MASTER

COO-3077-159

COURANT MATHEMATICS AND COMPUTING LABORATORY

950 6918

NEW YORK UNIVERSITY

PROGRESS REPORT No. 55

October 1, 1978 to September 30, 1979

PREPARED FOR

THE U. S. DEPARTMENT OF ENERGY

UNDER CONTRACT NO. EY-76-C-02-3077, TASK V

November 1, 1979

DISCLAIMER

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

REA

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

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

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Contents

I. ANALYTICAL AND NUMERICAL METHODS

A. Applied Analysis

1. ELASDYN

This project is aimed at understanding the radiation from seismic sources by numerical simulation with the ultimate aim of reducing seismic risk to sensitive structures.

During the year we continued the mathematical modeling of seismic slipping on a fault plane embedded in a 3-D uniform elastic whole space. We formulate the problem as a time dependent, two space dimensional integral equation over the slipping region. This obviates the introduction of artificial boundaries and reduces the dimensionality of the problem from 3 space plus 1 time to 2 space plus 1 time. The integral equation may be solved by an explicit step-by-step procedure in time, but at each step an integral over the previous values of the solution must be calculated.

Unfortunately the full elastic vector problem proved too difficult to set up numerically and we were concerned with completing the solution for a scalar analog.

The simulated motion on the fault plane is presented as a computer generated movie.

Pulse shapes and spectra are computed for the far field elastic radiation in various directions from the source. However, a numerical differentiation and a necessarily coarse discretization led to some difficulties which are still not fully resolved.

R. Burridge

2. Zero Dispersion Limit

We use the inverse scattering method to determine the weak limit of solutions of the Korteweg-de Vries equation as dispersion tends to zero. The limit, valid for all time, is characterized in terms of a quadratic programming problem which can be solved with the aid of function theoretic methods. The solution satisfies Whitham's averaged equation, at least for large t. For other values of time, the solution satisfies for one of a hierarchy of equations.

The KdV equation is the prototype of an approximation to equations describing undamped dispersive motion such as water waves, collisionless plasmas and nonlinear optics. The effect of small dispersion is to produce large amplitude waves whose wave length is proportional to the square root of the dispersion coefficient. When we are not interested in resolving phenomena on such a scale, the presence of such waves is an impediment to numerically resolving the larger scales which are of physical interest. In such cases, information of physical interest can be obtained out of the zero dispersion limit.

P. D. Lax

3. Reacting Flow Computations

a. We are developing and testing accurate and efficient numerical methods for mathematical modeling of combustion problems. The problem of the propagating one-dimensional deflagration wave has been chosen for preliminary analysis with a view towards model formulation. Numerical methods are being tested for the ozone flame system of equations and for wave solutions to nonlinear reaction-diffusion model equations. These model problems include stiff chemical kinetic source terms and permit comparisons to be made between numerical and analytical solutions.

Our results have emphasized the need for numerical methods with minimal numerical diffusion for combustion problems. Accordingly, two and three time level, second order numerical schemes have been devised and are being tested. In addition, stiffly-stable methods are being explored for the computation of the reaction terms. We have found a promising method in which the reverse reaction rate is treated semi-implicitly while the forward rate is computed explicitly.

Work is also in progress in the implementation of an Eulerian adaptive grid method which increases resolution in the flame zone where changes in the solution are the most significant. Results indicate that numerical errors can be minimized in this case by employing a logarithmic interpolation procedure between grid points in order to remap the grid. The interpolation can also be used to compute the physical diffusion terms in the equations. This method is also being adapted for convective terms in prototype nonlinear advection-diffusion equations for fluid dynamics problems.

b. Advanced computer codes are becoming available for the numerical 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 specie 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 intend to 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 specie evolution equations, and of fulfilling the requirement that the flow field be resolved accurately within the relatively thin energy release zone.

We are developing numerical methods focusing on these problems with the aid of model equations. We anticiate this research will then be extended to the coupled fluid dynamics and combustion equations, with complete chemical kinetic schemes, for the computation of multidimensional internal combustion engine phenomena.

c. 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. Capacitance Matrix Methods for Elliptic Equations

A major project, the extension of capacitance matrix methods to problems in three space dimensions, has been completed. These methods provide very efficient means for solving highly structured and finite element systems of linear equations that arise when certain special but important elliptic problems are discretized in general regions. Such programs can be used with profit, for example, as subprograms when solving fluid dynamic problems. The code for the three dimensioncal case is transportable and convenient to use. An improved mathematical framework for these methods has been provided through the work of my colleagues and myself, and through recent work in the Soviet Union, that of G. P. Astrakhantsev in particular. The development of finite element capacitance matrix methods has been actively pursued and considerable experience has been gained concerning their performance and the proper design of codes.

O. Widlund

2. Conjugate Gradient Methods

Work has continued on conjugate gradient type methods. The theory for certain nonstandard methods of this kind has been improved, and a method has been developed for the computation of the eigen elements for large sparse systematic eigenvalue problems and generalized eigenvalue problems. Such methods provide very flexible and useful tools for very large linear algebra problems. To our knowledge the use of preconditioned conjugate gradient methods for the systematic indefinite linear systems of Rayleigh quotient iteration and the development of a theory to explain the performance of these methods has not been previously carried out.

O. Widlund

3. Navier Stokes Equations

Work has begun on the further development of a theory for the vortex methods introduced by A. Chorin. We have simplified a theory previously developed by O. H. Hald for Euler's equation in two dimensions and begun work on three dimensional cases. Some work on algorithmic aspects of finite difference approximations of the Navier Stokes equation in three dimensions has also been done with special emphasis on problems relating to data flow and to the impact of new computer designs.

O. Widlund

4. Numerical Methods in Reaction-Diffusion Equations

In a slow burning deflagration system, some components of the solution may be approximated as traveling waves. We studied a numerical method for dealing with such solutions by treating the one dimensional Fisher equation $L(u) \equiv u_t - u_{xx} - u(1 - u) = 0$ with initial and boundary conditions corresponding to the exact traveling wave solution that it has. This special solution has heights 0, 1 at $x = -\infty, +\infty$ respectively. For a coarse spatial interval of size 2, the Crank-Nicolson scheme with a time interval of 1 produced a solution within 5% accuracy for the wave speed, that is, $5/\sqrt{6}$. Here the wave amplitude undergoes about 80% of its variation over a spatial range of 10 units (5 spatial intervals). The solution of the implicit equations in the Crank-Nicolson scheme is obtained by first using the standard explicit scheme to get a first estimate of the solution, and second using two Newton iterations to improve the estimate.

We investigated techniques for improving upon the accuracy of any algorithm for solving $L(u) = 0$, by conserving certain functionals of u. One such technique does not require finding the gradient of the reaction term $u(1-u)$, and may thus be useful with practical models.

Studies were begun with Burger's equation, again for the purpose of getting efficient schemes that are accurate.

E. Isaacson

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. The primary objective is to study three dimensional and nonlinear effects.

Notable progress has been achieved in three different areas. First, we improved the code specially in regard to the stability analysis. A much more accurate method of computing eigenvalues by using variational analysis has been implemented, and a more accurate treatment of the magnetic axis has been effected.

Second, we have written a fully vectorized version of the code to be run in the CRAY computer at Livermore. This code increases computational speed 30-fold and allows us to explore problems that before could not be resolved.

Third, we have documented our work in a short book, "A Computation Method in Plasma Physics," Springer-Verlag, New York, 1978. It contains a detailed analysis of the theory as well as a manual and a listing of our code, which should be useful to the scientific community.

The computational method has been applied in two different areas. The first has been a study of new stellarator concepts. We have found stellarator equilibria for a range of beta up to 10%, which are also stable to the fundamental mode $m = 1$, $k = 0$ and $m = 1$, $k = 1$. This work has been done in collaboration with the group headed by Leon Shohet at the University of Wisconsin.

The second application, still in progress, has been the study of nonlinear stability for Tokamaks. Here the fundamental question to be answered is in what manner does global stability analysis differ from common linear analysis and what are the implications of the difference for future experiments.

O. Betancourt

2. Low Speed Magnetohydrodynamic Flow

We have developed a numerical method for low speed magnetohydrodynamic flow to compute equilibria for magnetically confined plasmas and to determine their nonlinear stability by the solution of initial boundary value problems. We have exploited our freedom to evaluate the terms in the difference equations at any time between t and $t+\Delta t$ to construct a semi-implicit formulation in which the fastest waves are represented by a simple, easily solved implicit equation for a scalar pressure.

We have computed the resolution of an initial shear discontinuity in one dimension and our comparisons with analytic solutions indicate that the method is applicable whenever $(\nabla \cdot u)\,\Delta t$ is small. We have also implemented the method to solve the equations in three dimensions and have been able to solve equilibrium problems between two and three times as fast as with a previous, fully implicit formulation.

Because of the simplicity of the method and its applicability to more general problems with transport, we expect that it will find wide application in the study of confined plasmas.

J. U. Brackbill

3. Combustion Calculations

We have developed a method for solving diffusion, reaction problems by solving difference equations on a rezonable, Lagrangian mesh. This approach is used to concentrate resolution in the reaction front, where it is needed.

To simplify an earlier two-step method, ALE, the solution of the dynamical equations and convective transport are combined into a single step. In this step, the equations are written in generalized Eulierian form. For example, the energy equation is written:

$$\frac{\partial \rho_e}{\partial t} + \nabla\cdot[\rho e(\underset{\sim}{u} - \underset{\sim}{u}') - \underset{\approx}{Q}\cdot\underset{\sim}{u} - \rho\kappa\,\nabla i] + \rho e(\nabla \cdot \underset{\sim}{u}') = 0 ,$$

where $\underset{\approx}{Q}$ is the stress tensor, $\underset{\sim}{u}$ the fluid velocity, i the specific internal energy, $e = \tilde{I} + (1/2)u^2$ is the specific total energy, ρ the density, κ the conductivity, and $\underset{\sim}{u}'$ the grid velocity. Because we determine $\underset{\sim}{u}$ and $\underset{\sim}{u}'$ independently, we can move the grid arbitrarily with respect to the fluid. Thus, where $\underset{\sim}{u}"$ is the velocity defined by

$$- \nabla \cdot (\rho i \underset{\sim}{u}") = \nabla \cdot \rho\kappa\,\nabla i ,$$

the energy equation can be written

$$\frac{\partial \rho_e}{\partial t} + \nabla\cdot[\tfrac{1}{2}\rho u^2(\underset{\sim}{u}-\underset{\sim}{u}') + \rho i(\underset{\sim}{u}+\underset{\sim}{u}"-\underset{\sim}{u}') - \underset{\approx}{Q}\cdot u] + \rho e(\nabla\cdot\underset{\sim}{u}') = 0.$$

When we choose $\underset{\sim}{u}' = \underset{\sim}{u}"$, the mesh will move with the diffusion wave through the fluid.

In a computational test, we have solved a modified form of Fisher's equation,

$$\frac{\partial \phi}{\partial t} = \kappa \frac{\partial^2 \phi}{\partial x^2} + (\phi - \varepsilon)(1 - \phi)$$

with $\phi = \varepsilon$ ahead of the wave. By the definition above, $\underset{\sim}{u}"$ is zero everywhere except where $\partial\phi/\partial x \neq 0$, and the mesh points are caught up in a wave which displaces them a finite amount, first concentrating them in the wave front, then leaving them spread out behind. In combination with a smoothing or other similar rezoning prescription, the dynamic prescription $u' = u"$ can be extended to calculations in two and three dimensions, where the efficiency of the adaptive zoning will make quite ambitious calculations possible.

J. U. Brackbill

4. A Mesh Generator for Arbtirarily Shaped Domains

With several other investigators, we have been using a mesh generator for arbitrarily shaped domains that is derived by minimizing the integral

$$I = \iiint \left\{ (\nabla\zeta)^2 + (\nabla\eta)^2 + (\nabla\nu)^2 \right\} dx\, dy\, dz ,$$

where (x,y,z) are images in physical space of the natural coordinates (ζ,η,ν). The computation mesh in natural coordinates consists of a regular, rectilinear array. The corresponding mesh in physical space is the smoothest mapping consistent with the boundary conditions.

Although the smoothing algorithm is effective in generating a mesh, since the solution depends only on the boundaries, it does not use any information from the interior of the mesh. Because this is sometimes a real handicap, we have modified the method to allow either the specification of the volume of the cells or the minimization of their variation in volume by the penalty method. The new integral to be minimized is written

$$I = \iiint \left\{ (\nabla\zeta)^2 + (\nabla\eta)^2 + (\nabla\nu)^2 + \lambda w(x,y,z) J^2 \cdot \langle J \rangle \right\} dx\, dy\, dz,$$

where $J = \partial(\zeta,\eta,\nu)/\partial(x,y,z)$, $\langle J \rangle$ is the average value of J over the mesh, w is a prescribed function whose average value is $O(1)$, and λ is the penalty factor.

The advantage of using the penalty method over the method of constraints is the freedom to weigh the requirements for increases in smoothness in order to increase the accuracy of the difference equations against decreases in the variation in volume as a means to decrease the cost of the calculation. The disadvantage is that the optimum value of λ for a given problem must be determined by trial and error.

The new algorithm has been tested in two dimensions. A first practical application will be to rezoning in a rezonable Lagrangian calculation of laser target dynamics.

J. U. Brackbill

5. Combustion

Work has continued on an investigation of methods to be used to compute the exothermal energy release behind a propagating shock wave moving through a combustible mixture. A locally shock centered mesh, moving with the shock and imbedded in the global computational mesh, is used to define the shock layer; the motion of this layer is carried out using the method of Glimm so that the shock profile is sharp

with no temperature overshoot. The reaction model is constructed using a simple two step kinetic mechanism for gaseous premixed hydrogen-oxygen. The associated rate equations are solved using the Gear package.

In order to understand the interaction process in compressible reactive flows, for example, the mechanism controlling the transition process of deflagration to detonation, efficient computational methods must be developed. The difficulty in obtaining solutions to such problems centers around the various spatial scales, or temporal scales, associated with stiff equations of chemical rate theory; such scales are usually much smaller than hydrodynamic time scales. Our objective is to develop an automatic numerical procedure that will account for the development and subsequent propagation of detonation waves. We hope to accomplish this task by constructing an efficient algorithm which allows computational grids to be multiple defined in terms of the gradients of the field variables defining the rate processes.

The ability to design energy transformation devices which map exothermal heat release from fossil fuels into work is a major concern to DOE. The application to design, of the above numerical methods, runs from closed cyclic combustion systems through open "steady" (fluctuating) combustors.

S. Z. Burstein

6. Molecular Computations of Inhomogeneous Systems

In earlier work we examined the microscopic structure of liquid-vapor interfaces. This gave evidence of a much richer dynamical behavior than had been anticipated. In particular, the correlations associated with free capillary waves manifested themselves strongly over a large spatial domain.

In the past year, we investigated the structure of the interface when a hard wall is introduced into the transition region. Both longitudinal and transverse correlations are compared to those observed in a free interface. The density profile shows a transition from an oscillatory profile to a smooth monotonic one when the position of the hard wall is varied. Vestiges of the two phase behavior persist even when the pressure at the wall equals that in the bulk. We plan to study the system at much higher pressure.

M. H. Kalos et al.

7. Chemical Kinetics

The study of $C(^1D) + H_2$ has been completed and work has commenced on hydrocarbon rearrangement reactions. Calculations on oxygen atoms reacting with simple alkanes has been planned.

P. A. Whitlock

8. Kinetics of Binary Alloys and Nucleation

We have found an interesting scaling law for the structure function of the grains in an alloy following quenching; $\bar{S}(k,t) = K^{-3}F(k/K)$ with $K(t) \propto t^{-a}$ and $a \cong 0.25$ at late stages of the evolution. During the same period the mean cluster size grows linearly with time.

M. H. Kalos, J. L. Lebowitz, J. Marro

9. Theory of Critical Clusters

A new thermodynamic analysis was made for the equilibrium between a liquid cluster and the surrounding supersaturated gas phase in a finite constant volume. Such clusters are stable at intermediate volume, unstable in the thermodynamic limit. Observation of the critical cluster size ℓ^* yields information on the surface free energy of the liquid cluster.

The theory was used to analyze Monte Carlo simulations of the two-dimensional lattice gas model at low temperatures for clusters up to 500 atoms. In addition the mechanisms for cluster diffusivity have been considerably clarified.

K. Binder and M. H. Kalos

10. Equation of State of an FCC Binary Alloy

Monte Carlo and other theoretical work aimed at elucidating the equation of state of an FCC binary alloy has continued. In spin language the Hamiltonian is

$$H = J \sum_{nn} \sigma_i\sigma_j - \alpha J \sum_{nnn} \sigma_i\sigma_j - h \sum \sigma_i$$

J is positive so that the nearest neighbor (nn) interaction is antiferromagnetic. For $\alpha < -1/2$ the transition seems still to be first order. Renormalization group methods predict a first order transition for $\alpha < 0$, but second order in the limit of $\alpha \to -\infty$.

We have also investigated the phase diagram in the temperature-concentration (T-c) plane for $\alpha = 0$ and $\alpha = -0.25$, where cluster variational data were available. For $c = 0.5$ and 0.75, the agreement is good. For stoichiometric compositions, there is a significant discrepancy.

M. H. Kalos, J. Lebowitz, M. Phani

11. Kinetics of Order-Disorder Transitions

Analysis continued of data from computer modeling of the ordering of an antiferromagnetic alloy quenched from the melt. In the time regime where independent locally ordered domains grow — so there is as yet little long range order — we confirm a prediction of Cahn and Allen that the short range order $\sigma(t)$ obeys

$$\sigma(\infty) - \sigma(t) \propto t^{-1/2}$$

while the long range order grows linearly with time.

M. H. Kalos, J.L. Lebowitz, M. Phani

12. Collapse Transition in Polymer Melts

In studying the equilibrium conformational and scaling properties of continuum models of polymers, we have searched for the transition to a collapsed state in a dilute solution. That is, the characteristic nonideal conformation of polymers with excluded volume interactions is reversed at low temperatures. At an intermediate value — the Θ temperature — isolated chains behave in a nearly ideal (i.e., Gaussian) way. Our preliminary results confirm the general features of this view but do not as yet define a unique Θ temperature. We have been able to confirm important features of universal scaling laws as applied to these systems.

M. H. Kalos, J.L. Lebowitz, I. Webman

13. Properties of Models of Polymer Melts

Partly as a prelude to dynamical studies, the "reptation" Monte Carlo method developed here has been used to study conformation properties of ensembles of simple ball on spring models of polymers. At low densities previous results for isolated chains are recovered, but at effective densities of 0.3 and 0.5 the chain conformations are compressed. For example, as a function of ℓ, the number of bonds per chain, the squared end-to-end distance $\propto \ell^{1.07}$, whereas the excluded volume effects for an isolated chain force a behavior more like $\ell^{1.2}$.

M. H. Kalos et al.

14. Crossover Between Dimensionalities in Polymers

The conformational properties such as the squared end-to-end distance of a polymer constrained to lie in a slab exhibit a crossover from three- to two-dimensional behavior. With our usual bead-on-spring model and reptation Monte Carlo, we have determined the crossover behavior as a function of slab thickness measured in units of the unconstrained three-dimensional size and have confirmed a conjecture of de Gennes and Daoud.

M.H. Kalos, J.L. Lebowitz, I. Webman

15. Fluid and Crystal States of He-4

The work on fluid and FCC phases of He-4 using Lennard-Jones forces was completed and the paper based on it is about to appear. Calculations of the HCP phases of the crystal showed, as expected, little departure from the equation of state for FCC; a brief note on this is in preparation.

Calculations with more modern pair potentials for the He-He interactions are underway. At the equilibrium density of liquid He-4, the ESSMSV potential is effectively too weak, the MS12G6 proposed by Aziz et al. is too strong, but their HFDHE2 potential gives a very good binding energy of -7.1 K.

G.V. Chester, M.H. Kalos, P. Whitlock

16. Quantum Systems at Finite Temperature

Work was concentrated on variational methods for the Block equation which are capable of being handled by Monte Carlo quadrature. One very promising candidate has been explored. A critical evaluation of alternative methods of integration tentatively established the Green's function Monte Carlo algorithm as the most effective when exchange effects must be considered.

M.H. Kalos and P. A. Whitlock

17. Many-Fermion Problems

A new algorithm has been found for the exact integration ground state problems of this kind. Exploration on model problems is planned.

D.M. Ceperley and M.H. Kalos

II. ADVANCED COMPUTER CONCEPTS

A. Software Engineering

We have made good progress in demonstrating portability of large software systems by porting the 100,000-line SETL system from the CDC 6600 to the VAX. This effort has put us into position to link SETL to high efficiency numerical languages like FORTRAN. The resulting symbolic/numerical software package, which we hope to start distributing during the coming year, should be of considerable interest to DOE users who need powerful symbolic manipulation routines (which can be written in SETL) to set up large numerical calculations (for which existing FORTRAN codes can be used). The package we will release will have something of the flavor of the earlier Argonne SPEAKEASY effort, but will provide considerably more semantic power because of the very high level operations available as primitives in SETL.

The VAX provides an essential environment for this effort, in at least two regards:

(a) The virtual memory environment available on the VAX makes it feasible to link the SETL run-time support library, which is already large, together with large FORTRAN codes.

(b) The memory protect features available in the VAX, and in particular the existence of a system call that will temporarily cause a collection of pages to become read-only, allows us to call FORTRAN in a protected way without having to fear that the rather sensitive garbage-collected SETL run-time environment will be mangled.

We hope to complete the software links necessary for this effort during the next few months, following which we will make an experimental demonstration of its use to set up sizeable eigenvalue computations symbolically before they are solved numerically.

J. T. Schwartz

B. Distributed Systems

1. ARPANET Applications

At present, about 40 DOE and government scientific researchers use the CMCL system to obtain access to a variety of remote sites. A number of ARPANET applications reported last year have continued and are summarized here.

The principal interest of the CMCL in the use of network technology is that of gaining convenient access to large scale computers. The ARPANET provides this access to the CRAY and CDC-7600 computers of the MFECC at Lawrence Livermore Lab.

Computerized teleconferencing is being used extensively by researchers in the fields of Distributed Systems and Very High Level Languages. Information exchange between large numbers of remotely located researchers often approaches, in speed and richness of interaction, that which can be achieved by face to face meetings. In several instances, this means of communication has been a significant tool in support of collaborative computer program development and interlaboratory system design and specification.

Researchers from other institutions use the NYU facilities to access their home computers while visiting the New York area.

Courant Institute researchers use the network both to communicate with colleagues through the electronic mail facilities and to exchange programs and data.

Maintenance and development of the PDP-11 network access programs are done on off-site PDP-10 computers.

The recently acquired VAX 11/780 computer system has been connected to the ARPANET. This is the first VAX system to be so connected. Access to our system should be an aid to DOE researchers and laboratories that are contemplating acquisitions of similar systems.

E. Franceschini and M. Goldstein

2. Multicomputer Facilities

The CMCL activity is focused on the implications of a geographically dispersed, multicomputer environment of scientific users. In addition, the role of the small computer in large scale computational modeling is being studied. In this report period, a VAX 11/780 computer system has been acquired to assist in these activities.

a. Relative Performance Evaluation of Computer Systems

Several typical CMCL programs have been run on the VAX and comparisons made to CDC-6600 performance. Several small test programs were written to exercise specific features of the VAX systems. The effects of the virtual memory architecture on program performance have been particularly scrutinized.

b. Computer Program Profiles

The attempt to study the performance of programs across a broad spectrum of computer architectures has revealed the desirability of a means to analyze program structure. We have

begun the analysis of typical CMCL codes and are working towards the specification of a standard profile of the static and dynamic properties of typical DOE scientific programs. We are using existing tools and developing new ones to assist in the characterization of FORTRAN programs.

c. VAX Utilities

Several programs and procedures have been written to assist in the conversion of CDC-6600 programs to the VAX FORTRAN language, and to facilitate the movement of programs and data between the two machines.

d. Distributed System Node Development

Central to the study of the impact of multicomputer environments is the design, construction and evaluation of a model node for a distributed system environment. The CMCL node will consist of a cluster of several computational elements. At this time the design of the interconnection protocols and user level interfaces are close to completion.

e. Remote Connections to Distributed Systems Node

At this time no universal interconnection methods for geographically separated computers exist. The CMCL node will be provided with a variety of methods to connect to remote computers.

Connection has been made to the ARPANET.

Connection to a public packed switched network is being studied.

Remote job entry implementation schemes are being considered for those cases where a computer system is only accessible by direct telephone line.

In each of these cases strong emphasis is being placed on providing facilities that are easy to use and consistent with traditional practices of the vast community of DOE computer users who are not computer specialists.

E. Franceschini and M. Goldstein

3. Remote Access Graphics Capability

With the increasing variety of computer systems in use by CMCL researchers, a need exists for integrating the means of producing graphic output. Two important steps towards this goal are the standardization of the user interface language and the generation of a common, device-independent command

stream by the language processors. At this time no such broadly based standards exist. We are adopting the CALCOMP user interface as a local standard. This is a reasonable choice because it is used by several suppliers of graphics devices. Towards device independence, we are developing the necessary language processors to produce a generalized intermediate output. Specific utility programs are being written to translate the intermediate output to the command streams of various devices such as ink plotters, printer/plotters, COM devices, and interactive graphics terminals.

E. Franceschini and M. Goldstein

C. High Performance Systems

1. 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.

The first PUMA, together with a minimal operating system, was completed in June of 1978. The system has seen steadily increasing use since that time, and is now running about 300 hours/month of production programs. The engineering group has nearly completed two additional PUMA's; these systems utilize greatly improved packaging and will in consequence be somewhat faster than the first unit.

Modest improvements have been made during the year in the original PUMA operating system. At the same time, we have begun development of a much more comprehensive operating system, which will include most of the facilities of Control Data's operating systems.

Several improvements and additions have been made to our set of design automation tools over the past year: a new wire routing program for a new series of circuit boards; a program for the automatic selection of chip placements on circuit boards; and a program for generating circuit diagrams from circuit descriptions.

Finally, we have been working on the automatic optimization of horizontal microprograms. The PUMA and many other large processors are horizontally microprogrammed: instruction interpretation is controlled by a microprogram that is capable of specifying the concurrent execution of microoperations in the various units of the processor. Scheduling these micro-

operations to maximize processor speed, particularly for highly branched microprograms, is a very time-consuming task. We have compared various techniques for scheduling within basic blocks (straight-line code), and have developed new techniques for use outside of basic blocks.

Our work is already having a direct benefit in terms of the computing power available for DOE applications. In addition, we expect that our design automation tools and experience will be valuable in the construction of processor prototypes and emulators as part of a research effort in high-performance processors.

R. Grishman

III. Relationships to Other Projects

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

Applied Analysis

P. D. Lax is 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.

R. D. Reitz has information exchanges with the DISC Engine Program group, the cooperative research 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.

Computational Mathematics

O. Widlund sent DPOLE, a major piece of computer code, to the National Energy Software Center. Presented a paper at the NRCC Workshop in Chemistry at Santa Cruz, Calif., Aug. 1978. Maintains the following contacts: (1) numerical analysis group at Stanford, particularly Gene Golub and Michael Saunders; Alexander Chorin, Ole Hald, and Paul Concus and others at Berkeley; (2) J. Cullum and R. W. Willoughby, IBM Yorktown Heights; (3) D. P. O'Leary, Univ. Maryland, W. Proskurowski, Univ. Southern California, and D. M. Young, Jr., Univ. Texas-Austin; (4) B. Mercier, Centre d'Etudes de Lineil, Paris; Harwell mathematical software group, U.K. Atomic Energy Authority; computer science departments of the Universities of Stockholm and Uppsala.

Numerical Methods for PDE's

O. Betancourt and colleagues sent their three-dimensional MHD Equilibrium and Stability code to John T. Hogan, Oak Ridge National Laboratory. Collaboration continues with Leon Shohet's group, Univ. Wisconsin-Madison, and the Max Planck Institute, Garching, Germany.

J. U. Brackbill collaborates with MIT and Univ. Wisconsin investigators on low beta stellarator calculations. His code MALICE is being used at Livermore and Los Alamos. Active exchange with the Princeton Plasma Physics Laboratory theory group. Consultation with the laser fusion group at Los Alamos.

S. Z. Burstein continues his exchanges with W. Noh and W. P. Crowley, Lawrence Livermore Laboratory, and with G. Sod, Univ. North Carolina.

M. H. Kalos' team maintains numerous contacts. (1) Molecular Computations: Rahman, ANL; Raveche, NBS, Henderson, IBM-San Jose. (2) Chemical Kinetics: Muckerman, BNL; Butler, Naval Research Laboratory; hot-atom chemistry group, BNL. (3) Properties of Ordering Alloys: neutron and X-ray scattering facilities at BNL, ANL, ORNL; Cahn, NBS; Kikuchi, Hughes; IBM Yorktown Heights and San Jose. (4) Polymers: Ceperley, NRCC (LBL); Goad, LASL; Verdier and Mazur, NGS; Bell Telephone Laboratories. (5) Quantum Many-Body: Adler, LLL; Coester and Day, ANL; Ginocchio, LASL. And innumerable contacts with academic institutions both here and abroad.

Distributed Systems

E. Franceschini and M. Goldstein routinely use the electronic mail for communications with other Applied Mathematical Science program participants and Washington Headquarters, and are very much involved in DOE Computer Conferences dealing with distributed systems research, small computers for scientific use, command language standards, etc. They participate in the Semi-Annual AESOP Conferences, AMS Program Planning Workshops, TELENET User Group Meetings, and UNIX User Group Meetings.

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

CIMS PL/I	P. Abrahams
Bubble Deformation due to Flow	J.M. Broeck, J.B. Keller
Models of Morphogenetic Movement	S. Childress
Magneto-Fluids Dynamics	H. Grad
Natural Language Interfaces for Data Base Retrieval	R. Grishman
Multi-Microprocessor Software	M.C. Harrison
Inverse Reflection Problems in Seismic Prospecting	F. Karal
Cavitation Bubble Oscillations	J.B. Keller, M. Miksis
Computer Test Chamber for Prosthetic Mitral Valves	D.M. McQueen, C.S. Peskin
Shock-Sonic Line Connection	C. S. Morawetz
Facilitated Diffusion Across a Membrane	J. Nedelman
Aortic Sinus Vortex	C.S. Peskin, A.W. Wolfe
Meteorology	C.B. Sensenig

2. New York University

Nucleic Acid Molecules	S. Broyde
Effect of the Non-Additive Potential on the Structure of Water Polymers; A Molecular Model for the Dielectric Properties of Ice	E.S. Campbell
Organic Astrochemical Evolution	Y.E. Rhodes
Bed Expansion and Heat Transfer Modeling and Correlation Studies in a Pressurized Coal Fluidized Bed	V. Zakkay et al.
Employing Vaporized Fuel for the Enhancement of the Hydrocarbon Efficiency	V. Zakkay et al.

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 1979, time available on the 6600 was allocated as follows:

Courant Institute/DOE	78.8 %
DOE Research Divisions	3.3
NYU/Federal Government Affiliations	5.2
Other Universities/Federal Government	3.7
Federal Government Agencies	9.0
	100.0 %

About 36 non-DOE Federal agency contractors were allocated 1500 hours of computer time as follows:

Defense Nuclear Agency (DNA)	24.0 %
Environmental Protection Agency (EPA)	4.9
National Aero. & Space Adm. (NASA)	9.8
National Cancer Institute (NCI)	11.9
National Institute of Health (NIH)	7.3
National Science Foundation (NSF)	17.0
Office of Naval Research (ONR)	10.5
All Others	14.6
	100.0 %

IV. SEMINARS

During fiscal year 1979, CMCL sponsored a series of seminars in Numerical Analysis and Computer Science. The titles of the talks and the name of the speakers follow.

Numerical Analysis Seminars

"Numerical Computation of Shocks"
Andrew J. Majda
University of California at Los Angeles
October 13, 1978

"A Survey of Almost Incompressible Flow Calculations at Los Alamos: Part II, Generalization and Applications"
Jerry Brackbill
CIMS
October 27, 1978

"The Construction of Initial Data for Hyperbolic Systems from Incomplete Measurements"
Kenneth Bube
CIMS
November 2, 1978

"Capacitance Matrices, Potential Theory and Finite Elements"
Olof Widlund
CIMS
November 10, 1978

"Almost Integral Polyhedra"
Prof. Manfred Padberg
G.B.A. at N.Y.U.
November 17, 1978

"On Hald's Work on Vortex Methods"
Olof Widlund
CIMS
November 22, 1978

"Multgrid Methods, A Survey"
Jacob Steinberg
Technion and CIMS
November 29, 1978

"Multi-Level Adaptive Techniques for Partial Differential Equations"
Prof. Achi Brandt
University of Wisconsin
December 1, 1978

"Multigrid Methods, A Survey, Part II"
Jacob Steinberg
Technion and CIMS
December 6, 1978

"Eigenvalue Problems for Schrodinger Operators"
David Isaacson
Rutgers University
December 8, 1978

"Transonic Flow Calculations"
Antony Jameson
CIMS
December 14, 1978

"Topics in Two Dimensional Modeling of Semiconductor Devices"
Daniel D. Warner
Bell Labs
December 15, 1978

"Transonic Flow Calculations"
Antony Jameson
CIMS
December 20 and 21, 1978

"Fourth Order Compact Implicit Methods for Hyperbolic Conservation Laws"
Amiram Harten and Hallen Tal-Ezer
ICASE
February 9, 1979

"A Projected Lagrangian Algorithm for Solving the Nonlinear Minimax Problem"
Michael Overton
Stanford University
February 14, 1979

"An Algorithm for Computing the Numerical Range of a Matrix"
Charles Johnson
University of Maryland
February 23, 1979

"Spectral Methods for Free Surface Flows"
Steven Orszag
MIT
March 2, 1979

"Implicit Schemes and Lu Decompositions for Hyperbolic Equations"
Eli Turkel
CIMS
March 9, 1979

"Two Phase Flow on Ill-Posed Problem Well Treated"
Bruce Stewart
Brookhaven National Laboratory
March 16, 1979

"Lagrangian Hydrodynamics Using a Reconnectable Triangular Grid"
Martin Fritts/Jay Boris
Naval Research Laboratory
March 23, 1979

"A Lagrangian Method for the Navier-Stokes Equations with Large Deformations"
Charles S. Peskin
CIMS
April 6, 1979

"Computer Science Aspects of a Lagrangian Method for the Navier-Stokes Equations"
Charles S. Peskin
CIMS
April 20, 1979

"A New Fast High Order Laplace Solver for General Regions"
Anita Mayo
CIMS
April 27, 1979

"Nonlinear M.H.D. Stability"
Paul Garabedian
CIMS
May 4, 1979

"Gradient Methods for the Solution of Unsymmetric Linear Systems"
Martin Schultz
Yale University
May 11, 1979

"Numerical Methods for Singular Perturbation Problems"
Heinz-Otto Kreiss
Cal. Tech.
May 18, 1979

"Relaxation Methods for Fluid Flow Calculations"
J.J. Chattot
ONERA (France) and NASA Ames Research Center
May 25, 1979

Computer Science Seminars

"Register Allocation via Graph Coloring"
Gregory Chaitin
IBM
October 20, 1978

"Almost Integral Polyhedra"
Manfred Padberg
GBA at NYU
November 17, 1978

"The Unix Programming Environment"
Brian W. Kernighan
Bell Telephone Labs.
December 1, 1978

"Ultracomputers"
Jacob T. Schwartz
CIMS
December 15, 1978

"Equivalence of Relational Database Schemes"
Alberto O. Meldelson
Princeton University
January 5, 1979

"Automatic Storage Optimization"
Janet Fabri
IBM
January 26, 1979

"On Knowledge of Knowledge"
Ian Filotti
Columbia University
February 9, 1979

"Toward a Methodology for Software Engineering"
J. R. White
University of Connecticut
February 23, 1979

"Semantics of Encapsulated Data Types"
Samuel Kamin
SUNY at Stoney Brook
March 9, 1979

"Scheduling with Release Time and Deadlines"
Barbara Simons
University of California, Berkeley
March 23, 1979

"Program Verification in PL/CV Logic"
R. Constable
Cornell University
April 6, 1979

"Computable Queries for Relational Data Bases"
David Harel
IBM
May 4, 1979

"The Impact of Very Large-Scale Integration on
High Speed Computers"
Harold S. Stone
University of Massachusetts
May 18, 1979

V. PUBLICATIONS

1. P. W. Abrahams.
The CIMS PL/I Compiler.
SIGPLAN Notices 14: 107-116, Aug. 1979.

2. F. Bauer, O. Betancourt and P. R. Garabedian.
A Computational Method in Plasma Physics.
Springer-Verlag, New York, Sept. 1978.

3. O. Betancourt, P. R. Garabedian and F. Herrnegger.
Stability Effects of $\ell = 2,3$ Helical Fields on High-Beta Stellarator Configurations.
Plasma Physics and Controlled Nuclear Fusion Research 1978, Vol. 2, p. 355-362, Vienna, International Atomic Energy Agency, 1979.

4. S. Z. Burstein.
Numerical Methods in Chemically Reacting Fluid Flows.
Planned publication.

5. D. Ceperley.
Ground State of the Fermion One-Component Plasma: A Monte Carlo Study in Two and Three Dimensions.
Phys. Rev. B 18: 3126-3138, Oct. 1978.

6. M. Davis and J. T. Schwartz.
Mathematical Extensibility of Theorem Verifiers and Proof-Checkers.
Computers and Math. 5: 217-230 (1979).

7. J. A. Fisher.
The Optimization of Horizontal Microcode Within and Beyond Basic Blocks: An Application of Processor Scheduling with Resources.
Courant Mathematics and Computing Laboratory, R&D Report, COO-3077-161, Oct. 1979.

8. R. Grishman.
The Structure of the PUMA Computer System; Overview and the Central Processor.
Courant Mathematics and Computing Laboratory, R&D Report, COO-3077-157, Nov. 1978.

9. M. C. Harrison and N. Rubin.
Another Generalization of Resolution.
Assoc. for Comp. Mach. Jour. 25: 341-351, July 1978.

10. J. M. Hyman.
MOL1D: A General Purpose Subroutine Package for the Numerical Solution of Partial Differential Equations.
LA-7595-M Manual, Los Alamos Scientific Laboratory, March 1979.

11. A. Jameson.
Numerical Calculation of Transonic Flow Past a Swept Wing by a Finite Volume Method.
Lecture Notes in Physics, 91; Ed. by R. Glowinski and J. L. Lions, Springer, 1979.

12. A. Jameson.
Transonic Flow Calculations, pp. 1-87.
Numerical Methods in Fluid Dynamics; Ed. by H. J. Wirz and J. J. Smolderen, McGraw-Hill, 1978.

13. M. H. Kalos et al.
Computer Experiments on Phase Separation in Binary Alloys.
Adv. Colloid and Interface Sci. 10: 173-214, June 1979.

14. M. H. Kalos et al.
Computer Modeling of Quantum Liquids and Crystals, pp. 219-230.
Computer Modeling of Matter; Ed. by P. Lykos, American Chemical Soc., 1978 (ACS Symposium Series, 86).

15. M. H. Kalos et al.
Computer Simulation of the Time Evolution of a Quenched Model Alloy in the Nucleation Region.
Phys. Rev. Lett. 43: 282-285, July 1979.

16. M. H. Kalos et al.
Growth of Clusters in a First Order Phase Transition.
Jour. Statl. Phys. 19: 243-267, Sept. 1978.

17. M. H. Kalos et al.
Molecular Dynamics of Polymeric Systems.
Jour. Chem. Phys. 70: 1299-1304, Feb. 1979.

18. M. H. Kalos.
Monte Carlo Studies of Relaxation Phenomena: Kinetics of Phase Changes and Critical Slowing Down, pp. 225-260.
Monte Carlo Methods in Statistical Physics; Ed. by K. Binder, Springer, 1979. (Topics in Current Phys., 7.)

19. M. H. Kalos et al.
Monte Carlo Studies of Crystalline Helium.
Jour. de Physique 39: 1298-1302, Aug. 1978.

20. M. H. Kalos et al.
Monte Carlo Study of an Ordering Alloy on an FCC Lattice.
Phys. Rev. Lett. 42: 577-580, Feb. 1979.

21. M. H. Kalos and D. Ceperley.
Quantum Many-Body Problems, pp. 145-194.
Monte Carlo Mehods in Statistical Physics; Ed. by K. Binder, Springer, 1979. (Topics in Current Phys., 7.)

22. D. G. Korn.
Numerical Design of Transonic Cascades.
Jour. Computational Phys. 29: 20-34, Oct. 1978.

23. P. D. Lax.
Accuracy and Resolution in the Computation of Solutions of Linear and Nonlinear Equations, pp. 107-117.
Recent Advances in Numerical Analysis, Proceedings of a Symposium conducted by the Mathematics Research Center, University of Wisconsin-Madison, 1978; Ed. by C. de Boor and G. H. Golub, Academic Press, 1978.

24. P. D. Lax.
Recent Methods for Computing Discontinuous Solutions, pp. 3-12.
Lecture Notes in Physics, 91, Computing Methods in Applied Sciences and Engineering, 1977, II; Third International Symposium, IRIA Labonia; Ed. by R. Glowinski and J. L. Lions, Springer, 1979.

25. P. D. Lax and D. Levermore.
The Zero Dispersion Limit for the KdV Equation.
Proc. Natl. Acad. Sci. Vol. 76, No. 8, pp. 3602-3606, Aug. 1979.

26. G. B. McFadden.
An Artificial Viscosity Method for the Design of Super-Critical Airfoils.
Courant Mathematics and Computing Laboratory, R&D Report, COO-3077-158, July 1979.

27. C. S. Peskin and M. F. McCracken.
A Vortex-Grid Method for Blood Flow Through Heart Valves.
Lecture Notes in Physics, 90, pp. 377-384, Springer, 1979.

28. J. T. Schwartz et al.
Automatic Data Structure Selection in SETL.
SIGACT Symposium on Principles of Programming Languages, Sixth, San Antonio, Texas, 1979, ACM, 1979.

29. J. T. Schwartz.
Probabilistic Algorithms for Verification of Polynomial Identities.
NYU Comp. Sci. Dept. TR-004, Oct. 1978.

30. J. T. Schwartz.
The Interplay Between Mathematics and Computer Science.
ACM Proceedings of the 1978 Annual Conference, Wash. D. C., Vol. 1, New York, 1978.

31. J. T. Schwartz et al.
Programming by Refinement as Exemplified by the SETL Representation Sublanguage.
ACM Trans. Prog. Lang. and Systems 1: 27-49, July 1979.

32. G. A. Sod.
A Hybrid Random Choice Method with Application to Internal Combusion Engines.
Lecture Notes in Physics, 90, Springer, 1979.

33. P. A. Whitlock and M. H. Kalos.
Monte Carlo Calculation of the Radial Distribution Function of Quantum Hard Spheres at Finite Temperatures.
Jour. Comp. Phys. 30: 361-388, March 1979.

34. P. A. Whitlock et al.
Properties of Liquid and Solid ^{4}He.
Phys. Rev. B 19: 5598-5633, June 1979.

35. O. Widlund and W. Proskurowski.
A Finite Element Capacitance Matrix Method for the Newmann Problem for Laplace's Equation.
Planned publication.

36. O. Widlund and D. B. Szyld.
Applications of Conjugate Gradient Type Methods to Eigenvalue Calculations.
Proceedings of the Lehigh Univ. Conf. on Computer Methods for Partial Differential Equations, June 1979.

37. O. Widlund and D. P. O'Leary.
Capacitance Matrix Methods for the Helmholtz Equation on General Three-Dimensional Regions.
Math. of Comp. 33: 849-879, July 1979.

38. O. Widlund and D. P. O'Leary.
Capacitance Matrix Methods for the Helmholtz Equation on General Three-Dimensional Regions.
Courant Mathematics and Computing Laboratory, R&D Report, COO-3077-155, Oct. 1978.

39. O. Widlund.
On Certain Nonstandard Conjugate Gradient Methods for Systems of Linear Equations.
Planned publication.

40. O. Widlund.
On the Convergence of Chorin's Vortex Methods for Euler's Equations.
Planned publication.

41. O. Widlund and D. B. Szyld.
Rayleigh Quotient Iterations and Preconditioned Gradient Type Methods for Systematic Generalized Algebraic Eigenvalue Problems.
Planned publication.

42. O. Widlund.
Remarks on Iterative Methods for the Solution of Large Systems of Linear Algebraic Equations.
Proceedings of the NRCC Conference in Santa Cruz, CA, Aug. 9-11, 1978.
LBL Report 8158, UC-32 CONF 780878.

43. O. Widlund and D. P. O'Leary
Solution of the Helmholtz Equation for the Dirichlet Problem on General Bounded Three Dimensional Regions.
Submitted to ACM Transactions and Mathematical Software.