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INTRODUCTION

The Institute for Computer Applications in Science and Engineering (ICASE) is operated at the Langley Research Center (LaRC) of NASA by the Universities Space Research Association (USRA) under a contract with the Center. USRA is a nonprofit consortium of major U. S. colleges and universities.

The Institute conducts unclassified basic research in applied mathematics, numerical analysis, and computer science in order to extend and improve problem-solving capabilities in science and engineering, particularly in aeronautics and space.

ICASE has a small permanent staff. Research is conducted primarily by visiting scientists from universities and from industry, who have resident appointments for limited periods of time, and by consultants. Members of NASA's research staff also may be residents at ICASE for limited periods.

The major categories of the current ICASE research program are:

a. Numerical methods, with particular emphasis on the development and analysis of basic numerical algorithms;

b. Control and parameter identification problems, with emphasis on effective numerical methods;

c. Computational problems in engineering and the physical sciences, particularly fluid dynamics, acoustics, and structural analysis;

d. Computer systems and software, especially vector and parallel computers.

ICASE reports are considered to be primarily preprints of manuscripts that have been submitted to appropriate research journals or that are to appear in conference proceedings. A list of these reports for the period October 1, 1983, through March 31, 1984, follows a brief description of research in progress in the next section.

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RESEARCH IN PROGRESS

Saul Abarbanel and David Gottlieb

In many problems in fluid mechanics it is the steady state that is desired. Approaching the steady state via the finite difference approximation to the time dependent partial differential equations can be very costly in terms of computer machine time. This is true especially in problems where coordinate stretching or source terms impose severe restriction on the stability criteria for time-stepping.

In using such algorithms to reach steady state many researchers relax the time-consistency restriction and advance the calculation using a time step, \( \Delta t \), that arises from one grid point to another. The criterion for choosing the local time-step is formulated so that one does not exceed the Courant number indicated by linear stability theory.

We have shown that one can dispense even with the more relaxed restriction of constant CFL and vary spatially the Courant number in such a way that convergence to steady state is greatly enhanced. For linear hyperbolic systems one can predict a priori the optimal "time-steps." For nonlinear systems the optimality algorithm is equivalent to using Newton-Raphson iteration but without the need of inverting the matrix coefficients of a linearized problem.

Preliminary numerical results are very promising and the method is now being used to modify existing large programs being used at LaRC.

Loyce M. Adams

Work concerning the convergence questions of parallel (multi-color) SOR was done in conjunction with H. Jordan (University of Colorado). We were able to construct multi-color SOR schemes (for a wide range of stencils used to discretize partial differential equations) with the same rate of convergence as the corresponding natural rowwise ordered SOR scheme. Currently, unanswered questions that were stimulated by this research, such as the convergence rate of multi-color SSOR, are being pursued.
H. Thomas Banks

We are continuing (in collaboration with K. Kunisch (Technische Universität Graz) and K. Ito) our investigations of stable optimal distributed feedback controls for parabolic and hyperbolic systems. Numerical studies as well as theoretical questions are being pursued. Splines and tau-Legendre approximation schemes are being used.

In joint efforts with K. Murphy (Southern Methodist University) and K. Ito, we are developing methods for estimation of boundary parameters as well as spatially varying (and possibly discontinuous) coefficients in hyperbolic systems.

H. Thomas Banks and I. Gary Rosen

We have been developing numerical approximation schemes for the identification of hybrid systems involving the transverse vibration of flexible beams with attached tip bodies. Our methods are cubic spline based and center upon the finite dimensional approximation of the coupled systems of ordinary and partial differential equations which describe the dynamics of the system. Abstract operator formulations of the problem as well as mesh variational formulations are being used with the approximation schemes to develop a theoretical framework. Numerical studies are underway and initial findings are quite promising.

H. Thomas Banks and James M. Crowley

We have developed methods for estimating spatially varying parameters (density, stiffness, and damping) from discrete data in the Euler-Bernoulli model for vibrations of a flexible beam. These methods use Galerkin-projection approximations of the state and splines approximation of the parameter functions.

A general procedure was developed for computing the gradient of the cost functional with respect to the coefficients in the spline approximation using
an adjoint or costate equation. The resulting gradient was implemented in both conjugate-gradient and BFGS (quasi-Newton) methods for optimization. Numerical results were obtained and in some situations a substantial improvement was obtained when compared with the Levenberg-Marquardt algorithm (with finite difference Jacobian) used previously.

Stephen F. Davis

Work has continued on the application of upwind difference methods to the numerical solution of systems of hyperbolic partial differential equations. Particular emphasis has been focused on methods for computing discontinuous solutions of the Euler equations, i.e., solutions containing shocks.

A recently completed study has examined the question of whether it is possible to construct a total variation diminishing (TVD) finite difference scheme which does not require the determination of an "upwind" direction. Such a scheme was constructed by showing that the TVD upwind scheme studied by Sweby was equivalent to the Lax-Wendroff method plus an upstream weighted artificial dissipation term and that this term could be modified in such a way that the scheme remained TVD but no longer depended on the upwind direction. The resulting scheme does not contain any problem dependent parameters but is more dissipative than the upwind method. Fortunately, numerical experiments show that the results obtained using this method are almost indistinguishable from those obtained using the upwind method.

At this time additional numerical experiments are being conducted and an ICASE report on this work is being written. Future work will involve the implementation of these ideas in existing Langley computer codes and the construction of a rotationally biased version of this scheme.

A study is being conducted with T. N. Phillips on iterative methods for the solution of the large sparse linear systems which arise from the implicit upwind discretization of hyperbolic partial differential equations. The linear systems which result from such a discretization are diagonally dominant but not symmetric and not positive definite. Thus far we have examined two conjugate gradient type algorithms, namely, the biconjugate gradient method of
Fletcher and the minimum residual algorithm. Both algorithms were programmed for some simple problems involving a linear advection equation in two dimensions and Burgers' equation in one and two dimensions. Both algorithms converged for these problems in about the same number of steps. Since the biconjugate gradient method requires about twice the computation per step and is very difficult to precondition, we may not study it further. In the future we expect to apply these methods, with and without preconditioning, to some realistic problems and compare them with other methods.

Work has continued (in collaboration with J. Flaherty) on the adaptive finite element method that was first reported in ICASE Report No. 81-13. With the recent construction of a computable estimate for the time discretization error and its implementation in a time step selection algorithm, we were able to study the solution of reaction-diffusion equations which model ignition and combustion. Currently, we are studying how the small time steps required to solve such problems affect the choice of an algorithm for moving the spatial grid.

Work is underway (in collaboration with J. P. Drummond, LaRC) on numerical methods for problems involving the interaction of fluid dynamics and finite rate chemistry. At present we are conducting a study to determine which of the many methods that have been developed for stiff ordinary differential equations could be practically adapted to large problems involving partial differential equations.

**Stefan Peyock**

Work has continued on syntax programming, the use of syntax analysis techniques as a programming and problem-solving tool in a manner analogous to logic programming. The feasibility of syntax programming has now been definitely established, and the characteristics of this approach have been explored. It has become clear that the absence of the built-in backtracking capability central to logic programming poses few problems for the syntax programmer. It appears, in fact, that the control structures offered by
syntax programming allow for considerably more elegance and efficiency than is possible in logic programming.

A number of applications of syntax programming are presently under development, including an in-flight pilot aid system for failure diagnosis, and the addition of reasoning capabilities to database systems by means of syntax programming. The use of less formal parsing techniques, such as transition diagrams, is being investigated in conjunction with the latter application.

Dennis B. Cannon and John Van Rosendale

One of the central issues in parallel computing research is the treatment of problems having irregular structure, such as finite element discretizations on general irregular grids. The approach to this issue being explored here is the use of a flexible architecture that can adapt to such problems. The proposed architecture consists of 16 or more clusters of processors, each cluster being similar to the future Blue CHiP machine. These clusters are then interconnected by a packet switched communications network. Applications for which this architecture is well-suited include adaptive grid calculations, robot path planning, and cellular automata simulation. A compiler-driven, instruction-level simulator has been written, which executes a parallel dialect of C, and the performance and generality of this architecture is being studied.

This research effort is closely tied to the Blue CHiP project, which is a research project headed by L. Snyder of the University of Washington. The goal of the Blue CHiP project is the design and construction of highly parallel computers based on wafer-scale VLSI technology. One current research topic is the relative utility of machines based on circuit-switched processor interconnections with no shared memory. A related question is the ease of use of the Poker programming environment, designed for the future CHiP machine, and its current hardware emulator, Pringle. These questions are being explored through the design of a number of algorithms being programmed through Poker and executed on Pringle.
J. Steven Gibson and I. Gary Rosen

We have been investigating numerical approximation schemes for the closed loop solution of infinite dimensional discrete time linear quadratic regulator problems. Our effort has involved the study of finite dimensional approximations for the resulting discrete time operator Riccati equations and the related convergence questions. Several examples involving a variety of system types (e.g., parabolic, hyperbolic, delay, etc.) are being considered.

David Gottlieb

In collaboration with S. Abarbanel the behaviour of high order methods, in particular spectral methods, when applied to problems that contain shock waves has been studied. These methods yield oscillatory solutions and in the case of spectral methods the oscillations are global. Therefore the point values of the numerical solutions do not approximate well the values of the exact solution. However, we have found that more information is contained in the numerical solution obtained by high order methods than in the one obtained by lower order methods. In fact this information is hidden in the structure of the wiggles. We have shown that in general the numerical method approximate, to a high order accuracy, an oscillatory projection of the exact solution, and therefore must contain wiggles.

As an illustration we simulated a flow around a wedge by the pseudo-spectral Chebyshev method using a $9 \times 9$ grid. By using the structure of the oscillations we locate the shock to a very high accuracy, in fact one would need a grid of at least $1000 \times 1000$ points for a low order finite difference scheme to obtain the same accuracy.

With E. Tadmor a filter that yields accurate point values from a finite Fourier sum of a discontinuous function has been developed. We have shown that those point values can be obtained with spectral accuracy away from shocks.
The calculations of the boundary layer flow over an embedded cavity have been completed and reported. This work is continuing (in collaboration with T. Gatski, LaRC). In particular a series of calculations have been initiated whose purpose is to examine the effect of embedded cavities on separating flow. Also, large scale turbulent structures are being modeled in these flows by using Stuart vortices.

A two-dimensional Navier–Stokes code in elliptic–hyperbolic coordinates has been developed from the two-dimensional velocity-vorticity code in Cartesian coordinates. The new code is being used to calculate the impulsive start-up of a slender elliptic cylinder. The objective of this work is to study the time evolution of the flow past this slender, blunt-nosed body — particularly the development in time of the separation region at the rear of the body, as a function of slenderness ratio and Reynolds number. The results of the calculation will be compared with the predictions of classical boundary layer theory and with those of triple-deck theory. It is also planned to calculate the flow due to the interaction of vortical disturbances in the free stream ahead of the body with the blunt leading edge.

The two-dimensional Navier–Stokes code has also been adapted, with P. Hall, to polar coordinates. The code will be used to study the unsteady separation on a circular cylinder undergoing a harmonic oscillation along a diameter. The code is now being tested — in particular for its phase accuracy — by calculating the flow between concentric cylinders when the outer cylinder is stationary and the inner cylinder rotates harmonically about its axis. This problem was chosen as a test because it has a known exact solution of the unsteady Navier–Stokes equations.

Finally, in collaboration with T. Gatski a three-dimensional Navier–Stokes code in vorticity and velocity variables using compact schemes is under development. A preliminary version of this code is now being tested by calculating the time evolution of the Taylor–Green vortex.
Max D. Gunzburger and Roy A. Nicolaides

Numerical studies of incompressible separated flows are undertaken using codes implementing finite element methods for the Navier-Stokes equations. For the most part, two types of problems are considered. The first is boundary layer flows over irregular obstacles such as ramps, curved ramps, steps, cavities and combinations of these. Here a careful study of the effects of outflow boundary conditions has been carried out. The purpose of the calculation is to study the effects of the various obstacles on separation and hopefully to predict the appearance of transition regions. The calculations will be compared with experiments being conducted by B. Holmes (LaRC). The second project, which is in a preliminary stage, is the calculation of flows around airfoils at high angles of attack. The initial efforts have concentrated on a study of turbulence models which may be incorporated into the finite element codes in an efficient manner. In addition to the above personnel, the project has involved various students at Carnegie-Mellon University.

Philip Hall

The instability of a three-dimensional attachment line boundary layer is being investigated in some work with M. Malik (High Technology Corporation). The linear results presented in ICASE Report No. 84-5 are being extended into the nonlinear regime using perturbation and spectral methods. The purpose of the work is to understand the origin of the large amplitude disturbances which are observed experimentally for this flow. The effect of three-dimensionality of the basic flow on Gortler vortices is being considered; this problem is relevant to instability and transition on swept laminar flow wings. The effect of modulation on the instability of some convection problems is being investigated. A nonparallel flow analysis of crossflow instability is being undertaken in order to understand how boundary layer growth modifies the instability mechanism.
High Reynolds number turbulent shear flows have a great range of temporal and spatial scales. It is almost impossible to simulate them on presently available or projected future computers. Large eddy simulation (LES) provides a viable alternative. This is based on the assumption that the velocity field can be divided into large and small eddies, and the motions of the large eddies are not sensitive to the details of the small eddies (smaller than the grid size of a sufficiently fine mesh). The small eddies are assumed to have a universal character (there is evidence to this effect) and hence to be amenable to small grid scale modelling (SGS). The purpose of the present study (being carried out in collaboration with M. Y. Hussaini and D. Bushnell (LaRC)) is to put the SGS modelling within the framework of classical closures.

It is well known that free stream turbulence, entropy disturbance in tunnel acoustic field, triggers unstable waves in a boundary layer. But the mechanism by which an external disturbance environment enters the boundary layer and the nature of its signature in the perturbed flow are not well understood. The object of the present research effort is to perform controlled numerical experiments to get some insight into these mechanisms. With this purpose in mind, we are constructing an algorithm for VPS-32 for solving three-dimensional Navier-Stokes equations. Among the physical problems we intend to study are: response of a boundary layer to a stationary or moving acoustic wave and a convected array of counter rotating vortices.

The impingement of a shock wave on a boundary layer causes its separation leading to adverse aerodynamic effects. A conventional way of preventing separation is to provide suction at the wall. Recently, D. Bushnell (LaRC) proposed a novel device to prevent shock-induced separation. This device consists of a short control surface placed in the outer portion of the boundary layer (where the momentum is large) in such a way that the shock reflects from this control surface rather than from the wall. The preliminary
computations based on the two-dimensional Navier-Stokes equations confirm the validity of this approach. A detailed parametric study of this problem is underway.

The program of research in hydrodynamic stability and transition to turbulence has continued. Some of the classical problems such as Rayleigh-Benard flow and Taylor-Couette flow are revisited in view of the increased resolution which will be available on the Control Data Corporation VPS-32 computer. The idea is to verify the refined computational results and the bifurcation theory results against one another. Furthermore, a parametric study is being carried out to bring out the effects of various parameters such as heating and suction on the transition processes.

Kazufumi Ito

Research on delay differential equations is continuing. An ICASE report has been completed which describes the use of the Legendre-tau approximation for constructing the optimal feedback solution to linear quadratic regulator problems (LQR). An interesting relationship between the Legendre-tau approximation for delay differential equations and the Pade approximation to the exponential function has been obtained, which may resolve the stability property of Legendre-tau approximation. The advantage of using the dual state-space concept for the LQR problem has been investigated (see ICASE Report No. 82-3). It leads to an alternative numerical method for solving the LQR problem and numerical computations involving Legendre-tau and spline-based approximations are currently being made.

Research has continued (in collaboration with H. T. Banks on the development of computational methods for LQR problems for systems governed by PDEs. Preliminary numerical results for one-dimensional diffusion equations using spline-based finite element and Legendre-tau approximations appear promising. Our main goal is in the development of algorithms to design a finite-order compensator for distributed parameter systems. The study also involves development of efficient algorithms to solve the algebraic Riccati equation.
An iterative method for solving systems of indefinite linear equations has been developed. An ICASE report describing the method has been completed. The method involves the successive use of a modified version of the conjugate (or minimal residual method). The application of the method for solving elliptic and Helmholtz equations is being investigated.

David A. Kopriva

A method has been devised for patching together two (or more) Chebyshev grids so that increased resolution can be obtained in different parts of a hyperbolic flow. Numerical tests have been performed which indicate that with the very simple procedure spectral accuracy can be retained. Work is continuing to study the stability and range of applicability of the method.

Development of a spectral collocation code to compute two-dimensional shock-fitted flows over bodies is continuing. Shock-fitting and shock detection algorithms have been tested for both the two-dimensional code and a one-dimensional nozzle problem. The mesh patching strategy above will be incorporated into the final code. The program will be used to perform benchmark calculations against which finite difference solutions will be compared.

William D. Lakin

Integrating matrices have been shown to form the basis of a fast efficient numerical technique for the solution of vibration and buckling problems associated with rotating flexible beams such as propeller blades. However, the method has previously been limited to equations in one-space variable for cantilevered beams. The present work has extended the technique to beams with more general boundary conditions by employing both integrating and differentiating matrices on non-uniform grids which include near-boundary points. A generalization to problems in two-space variables has also been accomplished, and the free vibrations of a simply-supported rectangular plate are being examined as a test case.
Patricia Daniel Lamm

We have continued our efforts (in collaboration with E. Armstrong (LaRC) and H. T. Banks) on the problem of estimating spatially varying parameters appearing in static models for the surface of the maypole hoop/column antenna. Our work has involved the further development and testing of software packages that approximate both the surface shape and functional parameters representing elastic properties of the surface.

We have also carried out theoretical and computational investigations into the problem of estimating discontinuous coefficients in parabolic distributed systems. This work, partly motivated by reservoir engineering problems, uses linear and cubic spline approximations to estimate state variables and unknown coefficients. A desirable feature of the resulting algorithm involves the ease with which both the functional shape and points of discontinuity in the coefficients are estimated. These ideas are currently being extended to hyperbolic distributed systems.

Mala Mehrotra and John Van Rosendale

Tree searching is a fundamental computer science technique with applications in computer game-playing, robotics, combinatorial optimization and numerical analysis. Our research focuses on the problem of mapping tree searching algorithms to highly parallel architectures consisting of a thousand or more microprocessors. Though tree searching algorithms have a great deal of parallelism, it can be difficult to exploit on such highly parallel, loosely coupled machines. Among the issues currently being addressed are:

1. The amount of interprocessor communication necessary to achieve a balance load distribution.

2. Alternate approaches to imbedding tree searching in loosely connected processor arrays, and the effect they have on performance.

3. Alternate network topologies, including the use of packet switched interconnection networks.
A microprocessor simulator written by D. Gannon and executing a parallel dialect of the C language is being used to address these issues, and a number of practical tree traversal algorithms are being studied.

Piyush Mehrotra and John Van Rosendale

Software technology lags behind hardware technology in many areas, including parallel computing. The most common approach to parallel programming is to supplement current languages with parallel constructs, such as message passing primitives. Other approaches include "borrowing" high level systems programming primitives, such as monitors, to express parallelism, and the data flow approach, in which specialized architectures implement novel functional languages. Each of the above approaches has its advantages and disadvantages.

In our research we are investigating the use of dataflow at the function level to express parallel algorithms. Using functional procedure calls allows the user to specify his algorithm without having to worry about the particular communication constructs implemented in hardware. There are several unresolved research issues here, such as whether the system can efficiently schedule tasks, which we are currently exploring. Current research is aimed at answering such questions and also at finding a natural syntax for this type of language.

Piyush Mehrotra

Many data bases and dictionary systems use B*-trees as the underlying data structure. In a multi-user or a multiprocessor environment, these data structures need to be manipulated concurrently. Algorithms for concurrent retrieval, insertion and deletion of records from B*-trees were investigated. The algorithms were shown to be free from deadlock and starvation while performing the operations in a manner which preserved the integrity of the data structure.
A model of a general class of asynchronous, iterative solution methods for random, sparse linear systems is being developed. In the model, the system is solved by creating several cooperating tasks that each compute a portion of the solution vector. A data transfer model predicting both the probability that data must be transferred between two tasks and the amount of data to be transferred is included. This model is used to derive an execution time model for predicting parallel execution time and an optimal number of tasks given the dimension and sparsity of the coefficient matrix and the costs of computation, synchronization, and communication.

The suitability of different parallel architectures for solving randomly sparse linear systems is being considered. Based on the complexity of task scheduling, one parallel architecture, based on a broadcast bus, is being developed and analyzed.

Timothy N. Phillips

Research on the application of the spectral multigrid method to elliptic problems has continued. In joint work with M. Y. Hussaini and T. Zang (LaRC), investigations are in progress to compare various relaxation schemes for spectral discretizations of equations possessing a variety of boundary conditions.

In preliminary work on fibre-reinforced composite materials with M. Rose the coefficients in the stress-strain relationship were determined for an arbitrary orientation of the material fibres.

Research (in collaboration with M. Hafez (Computer Dynamics, Inc.)) is underway in the following areas:

1. Modified least squares for a system of first-order equations. This technique is used to obtain second-order equations in terms of auxiliary variables similar to potential and stream functions. The additional boundary conditions are determined and numerical results are presented for the Cauchy-Riemann equations. Details will appear in a forthcoming ICASE report.
2. Conservative calculations of nonisentropic flows using a potential function and correcting for the entropy generated by the shock. The flow is assumed to be irrotational and the model is a good approximation to the Euler equations provided that the vorticity due to the shock curvature is small.

3. Preconditioning techniques for periodic problems. Incompressible lifting flows are used as a test case for examining the effect of including the periodicity in the preconditioning matrix. For subsonic flows the minimal residual method is used. Extension to transonic flows is intended, as well as simulation of flows inside a wind tunnel.

Terrence W. Pratt

The programming of scientific and engineering problems for MIMD parallel computers is hampered by the lack of suitable programming environments. In particular, it is desirable to experiment with programming complete codes involving parallel algorithms. Performance comparisons for the same programs running on a variety of parallel machine architectures are particularly desirable, given the range of architectures that are presently under construction or proposed.

Efforts have begun to construct an appropriate parallel programming environment. The base programming language will be Fortran 77, extended to include parallel constructs. Initially the system will be implemented under UNIX on the ICASE VAX-750, with the intention of moving the implementation to a parallel machine when one becomes available at LaRC. The system is known by the acronym PISCES (Parallel Implementation of Scientific Computing EnvironmentS).

The Pisces design is based on a formally specified "virtual machine." The virtual machine provides parallel operations of five different "granularities," ranging from vector operations (instruction-level parallelism) to asynchronous tasks that communicate through messages. The new statements and declarations in Pisces Fortran provide access to the various
capabilities of the Pisces virtual machine. Each implementation of the virtual machine on a particular parallel architecture is expected to directly provide parallel operation at one or more of the granularity levels and simulate the other levels with ordinary sequential execution. Thus the same program may be run on several different implementations without major change in the code, but with potentially major performance differences due to differences in the underlying parallel architecture. By using Fortran as the base sequential language, the sequential parts of many programs may be carried over intact into the parallel environment without reprogramming.

Milton E. Rose

A general approach to finite volume methods for both stationary and time-dependent partial differential equation is being developed. For rectangular volumes the method produces the types of compact finite difference schemes treated earlier. It is believed that the approach can provide a computationally efficient alternative to certain finite element methods.

Nancy E. Shoemaker

The winter of 1983-84 saw a few changes in the computing environment at ICASE. We installed Macsyma from Symbolics, Inc., and Emacs from UniPress as software packages on the VAX. After identifying some problems that were corrected with new EPROM's, Jim Stanley worked on software to allow the use of the Anadex printer as an output device for documents prepared with nroff and neqsn. Some local software was modified to account for the transition in the Langley switching system from TRAN to MICOM.

A relatively minor addition to the hardware (an auto dialing modem) made a large change in the environment, since it connected the ICASE VAX to the dial-up network of UNIX machines. The University of Virginia (uvacs) is used as the link for news and there are mail-only connections with Purdue University, the University of Illinois (uiucdc), NASA Ames, and AT&T Technology Center.
A restricted VAX account was established for the Langley Artificial Intelligence group to give them access to the network news on AI. Preliminary work was done to investigate the feasibility of linking the UNIX mail system to the RAS mail system running on the Cybers. Implementation of such a link was deferred pending improvements in the general communications between the VAX and the Cybers. After a canvas of VAX users at NASA found little general interest in CSNET, ICASE applied for membership in CSNET at a reduced annual fee.

Experiments have been performed to test the feasibility of using the VAX as a front end processor for the VPS/32 (the upgraded CY-200 to be installed at Langley in the second half of 1984). Working with Jay Lambiotte (LaRC), a UNIX command, 200ftn, was developed that shipped a VAX file (of Cyber 200 Fortran statements) to the CY-203 for compilation and returned the listing to the VAX. After seeing the results of an experiment in executing this 200ftn command, the CY-200 System Enhancement Working Group recommended that "pseudo-interactive" access to the VPS/32 be recognized as a valid access method and be considered as decisions are made in tuning the new system. As the transition is made to the VPS/32, further work will be done to use the available UNIX utilities to build tools to simplify ICASE's interaction with the VPS/32 so that they can use both the rich interactive environment of the VAX and the vast computational power of the VPS/32.

Sivaguru S. Srintharan

The grid generation method of J. Thompson, F. Thames, and W. Mastin for two-dimensional multiply connected bodies, the Gaussian Method of three-dimensional grid generation by Warsi, and the grid generation problem in certain analytic surfaces can be studied from a unified point of view by considering certain harmonic mapping problems on an analytic Riemannian manifold. This project is in collaboration with P. Smith (Old Dominion University) and a preliminary version of the theory is reported in ICASE Report No. 84-12.
The plausibility of developing a code to compute incompressible unsteady fluid motion in a bounded but arbitrary domain is being studied in collaboration with A. Hassan (Arizona State University). A finite difference formulation of the fractional step type (related to the methods of A. Chorin and R. Temam) is being considered for the equations in primitive variables. Efficient ways to handle various geometrical terms in order to save time and storage are being investigated.

The invariant manifold theory relates the finite dimensional dynamical systems theory to infinite dimensional systems. A numerical method is being developed to compute invariant manifolds in Navier-Stokes equations. Group representation theory is employed to obtain computational efficiency for domains with certain group symmetry.

Hillel Tal-Ezer

Spectral methods have become a very useful and efficient tool for solving hyperbolic and parabolic problems. Stability analysis for nonperiodic problems results in a very severe restriction on the size of the time step. $\Delta t$ has to be proportional to $N^{-2}$ (N is the space resolution) in order to get a stable scheme. In our research we try to overcome this drawback. Using results obtained by M. Dubiner (Tel-Aviv University) it is possible to produce schemes with much improved $\Delta t$. $\Delta t$ has to be proportional to $N^{-11/9}$ in order to have stability.

Eli Turkel

Work has continued on investigating the properties of the Runge-Kutta time stepping scheme for solving the Euler equations. The enthalpy damping is being analyzed to determine why and how it accelerates the convergence to a steady state, both for the standard scheme and for multigrid versions. The
effect of mesh stretching and grid generation on the accuracy of solutions is also being investigated.

This basic work is being extended in two directions. In collaboration with B. van Leer, the central differences together with the artificial viscosity have been replaced by flux vector splitting. Both a standard Runge-Kutta scheme and a multigrid version are currently working. Comparisons are being conducted for a range of cases. A paper has been accepted by the Ninth International Conference on Numerical Methods in Fluid Dynamics. A second generalization has been to include a thin layer Navier-Stokes model. This work has been done together with C. Swanson (LaRC) and V. Vatsa (LaRC). Both laminar and turbulent flows over a flat plate and a NACA-0012 are being computed. Special attention is being paid to factors affecting the accuracy of the steady state solution.

Other work is being continued on ways of preconditioning the Euler equations. This speeds up the convergence to a steady state and is scheme independent. For highly subsonic flow one can make the time step independent of the speed of sound. Generalizations to incompressible flow are also being considered. Another application is to supersonic flow where an appropriate time step can be chosen for each equation by diagonalizing the system. A paper has been accepted by the Ninth International Conference on Numerical Methods in Fluid Dynamics.

There has also been work on the ongoing project on efficient methods to solve the Helmholtz equation. This has been a continuing effort with A. Bayliss and C. Goldstein (Brookhaven National Laboratory). A code has been developed that can be used for waveguides or underwater acoustics. A paper is being prepared for a conference in underwater acoustics. In addition, a preconditioner based on a partial multigrid solution to a Laplacian has been introduced in collaboration with J. Gozani (Tel-Aviv University) and A. Nachson (Tel-Aviv University). This work will appear in the proceedings of the Fourth IMACS Conference. A heuristic analysis of why this works is being studied with A. Bayliss and C. Goldstein and is incorporated in a forthcoming ICASE report.
Robert G. Voigt

Preparation of an extensive review of the state of parallel numerical algorithms for partial differential equations has continued in collaboration with J. Ortega. The work will include an overview of the architectural issues of parallel and vector computers that influence algorithm performance. Both direct and iterative techniques are considered along with an indication of the kinds of applications that have been addressed. An extensive bibliography will also be included.

Another effort with J. Oliger involves studying the nature of high performance scientific computing. This involves many stages and disciplines: problem definition—engineering and the sciences; mathematical formulation—engineering, the sciences and applied mathematics; discretization and algorithm formulation—numerical and algorithmic analysis; algorithm description and implementation—computer languages and systems; execution of the calculation—computer hardware; and interpretation of the results—data base management graphics, etc. A central theme is that synergism between these phases and disciplines is necessary to produce a computational environment which will be easily used, take advantage of modern technology exploit parallelism to a high degree, and take advantage of sophisticated efficient algorithms. Several other researchers have been asked to write on various aspects of the process and the result is intended as a volume in the SIAM Frontiers of Applied Mathematics series.

The theory of spectral methods for time dependent partial differential equations is reviewed. When the domain is periodic Fourier methods are presented while for nonperiodic problems both Chebyshev and Legendre methods are discussed. The theory is presented for both hyperbolic and parabolic systems using both Galerkin and collocation procedures. While most of the review considers problems with constant coefficients the extension to nonlinear problems is also discussed. Some results for problems with shocks are presented.


We consider the centrifugal instability of the viscous fluid flow between concentric circular cylinders in the small gap limit. The amplitude of the Taylor vortex is allowed to depend on a slow time variable, a slow axial variable, and the polar angle. It is shown that the amplitude of the vortex cannot in general be described by a single amplitude equation. However, if the axial variations are periodic a single amplitude equation can be derived. In the absence of any slow axial variations it is shown that a Taylor vortex remains stable to wavy vortex perturbations. Furthermore, in this situation, stable non-axisymmetric modes can occur but do not bifurcate from the Taylor vortex state. The stability of these modes is shown to be governed by a modified form of the Eckhaus criterion.


In this paper we describe some of the considerations that went into the design of the Finite Element Machine, a research asynchronous parallel computer under development at the NASA Langley Research Center. The
present status of the system is also discussed along with some indication of the type of results that have been obtained to date.


The eigenvalue problem for the linear stability of Couette flow between rotating concentric cylinders to axisymmetric disturbances is considered. It is shown by numerical calculations and by formal perturbation methods that when the outer cylinder is at rest there exist complex eigenvalues corresponding to oscillatory damped disturbances. The structure of the first few eigenvalues in the spectrum is discussed. The results do not contradict the "principle of exchange of stabilities"; namely, for a fixed axial wavenumber the first mode to become unstable as the speed of the inner cylinder is increased is nonoscillatory as the stability boundary is crossed.


A conceptual model for parallel computations on large arrays is developed in this paper. The model provides a set of language concepts appropriate for processing arrays which are generally too large to fit in the primary memories of a multiprocessor system. The semantic model is used to represent arrays on a concurrent architecture in such a way that the performance realities inherent in the distributed storage and processing can be adequately represented. An implementation of the large array concept as an Ada package is also described.


A design technique is proposed for linear regulators in which a feedback controller of fixed structure is chosen to minimize an integral quadratic objective function subject to the satisfaction of integral quadratic constraint functions. Application of a nonlinear programming algorithm to this mathematically tractable formulation results in an efficient and useful computer-aided design tool. Particular attention is paid to computational efficiency and various recommendations are made.
Two design examples illustrate the flexibility of the approach and highlight the special insight afforded to the designer.


First- and second-order explicit difference schemes are derived for a three-dimensional hyperbolic system of conservation laws, without recourse to dimensional factorization. All schemes are upwind biased and optimally stable.


This paper derives the three-dimensional lambda-formulation equations for a general orthogonal curvilinear coordinate system and provides various block-explicit and block-implicit methods for solving them, numerically. Three model problems, characterized by subsonic, supersonic and transonic flow conditions, are used to assess the reliability and compare the efficiency of the proposed methods.


A mathematical model has been developed for spinning mode acoustic radiation from a thick wall duct without flow. This model is based on a series of experiments (with and without flow) conducted by Richard Silcox [Silcox] of the Noise Control Branch at Langley Research Center. In these experiments a nearly pure azimuthal spinning mode was isolated and then reflection coefficients and far field pressure (amplitude and phase) were measured. In our model the governing boundary value problem for the Helmholtz equation is first converted into an integral equation for the unknown acoustic pressure over a disk, S1, near the mouth of the duct and over the exterior surface, S2, of the duct. Assuming a pure azimuthal mode excitation, the azimuthal dependence is integrated out which yields an integral equation over the generator C1 of S1 and the generator C2.
of S2 (see Figure 2). We approximate the sound pressure on C1 by a truncated modal expansion of the interior acoustic pressure. We use piecewise linear spline approximation on C2. We collocate at the knots of the spline and at zeros of the first term excluded in the truncated modal expansion. Finally, we compare numerical and experimental results.


In this paper we consider acoustic shock waves in a variable area duct which contains near sonic flows. The problem we treat here is modelled after an aeroengine inlet. It is known experimentally that area variation of a duct and high Mach number mean flow can reduce acoustical energy yielding substantial noise reduction. One possible reason for this is acoustic shocks. We describe the use of an explicit numerical method which is very accurate and also captures shocks reasonably well. Comparisons of the results are made with an existing asymptotic theory for Mach numbers close to unity. When shock occurs reduction of sound pressure levels are shown by examples.


The numerical solution of the laminar boundary-layer flow over an embedded cavity is studied. The purpose of the study is to examine the relevant drag characteristics of laminar cavity flow. The solution field is obtained in terms of velocity and vorticity variables, with the stream function and pressure derivable from the directly computed variables. An analysis and comparison is made among four square cavities, ranging in size from 0.25 to 1.00 boundary-layer thicknesses deep. The dominant flow features are examined in the vicinity of the cavity by means of the stream function and iso-vorticity contours. The dominant physics in the overall drag characteristics of the flow is examined by an analysis of the pressure and wall shear stress distributions in the cavity, and upstream and downstream of the cavity. Pressure forces and frictional forces in, and in the vicinity of, the cavity are determined. Stress relaxation distances, both upstream and downstream of the cavity, are calculated and analyzed. The flow dynamics of the boundary-layer flow over an embedded cavity is summarized. Finally, the relevance of the present results to the control of flow separation in such flows is discussed.

An overview of some of the recent major developments in the theory and applications of pseudospectral method is provided. The article is divided into two parts - theory and application to Fluid Dynamics. The part on theory summarizes the results pertaining to the basic principles of pseudospectral methods, their implementation and the relevant error estimates. The part on applications is divided into two sections - incompressible and compressible flows. The section on incompressible flows is confined to the simulation of stability transition and turbulence by spectral methods. The compressible flows section presents a fairly up-to-date review of spectral methods as applied to Potential and Euler equations. The last subsection discusses briefly a spectral algorithm for compressible Navier-Stokes equations.


A model for the execution time of parallel algorithms on processor arrays is described. The model is validated for the conjugate gradient algorithm on the eight processor Finite Element Machine at NASA Langley Research Center. Model predictions are also included for this algorithm on a larger array as the number of processors and system parameters are varied.


A compact difference scheme is described for treating the first-order system of PDE's which describe the equilibrium equations of an elastic body. An algebraic simplification enables the solution to be obtained by standard direct or iterative techniques.

Spectral methods for compressible flows are introduced in relation to finite difference and finite element techniques within the framework of the method of weighted residuals. Current spectral collocation methods are put in historical context. The basic concepts of Fourier spectral collocation methods are provided. Filtering strategies for shock-capturing approaches are also presented. Fourier shock capturing techniques are evaluated using a one-dimensional, periodic astrophysical "nozzle" problem.


The Chebyshev spectral collocation method for the Euler gas-dynamic equations is described. It is used with shock fitting to compute several two-dimensional gas-dynamic flows. Examples include a shock/acoustic wave interaction, a shock/vortex interaction, and the classical blunt body problem. With shock fitting, the spectral method has a clear advantage over second order finite differences in that equivalent accuracy can be obtained with far fewer grid points.


The instability of an infinite swept attachment line boundary layer is considered in the linear regime. The basic three-dimensional flow is shown to be susceptible to travelling wave disturbances which propagate along the attachment line. The effect of suction on the instability is discussed and the results suggest that the attachment line boundary layer on a swept wing can be significantly stabilized by extremely small amounts of suction. The results obtained are in excellent agreement with the available experimental observations.


It has been realized recently that in order to have a high level of maneuverability, supersonic delta wings should have a cross flow that is free of embedded shock waves. The conical cross flow sonic surface differs from that of plane transonic flow in many aspects. Well-known properties such as the monotone law are not true for conical cross flow.
sonic surfaces. Using a local analysis of the cross flow sonic line, relevant conditions for smooth cross flow are obtained. Using a technique to artificially construct a smooth sonic surface and an efficient numerical method to calculate the flow field, cones with smooth cross flow are obtained.


We present spline-based techniques for estimating spatially varying parameters that appear in parabolic distributed systems (typical of those found in reservoir simulation problems). In particular, we discuss the problem of determining discontinuous coefficients, estimating both the functional shape and points of discontinuity for such parameters. In addition, our ideas may also be applied to problems with unknown initial conditions and unknown parameters appearing in terms representing external forces. Convergence results and a summary of numerical performance of the resulting algorithms are given.


A pseudospectral numerical scheme for solving linear, periodic, hyperbolic problems is described. It has infinite accuracy both in time and in space. The high accuracy in time is achieved without increasing the computational work and memory space which is needed for a regular, one step explicit scheme. The algorithm is shown to be optimal in the sense that among all the explicit algorithms of a certain class it requires the least amount of work to achieve a certain given resolution. The class of algorithms referred to consists of all explicit schemes which may be represented as a polynomial in the spatial operator.

Wong, Yau Shu: Newton-like-minimal residual methods applied to transonic flow calculations, ICASE Report No. 84-9, February 16, 1984, 32 pages. To appear in AIAA J.

A new computational technique for the solution of the full potential equation is presented. The method consists of outer and inner iterations. The outer iterate is based on a Newton like algorithm, and a preconditioned Minimal Residual method is used to seek an approximate solution of the system of linear equations arising at each inner
iterate. The present iterative scheme is formulated so that the uncertainties and difficulties associated with many iterative techniques, namely the requirements of acceleration parameters and the treatment of additional boundary conditions for the intermediate variables, are eliminated. Numerical experiments based on the new method for transonic potential flows around NACA 0012 airfoil at different Mach numbers and different angles of attack are presented, and these results are compared with those obtained by the Approximate Factorization technique. Extension to three-dimensional flow calculations and application in finite element methods for fluid dynamics problems by the present method are also discussed.


Semi-discrete generalizations of the second order extension of Godunov's scheme, known as the MUSCL scheme, are constructed, starting with any three point "P" scheme. They are used to approximate scalar conservation laws in one space dimension. For convex conservation laws, each member of a wide class is proven to be a convergent approximation to the correct physical solution. Comparison with another class of high resolution convergent schemes is made.

**Trefethen, Lloyd N.:** Stability of finite difference models containing two boundaries or interfaces, ICASE Report No. 84-11, March 18, 1984, 46 pages. Submitted to Math. Comp.

It is known that the stability of finite difference models of hyperbolic initial boundary value problems is connected with the propagation and reflection of parasitic waves. Here the waves point of view is applied to models containing two boundaries or interfaces, where repeated reflection of trapped wave packets is a potential new source of instability. Our analysis accounts for various known instability phenomena in a unified way and leads to several new results, three of which are as follows. (1) Dissipativity does not ensure stability when three or more formulas are concatenated at a boundary or internal interface. (2) Algebraic "GKS instabilities" can be converted by a second boundary to exponential instabilities only when an infinite numerical reflection coefficient is present. (3) "GKS-stability" and "P-stability" can be established in certain problems by showing that all numerical reflection coefficients have modulus less than 1.

Harmonic grid generation methods for multiply connected plane regions and regions on curved surfaces are discussed. In particular, using a general formulation on an analytic Riemannian manifold, it is proved that these mappings are globally one-to-one and onto.
ICASE co-sponsored the 1983 SIAM meeting in Norfolk, VA in November 1983. This three day meeting focused on computational aerodynamics, parameter estimation and control, and parallel processing. A special two day follow-on meeting expanded on the theme of parallel processing. These meetings were attended by over 400 researchers.

In October of 1984 ICASE plans to host a small workshop which will address the various theoretical approaches to studying turbulence.
ICASE STAFF

October 1, 1983 through March 31, 1984

I. ADMINISTRATIVE

Milton E. Rose, Director
Ph.D., Mathematics, New York University, 1953
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Susan B. Ruth, Personnel/Accounting Secretary

Emily N. Todd, Visitor Coordinator/Correspondence Secretary

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C. William Gear, Professor, Department of Computer Science, University of Illinois at Urbana.

Anthony Hearn, Department Head, Department of Information Sciences, Rand Corporation.

Seymour Parter, Professor, Department of Mathematics, University of Wisconsin.
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Herbert E. Keller, Professor, Department of Applied Mathematics, California Institute of Technology.

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VII. CONSULTANTS


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J. Christian Wild - Ph.D., Rutgers University, 1977. Assistant Professor, Department of Computer Science, Old Dominion University. Concurrent Computing Systems.

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Mark H. Dunn - Graduate Student at Old Dominion University. (November 1980 to December 1983)

Mala Mehrotra - Graduate student at the College of William and Mary. (July 1983 to present)

Eiichi Oka - Graduate student at Old Dominion University. (February 1984 to present)

Peter L. Spence - Graduate student at Old Dominion University. (June 1982 to December 1983)

James M. Stanley - Graduate student at the College of William and Mary. (January 1984 to present)
GRADUATE FELLOWS

Hillel Tal-Ezer - Student at Tel-Aviv University, ISRAEL. (January 1984 to March 1984)
ICASE SEMINAR PROGRAM

October 1, 1983 through March 31, 1984

October 11  Dr. Robert J. Gelinas, Science Applications Inc.: Moving Finite Element Methods for the Solution of Large Gradient PDE Problems

October 14  Dr. Christian Klingenberg, Courant Institute of Mathematical Sciences: On the Stability of Triple Deck Flow

October 20  Dr. Paul Concus, Lawrence Berkeley Laboratory: Block Incomplete Cholesky Preconditionings for the Conjugate Gradient Method

October 25  Dr. William E. Pinebrook, Consultant: Optimization Through Evolution

November 16  Professor Farrokh Mistree, University of Houston: Optimization of Large, Complex Structural Systems

November 18  Dr. Mary Hace, Duke University: Data Storage for Supercomputers

November 22  Dr. Loyce Adams and Dr. John Van Rosendale, ICASE: Overview of the HEP- E

November 28  Dr. Ahmed F. Ghoniem, Massachusetts Institute of Technology: Numerical Simulation of Viscous Flow Using Vortex Methods

December 5  Dr. Philip Hall, ICASE: The Instability of a 3 Dimensional Boundary Layer Attachment Flow

December 13  Professor James Geer, State University of New York: Multiple-Time Scale Analysis Using Symbolic Computation

December 20  Professor Sudhakar G. Pandit, Christopher Newport College: Differential and Integral Equations Containing Impulses

January 6  Professor Harry F. Jordan, University of Colorado: Effective Utilization of a Pipelined Multiprocessor

January 11  Dr. Carl Gardner, Bowdoin College: Transition to Turbulence in Cylindrical Couette Flow: Numerical Methods, Stability of Wavy Vortices, and Renormalization Group Methods

January 30  Dr. Roland Glowinski, Institut National De Recherche en Informatique et en Automatique, France: Finite Element Solution of Transonic Flow Problem

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March 14  Mr. Manuel D. Salas, NASA Langley Research Center: Local Stability Analysis for a Planar Shock Wave or What You Don't Know Can Hurt You

March 16  Mr. Thomas J. Bridges, The Pennsylvania State University: Analysis of Forced Transition in a Boundary Layer

March 20  Professor James Hubbard, Massachusetts Institute of Technology: Distributed Parameter Control of Flexible Structures Using Polyvinylidene Fluoride (PVDF)

March 21  Professor Dennis W. Brewer, University of Arkansas: Parameter Estimation and Dependence in Evolution Equations
This report summarizes research conducted at the Institute for Computer Applications in Science and Engineering in applied mathematics, numerical analysis and computer science during the period October 1, 1983 through March 31, 1984.