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DISCLAIMER

Contents

I. APPLIED MATHEMATICS

A. Computational Fluid Dynamics

1. Computational Methods in Combustion

The present work centers on one dimensional calculations of a simple exothermic reaction model of a reactive compressible gas; by virtue of the parameters chosen, a steady progressive detonation wave is one possible solution connecting two uniform states through a discontinuity. The calculation is initiated by propagating a steady progressing shock wave through a reactive mixture of gas. The shock is allowed to reflect off a wall which results in a pressure and temperature rise of the gas above its ignition limit; combustion proceeds behind the reflected wave. Operator splitting is being tested as a method to capture the detonation wave dynamics. However, it appears that unsplit operators or the use of shock fitting methods may be required to resolve correctly the spatial and temporal distribution in these waves.

The nonlinear equations of compressible fluid dynamics are written in conservation form and are cast into difference equations by writing the flux terms as centered spatial difference quotients. The O.D.E. rate equations are solved at all mesh points defining the region of integration; after an arbitrary number of cycles of such computation, the graphical distribution of dependent variables are outputted.

S. Burstein

2. Transonic Fluid Dynamics

Work continued on updating the design code K. We designed a new turbine blade with larger turning angle and supersonic zone than in the blade presented in "Supercritical Wing Sections III." This was done by modifying the paths of integration. We improved (a) on a new compressor blade designed by Harry Stevens of Pratt-Whitney Aircraft, and (b) on the design of an airfoil for Ray Hicks of Ames, which will be tested at Ohio State University.

Improvements were also made to the transonic analysis code H.

F. Bauer

3. Numerical Methods in Climatology

A fully implicit difference scheme was developed and tested for solving the long-wave (shallow water) incompressible, hydrostatic, single fluid layer model of the atmosphere over

a spherical earth. The scheme is an adaptation of Beam and Warming's method used in aerodynamic calculations. With second order accuracy in the time variable and fourth order accuracy in the space variables, the solution of a simple initial value problem based on using one hour time steps is found to have accuracy corresponding to that of the solution of an explicit scheme based on using six minute time steps. In these cases the spatial interval was (360°/64). "Splitting" is used to factor the implicit operator so as to produce "tridiagonal" periodic linear systems.

Since the time step of the fully implicit scheme does not have to be decreased in proportion to any decrease of the space step, the fully implicit scheme requires relatively less computer time than the explicit scheme, when the spatial interval is reduced. For the spatial intervals required in meteorological problems, the fully implicit method may prove to be more efficient than the explicit method.

E. Isaacson et al.

4. Climate Models

Attempts were made to find nearly stationary subtropical highs in the model atmosphere. These would correspond to the observed Bermuda, Pacific, and Asiatic highs, which had been simulated by the stable equilibrium positions of three point vortices in simpler models developed by Bauer and Morikawa, Peters, and Stewart. Given an initial height of the fluid consisting of three uniformly spaced subtropical highs symmetrically situated about the equator and centered at $\pm 30°$ latitude, we found an initial velocity field by balancing the Coriolis force and the pressure gradient. This "geostrophic" choice produced a slowly moving and deforming flow. When mountains were introduced, the highs still deformed. Introduction of the effect of variable albedo over land and ocean, by prescribing that the density change appropriately, did not appreciably affect the slow movement and deformation of the highs. We now believe that the highs may be made more stationary by modifying the initial velocity so that the total derivative of the height is initially zero everywhere and so that only the east-west component of the velocity is geostrophically determined initially.

E. Isaacson, J. J. Stoker, and G. Zwas

5. Numerical Methods

For a given asymptotic order of accuracy, difference schemes are not uniquely determined. By modifying standard difference schemes so as to conserve certain functionals,

it is found possible to improve the "accuracy" of the solution obtained for "finite" interval calculations. This modification method was used to improve the accuracy of (a) the DuFort Frankel scheme for the heat equation, (b) the Lax-Friedrichs and the Lax-Wendroff schemes for a simple first order hyperbolic equation, and (c) the Lax-Friedrichs and the centered leap-frog scheme for the shallow water model of channel flow over a mountain. In case (c), the conserved functionals were total mass, total energy, and total potential enstrophy.

S. Cohn, D. Dee, and E. Isaacson

B. Numerical Analysis

1. Capacitance Matrix Methods for the Helmholtz Equation on General Bounded Three-Dimensional Regions

In this work the theory of capacitance matrix methods and various aspects of their implementation have been considered in great detail. Extensive numerical experiments have shown that our method requires a computer time that grows linearly with the number of mesh points used. Versions of these methods have been designed that only require an allocation of core storage proportional to the number of mesh points with neighbors outside the boundary of the region. This feature makes it possible to employ very fine meshes when solving Helmholz's equation on a general bounded three-dimensional region. In contrast to the traditional iterative methods for elliptic problems, our method applies equally well to operators that have both positive and negative eigenvalues.

During our work with this project a number of new efficient fast Poisson solvers have been developed for regions that allow separation of the variables. These solvers serve as important subroutines in our codes. The codes can easily be upgraded by exchanging this central module when a faster one becomes available. Methods to compute compact representations of approximate inverses of capacitance matrices have also been explored.

D. P. O'Leary and O. Widlund

2. Capacitance Matrix Methods for Finite Element Problems

Previous work on capacitance matrix methods has concentrated on applications using classical finite difference schemes. In this work, done jointly with Dr. Wlodzimierz Proskurowski of the Lawrence Berkeley Laboratory, we have developed a very fast method for solving the linear systems of equations arising when Helmholtz's equation is discretized using finite element methods.

A FORTRAN program has been developed for piecewise linear finite elements and general bounded two-dimensional regions. Methods have also been designed for a very general family of finite elements on meshes that are highly regular in the interior of the region. For problems in which this limitation on the choice of the mesh is acceptable, our methods require considerably fewer computer resources than other methods in current use. For positive definite cases, a new variant of the conjugate gradient method has allowed us to cut the work per iteration in half in comparison to our previous algorithms.

W. Proskurowski and O. Widlund

3. Conjugate Gradient Type Methods

The work reported in our August 1978 J. SIAM Numer. Anal. paper has continued along several different lines. Particular attention has been paid to the powerful idea of preconditioning and special families of operators that fail to be positive definite and symmetric. New error bounds have been obtained for the case treated in the paper mentioned above, and we have also shown that an interesting algorithm due to Paige and Saunders can be analyzed by using the same techniques. This work will soon result in a publication.

Experimental work applying preconditioning and the Paige-Saunders algorithm to large sparse symmetric eigenvalue problems is well advanced. The basic algorithm is a combination of inverse and Rayleigh quotient iterations. The resulting sparse, indefinite symmetric linear systems of equations are solved by a preconditioned version of the algorithm due to Paige and Saunders

D. B. Szyld and O. Widlund

4. Solution of Stationary Navier-Stokes Equations by a Lanczos Method

The algorithm analyzed in our August 1978 J. SIAM Numer. Anal. paper has been used to solve the nonlinear systems of algebraic equations that arise when the stationary Navier-Stokes equation is discretized by finite difference and finite element methods. The special structure of the Navier-Stokes operator, which is used in very important ways in existence and uniqueness theory, is retained by carefully chosen discretizations and our method is very well suited to take advantage of this structure. The well known square-cavity flow problem has been solved successfully using two different discretizations. The first one employs nonconforming, piecewise linear, divergence-free finite elements and the velocity variables, while the second uses a more traditional

13 point finite difference approximation of the problem in its stream function-vorticity formulation.

D. Rapoport and O. Widlund

5. Sparse Matrix Work on the Leontief World Model

Assistance has been provided to W. W. Leontief's group on sparse matrix problems arising when their models are implemented on the computer. Attention focused on the special block structure of the matrices, the possibility of storing large off-diagonal blocks without using the numerical values of their elements and the use of existing high quality numerical software. The problem of updating these matrices when groups of rows and/or columns are exchanged, without recomputing the entire factorization, has also been considered.

D. B. Szyld and O. Widlund

6. Computation of Discontinuous Solutions of Linear Hyperbolic Equations

We have tackled the problem of computing solutions of linear hyperbolic equations whose initial values are piecewise smooth. It is known that solutions of such problems are piecewise smooth, and that discontinuities occur across characteristic surfaces issuing from the discontinuities of the initial data. When a high-order difference method is used to compute approximately such a solution, the truncation errors across the discontinuities introduce large errors even in the smooth regions. In the paper with Mock, on "The Computation of Discontinuous Solutions of Linear Hyperbolic Equations," we show how to remove this error by appropriately preprocessing the initial data; this guarantees high-order accuracy for moments of the solutions. We show further that by post-processing the approximate solution, the solution can be recovered with high accuracy pointwise as well.

Discontinuous solutions of linear hyperbolic equations occur in many applications dealing with small amplitude wave motion (such as acoustics, etc.). The methods developed here are of practical, as well as theoretical interest.

P. D. Lax

7. Toeplitz Matrices

Classical asymptotic formulas on determinants of Toeplitz matrices have been extended via a multiple scattering expansion. These results imply an analogous expansion for the inverse of a Toeplitz matrix.

J. K. Percus

II. COMPUTATIONAL MAGNETOHYDRODYNAMICS

A. Magnetic Fusion Energy

One of the principal goals of CMCL is to develop methods for the numerical analysis of partial differential equations in three independent space variables and time. Under investigation are several three-dimensional codes for the CDC 6600 computer. It turns out that over the past ten years the advances in supercomputers and in their software have been at such a slow pace that one is at little disadvantage using a machine as old as the 6600. This would appear to be a field where considerable progress can now be made and where mathematical methods and imaginative algorithms can play a significant role.

One of our most successful codes is concerned with magnetic fusion energy using confinement in toroidal geometry. Equilibrium and stability of a relatively dense plasma are analyzed by a modified version of the standard variational principle of ideal magnetohydrodynamics. The energy is minimized over a three-dimensional grid of typically $20\times24\times24$ mesh points. The conjugate gradient method suggests a new and simplified hyperbolic system of partial differential equations describing the physics of the model. Adequate resolution for the design of experiments has been obtained by extrapolating to zero mesh size.

There are basically two different kinds of devices to achieve toroidal confinement. The device presently most favored by experimentalists is the Tokamak. For this configuration, heating and equilibrium are obtained by means of a strong toroidal current, and a torus of small aspect ratio is required to maintain ideal MHD stability. Only plasmas of relatively low and inefficient density can be achieved in the laboratory, and unfortunately the toroidal current has been found to lead to fatal resistive instabilities on a longer time scale.

The other kind of device for toroidal confinement, which was in favor earlier, is the stellarator. Here equilibrium is maintained by means of helical windings that result in complicated three-dimensional geometry. For stellarator plasmas of relatively high density our computer code has proved to be a decisive theoretical tool. Important three-dimensional and nonlinear effects can be analyzed that eluded previous simplified models. By running the code we have discovered high density stellarator configurations with triangular cross sections that are stable to the most important ideal MHD modes.

At the Max Planck Institute for Plasma Physics at Garching, Germany, an experiment called INTEREX is under construction to test our theory. We have made extensive runs to substantiate this experiment. A thorough analysis of numerical errors

indicates that the outcome should be successful. The experimental work is essential to validate the mathematical model on which the code is based. Even more interesting is the possibility that a spectacularly successful experiment might lead to a revised attitude toward the stellarator as a desirable concept for fusion reactors.

Further research on the MHD code has been initiated to enhance the resolution so that low density plasmas such as occur in Tokamaks can be investigated, too. Thought has also been given to vectorizing the code so that it can be run effectively with finer meshes on supercomputers such as the STAR and the CRAY.

P. R. Garabedian

B. Equilibrium and Stability in MHD

Work on equilibrium and stability problems in MHD continued in three areas: (a) A new code with better treatment of the vacuum region and with enhanced resolution was developed. (b) We collaborated on the book "A Computational Method in Plasma Physics," which includes the theory as well as extensive documentation for the use of the code, with examples and error analysis. (c) More calculations were done related to the new INTEREX experiment that is being built in Garching, and which will include a test of our stability results for the $m = 1$, $k = 0$ mode in high beta stellarators.

O. Betancourt

C. Stabilizing Effects of Helical Fields on High-Beta Stellarator Configurations

A computer code developed by O. Betancourt and P. R. Garabedian is applied to investigate magnetohydrodynamic equilibrium and stability of straight and toroidal high-beta stellarator configurations including a vacuum region outside. The code takes into account the important flux constraint of prescribing the rotational transform, an arbitrary pressure profile, and an arbitrary shape of the outer conducting wall.

It turns out that the flux constraint of prescribing the rotational transform μ is very important for the stabilization mechanism, in particular for small μ values as in the high-beta stellarator configurations. The geometrical and plasma parameters considered here are relevant to the INTEREX experiment which is now under construction in Garching, Germany. It has been shown that the rate of change of stable and unstable modes can be computed by the code.

The convergence study for the rate of change shows that the stabilizing effect due to the $\ell = 3$ field is significantly larger than the truncation error of the method.

Moreover, toroidal $\ell = 0,1,2$ high-beta stellarator equilibria with diffuse pressure profile have been computed. Extrapolation with mesh size for the restoring forces led to an excellent agreement between the numerical and experimental results; therefore, the code can be used to design experiments.

F. Herrnegger

D. Plasma Physics

Via ARPANET we used the CDC 7600 at LBL to verify further the equilibrium and stability results obtained with O. Betancourt's diffuse plasma code. At LBL we were able to run problems with finer meshes than on the CDC 6600 here at Courant. We studied a long straight case with 12 periods using a 16×16×192 mesh. On the CDC 6600 a similar case had to be run with only a 16×16×24 mesh. We were also able to run cases with one period using a 24×44×56 grid as compared with a 16×30×30 grid on the Courant computer.

During the year, O. Betancourt wrote a code with an improved treatment of the vacuum region. We used this code extensively to study equilibrium and stability. Improvements were made so that reliable growth rates could be obtained. Many runs were made to study the behavior of the proposed Garching INTEREX experiment using the triangular cross section. Franz Herrnegger, a visitor from the Max Planck Institute, carried out some detailed studies of the German experiments ISAR-T1-B, HBG, and INTEREX.

F. Bauer

III. COMPUTATIONAL PHYSICS AND CHEMISTRY

A. Materials Science

1. Growth of Clusters in a First-Order Phase Transition

The results of computer simulations of phase separation kinetics in a binary alloy were analyzed. The concentration of minority atoms was $\rho = 0.075$, about five times their largest possible single-phase equilibrium concentration at the temperature used. Both small ("gas phase") and large (nucleating) clusters were observed. The size distribution of small clusters was fitted approximately by $c_1 \cong (1-\rho)^3 W(t)$ and $c_\ell \cong (1-\rho)^4 Q_\ell W(t)^\ell$ for $2 < \ell < 10$, where Q_ℓ are known "cluster partition functions" and $W(t) = 0.015(1 + 7.17t^{-1/3})$. For $\ell > 20$, the distribution is fitted approximately by a distribution of the type proposed by Lifshitz and Slyozov, $c_\ell(t) = -(d/d\ell)\psi[\ell n\, t + \phi(\ell/t)]$, where ϕ was given by those authors and ψ is

$$\psi(x) = C_0 e^{-x} - C_1 e^{-4x/3} - C_2 e^{-5x/3}$$

C_0, C_1, C_2 being constants determined from the simulation.

M. H. Kalos et al.

2. Stochastic Simulation of Polymers

We have been modeling the dynamical properties of dilute solutions of macromolecules by computer simulation. Our preliminary investigation used the elementary bead-spring model in the "free-draining" limit (hydrodynamical effects are ignored). The polymer executes a stochastic motion due to the fluctuation of the surrounding solvent; this motion is simulated by an original Monte Carlo procedure. We have confirmed the predictions of the Flory theory for the static correlation functions and shown how to extend scaling to the time-dependent correlation functions. A paper on this work has been accepted for publication in Physical Review Letters.

We are now extending these simulations to consider more complex problems: inclusion of hydrodynamical effects, and of attractive interaction between different segments of a polymer, and investigation of concentrated solutions of polymers.

D. M. Ceperley, J. L. Lebowitz and M. H. Kalos

3. Molecular Dynamics Simulations of Polymeric Systems

We have developed a microscopic model of a polymer immersed in a solvent. All particles in the system interact via a shifted Lennard-Jones 6-12 repulsive potential.

In addition, atoms are linked into a polymer via a modified harmonic potential. So far we have examined two systems: one 5 unit chain in 120 solvent particles and one 10 unit chain in 990 solvents. In both simulations all particles are initially placed on a lattice consistent with a prescribed reduced number density, ρ^* of 0.3, and assigned a Maxwellian velocity distribution with reduced temperature, T^*, equal to 10.

Periodic boundary conditions are imposed. Verlet's integration scheme is used to solve Newton's equations. Time-step trials demonstrated that $\Delta t = 0.00463$ was appropriate for solving the differential equations. The trajectories provide both static and dynamic information about the system. We have calculated the pressure, the inter- and intra-chain pair-correlation functions, the diffusion coefficient, the square of the end-to-end distance, the radius of gyration and the moment of inertia tensor.

M. H. Kalos et al.

4. Equation of State of an FCC Binary Alloy

We have carried out Monte Carlo calculations of a binary alloy on a FCC lattice with both nearest and next-nearest neighbor interaction. The Hamiltonian is

$$H = J \sum_{n \cdot n} \sigma_i \sigma_j + \alpha J \sum_{nnn} \sigma_i \sigma_j$$

with $J > 0$.

The transition was found to be first order for $\alpha = 0$, which is also predicted by Kikuchi's cluster variation (CV) method. The transition temperature that we get for our lattice of 2048 sites was about 6% lower than the CV value.

Energy, sublattice magnetization and specific heat have been calculated for α from 0 to -6. For $0 \gtrsim \alpha \gtrsim -0.25$ the transition is first order; for higher values of $|\alpha|$, the transitions seem to be second order. We have yet to locate the point where this crossover might take place. Such a point would be a "tricritical point". Computation has been done for $\alpha = 0.25$ where the transition is again first order, which is in agreement with Sanchez's CV calculation with the transition temperature differing by about 6%.

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

B. Quantum Many-Body Systems

1. Fluid and Crystal States of He-4

Calculations of the ground state of FCC phases of ^{4}He were completed. Much effort was expended in analyzing, applying various corrections to, and assessing the errors of these and the previously obtained fluid results. Estimates of three-body potential effects were made. Properties calculated included equations of state, pressure, speed of sound, momentum density, Bose condensate fraction, and the one-body displacement in the crystal. The melting and freezing densities were also calculated. Fluid structure, pressure, speed of sound, and momentum density are in rather good agreement with experiment. This extends our previous conclusion that the Lennard-Jones potential, while not entirely correct, predicts properties in better agreement with experiment than had been supposed. Except for properties related to the equation of state (for the very similar h.c.p. phase) few of these data have been measured for crystals.

D. M. Ceperley, M. H. Kalos,
and P. A. Whitlock

2. Quantum Systems at Finite Temperatures

The study of the two-body hard sphere problem at $T > 0$ using Green's function Monte Carlo was completed. Additional Monte Carlo calculations demonstrated that a better choice of importance function significantly reduced the variance of the final result. With the improved importance function, accurate high temperature exchange results were determined. The use of a numerical importance function was explored by accumulating information in tabular form from a series of the same random walks that solve the Bloch equation. This experiment successfully demonstrated the feasibility of fixing values or parameters of an importance function as an outcome of the Monte Carlo, without the necessity of predetermining the analytic function.

Work is now in progress on applying the Green's function Monte Carlo method to many-body systems at $T > 0$.

M. H. Kalos and P. A. Whitlock

3. Neutron Matter

Recently there has been a great deal of interest in the ground state of neutron matter, spurred in part, by the discovery of pulsars. Three different approaches, the Brueckner-Bethe-Goldsteon expansion, the Fermi hyper netted chain approximation and variational fermion Monte Carlo

developed here, now give very similar results for simple neutron matter potentials at low densities (less than 1 neutron/fermi^3). This year we have modified our computer program to calculate the ground state properties with a spin dependent neutron potential and pseudopotential, and have carried out calculations on the Bethe spin dependent (V_3) homework potential. The initial results are in considerable disagreement with the first results published using the FHNC method.

D. Arnow, D. M. Ceperley, and
M. H. Kalos

4. Electron Gas

We have completed a variational Monte Carlo calculation of the ground state properties of the electron plasma and found the Wigner crystallization density as well as the correlation energy at all densities. This work has been accepted for publication in Physical Review B.

D. M. Ceperley

5. Model Fermion Systems

A number of conditions on the two-body reduced density matrix of an interacting electron system have been found through the use of several classes of exactly solvable models. Both upper and lower bounds on expectation values are thereby obtained.

J. K. Percus

6. Non-Uniform Classical Fluids

The equilibrium density profile of both wall-bounded and two-phase classical fluids has been investigated by constructing a sequence of exactly solvable models with many-body interactions, and perturbing out unwanted higher order terms.

J. K. Percus

7. Renormalization Group Methods

Real space renormalization group techniques have been applied to the triangular Ising lattice in a magnetic field, primarily by using a large (7-spin) unit cell. Low order cumulant expansion results are highly accurate.

J. K. Percus

C. Chemistry

1. Chemical Kinetics

The study of the gas phase kinetics of the reaction of $C(^1D)$ atoms with hydrogen molecules through a classical trajectory calculation was completed. The carbon atom preferentially inserts into the H_2 at low collision energies, while the direct reaction of C abstracting an H atom does not become important until a collision energy of 1.0 eV is reached. The direct reaction never becomes the dominant reaction pathway due to collision induced dissociation occurring at energies above 5.0 eV. Experiments with hot $C(^1D)$ atoms have shown that insertion is the primary reaction pathway in collisions with alkanes at low collision energies.

A second classical trajectory calculation of the gas phase kinetics of the reaction $O(^1D) + H_2$ was completed. The calculated reaction rate constant is in agreement with that measured in experiment. In contrast to the carbon reaction both insertion and direct reactions occur at all collision energies studied down to 0.25 Kcal/mole. The insertion reaction involves a long-lived complex that breaks up into an H atom plus an OH radical with a statistical distribution of vibrational states. The direct reaction produces OH radicals with a population inversion of the vibrational levels, which may account for the experimentally observed lasing of OH produced in the reaction of $O(^1D) + H_2$.

P. A. Whitlock

2. Quantum Chemistry

We have generalized our variational Monte Carlo method of computing ground state properties of fermion systems to treat molecular systems, that is, to calculate the correlation energy and electron density with the Born-Oppenheimer approximation. Preliminary results were somewhat disappointing in that the error in the energy, from a short calculation with an extremely crude trial function, was only somewhat less than that of Hartree-Fock.

We hope improvements in both the trial function and the sampling techniques will make Monte Carlo a viable alternative for doing quantum chemistry with large molecules.

D. M. Ceperley

3. Structure of Water

Novel, more efficient, Monte Carlo methods developed here have been applied elsewhere, but with close consultation with

Courant, to the simulation of the structure of liquid water. The new method, applied in the most straightforward way, is 2 to 5 times faster than conventional methods.

M. H. Kalos

4. Interfaces in Classical Fluids

Investigations continued on the nature of the interaction between a hard wall and a phase transition zone in a classical (argon-like) fluid. Most attention has been given to development of improved Monte Carlo methods.

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

IV. COMPUTER SCIENCE

A. CIMS PL/I, Version II

Work continued on Version II of the CIMS PL/I system. Development of the new system is intended to serve two goals: producing a product that is useful in its own right, and exploring the software engineering aspects of creating a large program.

The following progress was made during the year on the system:

1. The declaration-processing pass was written, and debugging of it was started.

2. A design was developed for the intermediate language that describes a virtual PL/I machine, and is used as the target of the code generator.

3. Some preliminary sketches of the code generator were written.

4. An extensive set of input-output facilities to allow communication between PL/I and CDC Record Manager was developed and debugged.

5. The parser was debugged to the point where most programs will pass through it correctly. In addition, a printer routine was developed to print back the output of the parse so that it could easily be checked.

P. Abrahams

B. Distributed Systems and Resource Sharing

1. ARPANET Implementation

Several new facilities have been added to the ARPANET access system.

The User File Transfer service was added. This had been omitted from the first stage of implementation by agreement to an initial subset with other DOE contractors. The User File Transfer service is particularly useful for the submittal of batch jobs to other sites. This is especially true where the server site does not itself have the User File Transfer protocol implemented.

Network mail (receive only) has been implemented so that Courant CDC-6600 users can receive ARPANET electronic mail here.

The new standard ARAPNET HOST to IMP protocol has been implemented. This protocol permits the number of IMP's on the network and the number of HOST's per IMP to exceed previous limits.

As a convenience for the testing and maintenance of the ARPANET access system, a facility has been implemented to enable the dumping of the contents of the memory of the front-end machine to a CDC 6600 file.

E. Franceschini and M. Goldstein

2. ARPANET Applications

A number of ARPANET applications reported during the previous fiscal year have continued and are briefly summarized here.

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

Computerized teleconferencing has been used extensively by the DOE 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 researchers use the network both to communicate with colleagues through the electronic mail facilities and for the exchange of programs and data.

Use of the ARPANET has increased somewhat. At this time, some thirty researchers use the Courant system to access a variety of remote sites on behalf of DOE and other government research programs.

Perhaps the principal area of interest at Courant in the use of network technology is a means of gaining convenient access to large scale computers. In the previous year, substantial work was done using CDC 7600 computers at other DOE sites. However, the further investigation of such possibilities has been curtailed by lack of funds to pay for outside computing.

E. Franceschini and M. Goldstein

3. Remote Access Graphics Capability

Courant researchers require computer output in graphic form. Neither the ARPANET nor available RJE terminals provide standardized remote graphics capabilities. At Courant, the following graphics capabilities have been implemented:

Courant batch jobs can be run on the LBL CDC 7600 via the ARPANET with output returned to the Courant CDC 6600. This output is prepared by suitable post-processing for display on local high quality ink plotters.

A system of programs has been written for the NASA-Langley STAR, CDC 6400 STAR front-end, and the Courant CDC-6600. These programs combine to provide local plotter output for jobs run on the STAR via the Courant remote job entry terminal.

These solutions are ad hoc and awkward. The experience gained will be used to determine longer range, generalized solutions, which perhaps may include adherence to some broad graphical standards.

E. Franceschini and M. Goldstein

4. Cooperation with Other Research Centers

Electronic mail is used routinely for communications with Applied Mathematical Sciences program participants both at contractor sites and at DOE headquarters.

We participate in several DOE Computer Conferences with other Applied Mathematical Sciences program participants on subjects of common interest, such as Distributed Systems Research, small computers for DOE scientific use, command language standards, etc.

A number of DOE meetings have been attended including the following:

Semiannual AESOP conferences,
Third Berkeley Workshop on Distributed Data Base Management and Computer Networks,
Applied Mathematical Sciences Program planning workshops,
Third Annual DOE Graphics Forum,
DOE Numerical Software Meeting.

E. Franceschini and M. Goldstein

5. Distributed Systems Research Planning

For some time, the Laboratory's increased computational requirements to support its very active and diverse program in large scale computation to develop methods applicable to energy research have not been adequately met by the in-house capabilities essentially dependent on the CDC 6600. Consequently, an exigent need exists to explore alternative means to augment the present capabilities.

The traditional economics and technology of computer services have encouraged the use of increasingly large computers and the concentration of resources in a few large centers. Although for many purposes, especially those of highly production-oriented environments, such organizations are highly successful, some benefits are being lost for research and development activities. Particularly the nature of services available to computer users is sometimes determined more by geography and the apparent economics of scale than by technical needs.

Recent innovations suggest a more varied and versatile approach to the organization of computer services in which greater flexibility in the matching of tools to tasks can result in customized services and improved economics for classes of applications. Among the technical advances that make this concept feasible are:

Cost/performance of small computers for general purpose computing.
Data communications,
Computer networks,
Inexpensive array processors,
Simplification in design and construction of specialized computer elements.

An example of a special case of successful application of principles implied by these innovations is the MFENET, in which computer services are distributed between a large central facility and several remotely located smaller service centers.

Here at the Laboratory, we are undertaking a number of experimental activities to evaluate the pertinence of these concepts to energy related research as practiced here and at other DOE research centers.

We are investigating various new computational elements suitable for a distributed approach to scientific applications. These include the ARPANET, the MFENET, conventional remote job entry terminals, inexpensive array processors, and a microprogrammed emulation of the CDC 6600. As these elements are evaluated, an integrated system will evolve to provide both powerful, low cost local capabilities and convenient

access to remotely located supercomputers. The cornerstone of this research is the acquisition of a modern, low cost, large capacity minicomputer.

For many years the 16-bit minicomputer has been an extremely cost-effective means of providing many specialized data processing services. However, the 16-bit architecture, with its limitations in program size and in numerical performance, has discouraged the use of minicomputers for general purpose or numerical computing.

More recently, relatively low cost machines with fast floating point hardware have been introduced to the market. These systems have 32-bit architecture that provides large address spaces and support for large main memories. These factors permit the execution of large programs without the need to explicitly manage their address spaces. The likelihood of realizing the rated performance of the floating point hardware is increased, and the conversion of programs written for larger machines is facilitated.

In order to exploit the potential of such devices in energy related research programs, we have acquired a Digital Equipment Corporation VAX-11/780 computer.

Planning for this research activity is underway.

E. Franceschini and M. Goldstein

C. Computer Design

1. PUMA

The objectives of this research are the development of digital design automation tools at the Laboratory and the construction of digital systems that will be useful in the Laboratory's research. Our efforts have been focused for the past several years on the design and construction of an emulator for the CDC 6600 central processor. These efforts reached fruition in the spring of 1978 with the completion of a processor running at roughly one-third the speed of a 6600.

Approximately a year ago, in the spring of 1977, we completed an initial, slower version of the processor. Three major developments during the past year have greatly increased the power of the system:

1. Design and construction of a faster control unit, which made it possible to increase the processor speed more than threefold (from 4 MHz to 13 MHz clock rate),

2. Installation and interfacing of a 131,072 word (× 60 bit memory),

3. Installation and programming of a PDP-11/34 minicomputer, which interfaces the central processor to peripherals and monitors central processor execution.

This system began running "production" jobs on a limited basis in June 1978, and we expect this usage to gradually increase in the coming months. We are currently beginning construction of a second unit of similar design; because of packaging improvements, we expect some further increase in processor speed. Most of our effort in the coming year, however, will be in software, gradually enhancing our currently rudimentary operating system.

R. Grishman

2. PUMA Operating System

During the last year, we have supported the PUMA operating system development by implementing a cross compiler for the LITTLE language to allow programs written in LITTLE to be run on the Digital Equipment Corporation PDP-11 series mini computers. This cross compiler was initially checked out on the IBM System/370, but is currently being moved to both the CDC 6600 and DEC-10 computer systems in addition to the IBM 370. Since the first two phases of the LITTLE compiler are the same regardless of the target machine, only the code generation phase of the compiler need be written. The code generator for the PDP-11 (ASMS11) was based on the previously developed code generator for the IBM System/370 (ASMS37) as the "superstructure" of ASMS37 was sufficiently general to be used on machines other than the IBM 370. This same strategy was used for the code generator for the DEC-10, which is currently being developed in cooperation with our group at Leeds University in England via ARPANET.

When development of ASMS11 had proceeded to the point where object programs were being produced, the run time library and the LITTLE written utilities were compiled and shaken down. Following the successful shakedown of the utilities, the PUMA Operating System (POS) was compiled and shaken down on the PDP-11.

Examination of the object code produced by ASMS11 for POS and other programs indicated the existence of a requirement for the generation of more efficient object code. The problem is that what appears to be very efficient code when generated by the code generator may not be efficient when examined in a more global context. For example, the code generator attempts to minimize storage references by keeping variables in registers for the duration of a basic block. Sooner or later, the code generator will run out of registers and be forced to preempt an already occupied register. As a result, the object code will frequently contain "dead" copy operations from one register to another. To attempt to remedy inefficiencies of this nature, work is currently proceeding on a compiler phase to reexamine the object code produced by the ASMS11 and manipulate it to obtain better code.

R. Gezelter

3. PUMA Operating System

Another PUMA support activity this year consisted in modifying the PUMA operating system to run on the PDP-11/34 and doing work with RSX11M.

The PUMA operating system was written in LITTLE and was run on the Honeywell 316 to run jobs on the PUMA. The operating system was first modified to be more portable so that it could run on the PDP-11.

Once the PUMA operating system (POS) ran on the PDP-11, it was used to run some light production-type work. It is important to note that the process of getting POS to run on the PDP-11 was hindered by the fact that the PDP-11 LITTLE compiler was not quite bug-free and the maintainer was not available to correct bugs.

At this point some features that will be needed for the "real" POS and that would make use of the 11 easier during development were added to the operating system (RSX11M0).

Once this was done, it was decided to fix up POS to support more features such as using the PDP-11 print spooler to process output and to support a COMMON file facility.

When the fixes mentioned were completed, it was possible to widen the scope of the "production" being done on the PUMA and support a few more applications.

Effort was also spent to produce a version of the 370 LITTLE compiler which would produce code for the DEC system-10. This code generation produced an output language called T10 which are assembler macros that expand to DEC-10 assembler language. Tony McCann of the University of Leeds, England, has agreed to try to run the generated code on his DEC-10 to try to bootstrap LITTLE on that machine. As of this date, McCann's effort has gone remarkably well and he found only a few minor bugs in the translation. We expect to use this translator to produce a VAX LITTLE with only a few days work. Ed Schonberg is using this same program as the basis for a LITTLE code generator for the Prime 400.

R. Kenner

D. SETL

Since April intensive debugging of the run-time library has been in progress. For this purpose, a comprehensive set of test programs has been designed and is currently being implemented. We intend to create an industrial grade library of standard test programs which will satisfy the following requirements: first, the library has to be modular so that additional tests can easily be added to it, and furthermore it must allow full or partial execution of all modules; second, each test has to check its results automatically, as much as possible, since the projected size of the test library makes it prohobitive to check the results manually.

The overall design of the test library has been completed, and much of it has been implemented with some changes still to be made to include existing stand-alone tests into the library.

Some preliminary effort aimed at installing SETL on the IBM 370 has been undertaken. A first attempt to run part of the compiler has been made; it pointed out some necessary changes both to the IBM LITTLE implementation and to the SETL source code. Most of these changes have been made on the SETL source at this time.

S. M. Freudenberger

E. Algorithmic Combinatorics

Work proceeded on two topics of interest in the area of algorithmic combinatorics. The first topic concerns chordal bipartite graphs. Two new theorems were discovered that generalize results of G. A. Dirac on triangulated graphs. The second topic involves the inductibility of hypergraphs. In this problem one tries to determine the maximum number of ways in which a hypergraph H with k vertices can appear as an induced subhypergraph of a hypergraph with n vertices, for $n \geq k$. It was discovered that many results of the inducibility of graphs generalize to hypergraphs.

M. C. Golumbic

V. SYSTEMS PROGRAMMING AND USER SERVICES

A. Operating System Development

In this period two major corrective code releases were applied to the NOS operating system. The principal effort in such cases is the reconciling of existing local modifications with changes introduced by the corrective code.

The execution time memory requirement of the remote job entry system had been growing, primarily as a result of ARPANET support extensions. A substantial reorganization and optimizing effort has been made to reduce the size of the code and of the memory requirement.

A new software package for the Zeta incremental plotter was installed.

A high level graphics package was installed. This system was acquired from the University of London Computer Centre.

An effort is being made to simplify the maintenance, and use of graphics packages. The approach is to achieve a degree of device-independence of plot data representation at an intermediate level. A final process generates input for selected, specific plotting devices.

E. Franceschini and M. Goldstein

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 the implementing modifications for improved system performance. The major systems and programs maintained were:

NOS 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 mini-computers
Compilers for various languages, e.g., FORTRAN, BASIC, ALGOL, SNOBOL, LISP.

E. Franceschini and M. Goldstein

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 and M. Goldstein

VI. RELATIONSHIPS TO OTHER PROJECTS

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

P. D. Lax continues his active role as a member of the Advanced Code Review Panel of the Nuclear Regulatory Commission. He is also a member of the Review Committee of the T Division at LASL.

P. R. Garabedian and his team during the past year have supplied the Transonic Airfoil Design Code to Pratt-Whitney Aircraft and Lockheed-California and have also made available the Two-Dimensional Analysis Code to Fairchild-Republic, Hamilton Standard, Lockheed-California and Canadair. Garabedian's team also improved on the design of an airfoil for NASA-Ames.

Collaborative effort has continued with the Max Planck Institute in Garching, Germany. An experiment designated INTEREX is under construction there that will test our MHD computational model of equilibrium and stability of a plasma in toroidal geometry.

O. Widlund exchanges information on PDE's with A. Chorin and P. Concus of LBL, and with G. Golub of Stanford University. Widlund's work on capacitance matrix methods for finite elements is done jointly with W. Proskurowski of the University of Southern California, and for the Helmholtz equation with D. P. O'Leary of the University of Maryland. On fast solvers for special elliptic problems on general regions, consultation by industry takes place with Celanese, RCA Sarnoff Laboratories, etc. International contacts are maintained with IRIA at Paris, France, with the Universities of Stockholm and Uppsala, Sweden, and with the Atomic Energy Research Establishment, England.

M. H. Kalos' work on chemical kinetics is done in collaboration with J. Muckerman, BNL. The work on quantum many-body problems is shared with B. Alder, LLL. On nuclear and neutron matter there are exchanges with Argonne. Relating to polymers and alloys there have been reciprocal visits with the National Bureau of Standards, and in this task we have also collaborated with a Rutgers University project supported by the Air Force Office of Scientific Research. In the modeling of quantum crystal and fluid systems, Kalos' group has collaborated with the Cornell University Laboratory of Atomic and Solid Physics.

S. Burstein reciprocally shares information on numerical methods in the solution of PDE's with energy sources with P. Crowley and W. Noh, LLL, and with G. Sod, North Carolina State University.

R. Grishman's PUMA project has ramified. BNL is designing and building an emulator for CDC 6600 processors. This emulator will be used together with the PUMA central processor to provide a complete emulation of the CDC 6600 computer system.

P. Abrahams' PL/I system has now been distributed to about 60 sites, including BNL and LBL. PL/I, Version II is being developed in collaboration with Control Data Corporation.

E. Isaacson explained the conservative modification method at LASL (the technique for improving any given algorithm for solving partial differential equations), where J.M. Hyman implemented it successfully. On climatology modeling, Isaacson maintains contacts with NASA Goddard Space Flight Center, Maryland.

B. Courant Institute and New York University

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

Courant Institute of Mathematical Sciences

1. Local Solution of Transonic Flows with Shocks

In most transonic flows with shocks there is a point where a shock becomes infinitely weak and merges with the sonic line. It is easy to see that the flow cannot be described by a Taylor expansion. In particular the local contribution to drag is not directly estimable.

We have determined numerically a local flow by finding a similarity solution for the small disturbance equation. Thus we are solving a nonlinear ordinary differential equation with singular coefficients and a jump condition.

The equation may be written as a system

$$\phi_x^2 = -\psi_y$$

$$\phi_y = \psi_x$$

and the shock conditions are ϕ, ψ continuous, ϕ_x increases across a shock (entropy condition). We set $\phi = \Omega_x$, $\psi = \Omega_y$ and the equation becomes

$$(\Omega_{xx})^2 + \Omega_{yy} = 0$$

Ω_x, Ω_y continuous. The solution sought is of the form

$$y^{\alpha} F(xy^{\gamma})$$

or

$$x^{\tilde{\alpha}} \tilde{F}(x^{\tilde{\alpha}}y)$$

with appropriate transformations as the quadrant changes.

The program by Mike Pilant is now able to compute a solution from a characteristic in the lower left quadrant across a sonic line, through the upper half plane, across a shock in the lower right quadrant and ending on the same

characteristic with the initial values of F and $\dot{F}$. It is now necessary for completion of the project to adjust the parameters, improve the iteration scheme, and the match.

If successful we shall try to find the full range of parameters for this flow.

C. S. Morawetz

2. Automotive Engine Modeling with a Hybrid Random Choice Method

Recently a numerical procedure was introduced for solving the one-dimensional equations for an inviscid, radially symmetric flow. The idea of the method was to use operator splitting to reduce this system of equations to two systems of equations; the equations of gas dynamics in Cartesian coordinates and a system of simultaneous ordinary differential equations. This method has been generalized to treat the two-dimensional equations of gas dynamics for an inviscid fluid in a cylindrical geometry.

When considering the flow in the cylinder of an internal combustion engine viscous effects cannot be ignored. The effect of viscosity in two-dimensions is confined to regions near the boundaries. Viscosity results in the creation of a thin boundary layer, which later separates into the fluid.

A grid free method for approximating the incompressible boundary layer equation for a cylinder and a flat plate is used. The computational elements are pieces of vortex sheets. The desirability of a grid free method can be seen from analysis which implies that if a grid method is used then several grid points must fall within the boundary layer whose thickness is $O(R^{-1/2})$, where R is the Reynolds number. Thus a relatively low upper bound must be imposed on the Reynolds number.

The computational domain is divided into two regions, one the interior and the other the region near the boundary. Different assumptions about compressibility are made, as well as different numerical methods used, in the two regions. Near the boundary the flow will be considered viscous and incompressible and in the interior the flow will be considered inviscid and compressible. The assumption of incompressibility near the boundary is reasonable provided the Mach number near the boundaries is small.

In an internal combustion engine a flame, which may be ignited by a spark, propagates through a fuel-air mixture and along the cylinder walls toward the piston head. Since the cylinder walls are relatively cold and the gas temperature drops sharply in the boundary layer to the temperature of the

cylinder wall with that heat being too low to sustain oxidation reactions, the flame is extinguished as it approaches the walls. This is one form of flame quenching. A thin layer of partially reacted fuel is left. The phenomenon of flame quenching is of fundamental importance because it is one major source of unburned hydrocarbon components in pollution.

The thickness of this boundary layer is affected by many parameters; the air-to-fuel ratio, gas temperature, wall temperature, flame speed, and the chemical concentrations, which interact with one another. This interaction makes it difficult to experimentally vary the parameters and study the individual effects. However, using numerical methods one may be able to establish relationships that will define flame quenching over a wide range of conditions.

One way in which the layer of unburned hydrocarbons along the cylinder walls may be eliminated is to confine the fuel to a subregion of the cylinder away from the walls. This is known as the stratified charge concept. If this could be accomplished, the flame could consume all of the fuel before the mixing and diffusion processes cause the fuel to reach the cylinder walls or reduce the fuel concentration below the flammability limit. This would reduce the hydrocarbons in the exhaust. In practice it is difficult to stratify the charge and analyze the process. However, it is a reasonable problem for the computer.

This method is used to study the flow in a motored engine chamber during the intake and compression strokes. The engine is assumed to be axially symmetric, with a single intake-exhaust value located on the chamber axis. The piston motion and valve timing represent an engine timing of 2500 RPM.

This method assumes axi-symmetry and hence is not directly applicable to three-dimensional engine flow. However, this can yield important information concerning the relative efforts on the flow field of valve size, swirl rate, piston and head geometries, and engine speed.

G. A. Sod

3. ELASDYN

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

This fiscal year saw the completion of one project and the continuation of a second.

First project. By setting up a 2-D elastodynamic crack problem as an integral equation to be solved numerically, we were able to show that rapidly moving shear cracks are unstable (in that speed increases as load increases) for crack speeds v_c in the ranges $v_c < v_R$ and $v_S < v_c < \sqrt{2}\, v_S$. On the other hand shear cracks propagate stably in the range $\sqrt{2}\, v_S < v_c < v_P$. Here, v_R, v_S, v_P are respectively the Rayleigh, shear, and compressional wave speeds. Crack speeds $v_c > v_R$ had not previously been treated.

Second project. This concerns the mathematical modeling of seismic slipping on a fault plane embedded in a 3-D uniform elastic whole space. We formulate the problem as a time dependent, two space dimensional integral equation over the slipping region. This obviates the introduction of artificial boundaries and reduces the (space) dimensionality of the problem from 3 to 2. The integral equation may be solved by an explicit step-by-step procedure in time.

Previously an analog scalar problem was set up and solved. During this year we have made considerable progress in setting up the scheme for the full three-dimensional elastodynamic vector equations. This turns out to be a complex task which we hope to continue during the year 1978-79.

R. Burridge

4. Flow Patterns Around Heart Valves

This work involves the development of a computer test chamber for mitral valve dynamics. The Navier-Stokes equations are solved numerically in the presence of moving boundaries that interact with the flow. These boundaries include the muscular heart wall and the (natural or prosthetic) mitral valve.

Our recent work on the natural valve has focussed on the adjustment of the parameters of the model to achieve good agreement with experiments. Such agreement has been partially achieved, and this work is continuing in collaboration with the experimental heart valve research program at the Albert Einstein College of Medicine. Even incorrect parameter values are interesting, as they sometimes correspond to important pathological conditions. For example, we have replicated in the computer the condition mitral valve prolapse syndrome, in which apparently normal valve closure is followed by sudden incompetence of the valve apparatus. A more detailed computer study on the possible causes of this condition is planned.

Our work on prosthetic valves during the past year involved fundamental extensions of the numerical methods in which we

developed the tools needed to model (essentially) rigid valves of arbitrary geometry. In structures that resist compression, the Hessian matrix of the strain-energy as a function of configuration need not be positive definite. (This is related to the possibility of buckling.) This difficulty was overcome by using Murray's modification of Newton's method. To implement this algorithm, we needed a code for the column form of the Cholesky factorization in the profile storage scheme. Compared to the more natural factorization by rows (with respect to this storage scheme), this requires additional storage for pointers. Given these pointers, however, the factorization code is simpler (and faster) than before.

Having resolved the difficulties associated with structures that resist compression, we turned to the problem of modeling the bending rigidity of valves and of the cages that restrict their movements. Bending rigidity was achieved through the use of forces that are functions of the configurations of triples of points. Such forces are conveniently specified as derivatives of an energy function. This energy function must be invariant under translation and rotation to secure conservation of momentum and angular momentum. We have found a simple energy function that can be used to hold two line segments in a right-angle configuration, and we have found quadratic energy functions that can be used in the modeling of straight or curved beams. (For quadratic energy functions we have proved the unconditional stability of the method.) These ideas have been tested successfully in the modeling of ball and disc prosthetic valves, and we feel that this phase of the development of methods is essentially complete.

D. McQueen and C. S. Peskin

5. The Aortic Sinus Vortex

We have combined the vortex method of A. J. Chorin with conformal mapping to achieve a numerical method for the Navier-Stokes equations that resolves the singularities associated with corners of the domain where the interior angle is greater than π. The conformal mapping also gives an explicit formula for the vortex velocities so that Laplace's equation need not be solved numerically at each time step. We have applied this method to the problem of blood flow in the aortic sinus, and we have traced the development over time of the aortic sinus vortex and its motion during the deceleration of the main stream. This motion is important to the mechanism of aortic valve closure. The results agree with experiment. We are currently involved in an effort to include a flexible aortic leaflet in the computational model.

C. S. Peskin and A. Wolfe

6. Natural Language Interfaces for Data Base Retrieval

This research project consists in the development of a system to allow users to interrogate a data base by asking questions in English. We have at present a simple operational question-answering system, which is being used as a vehicle for studying specific aspects of these systems. Three facets of question-answering systems have been studied in this manner over the past year:

1. Anaphora resolution. Questions may contain pronouns referring to objects mentioned previously in the dialog. We have incorporated into our system a procedure for finding the appropriate antecedent for certain classes of anaphoric reference.

2. Inferencing. More sophisticated question-answering systems can respond to questions that are not directly answered by an entry or set of entries in the data base, but involve some deduction or calculation. We have introduced a simple inferencing component into our system in order to study its interaction with the other parts of the system.

3. Optimization of data base retrieval requests. The question-answering system ultimately generates a retrieval request for a data base system. The most straightforward translation of questions into retrieval requests can produce quite inefficient requests. Rather than complicate the translation process, we have introduced a simplification component prior to retrieval, which substantially improves the efficiency of the retrieval request.

R. Grishman

7. Lifting of a Membrane Glued to a Flat Surface

The lifting of a membrane glued to a horizontal rigid surface by concentrated loads is investigated. The deflection of the lifted membrane surface is governed by the Laplace equation while the boundary of the lifted surface is to be determined so that the normal stress is equal to the strength of the glue. The critical slope of the membrane at the boundary is thereby specified. For a single concentrated load the surface of the membrane detached from the rigid surface is a circular cone. For more than one concentrated load with sufficient strength, the detached surface of the membrane is connected. This is a free surface problem and will be solved by conformal mapping. The final solutions are obtained by numerical integration of the mapping functions.

We are constructing solutions for n-concentrated loads placed at the vertices of an n-sided regular polygon. Two solutions are possible depending on whether the neighborhood of the center of the polygon is detached from the rigid surface or not. We are in the process of defining the ranges of the parameters, n and the critical slope, in which one of the solutions is admissible.

L. Ting

NYU Department of Applied Science

1. The Effects of Fluidized Bed Dynamics on Sorbent Activity

The desire to obtain acceptable levels of sulfur retention in a coal fired fluidized bed of limestone or dolomite while attempting to design for efficient production of steam or hot gas may, under some conditions, lead to a dilemma of contrary purposes. On the one hand, the production of large quantities of steam or heated air leads to a design requirement to obtain a high heat transfer coefficient in all sections of the bed. It is well known that such a situation can only be accomplished if the geometry of the bed and heat exchanger are such as to allow for good bed circulation. Compact pressurized units require deep beds and high superficial velocities, and thus heat exchanger designs which allow one to obtain good circulation (and a more uniform bed temperature) are of prime interest. On the other hand, there is evidence that changes in flow regime aimed at achieving heat transfer coefficients can cause a degradation in the sulfur retention capability of the bed. Therefore, the effect of bed dynamics on sulfur removal must be properly understood if one is to attempt a design which meets the simultaneous requirements of high heat transfer and high sulfur removal.

As part of our program for DOE, an analysis and computer model which couples the effects of bed dynamics to fluidized bed sorbent activity is being developed. A model recently published by Hartman and Loughlin quantifies sorbent activity in terms of two simultaneous diffusion processes: one through the particle of sorbent and another through the grains of which the particle is composed. As the sulfation reaction proceeds, the macropores and micropores of the particle close down and the sulfur retention of the particle reaches its

limiting value. This model using average conditions and neglecting the effects of variations in the flow field on diffusion at the particle surface appears, at least as a first approximation, to give a proper representation of the phenomenon and over long exposure times, yields levels of conversion to sulfate in reasonable agreement with experimental observations.

This model is being incorporated into an available code which analyzes the mixing and reaction of solid particles in turbulent streams. The basis of this code is the development of a finite difference solution for the coupled fluid dynamic and chemical reaction processes which accounts simultaneously for variable rates of diffusion of gaseous and particulate species, the effect of the turbulent "washing" velocity which increases gas contact with suspended solids and the reaction mechanisms at the surface and interior of the particle. The resulting code will be used to determine sulfur retention as a function of bed dynamics under a variety of conditions, accounting for the effects of particle size, air distribution, pressure, bed geometry, etc. Solids circulation patterns will be imposed for a particular gas flow distribution at the grid and, as a first approximation, the coal will be assumed to be burned immediately yielding an initial gas composed of N_2 , O_2 , CO_2 and SO_2 in varying concentrations.

G. Miller and V. Zakkay

2. An Experimental Study of the Effect of Fuel Vaporization on Combustion Efficiency

The purpose of the investigation is to determine the effects of fuel oil vaporization on the overall combustion efficiency in home oil burners and to compare it with atomized fuel oil burners. The vaporized premixed combustion mode will permit operation with low excess air and low stack exhaust temperatures which will yield lower fuel oil consumption. The effects of this combustion mode on the emissions such as CO , NO_x , unburned hydrocarbons and soot, will also be investigated.

A computer program for determining the adiabatic flame temperature and the equilibrium composition of the combustion products of vaporized #2 oil (a hydrocarbon) with air, has been written and debugged. It has been used to give the variation of the adiabatic flame temperature, carbon dioxide, carbon monoxide, and oxides of nitrogen as a function of the fuel to

air mixtures and other operating conditions such as pressure, air inlet temperature, and fuel carbon to hydrogen ratio. An indication of the equilibrium conditions for soot formation was also determined. These results were compared with experimental data and have been presented in progress reports. This work has not yet been published.

Additional computer programs will be written to evaluate various fuel vaporization techniques and for determing the pryolysis and combustion of #2 fuel oil. The effectiveness of various fuel-air mix devices will also be evaluated analytically using available mixing codes. Vaporized and premixed combustion processes will be examined to determine actual combustion efficiency and emission with different imposed boundary conditions such as fuel distribution, and heat removal rates. The heat transfer process of the combustion products to the heating coil will also be evaluated to assess the overall thermal efficiency of the furnace. The ultimate goal is to model the home furnace in order to assess the heat losses due to incomplete combustion, excessive exhaust stack temperatures, chamber heatup, and furnace cycling.

A. Agnone, W. Brenner, and V. Zakkay

NYU Department of Chemistry

1. Atomic Coreless Hartree-Fock Pseudopotentials for Atoms K through Zn.

Using the coreless Hartree-Fock (CHF) pseudopotential approach we have generated pseudopotentials for the atoms K through Zn. Atomic calculations indicate that excitation energies and orbital energies using these pseudopotentials are in excellent agreement with ab initio Hartree-Fock calculations. Optimized small basis sets for use with these pseudopotentials are presented along with tests for these basis sets. When used in molecular calculations these CHF pseudopotentials should provide ab initio quality energies and wave functions while reducing the computational effort.

Ab initio valence-only molecular orbital calculations, using an ab initio pseudopotential to represent the cores, are reported for $(CH_3)_2Mg$, $(CH_3)_2Zn$, $ZnCl_2$, $MgCl_2$, CH_3MgCl, and ZnF_2, all at experimental (electron diffraction) geometries.

The calculations were performed in an attempt to study the effects on the bonding of the full 3d and 3p orbitals which distinguish these compounds. We find that, as expected, the bonding is nearly all of σ type; the d electrons in Zn seem unimportant for these bicoordinate species. Orbital energies and population analysis are contrasted with expectations based on electronegativities and Pearson's hard-soft principle; the latter seems slightly more helpful. The somewhat unusual bond distances reported in the literature are briefly discussed.

In collaboration with M. H. Kalos we have investigated the application of a Monte Carlo integration scheme to the numerical evaluation of the matrix elements of the Fock operator in a Gaussian basis. Only the valence electrons have been explicitly treated, the core electrons being replaced by atomic pseudopotentials. The advantages of such a numerical scheme are twofold: (1) It is possible to incorporate and test recently developed local exchange and exchange correlation potentials which show great promise in partially accounting for molecular correlation energies within a one electron model. (2) Within a numerical evaluation scheme, the matrix elements of the Fock operator show an n^2 dependence on the size of the basis. This leads to the possibility of constructing rapid and efficient programming algorithms. Preliminary results on the H_2 molecule have been very encouraging and further work is in progress.

J. W. Moskowitz

NYU Graduate School of Arts and Science Economics Department

1. Information through the Printed Word: The Dissemination of Scholarly, Scientific and Intellectual Knowledge

This project concerns the dissemination of scholarly (scientific, technical, intellectual) knowledge through primary and secondary publications, chiefly books, journals and other materials. It is a fact-finding study designed to throw light on the economic condition of publishing and library operations.

Various reports had contended that some segments in the book-publishing industry, especially university presses, were having difficulties covering costs, that purchases of books by libraries had been drastically reduced, that the number of scholarly journals had been rapidly increasing, and that various journals had suffered declining circulation. The project was designed to test these factual judgments and to see whether they may be confirmed for some subject groups but disconfirmed for others.

F. Machlup

NYU Institute for Economic Analysis

1. World Economy Model

The multiregional input-output computer simulation model of world economy was devloped at Brandeis University as a tool for simulating scenarios incorporating alternative hypotheses about economic development for the world as a whole and for the individual regions. The data corresponding to each region include an inter-industry matrix which represents the input requirements, or the technology, of each of its industries. This level of detail makes the model particularly useful -- and is used -- for studying issues like the production and consumption of energy.

A copy of the model and data base (currently about three million pieces of information) were brought to Courant in September 1977. Since then, we have participated by making the system operational and used it to produce the simulation results in our report to the United Nations entitled Preliminary Study of Worldwise Economic and Social Implications of a Limitation on Military Spending (An Input-Output Approach), March 1978.

Currently, we are involved in implementing our redesign of the model using sparse matrix technology and designing or choosing a data base management system. We are also working on an analysis of the production and consumption of minerals. One issue addressed in this study will be the future energy requirements of the mining and processing of non-fuel minerals.

F. Duchin

C. ADP Sharing

In addition to the research activities in applied mathematics and computer science conducted on behalf of the Department of Energy, the Laboratory maintains and operates a CDC 6600 computer system, which is shared with other DOE contractors and government agencies.

During FY 1978, time available on the CDC 6600 was allocated as follows:

Courant Institute/DOE	81.1%
DOE Research Divisions	2.9
NYU/Federal Government Affiliations	8.4
Other Universities/Federal Government	2.5
Federal Government Agencies	5.1
	100.0%

About 30 non-DOE Federal agency contractors were allocated 1400 hours of computer time as follows:

Defense Nuclear Agency (DNA)	13.3%
Environmental Protection Agency (EPA)	3.6
National Aero. & Space Admin. (NASA)	5.4
National Cancer Institute (NCI)	9.9
National Library of Medicine (NLM)	7.8
National Science Foundation (NSF)	33.0
Office of Naval Research (ONR)	10.8
All Others	16.2
	100.0%

VII. SEMINARS

During fiscal year 1978, CMCL sponsored a series of seminars in Numerical Analysis and Computer Science. The titles of the talks and the name of the speakers follow.

Numerical Analysis Seminars

"Some Conjugate Gradient Methods for Symmetric, Indefinite Linear Systems of Equations"
Olof Widlund
Courant Institute of Mathematical Sciences (CIMS)
September 22 and 23, 1977

"Existence Approximation and Algorithms for Solving Elasto-Plastic Problems"
Bertrand Mercier
Ecole Polytechnique and CIMS
September 30, 1977

"A Method for the Computation of Three Dimensional Steady Viscous Flows"
Peter Eiseman
United Technologies Research Center
October 7, 1977

"The Numerical Radius of Power Bounded Matrices"
Gideon Zwas
CIMS and University of Tel Aviv, Israel
October 14, 1977

"A Numerical Study of Cylindrical Implosion"
Gary A. Sod
CIMS
October 21, 1977

"Computation of Limit Load for Plates"
B. Mercier
Ecole Polytechnique and CIMS
October 28, 1977

"Application of Banach Space Interpolation to Finite Element Approximation"
Ridgeway Scott
Brookhaven National Laboratory
November 4, 1977

"Extrapolation to the Limit -- Algorithms and Applications"
Prof. Donald C. Joyce
Massey University, New Zealand
November 11, 1977

"Hierarchical Relaxation"
W. Miranker
IBM
November 18, 1977

"Computation of High Frequency Solutions of the Helmholtz Equation"
Alvin Bayliss
I.C.A.S.E.
December 16, 1977

"Finite Element Solution of the Integral Equations of Potential Theory"
J.-C. Nedelee
Ecole Polytechnique, Paris, France
December 16, 1977

"Computed Tomography"
Prof. Gabor T. Herman
S.U.N.Y. at Buffalo
January 6, 1978

"Operator Compact Implicit Methods for Partial Differential Equations"
M. Ciment
National Bureau of Standards
February 17, 1978

"Computing Traveling Wave Solutions of the Two-Dimensional Heat Equation to Represent the Motion of a Quench Front"
Burton Wendroff
Los Alamos Scientific Laboratories
February 3, 1978

"Nonreflecting Boundary Conditions"
Andrew Majda
University of California, Los Angeles
February 24, 1978

"Fast Algorithms for Manipulating Formal Power Series"
R. P. Brent
Australian National University
March 3, 1978

"A Method of Moments for the Numerical Solution of the Boltzmann Equation"
Adie Pridor
Rensselaer Polytechnique Institute
March 10, 1978

"A Vortex-Grid Method for Blood Flow through Heart Valves"
M. McCracken
University of Indiana
March 17, 1978

"An Automated Nested Dissection Algorithm for Irregular Finite Element Problems"
Alan George
Dept. of Computer Science, Univ. of Waterloo
April 7, 1978

"Differential Geometric Methods for Solving a System of Nonlinear Constraint Optimization Problems: Global Analysis"
Kunio Tanabe
Inst. of Stat. Math., Tokyo and Brookhaven National Lab.
April 14, 1978

"Efficient Time Stepping Procedures for the Heat Equation with Time Varying Coefficients"
J. Bramble
Cornell University
April 21, 1978

"The Computation of Discontinuous Solutions of Linear Hyperbolic Equations"
Peter D. Lax
CIMS, NYU
April 28, 1978

"The Finite Element Method of Nonsmooth Domains"
Prof. Alfred Schatz
Cornell Univ.
May 5, 1978

Computer Science Seminars

"Meta-Mathematical Extensibility for Proof Checkers"
Martin Davis
CIMS
October 14, 1977

"Satellite Graphics"
Peter Hartzman
CIMS
October 21, 1977

"An Automatic Test Data Selection System"
Lori Clark
University of Massachusetts
October 28, 1977

"Languages and Oracles"
Ronald V. Book
University of California
November 4, 1977

"A Unified View of Some Arithmetic and Algebraic Algorithms"
David Y. Y. Yun
IBM, T. J. Watson Research Center
November 11, 1977

"Constructing Programs from Examples"
Phillip D. Summers
IBM. T. J. Watson Research Center
November 18, 1977

"Computing the Discrete Fourier Transition"
Shmuel Winograd
IBM, T. J. Watson Research Center
December 2, 1977

"Answering Queries from Tables"
Alfred Aho
Bell Telephone Laboratories
December 9, 1977

"Logic of Programs"
Albert Meyer
Massachusetts Institute of Technology
January 6, 1978

"The Axiomatization of SNOBOL 4 Pattern-Matching"
Morris Siegel
Cornell University
January 31, 1978

"Temporal Semantics of Concurrent Programs"
Amir Pluelli
Univ. of Pennsylvania & Tel Aviv
February 10, 1978

"New Methods for Intractability Proofs"
K. L. Manders
University of California, Berkeley
February 24, 1978

"Distributed Simulation of Queueing Systems"
Prof. Thomas Christopher
Illinois Inst. of Tech.
March 6, 1978

"Computing Technology from Space to Medicine"
Dr. Aaron Finerman
S.U.N.Y., Stonybrook, CS Dept.
March 10, 1978

"A Survey of PL/M Programming for Microcomputers"
Daniel D. McCracken
Author and Consultant
March 27, 1978

"Splitting Recursive Sets"
Seth Breidbart
Yale & Univ. of Cal., Santa Barbara
April 3, 1978

"An Intermediate Language for the CIMS PL/1 Compiler:
A Case Study in Design"
Paul Abrahams
NYU, CS Dept., CIMS
April 14, 1978

"Science, Computers and Society"
Milton R. Wessel
Visiting Prof., NYU Law School
April 21, 1978

"The REFAL Language (Recursive Function Algorithm) Language"
Valentin F. Turchin
CIMS, NYU
April 28, 1978

"Data Flow Programming Languages and Machines"
Dr. Bruce D. Shriver
Univ. of Southwestern Louisiana
May 1, 1978

"Models of Operating System Security"
Elaine Weyuker
CIMS, NYU
May 5, 1978

"The PUMA Computer System: Our Next Main Frame"
R. Grishman
CIMS, NYU
May 12, 1978

"Computational Power of Two Level Grammars"
Robert K. Dewar
CIMS, NYU
May 19, 1978

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3. A. Banegas.
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4. F. Bauer, P. R. Garabedian, and D. Korn.
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Springer-Verlag, New York, Nov. 1977.

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A Computational Method in Plasma Physics.
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6. B. J. Berne, M. H. Kalos, and M. Rao.
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7. O. Betancourt, P. R. Garabedian, and F. Herrnegger.
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8. O. Betancourt, P. R. Garabedian, and F. Herrnegger.
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Stabilizing Effects of ℓ = 2,3 Helical Fields of High-Beta Stellarator Configurations.
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18. M. C. Golumbic and Y. Perl.
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19. R. Grishman and L. Hirschman.
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21. A. Jameson.
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25. J. K. Percus.
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