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DISCLAIMER

Contents

I. APPLIED MATHEMATICS
(Partial Differential Equations)

A. Computational Fluid Dynamics

1. Transonic Fluid Dynamics

Considerable progress has been made in the area of transonic aerodynamics with applications to turbomachinery. Our basic design code for shockless airfoils has been upgraded to become a reliable tool for work on cascades of compressor and turbine blades. The difficulties that have been overcome were related to the large turning angles that occur in turbomachinery.

At present, we are in the process of transferring this technology to the Pratt and Whitney Aircraft Division of United Technologies Corporation. An important advance has been made by Pratt and Whitney Aircraft in conducting tests of one of our early compressor blades. Since adequate facilities were not available in the United States the experimental work was performed by the DFVLR in Germany. The test data on the blade came up to expectations in the transonic range. More gratifying was that the blade performed well at subsonic speeds over twice the range for a comparison section.

There is now reason to hope that supercritical airfoil technology will gain wide acceptance by industry and will lead to significant fuel savings in the future.

F. Bauer, P. R. Garabedian

2. Numerical Design for Transonic Airfoils and Cascades

A major effort was made to improve the new design code developed by D. Korn. The code was tested by designing several new airfoils, turbines, and a compressor blade. In the design process important bugs were discovered and eliminated. The code as it now stands is more reliable and versatile.

Two of the new designs need more work to meet the desired specifications. All these new cases and the code will be included in the new volume on supercritical wing sections now in preparation.

F. Bauer

3. On Finite-Difference Approximations and Entropy Conditions on Shocks

Weak solutions of hyperbolic conservation laws are not uniquely determined by their initial values; an entropy condition is needed to pick out the physically relevant solution.

The question arises whether finite-difference approximations converge to this particular solution. This study shows that in the case of a single conservation law, the first order monotone schemes, when convergent, always converge to the physically relevant solution. Numerical experimentation and analysis reveal that this is not always so for higher order accurate schemes.

A. Harten, J. M. Hyman, P. D. Lax

4. Strong Shock Computations by Lagrangian Methods

A new program to be used in multidimensional hydrodynamic flows, incorporating interface and free surface fitting procedures, has been written. The basic conservation equations defining the interior of regions are cast in Lagrangian form and are integrated using multistep methods. Boundaries that separate differing materials are treated by coupling characteristic methods at the boundary with the conservation equations in the interior. Several test problems have been run; they include strong shocks propagating from the free surface (where they are generated) and shocks and rarefactions moving through contact surfaces. The methods developed in this one-dimensional model will be extended to a two-dimensional "free Lagrantian mesh" algorithm.

S. Z. Burstein, W. P. Crowley

5. Deformable Media

Programming effort has been expended to make the present second order accurate elastic-perfectly plastic code more flexible. Following the boundary of each domain, on a Eulerian mesh, requires keeping track of the crossings of the boundary with the Eulerian mesh coordinates. More efficient use of the 6600 memory was achieved by mapping two-dimensional arrays into one-dimensional arrays which allowed for variable storage. Wrinkles on boundaries induced through Taylor instability can now be tracked much further in time. Testing of methods designed to improve the calculation of boundary properties is continuing. Kreiss' suggestion of extrapolating characteristic variables to the boundary is now being tested and compared with other methods of boundary treatment.

S. Z. Burstein, E. Turkel

6. Climatology

To simulate the effect on the atmosphere of the sun's heating, a single layered incompressible spherical fluid layer model is given a prescribed variable density function. This density

decreases where the air is hottest, for example, over land and directly under the sun. Conversely the density increases with cold, with latitude. By choosing parameters that represent the range of temperature density effects for an ideal gas, it was possible to simulate a month of atmospheric motion (starting from a steady zonal flow as an initial state). In this initial experiment, the sun was constrained to move on an equatorial orbit; a strong single equatorial high developed and circled the globe from west to east with a period of about 1 1/2 days. Further experiments will be attempted to see how to induce the observed three "permanent" subtropical highs. This model was proposed by J. J. Stoker as the simplest that might produce physically reasonable "climatic" features of atmospheric flows.

S. Cohn, E. Isaacson, J. J. Stoker

7. Line Vortices in the Two Dimensional Flow

Line vortices in two dimensional flow in the presence of barriers, e.g., vortices in the plane slit along the positive x-axis, are being investigated. The questions being considered are (a) the motion of a single vortex, (b) the motion of two vortices, one fixed, the other movable, to determine the positions if any where the unconstrained vortex would be stationary, (c) more vortices and other types of domains.

These investigations it is hoped will throw light on the position of the observed more-or-less fixed vortices in the atmosphere, as they are conditioned by the distribution of land and sea and mountain barriers. The results obtained so far look promising.

S. Lopez, J. J. Stoker

B. Numerical Analysis

1. A Capacitance Matrix Method for Helmholtz' Equation on General Bounded Three Dimensional Regions

Work continued on a variant of the capacitance matrix method previously developed by Proskurowski and Widlund for problems in two dimensions. A number of serious new difficulties associated with the increase of the dimension has been successfully resolved. Extensive numerical experiments show that our method converges in a modest number of iterations, a number which does not increase when the mesh is refined. The usefulness of our capacitance matrix method for problems in three dimensions has thus been firmly established. A portable FORTRAN program which can be used even for Helmholtz' equations of indefinite type is now ready for publication. An important subroutine of this program is a fast Helmholtz solver

on a rectangular region. Our program can easily be upgraded by replacing this subroutine by an even better fast Helmholtz solver once such a program becomes available.

O. Widlund, D. P. O'Leary

2. Fast Poisson Solvers for Problems with Sparsity

Fast Poisson solvers, which provide the numerical solution of Poisson's equation on regions that permit the separation of variables, have proven very useful in many applications. In certain of these applications the data are sparse and the solution is only required at relatively few mesh points. We have developed algorithms for such problems, in two and three dimensions, that allow considerable savings in computer storage and execution speed. Modified versions of our FORTRAN code are now being used by others in important applications.

O. Widlund, A. Banegas

3. Some New Capacitance Matrix Methods

A survey has been written on capacitance matrix methods applied to Helmholtz' equation on general bounded regions in two and three dimensions. The use of new fast Helmholtz solvers in this work, which permits a drastic decrease in the use of core storage, is emphasized.

O. Widlund

4. Fredholm Integral Equations and Fast Poisson Solvers

The use of Fredholm integral equations for the numerical solution of Poisson's equation is widespread. If the solution is required at very many points, however, this method is quite expensive. An idea due to Charles Peskin has been developed and tried out in practice. The solution, obtained by solving the integral equation by a numerical quadrature method, is found at mesh points within a few mesh lengths of the boundary. After a simple transformation, these values provide data for a conventional fast Poisson solver which furnish an approximate solution on the entire mesh. The use of similar integral equation methods for the solution of certain free surface problems is currently being tested in practice.

O. Widlund, A. Mayo

5. A Lanczos Method for a Class of Nonsymmetric Systems of Linear Equations

Work was completed on a paper with this title. Let L be a real linear operator with a positive definite symmetric part M.

In certain applications, a number of problems of the form $Mv = g$ can be solved with less human or computational effort than the original equation $Lu = f$. An iterative Lanczos method, which requires no a priori information on the spectrum of the operators, is derived for such problems. The convergence of the method is established assuming only that $M^{-1}L$ is bounded. If $M^{-1}L$ differs from the identity mapping by a compact operator, the convergence is shown to be superlinear. The method is particularly well suited for large sparse systems arising from elliptic problems. Results from a series of numerical experiments are presented. They indicate that the method is numerically stable and that the number of iterations can be accurately predicated by our error estimates.

O. Widlund

6. Solution of Stationary Navier-Stokes Equations by a Lanzcos Method

The nonlinear systems of equations that arise when discretizing the stationary Navier-Stokes equation by finite differences or finite elements have a very special structure. Nonlinear versions of a Lanczos method, previously studied by Concus, Golub, Widlund and Young in the linear case, are being developed and tested on some standard test problems such as flow in a square cavity. New theoretical results for the linear case have also been obtained.

O. Widlund, D. Rapoport

7. Conjugate Gradient-Type Methods for Saddle Point Problems

Numerical methods for symmetric indefinite systems of linear equations have been studied intensively during the last few years. We have developed a unified theory for many of the methods of conjugate gradient type, which have been proposed in the literature, and found estimates on the rate of convergence. The most promising of these methods are being tested on the Stokes problem. The extension of these methods to nonlinear problems and the use of preconditioning to enhance the rate of convergence is actively being considered.

O. Widlund, F. Thomasset

8. Best Error Bounds for Approximation by Piecewise Polynomial Functions

Finite elements and polynomial splines are examples of families of piecewise polynomial functions that are widely used in many applications. We have continued our previous work and have obtained further precise results on the extent by which the rate of convergence suffers when we approximate functions that are not smooth enough to permit the use of standard error

estimates. In particular, we have new results for a large family of approximation procedures that characterize the approximation error for functions in the Hilbert spaces W_2^s.

O. Widlund

C. Other Applications

1. Periodic Forced Vibrations of Relaxation Oscillators

In our work with periodic forced vibrations of relaxation oscillators we have treated differential equations of the form:

$$\ddot{\vec{x}} + \mu f(\dot{\vec{x}}) + \vec{x} = \vec{F}(\vec{x},\dot{\vec{x}},t) \ .$$

The left-hand sides are all of the same form except that the nonlinear damping term may differ in each degree of freedom; however, they should all be qualitatively like the term $-\dot{x} + (\dot{x})^3/3$ which occurs in the van der Pol equation. The parameter μ is assumed to be arbitrarily large, that is, the nonlinearity in the damping is large. If the functions $\vec{F}$ are independent of $\vec{x}$ and periodic in t, it is proved that periodic forced vibrations exist having the period of the functions $\vec{F}$, and the period can be chosen arbitrarily. If the $\vec{F}$ depend on $\vec{x}$, then they should be such that $\lim \vec{F}(\vec{x}) \to 0$ when $|\vec{x}| \to \infty$; and in that case the same result is valid. It is a general result, but it is rather unsatisfactory from a physical point of view since almost all of the periodic solutions would be extremely unstable.

A more satisfactory result is obtained if the system has only one degree of freedom. In that case, again for large values of μ, if F is bounded when the velocity $\dot{x}$ is bounded, periodic forced vibrations are shown to exist having periods as close to those of the free nonlinear vibration as might be desired, and they are stable in the sense that all would lie in a narrow ring containing the limit cycle for the free vibrations. There exist also subharmonics of any order. These results require a peculiar geometric discussion combined with an unusual way of making use of the Brouwer fixed point theorem. All attempts to apply this to systems have failed.

K. Anand is working on a thesis dealing with a special case of the above system having one degree of freedom. It is assumed that $f(\dot{x})$ is piecewise linear so that the differential equation can be integrated explicitly in different regions, with piecing together by continuity at the breaks caused by discontinuities in $f(x)$. What is wanted, in part, is an asymptotic estimate, using the explicit solution, for the period of the forced vibration when μ is sufficiently large. As noted above, that period must be close to the period of

the nonlinear free vibration. What we previously did shows that such oscillations exist, but no estimate in terms of μ for the difference between the two periods is obtained. The problem should be solvable, although the calculations are extremely messy.

J. J. Stoker

II. COMPUTATIONAL PHYSICS AND CHEMISTRY
(Partial Differential Equations)

A. Physics

1. Stabilization of the High Beta Stellerator

Using the ARPA net we have made large scale computations on the magnetohydrodynamics model of equilibrium and stability of a plasma in toroidal geometry. This is a fully three dimensional problem with an iterative scheme that simulates time. The resolution of the first version of our code was disappointing, and a new formulation has now been given that improves the accuracy by an amount comparable to one mesh refinement. This new version confirms earlier results concerning stabilization of high beta stellarators. We have now much more convincing evidence that triangular cross sections serve to stabilize the important $m = 1$, $k = 0$ mode. This effect is dependent on the magnetic structure within the plasma. Therefore, it is more significant in cases of low compression ratio.

Experiments in the favorable range of compression ratios are in the construction stage at the Max Planck Institute for Plasma Physics in Garching, Germany. We are in active correspondence with the group there, and a collaborative effort has been set up to work on the mathematical theory together with experiment. The prospect is that the better theory implemented in our computer code will bring the high beta stellarator into a range of operation competitive with current Tokamak research.

This is an example of a problem in energy research where progress could only be made through large scale computation on a genuinely three dimensional model.

O. Betancourt, P. R. Garabedian

2. One Dimensional Systems

The equilibrium statistical mechanics of classical one dimensional hard cores in an arbitrary external field was solved. It was verified that the pair direct correlation function remains of finite range in this case, and the properties of the higher direct and indirect correlation functions were examined.

The equilibrium statistical mechanics of the one dimensional Ising model in an arbitrary external field was solved completely. The signs and range of the higher direct correlation functions were determined, verifying a surmise of interest in constructive quantum field theory.

Similar techniques are now being used to study the statistics of linear chain polymers.

J. K. Percus

3. Nonuniform Fluids

A modified linear response theory of nonuniform fluids was developed. Numerical comparison with Monte Carlo calculations of both classical and Boson hard core fluids bounded by a wall was gratifying.

Similar techniques are being applied to the electron fluids of idealized closed shell atoms, regarded as nonuniform Fermion fluids. The cusp condition at the nucleus is found to hold exactly.

A sequence of models and model-generated restrictions on reduced density matrices is being applied to obtain both upper and lower bounds on the ground state energies and expectations of idealized atoms.

A quantum mechanical phase space formulation is being applied to obtain sequential approximations to the electron density of an idealized atom. Preliminary tests on harmonically bound electrons have verified that the required shell structure is rapidly built up in this fashion.

J. K. Percus

4. Two Phase Interface Region

The correlations existing in the transition region between gas and liquid phases of a simulated argon fluid have been investigated numerically and analytically. The picture which emerges is that of a hydrodynamically fluctuating sharply defined surface separating the two phases.

This investigation is being extended to the boundary region of a wall-bounded fluid, and to the interaction between wall and phase transition zone.

M. Kalos, J. K. Percus, M. Rao

5. Kinetics of Phase Transitions in Model Alloys

Study of the equilibrium properties and time evolution of model alloys has continued. Closer study of the simple cubic system undergoing phase segregation has shown clear evidence of a metastable state close to the coexistence line. The properties of the state observed in our computer experiments have been compared with appropriate theories. In the spinoidal region this metastability disappears.

We have continued the observation of the behavior of the ordering transition in the antiferromagnetic analog alloy system. This has been extended to square lattices and systems in which the diffusion of vacancies cause the atomic rearrangements.

In addition the more realistic case of an FCC lattice with next-nearest-neighbor and nearest-neighbor interactions has been modeled. Preliminary to doing studies of the kinetics, the previously unknown phase diagram is being mapped.

M. Kalos et al.

6. Theory of Quantum Many-Body Systems

Calculations on the ground state of liquid ^{4}He with Lennard-Jones potentials have continued. Results at densities from 0.9 to 1.2 times the observed equilibrium density are essentially complete and final corrections are being made. The energies agree well with the (less precise) values obtained previously by Kalos, Levesque and Verlet using Green's function Monte Carlo methods on the hard sphere quantum fluid and a perturbation theory connecting the latter with the Lennard-Jones system.

In addition to this confirmation, we find that the simple de Boer-Michels parameters agree substantially better with experiment than has been generally supposed. The equilibrium density is within 3% of the experimental and the minimum energy is only 4% too high. The structure function agrees well with experiment. It appears that neglect of three-body terms in the usual product wave function is responsible for the 16% overestimate of the energy obtained in variational methods.

Calculations of the solid phase have begun.

M. H. Kalos et al.

7. Quantum Systems at Finite Temperatures

The application of Green's function Monte Carlo to the study of quantum systems at $T > 0$ has been implemented in a study of the two-body hard sphere problem. We have determined the direct and exchange contributions to the pair correlation coefficients and the second virial coefficients. We use GFMC with ad hoc but powerful importance sampling and find very satisfactory agreement with published numerical results. In particular, we are able to estimate accurately the departure from unity of the direct pair correlation at high temperatures. We are presently testing various ways of improving the importance sampling still more.

M. H. Kalos, P. Whitlock

8. Theory of Classical Fluids

We continue the study of inhomogeneous argon fluid systems below the critical temperature. One simulation, for which a new Monte Carlo method has been devised, is of the structure of the fluid near a hard wall. It has proved possible to put the fluid near the wall in either the gas or the liquid phase.

Using Monte Carlo and molecular dynamics, we study small liquid clusters (up to 256 atoms) of argon in equilibrium with its vapor. Thermodynamical properties and the density and energy profiles have been determined. The distribution of small cluster sizes has been observed.

M. H. Kalos, J. K. Percus

B. Chemistry

1. Chemical Kinetics

A new program has been initiated to study the gas phase kinetics of the reaction of a $C(^1D)$ atom with a hydrogen molecule using computer solution of the classical equations of motion and Monte Carlo integration over initial conditions. This reaction can be considered as an approximate simulation of the primary attack of a free carbon atom on an alkane C-H bond. We will examine the reaction over a wide range of collision energies from thermal to 10 eV, calculating the reaction rate and observing any changes in the microscopic mechanism. Calculations have been completed at 0.5 and 1.0 eV.

P. Whitlock.

2. Dynamical Properties of Polymers

A new research program on polymers has been initiated. An existing molecular dynamics program has been adapted to the simulation of "atoms" interacting by Lennard-Jones forces together with intrachain harmonic forces.

M. H. Kalos et al.

III. COMPUTER SCIENCE

A. Programming Languages and Compilers

1. SETL

Work on the SETL very high level language has continued actively. Significant milestones attained during the past year were as follows:

a. A design of a full set of run time data structures, including data structures for a fairly wide choice of optimized set and vector representations, was completed. Coding of a library of set theoretic operations based upon these structures is now about 3/4 complete, and many of the operations have been tested successfully. A first draft compiler design has been written in full detail and extensively tested; this is now being reworked into its final form, and should be ready in the first quarter of 1978.

b. Two alternative techniques for semiautomatic data structure choice have been studied in considerable detail. Both techniques appear promising, and we are now in the process of studying them comparatively in order to choose one for implementation in the SETL optimize-system currently under development. Using these techniques, we now expect to be able to generate reasonably efficient data structures automatically for rather extensive classes of algorithms.

c. Detail drafts representing about 60% of the logic of the full optimizer system currently planned have been worked up. We are now proceeding to complete these drafts and to scrutinize them carefully for logical inconsistencies. This extensive collection of optimizer algorithms is written in SETL, and should therefore be executable, at least for testing, as soon as our new SETL system is complete.

d. Work has begun on a set of measurement utilities to be installed into the SETL system during its development, and to remain part of the completed system. By making these utilities available during development, we hope to be able to make a number of significant design improvements on the basis of objective measurements of system performance.

e. We have studied the possibility of increasing the efficiency of SETL by supporting its shortest (and most frequent) operations directly in microcode on the PUMA hardware. These operations should run 5-10 times faster when microcoded than they do on the 6600; this should speed the total system up by a factor of 2 to 4. We hope to make these estimates more precise by use of the measurement system described under (d) above. When this has been done, a full scale microcode effort may be undertaken.

f. The quality of code generated by the compiler for SETL's implementation language LITTLE has been substantially improved. LITTLE is now available as a production compiler for the 6600, IBM 370, and Honeywell 316, with a DPD-11 variant under development and a PDP-10 variant now being designed. The compiler handles approximately 9000 statements/sec. on the 6600 and 15,000 statements/sec. on the 370. The transportability of the language was tested quite successfully in the recent use of LITTLE to develop the PUMA operating support system (POS) on the CDC 6600 and then to transfer it with almost no code change to the Honeywell 316.

R. B. K. Dewar, J. T. Schwartz

2. PL/I Compiler

During the reporting period, work commenced on Version II of the CIMS PL/I system, under joint sponsorship of ERDA and the Control Data Corporation. Development of the new system is intended to serve two goals: to produce a product that is useful in its own right and to explore the software engineering aspects of creating a large program.

The first major accomplishment was the installation of facilities for formatted input-output in the existing system, but in a form that will carry over to Version II. The existence of these facilities removes the major functional limitation encountered by users of the existing system, although the large core requirements and slow compilation still remain. As part of the work on formatted input-output, we developed routines for the conversion of floating point numbers to character form, and conversely, that are fast, accurate, and clearly written. These routines should be quite helpful in scientific calculations involving large volumes of input-output. (They are also more compact than their FORTRAN counterparts.)

Beyond that, the parser for Version II has been written and compiled, but not yet debugged. Version II will implement full ANSI Standard PL/I and the parser is therefore capable of parsing the entire language -- nothing has been omitted. Part of our experimentation in software engineering is in having the debugging done by relatively inexperienced students, one of whom is now working on the parser. Our hypothesis is that while inexperienced programmers may damage the quality of a product if they actually write code, there is little damage that they can do in debugging well written code. It is important to distinguish debugging from testing here: debugging is the removal of known bugs, while testing is the search for the existence of bugs. It is still up to the author to be sure that the set of test cases is adequate. The debugger can also discover places where the code is correct but obscure; the appropriate remedy in this case is for the author to add appropriate clarifying comments.

This approach to software production has some subtle advantages. It removes the primary author from the time consuming process of tracking down obscure errors, and thereby shortens total production time of the program. Since the debugger reads the code, the quality of the code is improved by his insights. Moreover, since the job of debugger is not regarded as a long-term assignment, the motivational problems associated with it are largely avoided. It is in fact the kind of job that is satisfying over the short run -- since it is highly educational -- but not over the long run.

P. Abrahams

B. Other Applications

1. Digital Computer Design Automation -- PUMA

The objectives of this research are the development of digital design automation tools at the Laboratory and the construction of digital systems which will be useful in the Laboratory's research.

During the past year, considerable progress has been made in the design and construction of a small processing unit, identical in instruction set to the Control Data 6600 central processor, and about half as fast. This effort has utilized and furthered the development of an integrated system for design automation -- for circuit description, simulation, wiring, and testing.

An initial, slower version of the processor (about one-eighth the speed of a CDC 6600) was completed during the spring. With the assistance of the Laboratory's hardware group, this processor was interfaced to a small memory (4096 60-bit words) and a mini-computer for performing input and output. During the past few months (May-July) we have been debugging both the processor and the computer's operating system.

We expect that the processor will be available for use in August, although severely limited by the low processor speed, small memory, and slow input-output rate. We are currently designing a faster processor, and expect to assemble the new processor in the coming fall. A larger memory and faster mini-computer have also been ordered for the system and should be available towards the end of 1977.

R. Grishman

2. Natural Language Data Base Retrieval System

This research project is developing a system to allow users to interrogate a data base by asking questions in English. The particular type of data base on which we have been working

consists of natural language text (in some scientific or technical field) which has been transformed by computer into a tabular structure. Such structured or "formatted" data bases are currently being produced by the N.Y.U. Linguistic String Project.

An initial version of the system became operational in June; it can answer simple questions about a small data base of hospital X-ray reports. As an illustration of the system's capabilities, we present the following brief dialogue:

USER: Did every patient have a chest X-ray in 1975?

SYSTEM: No (PZ did not).

USER: Has PZ had any since 1975?

SYSTEM: No.

USER: How many has PY had since 4-1-75?

SYSTEM: 1 (T6)

USER: When was it taken?

SYSTEM: 8-10-75

Much still remains to be done in developing this system -- enlarging the domain in which questions can be asked and increasing the variety of question types which will be accepted.

R. Grishman

3. CIMMS Multi-Microprocessor Project

Development work on this project has continued. CIMMS.OS.1, Version 1 of the operating system, is now operational, though it has not yet received extensive testing. CIMMS.OS.1 provides a single virtual memory space of 64k bytes for each of the eight 6800 microprocessors, with the management of the virtual memory being done by the PDP-11. At the present time we have one 6800 which is fully operational under Version 1 with its own PROM to be written, and 6 other 6800's which need minor hardware modifications to operate.

In the development phase are projects to implement assembler under CIMMS.OS.1, to implement BASIC, and to get CIMMS.OS.2 operational. CIMMS.OS.2 will provide the same facilities as CIMMS.OS.1 but with more concurrency in its operation. In the planning stage is CIMMS.OS.3, which will provide multiple, system, and shared files.

Also under development is a version of BALM suitable for implementation in the microprocessors.

M. C. Harrison

4. Intelligent Terminal Graphics

A major project to provide an intelligent terminal for three dimensional graphics was concluded this year. Much of the effort was directed toward the study of the effects surrounding the distribution of work load between two machines for problems of a graphical nature.

The distribution of work has caused difficulties ever since it was realized that the use of refresh graphics devices is only practical when two computers are employed. This happens because, on the one hand, the device itself imposes enormous real time demands on the processor servicing it, and, on the other hand, the applications intermittently require substantial computational power. Since the real time requirements will drain the resources of very powerful machines, the inevitable solution is to shunt off display maintenance to a minicomputer. However, the problems only begin here, for one must then decide how much of the software will follow the refreshing facility to the minicomputer.

Early in this project we developed a compiler to produce code for our video terminal, a Honeywell 316 minicomputer driving a Vector General graphics display. The language, LITTLE, was designed by Jacob Schwartz with systems implementation in mind, and was already running on our mainframe CDC 6600. LITTLE's level (approximately between PL/I and FORTRAN) coupled with its efficiency provided a much more powerful vehicle for development of a graphics system than had been previously available. Perhaps even more important, however, is that LITTLE programs are easily transportable. The net result of this approach is the enabling of intelligent decisions about software distribution between the terminal driver and the powerful mainframe.

Starting with a design in the set theoretic language SETL and proceeding to an implementation in LITTLE, we built a sophisticated graphical system with a flexible, hierarchical data structure and a variety of manipulative functions for graphical entities. Of the many distribution alternatives perceived, we chose that of raising the intelligence level of the local terminal.

T. Stuart

IV. ARPA NETWORK

A. Network Access Method

The implementation portion of the ARPANET project was primarily a development effort to provide the tools for using the network for the purpose of studying its relevance to ERDA's computational needs. However, the NYU design approach has provided significant knowledge in two areas of network access technology.

1. Computer System and Operating System Independence

The high cost of system development makes a transportable design very attractive. The NYU time sharing access technique has demonstrated portability by being installed with a minimal effort at several ERDA computer centers and Navy laboratories. Independently, the TELENET Corporation has adopted a similar technique for their basic access method.

The file transfer subsystem, although not as easily transported as the time-sharing subsystem, provides the benefits of a standardized higher level protocol between the host and front-end systems. No actual installations have been made outside of NYU, but some of the Navy laboratories are considering it.

2. Front-End Minicomputer Architecture

Recently, the principle of off-loading the telecommunications tasks of large computer systems to small front-end computers has received wide acceptance. At NYU, experimentation with such methods began as early as 1966. We chose this approach for the ARPANET connection. Through a successful implementation, a great deal has been learned about the distribution of tasks between the front-end and host systems and about the impact of front-end software design on the efficiency of data transfer. In particular, it has become clear that elaborate and generalized front-end systems, such as ANTS II, ELF II, and UNIX, typically incur too much overhead to easily provide the necessary transfer rates for either large numbers of interactive users or high speed file transfers.

3. Implementation Status

The basic implementation of the network access capability has been completed. Time-sharing access to the network, time-sharing access to our CDC 6600 from the network, file transfer, and remote job submittal between sites are all operational.

Development activities to increase system efficiency and to simplify the user interface are either underway or planned.

All necessary program modifications have been made to accommodate the change in the CDC host computer to the NOS operating system.

Portions of the NYU network access system have been successfully installed at the Brookhaven National Laboratory and at several Navy research centers.

Ongoing maintenance is being provided for locally developed software. A plan for maintenance of the entire ELF system is being developed in conjunction with other user installations.

B. Network Applications

The ARPANET is being used routinely for several applications.

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

A group studying the application of computerized algebraic manipulation techniques in plasma physics regularly uses the network to access the MACSYMA system at MIT.

Computerized teleconferencing has been used extensively by the ERDA Working Group on Computer Networking to conduct its business. Of particular interest has been the success of this method in the preparation of a research report by this group of geographically separated collaborators.

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

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

Among the resource sharing problems potentially available to networking solutions, one of major concern to the ERDA community at this time is that of utilization of available computer time across laboratory boundaries. We have chosen this as a major focus of our experimental effort at this time.

In the recent past, the computer industry has seen remote computing practiced with a good deal of success. However, it is important to distinguish this kind of activity from the more complex activity suggested by the notion of sharing among the ERDA laboratories.

Current practice consists typically of a number of geographically dispersed users, with either conversational or remote job entry terminals, accessing a single centrally located computer. These users seldom have any significant local

computing power or data storage media other than punched cards or printed paper. Such a situation is quite different from that at the ERDA laboratories. Here we see large clusters of users with a great deal of local computing power, with familiar software to provide many program development support functions, such as editors, compilers, data managers, and subroutine libraries. In addition they have established working relationships with user services personnel at their own computing centers.

If these users are to use similar, but different, facilities at other sites, many questions are raised. Some are mentioned here by way of example. First, what is the impact on these users of the need to learn two or more sets of dictions for specifying similar functions at different sites? In cases when the programs are "identical", such as with the CDC FORTRAN Extended Compiler, how should we deal with the fact that different sites may have the compiler at different release levels and, therefore, containing different error populations? Second, if these users are to run at more than one site (even if one of these is their own), how should they manage their program and data libraries? Should they keep multiple copies or single copies to be shipped as needed? How difficult will it be to maintain multiple copies? Even among CDC sites there are important differences in the internal forms of data; a central issue here is that of the means of data transport. The economics and response times of different methods should be evaluated all the way from station wagons to packet switched networks. A third issue is that of special hardware, such as graphic output devices. Is it more convenient, or even necessary in some cases, to do plotting at home or at the site where the associated computations are done? If at home, what compatibility issues are raised between remote software and local hardware?

All questions raised may be viewed as instances of a general question relating to the distribution of labor over a distributed collection of resources. Whereas, in the traditional remote computing activity, the answers are pretty much dictated by the rigid distribution of resources between the central site and the remote terminals, the situation of the ERDA laboratories is something quite different that has not received any but ad hoc attention in the computing community at large, and which is deserving of serious study and experimentation.

In order to begin to answer this question we are performing some of our typical large scale calculations on the Lawrence Berkeley Laboratory CDC 7600 using the ARPANET as the prime data communications method. For comparison and in order to investigate compatibility issues we are running programs at the Brookhaven facility by standard remote job entry methods.

E. Franceschini, M. Goldstein

V. RELATIONSHIP TO OTHER PROJECTS

A. DOE Laboratories, Government Agencies and Industry

In cooperation with LASL and LLL, our Laboratory develops methods for calculating flows with shocks. The methods developed have proved useful for studying a wide variety of flow patterns.

In the use of our Transonic Analysis and Design Codes, assistance is provided to the NASA Langley and Ames Research Centers, National Research Council of Canada, Pratt and Whitney Aircraft of United Technologies, Sikorsky, Hamilton Standard, and Northrop Aircraft.

E. Isaacson and others at Courant maintain contact with NASA Goddard Space Flight Center, Maryland, on climatology modeling.

A collaborative effort has been set up to work on the mathematical theory together with experiment of the stabilization of the High Beta Stellarator with the Max Planck Institute for Plasma Physics in Garching, West Germany. We provided the group there with a copy of our MHD Equilibrium and Stability Code which they now use. This code has also been made available to Dr. L. Shohet and his colleagues at the University of Wisconsin.

The Laboratory conducts work on the development of numerical methods for modeling chemical and reacting flows occurring in combustion. Gary Sod periodically visits members of LLL and LBL, who are also engaged in this research.

Relative to reactor safety, some of the theoretical and numerical methods used to study the reflooding problem in a loss of coolant accident have been developed here at the CIMS. Peter Lax is an active member of the Advanced Code Review Panel of the Nuclear Regulatory Commission.

F. Tappert is a consultant to LASL for studies in laser fusion.

A portion of O. Widlund's work on elliptical partial differential equations is done in collaboration with DOE projects at LBL.

We have worked with Westinghouse regarding properties of radiation damage. In our work with alloys, we have collaborated with a project, supported by a grant from the Air Force Office of Scientific Research, at Yeshiva University. In the modeling of quantum systems and fluid systems, we have collaborated with the Cornell University Laboratory of Atomic and Solid Physics.

A code for the numerical calculation of transonic flows past swept wings, developed here, has had wide acceptance in the aerospace industry. In particular, it has been used at Grumman, Boeing, McDonnel Douglas, and Lockhead to analyze wings of current and future designs for medium and long range transport aircraft.

The CIMS PL/I compiler has now been distributed to about 50 different installations including LBL and BNL. During the past year work has begun on Version II of the CIMS PL/I system with support from Control Data Corporation.

Nine U. S. Navy computing centers are either using or plan to use a Server Telnet based on our Laboratory's software for access to the ARPA Network.

B. Magneto-Fluid Dynamics Division, Courant Institute and New York University

The Laboratory has many ties with other research groups within the Courant Institute and New York University. In particular, the Laboratory has strong interests in the controlled thermonuclear research program of the Magneto-Fluid Dynamics Division here at Courant. There are also many inter-relationships between our projects and those of the Courant Institute in the field of continuum mechanics and mathematical physics.

Reciprocal theoretical support, sharing of computational resources, and training of personnel to apply advanced mathematical and computer methods accompany these interrelationships. Within this purview, the Laboratory has given support to the following projects:

Magneto-Fluid Dynamics Division

1. Scope

The Magneto-Fluid Dynamics Division effort in Computational Fusion Research has, in the distant past, concentrated primarily on developing algorithms for the effective solution of novel and nonstandard computational problems such as free boundary equilibria, bifurcation of equilibria, computation of ill-posed or basically nonexistent equilibria and computation of composite (elliptic and hyperbolic) closed line equilibria. Algorithms for MHD and guiding center models of free boundary and distributed profile equilibria have found their way into everyday use in computational CTR plasma physics. Such research has fit ideally into the overall program of the Courant Institute and in particular was able to take advantage of the extensive facilities of the ERDA Computing Center also based in the Courant Institute.

In the past three years, the computing effort in the MFD Division has been enlarged to include simulation of fusion plasma phenomena. Large programs are underway in the development of efficient 2D + t diffusion codes including island structure, based on the prior development of a theory of adiabatic compression; also for numerical MHD and guiding center stability, also Alfvén wave heating guided from spectral theory. Efficient numerical algorithms and codes for computing MHD stability of highly elongated toroidal equilibria have also been developed. Each of the foregoing represents a significant advance in the relevant state-of-the-art.

2. Technical Progress in Fiscal Year 1977

Continued development and application to current interesting experimental configurations of a series of state-of-the-art 2D + t adiabatic and resistive diffusion codes was considered a major step forward in FY 1977. These codes represent a self-consistent treatment of the entire diffusive transition from an initial noncircular axisymmetric configuration to a fully formed doublet plasma. The numerical codes contain the basic ingredients of adiabatic compression, island formation, growth and saturation plus transport. Among the more recent technical advances made during the course of code development are:

a. Advances in treating a separatrix - a key improvement in accuracy has been the use of interpolation of specific inductance following the moving separatrix. The necessity became clear after mathematical analysis of the separatrix singularity. It turns out to be essential to closely place contours on each side of the separatrix. This is done effectively by a geometrically increasing spacing (with occasional extra contours, e.g., at the center if islation is about to occur or near the outer edge if the geometrical spacing is too large). Also, with growing or shrinking islands, the number of inner contours must be allowed to vary from step to step. Another important critical point is that for accuracy, interpolation (in either the 2D geometry computation or the 1D diffusion computation) must not be allowed across the separatrix.

b. Guidelines for noting changes in topology have been refined--the decision of when to dignify small islands by assigning contours to them inside, defining new inductance functions and adding new diffusion equations as they are needed is intricate but not difficult. The number of time steps at which the geometry is recomputed does not have to exceed two or three in a doublet or belt pinch problem so long as the topology does not change (the plasma shape can change considerably); an additional one or two subdivided steps are helpful during islation, until the islands grow to an appropriate size. A complete transition from belt pinch to doublet can be computed in under one minute of 6600 time.

c. An Eulerian 2D mesh is found to be more efficient than other codes using Lagrangian or flux coordinates; this is quite evident from the singularityand multivaluedness of Lagrangian independent variables (when even a simpler polar coordinate singularity requires special care and reduces the accuracy). Generally speaking, in a 1×2 rectangular domain, a 32×64 mesh gives an adequate answer, 64×128 is standard for the 2D mesh (and 128×256 is used for special purposes such as checking singular boundary layers and the low resistivity limit). Some 200 to 300 points are taken in the 1D diffusion mesh (approximately equal mesh size in the islands and outer regions). The number of contours varies from two (in an island at birth) to a standard number of 10 to 20 for the entire plasma.

d. The treatment of a free boundary at the plasma edge has been considered in detail and rules have been developed for such treatment. In the adiabatic problem, the volume of the plasma can be given a priori or it can be determined from given external flux or current constraints. A useful tool here (and in diffusion problems) is the inductance of the exterior vacuum field. This serves to connect boundary conditions at the edge of the plasma directly with the outer wall. There is no need to calculate more than one or two contours in the vacuum, and the value of L is given explicitly at each iteration step by the Poisson (or other) inversion. The resistive free boundary has a linear pressure profile (to $p = 0$) with an explicit formula for the boundary velocity. The free boundary with heat flow and resistivity ($\rho = p = 0$ at the edge) is handled in terms of the normalized volume, say $\xi = V/V_p(T)$ as independent variable. The boundary is always $\xi = 1$, but there is an artificial convection term involving $\dot{V}_p/V_p$ which has to be determined. We are able to monitor the exponents (e.g. $\rho \sim V^r$) to detect when the plasma leaves the wall or limiter, then use a very accurate feedback mechanism to determine $\dot{V}_p$ such that the plasma neither leaves the "wall" $\xi = 1$ nor leans on it too heavily. For ease in making comparisons, the codes are written so that it is easy to make changes in the type of interpolation and in types of explicit and implicit diffusion schemes. Essential for efficient computation is the optimizing of the 2D geometry mesh, numbers of contours inside and outside the separatrix, an inner and outer diffusion mesh, an interpolation mesh from 1D to 2D, and a judicious choice of backaveraging and accuracy limits in several parts of the calculation. Only a small amount of optimization has been attempted.

H. Grad, S. Liu, D. Stevens, E. Turkel

A major achievement was accomplished with the conversion of the numerical code for calculation of stability of highly elongated high-β tokamak plasmas to one for which any given form of the plasma current density profile can be used to generate the equilibrium flux surfaces. The equilibria are computed numerically and very quickly and the resulting magnetic field profiles

are then passed on to the stability code. Extensive studies of a variety of families of current density profiles and plasma-vacuum boundary shapes have been made to determine the effects of these functions on the stability of the most dangerous modes occurring in the system. Current density profiles yielding belt pinch and doublet like outer boundaries have been studied with the following general wisdom resulting:

a. Both plasma cross section and current density profile significantly affect the linear stability of high-β tokamak plasmas.

b. A peaked off-axis doublet-like current density and plasma cross section with reasonable outer wall separation appears to be advantageous.

c. An interesting point is that we have made a connection to earlier predictions concerning the possible advantage of low shear plasma profiles.

W. Grossmann, J. Tataronis, H. Weitzner

Significant progress was also made in the development of a computer code for treating the linearized dynamics of a Vlasov-fluid model of a plasma in straight cylindrical geometry. Many simplifications and reductions of the governing equations have been found resulting in algorithms which will facilitate the numerical computation. The code is being written initially to investigate certain linear θ-pinch questions such as the effect of finite Larmor radius on rotational instabilities.

C. Seyler

Courant Institute of Mathematical Sciences

1. Transonic Flow Calculations

In order to conserve fuel in commercial air transport operations it is important to optimize the design of swept wings for flight at speeds near the speed of sound. A code for the numerical calculation of transonic flows past swept wings has been developed at the Courant Institute. This code, released through NASA, has had wide acceptance in the aerospace industry. In particular it has been used at Grumman, Boeing, McDonnell Douglas, and Lockheed to analyze wings of current and future designs for medium and long range transport aircraft.

There is a need to analyze more complex configurations such as wing fuselage combinations and ultimately the complete aircraft. For this purpose a new scheme has been developed in which cubes are individually mapped to small volume elements by separate local transformations. Preliminary results indicate the promise of this method, which should be able to treat configurations of more or less arbitrary geometric complexity, given a sufficiently powerful computer.

D. Caughey, A. Jameson

2. ELASDYN

During the fiscal year one project was almost completed and another reached a significant stage of development. Both projects are concerned with the solution of integral equations arising in fracture mechanics and seismic source theory.

First Project. It had been noticed by Joe Andrews of the U.S.G.S., Menlo Park, that when a shear crack with finite cohesion accelerates, it at first smoothly approaches the Rayleigh wave speed v_R but then its speed discontinuously changes to a value slightly greater than $\sqrt{2}\ v_s$, where v_s is the shear wave speed. We conjectured that crack speeds between v_R and $\sqrt{2}\ v_s$ are unstable and were able to demonstrate this at least in the range $(v_s, \sqrt{2}\ v_s)$ by studying the steady motion of a crack under the influence of a following load. We found that in the rage $(v_s, \sqrt{2}\ v_s)$ the crack speed increased as the load diminished, whereas in the range $(\sqrt{2}\ v_s, v_P)$, v_P being the P wave speed, the crack speed increased as the load increased. The former regime we interpreted as unstable and therefore not arising in practice and so we partially explained Andrews' results.

Second Project. This project concerns the mathematical modeling of seismic clipping on a fault plane embedded in a uniform elastic whole space.

We formulate the problem as a time-dependent integral equation over the region of slip in the fault plane. This method obviates

the introduction of artificial boundaries and reduces the dimensionality of the problem from 3 to 2 space dimensions.

The singular integral equation may be solved step by step in time by an explicit scheme.

So far we have solved scalar analogs of the elastodynamic problem, i.e., we have used the scalar wave equation before setting up the computations for the full elastodynamic equations.

The work has progressed so well that we were able to show a computer movie of our seismic source model at the American Geophysical Union meeting in Washington, D. C., in June this year.

We intend to continue this project by performing the calculations for the full elastic wave equation in the 1977-78 fiscal year.

R. Burridge

3. Physiological Research

These projects involve not merely the application of existing methods but the development of new methods in the area of computational fluid dynamics, an important field of interest of ERDA/DOE in general and of the Mathematical and Computing Laboratory of New York University in particular. For example:

a. In the use of A. J. Chorin's finite difference method for the Navier-Stokes equations, we have developed a new method for coupling an immersed, moving, elastic boundary to the flow.

b. In the use of Chorin's vortex method, we have achieved a similar result, and we have also developed a new hybrid method (related to that of Shestakov) to deal with the practical limitations imposed by internal flows. In a different application, we have combined the vortex method with conformal mapping to achieve high resolution near sites of vortex shedding.

c. We have developed a new, fully Lagrangian method for the Navier-Stokes equations.

d. In research on the inner ear, we have developed a new method to deal with certain problems of wave propagation where the wave speed varies with position.

This work has had an impact on other ERDA/DOE research in which the treatment of boundary conditions was important. In particular, we were involved in the discussions that led to the accurate treatment of the boundary conditions in Chorin's recent vortex sheet method for the combustion problem.

This illustrates how diverse applications reinforce each other by stimulating the development of improved numerical methods. Both the combustion problem and the problem of blood flow in the heart involve the Navier-Stokes equations. Vortex dynamics, especially the interaction of vortices with boundaries, play a fundamental role in both areas, and computational experience in either application is important to both fields of investigation.

C. S. Peskin

4. Vortex Methods for the Heart Valve Problem

In an effort to extend our numerical studies of the flow of blood around heart valves into the regime of high Reynolds numbers, we are investigating the application of the vortex method of A. J. Chorin to this problem.

a. The aortic sinus vortex. The aorta bulges outward just beyond the aortic valve forming a sinus behind each of the valve leaflets. The function of the sinus is to trap a vortex which participates in efficient valve closure. There is a conformal mapping from a two dimensional model of the sinus region onto the upper half plane, which we use to determine the equilibrium position and strength for an inviscid point vortex in the sinus. The stability of this equilibrium is established by computing the vortex trajectories. Next, we use the vortex method for slightly viscous flow to study the formation of the aortic sinus vortex. The same conformal mapping automatically generates high resolution near the corners of the sinus in the physical plane. The results for a flow started impulsively from rest exhibit vortex shedding and streamline separation at the upstream border of the sinus. The point of reattachment of the separating streamline moves along the sinus wall until it encounters the downstream border of the sinus. The flow pattern then becomes steady, with a vortex in the aortic sinus and a nearly uniform flow in the aorta.

b. A hybrid vortex-finite difference method for the case of moving, immersed, elastic boundaries. As originally formulated the vortex method was applied to the case of rigid boundaries in an external flow. Vortices were generated to enforce the no-slip condition at the boundary, and the number of discrete vortices was held within bounds by ignoring the vortices that were swept away downstream. This was important since the computational work per time step increased as the square of the number of vortices. In the heart we must deal with moving, immersed, elastic boundaries (the valve leaflets) and with vortices which are not swept away downstream but which accumulate as the ventricle fills. We overcome these difficulties by combining the vortex method with finite difference methods as follows. First, we use the curl of the (singular) boundary force field as a source of vorticity. We retain each discrete vortex only for a fixed amount of time, after which we transfer its vorticity to a computational mesh.

We move the discrete vortices in a velocity field computed on a computational mesh. Because of this, the computational work grows only linearly with the number of discrete vortices. There are several variants of this method, which differ with respect to the precise algorithm for generating vorticity from the curl of the boundary forces. In the first such variant, the force at each boundary point is used to generate a vortex dipole. This method works well as long as the discrete vortices are retained for only a short time, but instability sets in when longer lifetimes are tried. We are now testing other variants in which the normal and tangential components of the boundary force are treated separately.

C. S. Peskin, A. Wolfe

5. Comparison with Heart Valve Experiments.

We are setting the parameters in our computational experiments to agree as closely as possible with the corresponding quantities in animal experiments. This will provide a test of the numerical methods, and will give us a reasonable standard case, against which computed results for prosthetic heart valves can be compared.

D. M. McQueen, C. S. Peskin

6. Polygon Method

This fully Lagrangian method for viscous incompressible flow with large deformations has been improved as follows. First, we have speeded up the construction of the polygons by devising a method which takes advantage of the fact that the configuration changes only slightly from one time step to the next. Second, we have combined the heat equation step and the Laplace equation step into a single step representing the Stokes equations. This removes a conflict in the boundary conditions, and it simplifies the algorithm. The Stokes equation step is followed by convection to complete one time step of the Navier-Stokes equations.

C. S. Peskin

7. Improved Graphics

We now produce cine films of the heart valve results in which fluid markers (rather than velocity vectors) are used to indicate the fluid motion. We also produce streamline plots of the fluid velocity field at selected time steps. This required a special program because the source in the atrium makes the stream function multivalued.

C. S. Peskin, A. Wolfe

9. Statistics of Normal Mode Amplitudes in a Random Ocean

A statistical theory of acoustic propagation in a random ocean, valid in the limit of low acoustic frequency, is presented. A random internal wave model gives sound speed fluctuations $\delta c(r,z,t)$ about a deterministic profile $\bar{c}(z)$. Using normal modes $\phi_n(z)$ of $\bar{c}(z)$ as a basis, the theory gives quantitative estimates of statistical moments of the mode amplitudes $\psi_n(r,t)$, which are randomly coupled via δc. Invoking a quasistatic approximation, the theory reduces time to a parameter. From any initial ($r = 0$) distribution of modal powers $|\psi_n|^2$, the evolution of their averages to an equilibrium is predicted by "coupled power" equations. The theory makes similar predictions for average fluctuations of the modal powers about their means. In the equilibrium limit, the theory gives the full probability distribution of the ψ_n.

Excellent confirmation of the theory came from a large-scale Monte Carlo computer simulation. At each of the acoustic frequencies 50, 100, 200, 500, and 1000 Hz, 100 independent realizations of the ψ_n were obtained. The sample moments then indicated that at least up to 200 Hz, the theoretical predictions were quite accurate. For 500 Hz and above the theory broke down, as expected for sufficiently high acoustic frequency.

L. B. Dozier, F. D. Tappert

10. A Numerical Study of a Converging Cylindrical Shock

A numerical procedure was developed for the solution of the one-dimensional equations of gas dynamics for a cylindrically or spherically symmetric flow. The method consists of a judicious combination of Glimm's method (a random choice method) and operator splitting. The method was applied to the problem of a converging cylindrical shock.

G. A. Sod

11. A Survey of Numerical Methods for Compressible Fluids

The finite difference methods of Godunov, Hyman, Lax-Wendroff (two-step), MacCormack, Rusanov, the upwind scheme, the hybrid scheme of Harten and Zwas, the antidiffusion method of Boris and Book, and the artificial compression method of Harten were compared with the random choice method known as Glimm's method. His methods were used to integrate the one-dimensional Eulerian form of the equations of gas dynamics for an inviscid fluid.

G. A. Sod

12. The Numerical Model of Unsteady Combustion Phenomena

The numerical modeling of a chemically reactive flow is complicated by the interaction of unsteady wave motion and fast energy release. The flow calculations are governed by acoustic time scale while the characterstic chemical reaction time scales can be several orders of magnitude smaller.

A numerical method is being developed which properly models wave interaction (including shock waves) with the process of fast energy release. The unsteady transport of chemical species, momentum, and energy is treated by Glimm's method, a random choice method. Operator splitting is applied to the chemical source terms in the species transport equations, resulting in a set of simultaneous ordinary differential equations.

As a test case, the method will be applied to the one-dimensional, shock induced detonations of methane and air.

G. A. Sod

13. LITTLE Programming System

The thrust of the work in this period was to complete the "consolidation" phase of language and compiler development. The language changes were minor, and consisted mostly of simplifications. Substantial changes were made in the operating system interface. This interface is now more portable and more efficient, and does not contain any implicit uses of the FORTRAN (FTN) library.

LITTLE input/output was simplified and the implementation largely redone. The run time support procedures are much smaller and more efficient. More of the conversions are now done in LITTLE, although an implementation has the option of providing certain well defined procedures in assembly language, to permit use of particular hardware features.

The LITTLE guide was revised to reflect the work of the last three years. The guide was moved to the System/370 at CUNY, and converted to upper and lower case. Two document processors -- LTLDOC and LTLPAD -- were written to assist in listing the GUIDE; these processors are now used for other documents also. The revised guide has been read by at least ten people, and seems to be in good shape. A number of copies have been sent in response to requests for more information on LITTLE.

The Boeing Aircraft Company requested a demonstration copy of LITTLE for the CDC 6600 in March 1977. The production of this copy provided an opportunity to revise and test the export procedures for LITTLE. This effort seems successful as Boeing reported that they had no difficulty installing LITTLE, and were very impressed by the simplicity of the installation process.

We wrote a syntax generator SYN which replaced the syntax generator TOPDOWN. TOPDOWN was written in BALM and required a supplementary program TDLINK written in FORTRAN and LITTLE. SYN is written entirely in LITTLE and is integrated into the LITTLE system. The LITTLE grammar and parser were converted to use SYN; work is underway to convert the SETL and GYVE grammars.

Work was begun on the addition of program measurement tools to LITTLE. These tools support the automatic generation of counters to count the number of times various events occur during execution. An experimental version was created and used to measure the LITTLE compiler. The measurements indicated several ways to improve the compiler performance. It seems clear that a relatively modest effort will permit the collection of measurements which are of great interest to the writers of the new SETL implementation.

One sign of success was the relatively small amount of time required to maintain the LITTLE system. Extensive use of LITTLE in writing the new SETL implementation and the POS operating system uncovered only a small number of bugs.

D. Shields

NYU Department of Applied Science

1. Modeling of a Flow Field in a Coal Fired Fluidized Bed Packed with Heat Exchangers

Work has begun on the modeling of the flow field in a full scale fluidized system with pressure and heat transfer effects included. Emphasis at the present time has been on the determination of the relevant equations of motion under steady state conditions, and the establishment of a numerical integration scheme for their solution. The analysis will be coupled to information determined from the experiments so that ultimately the analysis can be used to determine parametrically how variations in different flow properties and scale sizes will affect the efficiency of the operation.

Published work to date on bubble development and the gas flow patterns through them is at a stage where it is still not possible to attempt to predict the detailed effects of particle shape and size distributions on such development; or the effects of scale, internal surfaces and pressure (it has been pointed out that at pressurized conditions, the higher gas density causes the density ratio between particles and fluid to decrease, and thus the gas may act more like a liquid, inhibiting bubble development and growth). Thus the present analysis does not utilize the principles of bubble and emulsion phases, which have been utilized in many previous models.

To test some of the assumptions which will be utilized in our complete model, a preliminary analysis is being performed under the following assumptions:

a. Entering gas is unheated and incompressible (bed is operating at atmospheric pressure),

b. Particles are noninteracting except in the determination of the drag force acting on an individual particle (see below),

c. Gas distribution at entrance is axisymmetric (but can have a radial distribution),

d. No internal surfaces in bed,

e. Gas flow is laminar.

The assumption (b) is only true for $\lambda/d_p >> 1$ (where λ is the interparticle distance), which is not true here. Studies of friction factors in packed beds (where $\lambda/d_p << 1$, the other extreme) indicate that the equivalent 'C_D' (drag coefficient) would be on the order of 30, for 1/8 " limestone particles with a gas velocity of 2 ft/sec, a void fraction of .3 and a pressure drop of 1 psi. It is thus obvious that the C_D term (it is of course not correct to call it a single particle drag coefficient) will be a function of position. Near the top of the bed at the center, it can be expected that $C_D \approx 1$ while at the bottom $C_D >> 1$ near the walls, if a good circulation pattern is established. We plan to experimentally determine the drag force variation in a fluidized bed and establish correlations with Reynolds number, void fraction, and local pressure drop which will be incorporated into the analysis.

An integral technique has been developed for the solution of the flow properties, assuming that the following information is known from experiments:

a. Wall pressure distribution along bed (the radial distributions are calculated),

b. The height of the bed for a given experiment,

c. The gas velocity profile at the entrance,

d. The C_D distribution.

The resulting system is then solved by iteration. The system of equations are five first order ordinary differential equations which have been numerically coded and run on the CDC 6600 computer. The calculations indicate that the method gives an adequate representation of the flow field in the bed.

G. Miller

2. Dispersion of a Plume in an Urban Area

Wind speeds are smaller in the city than in the surrounding country at the same height, mainly because of the greater aerodynamic roughness of the city. The resulting horizontal convergence of the wind field results in mean vertical motion of the air over the city. It is easy to show by scale analysis that the main effect of the vertical motion should be to increase the effective height of a plume from a smoke stack by about the same proportion as the horizontal wind speed is reduced.

We used available information on the decrease of wind speed to calculate the corresponding vertical motions, and computed the effect of such vertical motions on concentrations at ground level, due to emission of pollutants from a typical stack. This was done by solving by finite differences the differential equation for a diffusing plume with varying horizontal and vertical mean wind speeds. The results agreed with what was expected from scale analysis. Decreases of surface concentrations of the order of 10% for a 100 meter stack were calculated for representative conditions.

R. Deland

3. Sonic Boom Propagation

We have been developing numerical programs for sonic boom propagation through the real atmosphere from wing-body configuration to the ground. We employ the nonlinear inviscid equations and shock equations. The real sonic boom problem is not axisymmetric because the nonuniformity in the atmosphere is nearly two-dimensional and the real airplane configuration is far from axisymmetric. We developed a numerical program for NASA Langley Research Center. The program computes the flow quantities in the vertical plane passing through the axis of the airplane and their second circumferential derivatives plus the first derivative of the circumferential velocity component w. The governing equations in the vertical plane involve one extra unknown, the third derivative of w. A closure condition is imposed. The program has been employed by NASA to study the asymmetric effects due to lift.

We are currently developing an extension of the program to include the effect of the lift and also the spanwise variation of the lift and volume distribution. The additional unknowns are the fourth circumferential derivatives of flow quantities in the vertical plane and the third derivative of the circumferential velocity component. We completed the subroutine for the bow shock and the characteristic points and are developing the subroutine for the formation of shock and for the embedded shock.

L. Ting

NYU Department of Chemistry

1. Atomic Pseudopotentials

Coreless Hartree-Fock (CHF) pseudopotentials have been generated for the atoms Be through Zn, and for the second and third row transition metal atoms Pd, Pt, Cd, and Hg. Atomic calculations indicate that excitation energies and orbital energies are in excellent agreement with ab initio Hartree-Fock calculations.

Recently developed ab-initio pseudopotentials have been employed for the calculation of electronic energy levels and internal rotation barriers in C_2H_6, CH_3SiH_3 and Si_2H_6. The results show that the errors caused by the use of the pseudopotentials are negligible compared to those of limited basis-set size, so that the pseudopotentials can indeed be used to replace the core electrons.

Ab-initio calculations have been performed for the $ZnCl_2$ and $(CH_3)_2Zn$ molecules employing pseudopotential methods. The orbital ionziation potentials are compared with those obtained from photoelectron spectra. There is excellent agreement between predicted and observed values for the outer valence orbitals.

Recently, we have begun a series of computations on the square planar complexes $PtCl_4^{2-}$ and Zeise's anion $Pt(C_2H_4)Cl_3^-$. Preliminary results indicate a large metal-ligand covalency and that the electronic d-d and ligand to metal charge transfer transitions fall in the right part of the spectrum. It should be pointed out that Koopman's theorem is not valid for those systems. However, when the ionization potentials are computed directly, the electrons of lowest ionization potential come from orbitals of mainly metal d-character in agreement with the X-ray photoelectron spectra.

J. W. Moskowitz

2. Photoelectron Spectroscopy

The photoelectron spectrometer for liquid systems designed and built in our laboratory uses high accuracy (5 1/2 decimal digits) analog-digital conversion of the output signal (photocurrent) measured typically in 300 steps per curve, 10 curves per experiment, one experiment per day. The data are communicated directly to a text file which, after conclusion of the experiment, is evaluated by separation of numerical and non-numerical data and proper format conversions. The data are smoothed and a numerical first and/or second order differentiation is performed. Ultimately, energy distribution curves of emitted electrons are plotted on a CALCOMP plotter in suitable form. In addition, a comparison between theoretical and experimental curves is performed.

Photoelectron spectroscopy of various liquids was investigated at variable photon energy up to 10 eV and with rare-gas resonance lines at 11.7 (ArI), 16.8 (NeI), and 21.2 (HeI) eV. Seven liquids were studied: N-methylaniline, N,N'-dimethyl-p-toluidine, formamide, hexamethyl phosphoric triamide, tetraglyme, ethylene glycol, and n-decanol. Energy distribution curves displayed at the higher photon energies a band structure matching the sequence of bands in the corresponding gas-phase photoelectron spectra. The bands were attributed to emission of unscattered electrons (no loss of kinetic energy to the liquid), whereas the underlying background was ascribed to scattered (in the liquid) electrons. Quantitative treatment based on this interpretation agreed with experiment. Energies characterizing either bulk or surface photoionization were determined within $\pm$0.1 eV. The gas-liquid red shift (0.9 to 1.4 eV) and bulk-surface blue shift (0.5 to 1.3 eV) in photoionization energies were interpreted in terms of electronic polarization of the liquid medium. This is, to our knowledge, the first investigation of liquids by ultraviolet photoelectron spectroscopy above 10 eV.

P. Delahay

3. Use of Charge Density Shifts to Interpret Shifts Upon Hydrogen Bonding

This research was undertaken to investigate the contradiction which Professor M. Low of this department found between the conventional inferences about shifts in electronic density upon hydrogen-bonding deduced from shifts in IR frequencies and similarly conventional inferences from NMR chemical shifts. The plan was to use minimal basis set Hartree-Fock wave functions available for some systems of interest to calculate density shifts. Programs have been written and tested. In a test of the shifts predicted by minimal basis set functions for H_2O and $(H_2O)_2$ against those predicted by functions of near Hartree-Fock accuracy, comparison showed the same qualitative function of distance and angles and justified the use of the minimal basis set functions. Because different normal modes show shifts of opposite sign, it is apparent that any correlation with density shifts must be angularly dependent. Since the shifts in normal frequencies are determined by alterations of the potential as a function of normal coordinates, any possible correlation should depend upon whether the functional dependence, which is determined globally by the nuclear framework, is reflected in local electronic density shifts along the normal coordinates. There was no such correlation and conventional inferences must be rejected -- a useful negative conclusion. Positively, the computed density shifts are of interest, both negative and positive results should be published.

E. S. Campbell

4. Molecular Dynamics Calculations on a Model of a Fused Salt

The potentials were chosen to approximate potassium chloride. For convenience in the calculation of correlation functions the system was made symmetrical in that the masses and intermolecular potentials (aside from the coulombic contribution) were taken to be the same for all particles. Thus the model is of an imaginary liquid similar to molten KCl.

The nominal temperature was 1045°K, the pressure was a few kilobars and the molar volume 48.00 ml.

A novel feature was the relatively large size of the unit cell (41Å^3), containing 1728 particles (108-216 is usual). The use of a "link" permitted a system of this size to be run without excessive demands on machine core (225 K_∞). The advantage of such a system is that the amount of computation time goes approximately as N, whereas the amount of two particle information used in correlation functions goes as N^2. On the other hand, long time effects are more expensive to study by this method.

Electrical conductivity was determined by several methods. The direct approach was based on the application of an electrical field and the determination of the resultant current flow. This is a nonequilibrium system and temperature was maintained by readjusting the velocities (thermostatting) at each step. Separate adjustments were made to the velocities parallel and perpendicular to the field direction. The energy extracted from the system to maintain uniform temperature was monitored and used in an alternative calculation of the conductivity. Both of these methods of determining the conductivity were used for the first time in this work.

The correlation function of the fluctuating current (normal to the applied field or in its absence) was used to calculate the zero field conductance.

The conductance was measured at five different (high) values of the nominal electric field to test for the linearity of the familiar Ohm's law under extreme conditions (10^7 v/cm).

Radial distribution functions and velocity autocorrelation functions were evaluated.

The diffusion coefficient was computed from the velocity autocorrelation function and from the Einstein relation. In the latter case the transition to the Brownian regime was observed.

The autocorrelation function of the polarization of the system was determined and utilized to estimate the polarizability of the system.

Since the cell was 41 Å on an edge, all of the dynamical properties correspond to this wavelength.

The basic data consists of eight sets of position and velocity data containing more than two million numbers each. A part of this material has been "mined" for various statistical results but a good deal of analysis remains to be done. A publication describing the results to date is in preparation and is expected to be ready within three months.

B. R. Sundheim

5. Spacial Distribution of Electrons in Reactive Molecules

For several years this research group has been studying experimentally the spacial distribution of electrons in reactive molecules and chemical intermediates and as a result we have developed empirical rules to rationalize these distributions. It became appropriate however to develop more fundamental explanations for our results and this necessitated the development of sophisticated programs to perform quantum mechanical calculations and to describe these results in a manner such that direct comparison between the calculations and experiments was possible.

This has been accomplished by using, first, calculations which are known to reproduce electron spin distributions with considerable reliability. These calculations involve the approximations of intermediate neglect of differential overlap (INDO) developed by J. A. Pople and coworkers.

The resulting eigenvalues and eigenvectors were translated into electron densities and electron spin densities using programs initially developed by R. A. Bader et al. and modified very substantially in this group by several graduate students. And finally the results were expressed graphically using the Courant Institute program PUREJOY.

These calculations yielded useful results which not only were in accord with experimental data, thus confirming the validity of the calculations and experiments, but led to information regarding spin densities not previously available. This has in turn suggested further experimental investigations.

An understanding of the distribution of electrons is fundamental to chemistry; it is electrons that hold molecules together and are responsible for all reactions. We have been able to rationalize numerous unusual reactions on the basis of these studies and have also been able to predict several otherwise unexpected reactions.

This work is continuing

G. Underwood

C. ADP Sharing

In addition to carrying out research in applied mathematics and computer science, the Laboratory maintains and operates a large scientific computing facility -- a Control Data Corp. 6600 computer system. The Laboratory shares the computing facility with other ERDA/DOE sites and Government agencies. In FY 1977, time available on the CDC 6600 was 7244 hours. This time was used as follows:

Courant Institute/DOE (formerly ERDA)	78.6%
ERDA Research Divisions	4.3
NYU - Federal Government Affiliations	7.9
Other Universities / Federal Government	3.8
Federal Government Agencies	5.4
	100.0%

Non-ERDA Federal agency contractors used 1408 hours as follows:

Defense Nuclear Agency (DNA)	12.4%
Environmental Protection Agency (EPA)	7.9
National Aero. & Space Adm. (NASA)	9.8
National Cancer Institute (NCI)	8.7
National Science Foundation (NSF)	29.9
Office of Naval Research (ONR)	10.8
All others	20.5
	100.0%

VI. SYSTEMS PROGRAMMING AND USER SERVICES

A. Operating System Development

Conversion to the NOS operating system for the CDC 6600 was accomplished in this period. This activity has consisted in the installation of the CDC supplied system and the accommodation of a number of non-CDC subsystems and programs to the new environment. The principal areas of local conversion effort have been:

Accounting programs
Software for NYU telecommunications control hardware & protocol
Support for non-CDC graphics devices
NYU library of applications programs, utilities and subroutines
NYU file maintenance system, CIMLIB
Indiana University permanent file management package
NYU KRONOS to NOS user conversion guide
Conversion aid consultation for users

B. Software Maintenance

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

NOS 1.1 Operating System
Remote entry system
Telecommunications control software
CIMLIB file maintenance system
Indiana University 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

C. 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 subroutines available at the Laboratory is kept in machine readable form for ease of maintenance.

E. Franceschini, M. Goldstein

VII. SEMINARS

During fiscal year 1977, the Laboratory sponsored a series of seminars in combustion theory and multiphase flow, numerical analysis, and computer science. The titles of the talks and the names of the speakers follow.

A. Combustion Theory and Multiphase Flow

"Chapman-Jouguet Theory of Deflagration and Detonation"
Gary A. Sod
Courant Institute of Mathematical Sciences (CIMS)
February 8, 1977

"Glimm's Difference Scheme"
Peter D. Lax
CIMS
February 15, 1977

"Reaction Kinetics"
Peter D. Lax
CIMS
February 22, 1977

"Glimm's Method with Chemistry and Its Implementation"
Gary A. Sod
CIMS
March 1, 1977

"One Dimensional Steady Laminar Flames"
Paul Berg
Stanford University
March 8, 1977

"Permanent Structures Among the Solutions of Reaction-Diffusion Equations"
Lou Howard
M.I.T.
March 15, 1977

"Survey of Combustion"
Ira Glassman
Princeton University
April 12, 1977

"Exothermic Centers of Gas Flow"
Alexandre J. Chorin
University of California, Berkeley
April 19, 1977

"Calculation of Bimolecular Rate Constants (Complexities of a Single Step in a Combustion Mechanism when Viewed at a Fundamental Level)
J. Muckerman
Brookhaven National Laboratory
April 26, 1977

"Combustion Instability"
Samuel Z. Burstein
CIMS
May 3, 1977

"Some Problems in Calculations of Flame Propagation"
William Sirignano
Princeton University
May 10, 1977

B. Numerical Analysis

"Higher Order Difference Methods for the Initial Boundary Value Problem"
Joseph Oliger
Stanford University
October 22, 1976

"Difference Methods for Dynamic Black Hole Interactions"
Larry Smarr
Harvard University
October 29, 1976

"Inverse Eigenvalue Problem and Numerical Quadrature"
Gene Golub
Stanford University
December 17, 1976

"Stiff Initial Value Problems in ODE's"
Rolph Jeltsch
University of Bochum, Germany
March 18, 1977

"Discrete Time Galerkin Procedures for Parabolic and Hyperbolic Initial Value Problems"
James Bramble
Cornell University
March 31, 1977

"Spectral Methods for Mixed Initial Boundary Value Problems"
Steve Orszag
M.I.T.
April 8, 1977

"Relaxation Methods for Time Dependent Conservation Equations of Fluid Dynamics"
H. J. Wirz
Institut von Karman de Dynamique des Fluides, Belgium
April 29, 1977

C. Computer Science

"Approximation Algorithms for Some Routing Problems"
Mathew S. Hecht
University of Maryland
November 12, 1976

"Computational Methods in Economic Input-Output Analysis"
Dietrich Fischer
New York University
November 19, 1976

"Assignment Commands and Array References"
Ravi Sethi
Bell Telephone Laboratories
December 10, 1976

"STRUCT: A Program which Structures FORTRAN"
Brenda Baker
Bell Telephone Laboratories
January 7, 1977

"Database Management Facility and Architecture for the Realization of Data Independence"
David W. Stemple
University of Massachusetts
January 14, 1977

"Bin Packing Problems in Operating Systems"
E. G. Coffman, Jr.
Columbia University
February 4, 1977

"An Overview of Medical Applications of Computer Science"
Aran Safir
Mount Sinai School of Medicine
February 11, 1977

"Encapsulated Data Types and Generic Procedures"
Allan J. Demers
Cornell University
February 18, 1977

"ESL: Clusters and Dialogues for Set Implementations"
Jacob Katzenelson
Technion-Israel Institute of Technology
February 25, 1977

"The Phrasal Lexicon and Parser for English"
James Rhyne
University of Houston
March 10, 1977

"A New Approach to Compiler Construction"
Fran Allen
IBM
March 18, 1977

"First Order Semantics"
Robert Cartwright, Jr.
Cornell University
April 1, 1977

"Symbolic Evaluation and the Global Value Graph"
John H. Reif
Harvard University
April 15, 1977

"The CMU RT-CAD System: An Innovative Approach to Computer Aided Design"
Daniel P. Siewiorek
Carnegie Mellon University
April 22, 1977

"CHOPP: A Self-Organizing Large Scale Multiprocessor"
David Klappholz et al.
Columbia University
April 29, 1977

"A Predicate-Calculus Based Semantic Network for Question-Answering Systems"
Jack Minker
University of Maryland
May 6, 1977

"Application of Programming Languages"
David Korn
Bell Telephone Laboratories
May 13, 1977

VIII. PUBLICATIONS

Barnes, J., Betancourt, O., Brackbill, J., Dagazian, R., Friedberg, J., Analytical and Numerical Studies of Scyllac Equilibria, Proceedings of the 6th IAEA Conference on Plasma Physics and Controlled Nuclear Fusion, 1976.

Betancourt, O., Garabedian, P. R., Equilibrium and Stability Code for a Diffuse Plasma in Three Dimensions, Proceedings of Annual Meeting on Theoretical Aspects of Controlled Thermonuclear Research, Madison, Wisconsin, April 1976.

Betancourt, O., Diffuse High Beta Stellarator Equilibrium, Bulletin of the American Physical Society, October 1976.

Betancourt, O., Garabedian, P. R., A Method of Computational Magnetohydrodynamics Defining Stable Scyllac Equilibria, Natl. Acad. Sci. Proc., 74: 393-397, February 1977.

Caughey, D. A., Jameson, A., Numerical Calculation of the Transonic Flow Past a Swept Wing, COO-3077-140, June 1977.

Franceschini, E., An Arpanet Front-End for Large Computers, Proceedings of the Berkeley Workshop on Distributed Data Management and Computer Networks, May 1976.

Franceschini, E. et al., General Purpose Computer Networks and Resource Sharing in ERDA, Volumes 1-4, Working Group on Computer Networking, Division of Basic Energy Sciences, ERDA, July 1977.

Garabedian, P. R., Transonic Flow Theory of Airfoils and Wings, Society of Engineering Sciences 13th Annual Meeting, Advances in Engineering Science, Vol. 4, NASA CP-2001, pp. 1349-1355, Hampton, Va., November 1-3, 1976.

Garabedian, P. R., Univalent Functions and the Riemann Mapping Theorem, Amer. Math. Soc. Proc. 61:242-244, December 1976.

Garabedian, P. R., Computation of Wave Drag for Transonic Flow, Journal d'Analyse Mathematique, Vol. 30, pp. 164-171, 1976. COO-3077-135.

Hyman, J. M., The Method of Lines Solution of Partial Differential Equations, COO-3077-139, October 1976.

Kalos, M. H., Kirkpatrick, S., Lebowitz, J. L., Marro, J., Sur, A., Monte Carlo Studies of Percolation Phenomena for a Simple Cubic Lattice, J. Stat. Phys., Vol. 15, No. 5, p. 345, 1976.

Kalos, M. H., Percus, J. K., Rao, M., Structure of a Liquid-Vapor Interface, COO-3077-141, January 1977.

Kalos, M. H., Lebowitz, J. L., Marro, J., Sur, A., Time Evolution of a Quenched Binary Alloy, IV: Computer Simulations of a Three-Dimensional Model System, Physical Review B, Vol. 15, No. 6, March 15, 1977.

Levesque, D., Rao, M., Surface Structure of a Liquid Film, The Journal of Chemical Physics, Vol. 65, No. 8, October 15, 1976, pp. 3233-3236. COO-3077-138.

McIntyre, Jr., E. A., Design of Transonic Cascades by Conformal Transportation of the Complex Characteristics, COO-3077-136, October 1976.

Percus, J. K., Model for Density Variation at a Fluid Surface, Journal of Statistical Physics, Vol. 14, No. 5, 1976.

Percus, J. K., Equilibrium State of a Classical Fluid of Hard Rods in an External Field, Journal of Statistical Physics, Vol. 15, No. 6, 1976.

Percus, J. K., One-Dimensional Ising Model in Arbtirary External Field, Journal of Statistical Physics, Vol. 16, No. 3, 1977, pp. 299-309.

Pereyra, V., Proskurowski, S., Widlund, O., High Order Fast Laplace Solvers for the Dirichlet Problem on General Regions, Math. of Comp., 36: 1-16, January 1977.

Proskurowski, W., Widlund, O., On the Numerical Solution of Helmholtz' Equation by the Capacitance Matrix Method, Mathematics of Computation, Vol. 30, No. 135, July 1976, pp. 433-468.

Sod, G., Numerical Study of a Converging Cylindrical Shock, COO-3077-144, May 1977.

Sod, G., A Survey of Numerical Methods for Compressible Fluids, COO-3077-145, June 1977.

Tappert, F., Diffractive Ray Tracing of Laser Beams, J. Opt. Soc. Am., Vol. 66, No. 12, December 1976, pp. 1368-1373.

Widlund, O., On Best Error Bounds for Approximation by Piecewise Polynomial Functions, Numerische Math. 27: 327-338, 1977.