).

9. J. Glimm, D. Marchesin, and O. McBryan.
   A Numerical Method for Two-Phase Flow with an Unstable Interface.
   J. Comp. Phys. To appear.

10. J. Glimm, D. Marchesin, and O. McBryan.
    A Shock Tracking Method for Hyperbolic Systems.
    Proceedings of Army Numerical Analysis and Computer Conference, Moffet Field, Calif., Feb. 1980.

11. J. Glimm, D. Marchesin, and O. McBryan.
Statistical Fluid Dynamics: Unstable Fingers.
Comm. Math. Phys. 74:1-18, June 1980.

12. J. Glimm, D. Marchesin, and O. McBryan.
Unstable Fingers in Two-Phase Flow.
Comm. Pure Appl. Math. To appear.

13. A. Gottlieb and C. Kruskal.
A Data-Motion Algorithm.
Ultracomputer Notes, N.Y.U., Jan. 1980.

14. A. Gottlieb.
Another Remark on the Planarity of the Shuffle-Exchange Network of Sizes 16 and 32.
Ultracomputer Notes, N.Y.U., May 1980.

15. A. Harten and P. D. Lax
A Random Choice Finite-Difference Scheme for Hyperbolic Conservation Laws.
Courant Mathematics and Computing Laboratory, R&D Report, DOE/ER/03077-167, May 1980.

16. E. Isaacson and G. Zwas.
Mountain Winds -- Revisited.
SIAM Jour. on Numerical Analysis, 1980. Accepted for publication.

17. M. H. Kalos et al.
Computer Simulation of Chains in Solution and Bulk State.
Jour. Macro-Molecular Science. In press.

18. M. H. Kalos and K. Binder.
Critical Clusters in a Supersaturated Vapor: Theory and Monte Carlo Simulation.
Jour. Stat. Phys. 22:363-396, Mar. 1980.

19. M. H. Kalos, J. L. Lebowitz, and I. Webman.
Elastic Properties of Polymer Chains.
Phys. Rev. A. Accepted for publication.

20. M. H. Kalos, J. L. Lebowitz, and I. Webman.
Excluded Volume Expansion of Polymer Chains:
A Monte Carlo Study of the Scaling Properties.
Phys. Rev. B, 21, 5540 (1980).

21. M. H. Kalos et al.
Investigations of Static Properties of Model Bulk Polymer Fluids.
Jour. Chem. Phys. 72:3228-3235, Mar. 1980.

22. M. H. Kalos et al.
Kinetics of Order-Disorder Transitions.
Phys. Rev. Lett. 45:366-369, Aug. 1980.

23. M. H. Kalos.
Monte Carlo Methods in Quantum Many-Body Problems.
Nucl. Phys. A 328: 163-168, Oct. 1979.

24. M. H. Kalos, J. L. Lebowitz, and M. K. Phani.
Monte Carlo Studies of an Ising Antiferromagnet into Nearest and Next Nearest Neighbor Interactions on an FCC Lattice.
Phys. Rev. B. In press.

25. M. H. Kalos, J. L. Lebowitz, and I. Webman.
Monte Carlo Studies of a Polymer between Planes, Crossover between Dimensionalities.
Jour. de Physique 41, 579, Paris, 1980.

26. M. H. Kalos.
Recent Developments in Monte Carlo Calculations of Quantum Systems.
Proceedings of the 4th Pan-American Workshop on Self-Consistent Theories of Condensed Matter.
In press.

27. C. Kruskal and L. Rudolph.
Observations Concerning Multidimensional Ultracomputers.
Ultracomputer Notes, N.Y.U., Jan. 1980.

28. P. D. Lax.
On the Notion of Hyperbolicity.
Comm. Pure Appl. Math. 33: 395-397, May 1980.

29. M. A. Lee et al.
Variational Monte Carlo Calculations of Liquid ^{4}He with Three-Body Correlations.
Phys. Rev. Lett. 45: 573-576, Aug. 1980.

30. O. McBryan.
Elliptic and Hyperbolic Interface Refinement.
Boundary Layers and Interior Layers -- Computational and Asymptotic Methods, J. Miller, ed., Boole Press, Dublin, 1980.

31. O. McBryan et al.
Front Tracking for Hyperbolic Systems.
Advances in Appl. Math. To appear.

32. M. Overton and W. Murray.
A Projected Lagrangian Algorithm for Nonlinear L1 Optimization.
Systems Optimization Laboratory Report SOL-80-4, Stanford Univ., Feb. 1980.

33. M. Overton and W. Murray.
A Projected Lagrangian Algorithm for Nonlinear Minimax Optimization.
Systems Optimization Laboratory Report SOL 79-21, Stanford Univ., Nov. 1979. Accepted for publication in SIAM Jour. on Sci. & Stat. Comput.

34. M. Overton with W. Murray.
Steplength Algorithms for Minimizing a Class of Nondifferentiable Functions.
Computing 23, pp. 309-331 (1979).

35. J. K. Percus and O. E. Percus.
Ethical Procedures in Comparative Evaluation of Drugs.
Courant Mathematics and Computing Laboratory, R&D Report, COO-3077-163, Feb. 1980.

36. J. K. Percus et al.
Structure of a Liquid-Vapor Interface in the Presence of a Hard Wall in the Transition Region.
Jour. Chem. Phys. 71: 3802-3806, Nov. 1979.

37. C. S. Peskin and D. M. McQueen.
Modeling Prosthetic Heart Valves for Numerical Analysis of Blood Flow in the Heart.
Jour. Comp. Phys. 37: 113-132, Aug. 1980.

38. C. S. Peskin and M. F. McCracken.
A Vortex Method for Blood Flow through Heart Valves.
Jour. Comp. Phys. 35: 183-205, Apr. 1980.

39. R. D. Reitz.
The Application of an Explicit Numerical Method for a Reaction-Diffusion System in Combustion.
Courant Mathematics and Computing Laboratory, R&D Report, COO-3077-162, Nov. 1979.

40 . R. D. Reitz.
Computations of Laminar Flame Propagation Using an Explicit Numerical Method.
Proceedings of the 18^{th} Symposium on Combustion, Aug. 1980.

41. L. Rudolph.
A Remark on the Planarity of the Shuffle-Exchange Network of Sizes 16 and 32.
Ultracomputer Notes, N.Y.U., Feb. 1980.

42. J. T. Schwartz.
The Burroughs FMP Machine.
Ultracomputer Notes, N.Y.U., Jan. 1980.

43. J. T. Schwartz.
A Remark on Nearly Planar Embeddings of Small Ultracomputers.
Ultracomputer Notes, N.Y.U., Dec. 1979.

44. J. T. Schwartz.
Ultracomputers.
ACM Transactions on Programming Languages and Systems.
To appear, Oct. 1980.

45. H. R. Strauss.
Linear and Nonlinear Studies of High Beta Tokamaks.
IAEA, J-1, Brussels, 1980.

46. R. H. Strauss et al.
Relation beween Tokamak Temperature Profiles and Localized Instabilities.
IAEA CN-38IM-2, Brussels, 1980.

47. H. R. Strauss et al.
Stability of High Beta Tokamaks to Ballooning Modes.
Nucl. Fusion 20, 638 (1980).

48. H. R. Strauss et al.
Stabilization of Trapped Electron Shear-Alfven Instabilities by Temperature Gradient.
Phys. Fluids 22, 2364 (1979).

49. H. R. Strauss.
Stellarator Equations of Motion.
Plasma Physics. To appear.

50. H. R. Strauss et al.
Unified Theory of Tearing Modes.
Phys. Fluid 22, 2364 (1979).

51. S. Topiol et al.
Implementation of the GAUSSIAN 78 Programs on the NYU VAX/11-780: A Probe into Basis Set and Correlation of the Effects on the Structure of Molecular Complexes.
Courant Mathematics and Computing Laboratory, R&D Report, DOE/ER/03077-166, April 1980.

52. P. A. Whitlock et al.
Properties of the HCP Phase of ^{4}He.
Phys. Rev. B21, 999 (1980).

53. P. A. Whitlock, J. T. Muckerman, and P. M. Kroger.
Reactions of the ^{1}D State of Oxygen and Carbon.
"Potential Energy Surfaces and Dynamics Calculations," edited by D. G. Trublar.
Plenum Press, New York. In press.

54. P. A. Whitlock, J. T. Muckerman, and E. R. Fisher.
Theoretical Investigations of the Energetics and Dynamics of the Reaction $O(^1D) + H_2$.
Preprint.

55. O. Widlund and D. B. Szyld.
Applications of Conjugate Gradient Type Methods for Eigenvalue Calculations.p. 167-173 in: Advances in Computer Methods for Partial Differential Equations III.
Proceedings of the 3rd IMACS International Symposium.
Lehigh Univ., Bethlehem, Pa., 1979.

56. O. Widlund and W. Proskurowski.
A Finite Element Capacitance Matrix Method for the Neumann Problem for Laplace's Equation.
SIAM J. Scientific and Statistical Computing.
Accepted for publication.

57. O. Widlund and D. P. O'Leary.
Solution of the Helmholtz Equation for the Dirichlet Problem on General Bounded Three-Dimensional Regions.
ACM Transactions on Mathematical Software.
Accepted for publication.