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TECHNICAL SUMMARY

MASTER

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I. Applied Mathematics and Mechanics

A. Computational Fluid Dynamics

1. Study of High-Order Difference Schemes for Shock Calculations

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. This defect can be corrected by the addition of very small amounts of artificial viscosity.

-- A. Harten, P. D. Lax

2. Numerical Methods for Compressible Flows

The numerical computation of steady compressible flows can be divided into two main parts. Firstly, it is necessary to construct a difference approximation which converges to the solution of the differential equation as the mesh width is decreased. Then an iterative method must be devised for solving the resulting set of nonlinear difference equations. Methods of accelerating the iterative scheme have been extensively investigated during the last year, and two new iterative methods have been developed. The first is a variant of an alternating direction method with a transition to a marching scheme in the hyperbolic region. This gives fast convergence if a suitable sequence of iteration parameters can be found. The second is a hybrid method in which relaxation sweeps are used in combination with steps in which a direct method is used to solve Poisson's equations, with the nonlinear terms treated as forcing terms. The Poisson method by itself is unsuitable for treating equations of mixed type, since it is divergent in the hyperbolic region. If it is stabilized by the use of a sufficient number of relaxation sweeps, however, it proves to be very effective.

-- A. Jameson

3. Numerical Analysis of Transonic Flows

The second volume on transonic flows entitled, "Supercritical Wing Sections II", F. Bauer, P. Garabedian, D. Korn and A. Jameson was completed and published by Springer-Verlag.

The turbulent boundary layer corrected analysis program was tested on an airfoil designed by R. Whitcomb. The comparison of analysis with the wind tunnel experiments is very good for a range of Mach numbers. Results were even quite good for a high lift case using our non-conservation form of the compressible flow equation.

We have attempted to improve the resolution at the shocks and improve the drag calculations. We restored the artificial viscosity parameter EP which we used for the flow calculations in Volume I to reduce the truncation error. This was done for both the non-conservation and the quasi-conservation formulations. We have also incorporated the full conservation form of the flow equations into our analysis program.

These modifications have not significantly improved the treatment of shocks and the drag prediction. We have also tried modifying the difference scheme at the shock. The investigation is continuing.

Jameson's three-dimensional infinite yawed wing program was modified using the parameter EP. The use of EP did sharpen the shock resolution.

We have started to incorporate the Jameson fast solver for solution of the flow equations in our program.

A paper on some of our results was presented at the Hartford AIAA meeting on Transonic Flows on June 20, 1975.

-- F. Bauer

4. Turbine Blades

Work continues on designing turbine blades so as to reduce friction losses. The aim is to eliminate shock waves in cases where the flow has become transonic and involves enclosed regions of supersonic flow.

Interesting examples have been calculated that show promise of reducing losses by as much as 20%. A detailed technical report on this subject is in preparation.

-- P. R. Garabedian, E. McIntyre

5. Numerical Design of Transonic Cascades

In the past six months we have begun work on an improved procedure for designing more efficient supercritical compressor and turbine blades. This procedure would allow the user to specify the desired pressure distribution, and it would compute the corresponding blade shape in a single run. The procedure uses our previous method as an inner loop. Since the trial and error aspect of our previous method is eliminated, this program could become a valuable industrial tool.

At present, we are debugging a computer program which will be used to design subcritical airfoils having a prescribed pressure distribution. This will be followed by supercritical airfoil design. Finally, we will modify the program to design supercritical compressor and turbine blades.

-- D. Korn

6. Climatological Calculations -- Conservative Modification Method

Three numerical methods were developed to calculate the motion of a shallow incompressible fluid layer over a rotating perfect sphere: a Mintz-Arakawa type scheme, a Kreiss-Oliger type scheme, and a rectangular stereographic coordinate scheme. The first two methods used uniform spherical coordinate meshes and filtering of the numerical solution on lines of latitude near the poles to overcome the Courant-Friedrichs-Lowy restriction on the time step. The third method covered the sphere by the overlapping images of two squares, each situated in one of the two polar stereographic planes. Here a uniform rectangular mesh is introduced in each square and the values of the height of the layer and the velocity of the fluid are advanced at the interior mesh points by

a two-step Lax-Wendroff method. The values of these quantities at the boundary points of a square are then found by interpolation, relative to the surrounding values at interior points of the opposite squares.

The stereographic coordinate scheme did not conserve the total mass of the fluid. In fact, it permitted an approximately linear increase in total mass of about 10% per year. Hence a conservative modification method was developed. At each step, the modification method produced a perturbation in the calculated values of height and velocity of at most cubic order in the time step, but conserved the linearized total mass and total energy constraints of the physical system. This dramatically improved the "accuracy" of the calculations. The conservative modification method is applicable to other situations and will be described in a paper by A. Bayliss and E. Isaacson to be presented at the summer 1975 meeting of the American Mathematical Society. A similar method has been developed by Y. K. Sasaki, in an unpublished manuscript.

The Kreiss-Oliger type method produced a small oscillation in the total mass, with a variation of about two parts in ten thousand and a half period of about 30 hours. It is planned to try the conservative modification scheme on this program.

In long runs, the numerical solutions are surprisingly accurate. For details see Final Report I, CIMS-NYU Report No. IMM 407, January 1975, and Final Report II, to appear, both by E. Isaacson and J. J. Stoker.

-- L. Bauer, A. Bayliss, M. Ghil,
E. Isaacson, D. Korn, C. Leiva,
J. J. Stoker

7. Flow Patterns Around Heart Valves

The aim of this work is to develop numerical methods which can be used to study the flow of blood in the heart and the interaction of this flow with the heart valves. Such methods will then be applied to the design of prosthetic heart valves. We are currently working on two methods for this problem. The first method, already operational, involves a finite difference method for the

solution of the Navier-Stokes equations for the fluid. The fixed fluid mesh is coupled to a moving (Lagrangian) representation of the valve leaflets and heart wall. The elastic and muscular properties of these tissues are included in this representation. The second method, now being developed, involves a Lagrangian representation of the fluid as well as the tissues. A collection of moving points represents the instantaneous configuration of the fluid and induces, at each instant, a polygonal partition of the fluid domain. The areas of the polygons are held constant, but the lengths of their edges change smoothly as the points of the fluid move. The topology is also free to change in a natural way. (This Lagrangian method also has potential geophysical applications because the usual difficulties associated with distortion of the coordinate system near the poles are completely avoided. The application of this method of flows on the surface of a sphere is being explored by B. Loerinc.)

-- C. S. Peskin

8. Wave Propagation and Frequency Analysis in the Cochlea

The inner ear contains an elastic plate separating two regions of incompressible fluid. The stiffness of the plate varies exponentially with distance, and this gives rise to a peculiar type of wave propagation in which waves of a given frequency peak at a given place. Since the auditory nerves are distributed along the plate, different neurons are effectively tuned to different frequency components of the sound signal. In our analysis of this problem we first reduce the problem to an integral equation along the plate. Upon discretization, this becomes a large system of linear algebraic equations which can be solved on the computer.

-- C. S. Peskin

9. Deformable Media

Several test calculations are being carried out using Eulerian coordinates for problems usually defined by Lagrangian coordinates. Two such problems are the compression of a soft metal by explosive compression waves

and the flyer plate problem. The geometry of the first problem is characterized by two concentric thick walled spheres. The outer sphere has thermodynamic properties of a detonable material. The inner has material properties of an elastic perfectly plastic metal. The dynamics of collapse of the inner sphere are dependent on the mode of initiation of the detonation in the explosive. In the second problem various flyer plate properties are being studied.

Motion pictures are being generated for both problems and an ERDA R & D Report is being prepared.

-- S. Z. Burstein, E. Turkel

B. Controlled Thermonuclear Research

1. Computational Plasma Physics

Work has continued during the past year on three dimensional equilibrium and stability codes for magnetohydrodynamics. The sharp boundary code has been improved. It has been used to compute the equilibrium and stability of a number of configurations: circles, ellipses, trefoils, beans, etc. The code has been used in particular to study Scyllac, Stellarator, and axially symmetric Tokamak equilibria.

A new code has been written to analyze the equilibrium and stability of a diffuse plasma in three dimensions. The code is based on constructing paths of steepest descent associated with the variational principle of magnetohydrodynamics. The potential energy of the confined plasma is approximated by a discrete sum found through an application of the finite element method. The discrete sum is minimized with respect to the values of a coordinate transformation at the vertices of a finite difference grid. Unstable cases are characterized by indefinite descent of the energy. Stable cases are characterized by convergence of the energy to a relative minimum. A typical run of the program requires 150K words of storage and one hour of running time on the CDC 6600 computer.

-- F. Bauer, O. Betancourt, P.R. Garabedian

C. Numerical Analysis

1. Numerical Secondary Bifurcation

Secondary transitions or secondary bifurcations occur frequently in many nonlinear stability problems. In hydrodynamic stability, secondary bifurcations are called secondary transitions; in elastic stability they are called secondary bucklings. Secondary bifurcation phenomena were known at least since the time of Poincaré. In fact, it was Poincaré who invented the term secondary bifurcation in his classical studies of the equilibrium states of rotating and self-gravitating liquid masses. Secondary bifurcation points and the corresponding secondary states were determined numerically. The nonlinear algebraic equations that result from difference approximations of the von Kármán equations were solved by an accelerated iteration procedure. The results of these computations and a comparison with the theory of secondary bifurcation of Bauer, Keller, and Reiss were reported at the SYNSPADE 1975 meeting. They are summarized in a paper of the proceedings of this meeting.

-- L. Bauer, E. Reiss

2. Wave-Guide Modes

The first 15 wave guide modes and propagation numbers for a hexagonal wave guide were determined by a previously developed numerical method.

-- L. Bauer, E. Reiss

3. Approximation Theory

Work was completed on a paper "On Best Error Bounds for Approximation by Piecewise Polynomial Functions." This theory is an analog of the well-known classical theory on best approximation by trigonometric polynomials as developed by Jackson, Bernstein and Zygmund. Important examples for which our theory applies are interpolation and best approximation by polynomials splines, Hermite functions, and finite elements.

-- O. Widlund

4. Fast Helmholtz Solvers on Nonrectangular Regions

A report "On the Numerical Solution of Laplace's and Helmholtz's Equation by the Capacitance Matrix Method" will appear in the very near future. Our algorithm represents a considerable modification of the capacitance matrix method as previously implemented. A discrete potential theory has been developed and used as a powerful guide in the development of the computer programs. Considerable evidence indicates that the operation count for the algorithm is only $\text{const.} \times N \log_2 N$, where N is the number of variables.

Our algorithms produces highly accurate solutions of the linear systems of algebraic equations which arise when Laplace's and Helmholtz's equations are discretized by using standard finite difference schemes on arbitrary regions in the plane.

-- W. Proskurowski, O. Widlund

5. Difference Correction Methods for Elliptic Difference Equations

We have further explored the difference correction method, developed essentially by Victor Pereyra, to enhance the accuracy of the finite difference solution of elliptic problems. In contrast to the related and better known Richardson extrapolation procedure, the difference correction method requires only one fixed mesh. A method proposed by Kreiss has been further developed. A series of successful computer experiments have just been concluded. Our program employs a variant of the capacitance matrix method. A publication is currently being prepared.

-- V. Pereyra, W. Proskurowski,
O. Widlund

6. Fast Helmholtz Solvers for Three-Dimensional Problems

Preliminary work has been carried out in order to extend the capacitance matrix method to three dimensions. While a direct extension of the method for two-dimensional problems is possible it would require an excessive amount of storage. Preliminary computer experiments with related problems from classical potential theory have been very promising. The development of fast, highly

accurate methods for the three-dimensional Helmholtz problem which would require only a modest amount of storage therefore seems quite feasible.

-- O. Widlund

7. Eigenvalue Calculations with the Capacitance Matrix Method

Work is in progress to develop a method to calculate the eigenvalues and eigenfunctions of the Laplace operator on general two-dimensional regions. It is based on the observation that the capacitance matrix is singular if and only if the original problem is singular. A linear eigenvalue problem with many variables is thereby converted into a much smaller nonlinear problem.

-- W. Proskurowski, O. Widlund

II. Computational Physics, Chemistry, and Biology

A. Physics

1. Diffractive Ray Tracing of Laser Beams

A method for extending conventional ray tracing techniques to include diffraction effects associated with focused laser beams has been developed. The main idea is to provide rays with a distribution of directions at each point in space, as in radiative transfer calculations. The Wigner phase space distribution function is used to obtain formulas for the spread of ray angles which yield the correct diffraction patterns for both coherent and partially coherent laser beams. This method is readily implemented numerically by means of computer programs that are used in Monte Carlo radiative transfer calculations.

-- F. D. Tappert

2. Moment Theory of Self-Trapped Laser Beams with Nonlinear Saturation

The moment theory of the quasi-optical equation was used to obtain simple analytical expressions for the relation between beam radius and power of stationary self-trapped light beams in passive nonlinear media with saturation of the index of refraction. Results were compared to recent numerical calculations giving good agreement. In addition, the stability of these self-trapped beams was determined.

-- F. D. Tappert

3. Filamentation of High-Power Laser Beams and Pulses in Plasma

The quasi-optical equation describing propagation of laser radiation has been solved numerically for time-independent beams in three space dimensions and time-dependent pulses in two space dimensions. Saturation of the index of refraction in accordance with the relativistic electron plasma nonlinearity and the ponderomotive plasma nonlinearity was taken into account. The quasi-optical equation was solved using the "split-step Fourier" algorithm which is exactly norm conserving, highly accurate (infinite order in spatial derivatives), and requires minimal storage. If the beam power is above a certain critical power, which has been determined numerically, then the beam or pulse becomes unstable

and breaks up into a large number of self-focusing filaments. These filaments are analogous to two-dimensional solitons. The manner in which these filaments interact nonlinearly with each other has been carefully studied numerically with the goal of using their special properties in laser fusion applications.

-- F. D. Tappert

4. Relativistic Nonlinear-Optic Instabilities of Electromagnetic Waves in Plasma

Relativistic electron plasma motion induced by high intensity electromagnetic waves results in a local (in space and time) nonlinear index of refraction which leads to the familiar self-modulation and self-focusing instabilities of the radiation field. Theoretical-numerical studies of this effect show temporal pulse compression with frequency broadening, transverse beam collapse and break up with angular broadening, and other fast-growing nonlinear effects.

-- F. D. Tappert

5. Properties of Non-Uniform Classical Fluids

A molecular dynamics program has been put into operation to study the properties of classical liquids. The program is used to study the physics of a self-supporting film of liquid argon in equilibrium with its vapor. The surface profile obtained will be compared to the Monte-Carlo results obtained by K.S. Liu. In addition, the time correlation functions are studied to understand the excitations in the liquid drop.

-- M. H. Kalos, D. Levesque,
M. Rao

6. Ground State of Quantum Systems

The exact code to study quantum liquids is used to model liquid helium with an interaction potential consisting of a hard sphere plus a square well. Energy variations with density are studied using a 64 particle system. At the equilibrium density the size dependence of energy is studied using 32, 64, 128 and 256 particles. The energy values obtained are much deeper than those obtained from a variational

calculation using the same trial functions as for a pure hard sphere system. We are investigating the deficiencies of this function.

-- M. H. Kalos, K. S. Liu,
M. Rao

7. Quantum Free Film

The same potential used above (hard sphere plus attractive square well) has been used to construct a self bound film of bosons with two free surfaces. We find a density profile with apparently well developed structure with a wavelength of about 4 Å and amplitude about 8%. Because the trial function used is not very accurate the statistics are uncertain; they are being analyzed now. For much the same reason the potential does not model the ${}^4\text{He}$ potential very well, but this is not likely to affect the nature of the density profile.

-- G. V. Chester, M. H. Kalos,
K. S. Liu

8. Two-Dimensional ${}^4\text{He}$ System

A variational study of fluid and crystal states of ${}^4\text{He}$, modeled by a Lennard-Jones potential, has been completed. The lowest energy state is fluid, but at higher densities the system crystallizes. The melting density we find ($p\sigma^2 = 0.5$; $\sigma = 2.55 \text{ \AA}$) is rather close to that observed experimentally for monolayers of ${}^4\text{He}$ absorbed on Grafoil.

-- G. V. Chester, M. H. Kalos,
K. S. Liu

9. Models of Nuclear Matter

The work of Kalos, Levesque, and Verlet in solving the many body Schrodinger equation for hard sphere bosons has been extended to a continuous potential. A repulsive Yukawa potential that models the interaction

between neutrons at high densities was studied. There is considerable interest as to whether the ground state of this system is liquid or solid. A number of techniques have been discovered and implemented to improve the accuracy of the exact solution of the ground state. For example, the energy of the ground state can be estimated within .1% with 1 hour of computing time.

To solve the Schrodinger equation one starts with a trial wave function and the better the trial wave function is the more accurate statistically the exact solution is. It was found that the Jastrow wave function of Cochran and Chester is a very good approximation to the ground state of the Yukawa neutrons. The best Jastrow 'pseudo-potential' was found accurately and quickly by reweighting the configurations sampled from a nearby Jastrow and determining the change of parameters which would lead to minimum energy. The variational energy of this wave function is almost exactly right for this potential; however, other expectation values such as the zero momentum or condensate fraction and kinetic energy are off considerably.

A new trial solid wave function similar to a Wannier periodic wave function has been used to determine if this system will crystallize. Other workers have assumed that in the solid, particles will not interchange their lattice sites and have chosen a wave function where particles are tied to their lattice sites by a harmonic force. The assumption is probably justified for helium, but for a soft-core potential like the Yukawa it is better to have a wave function which is symmetric. In fact, the symmetric wave function lowered the energy of the crystal enough so the metastability found for the harmonic solid disappeared. We have found, in agreement with most other researchers on this problem, that the model neutron system is a liquid.

The real neutrons are, of course, fermions and it would be highly desirable to solve this model Yukawa problem with an antisymmetric wave function. The first attempt was to use Feymann's theorem to compute the variational energy of ψ_B^F where ψ_B is the ground state

of the boson system and F is a Slater determinate of plane waves.

Since the particles in the boson system have no spin, one is forced to do a walk in spin coordinate space in order to compute this energy. It was found that this walk is hard to do in reasonable amounts of time without introducing a bias. Recently, a program has been written to sample $\psi_J F$ where ψ_J is a symmetric Jastrow wave function. The program uses a Metropolis walk in coordinate space where all the particles are moved simultaneously. This technique has been checked out on the interacting boson system as well as the ideal gas fermion problem. Preliminary results indicate that it works well for this fermion system and for interacting fermions.

-- D. Ceperley, G. V. Chester,
M. H. Kalos

10. Quantum Systems at Finite Temperatures

The utility of several variational principles are studied to obtain the properties of quantum liquids at finite temperatures. We have developed a few plausible trial density matrix forms useful for the necessary importance sampling in the Monte Carlo estimation of many-body quantum systems. Very likely they can be used as they stand down to about the lambda transition in He like systems. Joining these to plausible very low temperature forms is more delicate and will probably require auxiliary variational calculations. We have begun the calculation of the second and third virial coefficients of a hard sphere fluid as a test of the methods. The second is known numerically and an asymptotic series for the third has recently been extended to the fourth term which can be verified.

-- M. H. Kalos, D. Levesque, M. Rao

11. Simulation of Kinetics of Binary Alloys

We have continued the simulation studies in several new directions. A thorough study of the three dimensional system (isomorphic to the Ising ferromagnetic system) was carried out for the case where equal numbers of each kind of particle are present. The evolution of various properties, especially energy and structure function, following quenching to a specified temperature has been

followed. Comparisons with theories of Langer and of Binder which predict specific properties (and which are partly based on our earlier results) have been made. With a plausible adjustment of the time scale our results are compatible with recent experiments on Al-Zn.

Studies of the two dimensional system have been extended to much longer times and carried out in a much larger system (200 x 200) to examine in detail the height and position of the peak of the structure function.

Three new areas of investigation were just begun. The two dimensional program was modified to follow the diffusion, growth, and joining of clusters after the nucleation has begun. The dynamics of the processes underlie Binder's theories.

We have begun the study of alloys which resemble antiferromagnetic spin systems.

The three dimensional program has been modified to model a system whose dynamics are controlled by the diffusion of a third component, usually thought of as a small fraction of vacancies.

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

12. Raman Spectra of Crystals

The high-frequency part of the two-phonon Raman spectrum of diamond, which shows some anomalous and controversial features has been analyzed. A careful calculation of the dispersion curves in diamond reveals a shallow maximum in the [100] direction for the LO branch. The two-phonon (overtone) density of states shows a sharp peak near twice the Raman frequency. This supports the interpretation of an observed peak in two-phonon Raman scattering as a simple overtone without the need to invoke a two-phonon bound state. The CDC 6600 computer was used for setting up and diagonalizing the dynamical matrix for various values of the phonon momentum and for calculating the density of states.

The results obtained thus far are only preliminary, and further calculations are required before they can be submitted for publication. We hope to be able to carry out these calculations in the coming year.

-- A. K. Agyei

B. Chemistry

1. Atomic Effective Potentials

Chemists have long known that the essential features of molecular structure are determined by the valence electrons. As a result a great deal of effort has gone into seeking ways of replacing the core electrons by a local effective or pseudopotential. Recently, an accurate Hartree-Fock effective potential has been developed by C. F. Melius, et al. (Chem. Phys. Lett. 28, 457 (1974)) for Ni and Fe. In collaboration with Melius we are developing potentials for the remainder of the first row transition metal atoms and are extending the method to the second row.

-- J. W. Moskowitz

2. A Molecular Complex Model for the Chemisorption of Hydrogen on a Nickel Surface

The chemisorption of hydrogen on nickel has been studied using a localized surface complex: $H_2 + Ni_2 \rightarrow Ni_2H_2$. The electronic structure was calculated using ab initio methods which included electron correlation, the core electrons of Ni being replaced by an ab initio quality effective potential. We find that the chemisorptive bond of H on Ni is formed primarily to the Ni 4s electron, the 3rd electrons remaining localized on the individual Ni atoms. The dissociative chemisorption process is explained in terms of Woodward-Hoffmann correlation diagrams, with the d electrons allowing the reaction to occur on an otherwise forbidden reaction path involving a biradical intermediate.

-- J. W. Moskowitz

3. The Electronic Structure of the Actinides

The role of the 5f electrons in the electronic structure and bonding of the actinide complexes has been studied. Self-consistent-field computations have been performed in the recently developed χ - α Scattered-Wave-
Approximation for UO_2^{++} , UF_6^- and UF_6^- .

-- J. W. Moskowitz

C. Biology

1. Cross-Bridge Dynamics in Muscle

The sliding filaments of skeletal and heart muscle have cross-bridges which cyclically attach, participate in shortening, and break. At any instant there is a population of cross-bridges, each cross-bridge being characterized by its state of strain. The equation governing the dynamics of this population resembles that of a birth-death process, and contains an unknown function giving the rate of breakage of cross-bridges as a function of strain. Lacker has been able to show that this function can be computed from data on the steady mechanical behavior of muscle, and he is using this result to predict the transient behavior.

-- H. M. Lacker, C. S. Peskin

2. Fiber Architecture of the Heart Wall

This work represents an attempt to predict the spiralling fiber geometry of the heart wall from equations of equilibrium of the pressure field with the fiber stress. Computational results reveal that a closed, heart-shaped structure is not possible without branching of the cardiac muscle fibers. Such branching is regularly observed in microscopic sections of cardiac (but not skeletal) muscle.

-- A. Jamgotchian, C. S. Peskin

3. Pattern Formation by Swimming Micro-Organisms

A numerical program devised in collaboration with R. Peyret of the University of Paris has been used to study the patterns formed in cultures of certain swimming micro-organisms. The program solves the Navier-Stokes equations in a rectangle with free upper boundary. The flow field is driven by N points or particles, representing the organisms, under the action of a gravitation field. The particles drift upward (negative geotaxis) but also execute an isotropic random walk relative to the ambient fluid. The results bear not only on bioconvection but also on insect swarming and other collective phenomena.

These computations are nearly complete, and a paper in preparation (with R. Peyret) will be submitted to the Journal de Mecanique in the near future.

-- S. Childress

4. Pattern Formation in Tissue

An exploratory series of computations have been made in an attempt to understand the properties of certain plausible systems of equations. The problem models biological differentiation at the cellular level as follows: each "cell" is an element of the spatial grid of the numerical scheme; cell states are determined by a time-dependent vector, representing the concentrations of a certain number of substances which determine cell type. If diffusion is allowed across cell boundaries, the resulting vector field satisfies a system of nonlinear parabolic equations.

Calculations to date have eliminated certain chemical kinetics. A more promising "activator" model has been studied. Restricting attention to one space dimension, we have been able to model regenerative tissue, with the property that an excised segment, when left to develop, reproduces a scaled-down pattern of differentiation equivalent to the original one.

At present we foresee further experimentation with one-dimensional case, but we intend to pursue the most promising kinetic models and eventually explore patterns of cellular differentiation in two and possibly three dimensions.

-- S. Childress

III. Computer Science

A. Computer Netting

1. ARPA Network

Implementation Status

The ARPA Network message processor (IMP) was delivered and installed. A PDP-11 minicomputer was acquired and connected to the IMP. The ELF system for ARPA network access was acquired, configured for our PDP-11 and installed. Thus, interactive user access to the network was achieved.

A final evaluation of available software for network access showed the ELF system to be best for our purposes. The ELF development effort by the ARPA sponsored Speech and Communication Research Laboratory had not advanced as much as we had hoped. The system did provide interactive network access for a number of users but had no file transfer capability and no work had been done to facilitate its use as a front-end for a larger server host system such as our CDC-6600. However, we learned that maintenance and on going development support was being provided by the Air Force Systems Command and that several different projects would be underway soon by various government agencies to extend the ELF system into a network front-end. Completion of these projects is not expected until well into fiscal year 1977. We decided that we could not wait so long, and, further we were concerned about depending on projects over which we could exercise no control. Accordingly, we undertook an implementation effort of our own. A two stage design strategy was chosen to give early completion of a limited but adequate facility and a natural extension to a more effective long term solution. Programming was begun to provide network access to our CDC 6600 time sharing system. Program design was begun to provide network file transfer and remote job entry facilities.

Network Experimentation

This activity is at its earliest stage. The preliminary investigation of various host systems is being undertaken in order to begin to discover and evaluate network characteristics and also to learn about

the various host facilities, such as, operating system command languages, programming languages and dialects, compiler performance, file organization, accounting methods, on-line and in person user services, etc.

Some attempts are being made in conjunction with other ERDA sites, to use the ARPA Network mail facility for correspondence. In addition, since the source files of the ELF system are at the Stanford Research Institute PDP-10 computer, and then cannot practically be kept at our own PDP-11, the programming development work which we are doing to the ELF system must be done at the SRI computer via the network. Thus, this work in itself provides an interesting network experiment.

ERDA Computer Networking Group

Two meetings of the Implementation Panel were held for the purposes of information exchange, implementation status reporting, and the discussion and finalization of specifications for a file transfer protocol. The decision was made to adapt a subset of the ARPA File Transfer Protocol. Notes of these meetings were prepared and distributed to panel members.

Meetings of the Objectives Panel of the networking group were attended.

Miscellaneous Network Activities

In keeping with our interest in alternatives to the ARPA Network we have received verbal briefings and have studied written documents concerning plans by the EDUCOM group to use the TELENET communications system. Of particular interest were the pricing policies and the technical details of the TELENET system architecture. We were also interested in the strategies for bringing different machines onto the network. At present, the orientation is essentially to IBM equipment and communications protocols.

-- E. Franceschini, M. Goldstein

B. Programming Languages and Compilers

1. GYVE Language

Development of full-scale operating systems has tended to be a particularly difficult, confused affair, as structured high level techniques in this area have been lacking. To address this area of programming, certain major problems of parallel process coordination, resource allocation, and protection must be faced. In a doctoral thesis currently under preparation, Mr. Phillip Shaw has taken a major step forward in this important area, specifically by devising a new programming language, designated GYVE, in which an exceptionally broad spectrum of crucial operating systems issues are faced, and which we expect will make it much easier to write operating systems of all sorts, including advanced network operating systems, and systems for the control of experiments in real time. We are currently beginning to explore the use of these techniques for operating systems specification, designing an implementation of GYVE, and studying ways in which it can be extended so as to solve problems which it currently does not address. Among these are: multi-level memory hierarchy control, system recovery after crash, system reliability and "graceful degradation," distributed computer networks with limited inter-node bandwidth, network reliability in the presence of occasional message loss, and multiple-object access techniques which can be guaranteed to be deadlock-free. This work, though relatively new, has already generated considerable interest at the Courant Institute, and several of our better graduate students have already become actively involved in it.

-- J. T. Schwartz

2. BALM Language

In the last year work has continued on the development of BALM, the extendable list-processing language developed here for the 6600, and subsequently implemented on other machines. A translator version was implemented for the 1108. In addition, work has been started on the implementation of a set of multi-tasking primitives which will permit (simulated) parallel processing, backtracking, etc.

-- M. Harrison

3. PL/I Compiler

Work has continued on the CIMS PL/I system, on the standardization of PL/I, and on examining issues in programming languages design and implementation that arose from prior work with PL/I.

The CIMS PL/I system has now been distributed to about fifty different installations, and experience with it is becoming available. A number of earlier problems have been solved, but some others, notably large core size required for compilation and lack of stream input-output, remain. However, both of these problems are on the way to solution.

Collaboration has continued with the Lawrence Berkeley Laboratory in connection with CIMS PL/I. The system has been used successfully at that Laboratory. In turn, their contributions have been of great help in improving the system.

The major improvement added during this year was a collection of facilities for scientific computation. These included a large collection of built-in functions; implementation of the exponentiation operator for the full range of cases; and installations of the floating input-output and constant handling that was previously lacking.

We have participated in the committee X3J1 of the American National Standards Institute, which is developing the national standard for PL/I that has recently been released for public comment.

-- P. Abrahams

C. Operating Systems, Micro-Processor Networks, and Modular Systems

1. Operating Systems

This work is concerned with a relatively new scheduling algorithm -- the Page Fault Frequency (PFF) algorithm. Initial simulations reported in the literature suggest that this may be superior to the standard "working set" algorithm. This thesis will

simulate the PFF and working set algorithms within a more realistic multi-programming environment. Initial results suggest that there may be flaws in the PFF algorithm which do not show up in an oversimplified simulation.

-- M. Harrison

2. Micro-Processor Networks

It is clear that developments in technology will have a profound effect on the architecture of computers. Currently, one of the most interesting developments is the availability of inexpensive micro-processors. It seems clear that such micro-processors could be used in many places in a computing system to replace hard-wired structures. This work is concerned with the possible use of networks of micro-processors. The techniques will be to simulate such a network, and then see what level of performance could be obtained with the network structured and programmed to provide the functions of various components in a computing system, such as multiplexors, etc.

-- M. Harrison

3. Modular Systems for Scientific Problem Solving

Experimentation continues with the design of advanced processors, use of microprogrammable units, minisystems, and graphic facilities with a view towards scientific problem solving. The advanced processors can be assembled from off-the-shelf logic chips. They will serve to do local computing, augment the power of a local computer, or will serve as processors for a local computer.

-- R. Grishman

IV. Systems Programming, User Services Activities, and Hardware Support

A. Systems Programming and User Services

Conversion to the KRONOS operating system for the CDC 6600 was completed and the system put into production. The principle tasks involved in this process were the following:

- Accounting programs
- Software for NYU telecommunications control hardware and protocols
- Support for non-CDC graphics devices
- Conversion of NYU program and subroutine library
- Conversion of NYU file maintenance system, CIMLIB
- Installation of the Indiana University permanent file management package
- Various minor modifications to FORTRAN compiler
- NYU SCOPE to KRONOS user conversion guide
- Conversion aid consultation for users

Software maintenance was provided in the form of 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:

- KRONOS 2.1 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 mini-computers
- Compilers for various languages, e.g., FORTRAN, BASIC, ALGOL, SNOBOL, LISP

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

B. Hardware Support

Hardware support encompasses: the design and assembly of front-end, communications, and interfacing facilities, including attendant software, that are either unavailable from industry or too expensive to procure; the periodic upgrading of these facilities vis-a-vis advancing technology and the Laboratory's needs; the evaluation and selection for either purchase or lease of automatic data processing equipment (ADPE); the preventive and remedial maintenance of a substantial component of the Laboratory's ADPE complement.

In the Computing Laboratory's ADPE complement there are a variety and multiplicity of interfaces that are interposed between the CDC 6600 and its intrasite and remote terminals and between equipment items of different manufacture. All these interfaces (with the exception of the 6600/516 interface) were redesigned for the dual purpose of maintainability and improved performance using off-the-shelf multiple sourced TTL. These interfaces were built and tested.

The ARPA IMP and the IMP to Host interface were installed and are now functional.

The 32 port multiplexer was expanded to 64 ports, and a new 16 port synchronous multiplexer was built and tested. It was designed to accommodate two different I/O service routines. One scheme would satisfy the service routine now operational, while the other was to accommodate higher speeds and a more efficient interrupt handler.

In-house terminal service has been expanded to include more private line service and more shared dial up service.

An interface to connect Honeywell I/O interfaces to a DEC PDP-11 has been designed and is in the process of construction. With such a device all Honeywell minicomputers could be replaced with DEC PDP 11's and still maintain service to the Laboratory's intrasite and remote terminal users.

Periodic maintenance of all minicomputers, terminals, and communication lines have been performed. Investigations of remote service to the Brookhaven 7600 have been initiated. Communication equipment and line changes have been studied and some testing of such service will be tried during the next reporting period.

-- R. P. Bianchini

V. Publications

A. Issued

Anderson, D. T., O. L. Betancourt, Shohet, J. L., Tataronis, J. A., "Three Dimensional MHD Equilibria of Toroidal Stellarators", ECE-75-11 Report, University of Wisconsin, Madison, July 1975.

Bauer, F., Korn, D., Computer Simulation of Transonic Flow Past Airfoils with Boundary Layer Correction, AIAA meeting June 1975, Hartford, Conn.

Bauer, F., Garabedian, P., Jameson, A., Korn, D., Super-critical Wing Section II, Lecture Notes in Economics and Mathematics Systems, Vol. 108, Springer-Verlag, 1975, COO-3077-80.

Betancourt, O., Garabedian, P., Computer Simulation of the Toroidal Equilibrium and Stability of a Plasma in Three Dimensions, Proc. Nat. Acad. Sci., Vol. 72, No. 3, pp. 926-927, March 1975, COO-3077-89.

Bortz, A. B., Kalos, M. H., Lebowitz, J. L., A New Algorithm for Monte Carlo Simulation of Ising Spin Systems, J of Computational Physics, Vol. 17, No. 1, January 1975, COO-3077-79.

Bortz, A. B., Kalos, M. H., Lebowitz, J. L., Marro, J., Time Evolution of a Quenched Binary Alloy II: Computer Simulation of a Three-Dimensional Model System, Physical Review B, Vol. 10, pp. 535-541, July 15, 1974.

Burstein, S., Difference Methods for Transonic Flows about Airfoils, Fourth International Conference of Numerical Methods in Fluid Mechanics, Boulder, Colorado, June 1974 (Springer-Verlag).

Chester, G. V., Kalos, M. H., Liu, K. S., Variational Calculations of Liquid ^4He with Free Surfaces, Physical Review B., Vol. 12, No. 5, September 1, 1975, COO-3077-93.

Cooper, F., Frye, G., Schonberg, E., Landau's Hydrodynamics Model of Particle Production and Electron Position Annihilation into Hadrons, Physical Review D, Vol. 11, No. 1, pp. 192-213, January 1975.

Franceschini, E., Goldstein, M., Computer Sharing at NYU - From Internal System to ARPANET, presented at AESOP Conference, Vol. 12, March 25-27, 1975, St. Petersburg, Florida.

Garabedian, P. R., Computational Transonics, NASA Conference on Aerodynamic Analyses Requiring Advanced Computers, Langley Research Center, March 4-6, 1975.

Garabedian, P. R., On the Design of Airfoils Having no Boundary Layer Separation, Advances in Mathematics, Vol. 15, No. 2, February 1975, COO-3077-77.

Garabedian, P. R., The Existence of Green's Function Revisited, Rendiconti di Matematica (1) Vol. 8, Series VI, 1975, COO-3077-87.

Jameson, A., Accelerated Iteration Schemes for Transonic Flow Calculations Using Fast Poisson Solvers, March 1975, COO-3077-82.

Jameson, A., O'Malley, R. E., Jr., Cheap Control of the Time-Invariant Regulator, Applied Mathematics & Optimization, Vol. 1, No. 4, Springer-Verlag, 1975, COO-3077-76.

Jameson, A., Iterative Solution of Transonic Flows Over Airfoils and Wings, Including Flows at Mach 1, Comm. on Pure & Appl. Math., Vol. XXVII, 283-309 (1974), COO-3077-71.

Jameson, A., O'Malley, R. E., Jr., Singular Perturbation and Singular Arc - Part I, IEEE Trans. on Automatic Control, Vol. 20, No. 2, April 1975.

Jameson, A., Transonic Potential Flow Calculations Using Conservation Form, AIAA Meeting, June 1975, Hartford, Conn.

Korn, D. G., Numerical Design of Transonic Cascades, January 1975, COO-3077-72.

Korn, D., Transonic Design in Two Dimensions, Constructive and Computational Methods for Differential and Integral Equations, Lecture Notes in Mathematics, Vol. 430, pp. 271-288, 1974, COO-3077-81.

Kreiss, H. O., Parter, S. V., Remarks on Singular Perturbations with Turning Points, SIAM J. Math. Anal., Vol. 5, No. 2, April 1974, COO-3077-73.

Lax, P. D., Almost Periodic Behavior of Nonlinear Waves, Advances in Math., 16:368-379, June 1975.

Lax, P. D., Applied Mathematics and Computing Proceedings of Symposia in Applied Mathematics, Vol. 20, 1974, COO-3077-78.

Lax, P. D., Periodic Solutions of the KdV Equation, Comm. on Pure & Appl. Math., Vol. XXVIII, 141-188 (1975), COO-3077-90.

Lax, P. D., Phillips, R. S., Scattering Theory for Dissipative Hyperbolic Systems, J. of Functional Analyses, Academic Press, Vol. 14, No. 2, October 1973, pp. 172-235, COO-3077-88.

Melius, C. F., Moskowitz, J. W., Ratner, M. A., A Molecular Complex Model for the Chemisorption of Hydrogen on a Nickel Surface, April 1975, COO-3077-86.

Meyer, J., A Precis of GYVE, Tech. Report, Computer Science Dept., Courant Institute (1975).

Percus, J. K., Correlation Inequalities for Ising Spin Lattices, Comm. Math. Physics 40, pp. 283-308 (1975), COO-3077-84.

Schwartz, J., Shaw, P., A Brief Survey of the Principal Concepts of GYVE, a Language for the Description and Control of Multiple Processes Acting in Parallel, Tech. Report, Computer Science Dept., Courant Institute (1975).

Schwartz, J., Treatment of Multi-Computer Networks in the GYVE Language; Scheduling for Devices with Real-Time Constraints; Distributed Networks of Device Controllers, Tech. Report, Computer Science Dept., Courant Institute (1975).

B. Accepted

Belpaire, G., Hsu, Nai-Ting, Formal Properties of Recursive Virtual Machine Architectures, to be presented at the 5th Symposium on Operating Systems Principles, Austin, Texas, November 1975.

Ghil, M., Steady-State Solutions of a Diffusive Energy-Balance Climate Model and their Stability, Jour. of the Atmospheric Sciences.

Lam, J. F., Lippmann, B., Tappert, F., Moment Theory of Self-Trapped Laser Beams with Nonlinear Saturation, Optics Communications.

Owens, P. J., Schwartz, J. T., A Comprehensive Survey of Parsing Algorithms for Programming Languages, ERDA R & D Report.