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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, fluid mechanics, and computer science in order to extend and improve problem-solving capabilities in science and engineering, particularly in the areas of aeronautics and space research.

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

The major categories of the current ICASE research program are:

- Applied and numerical mathematics, including numerical analysis and algorithm development;
- Theoretical and computational research in fluid mechanics in selected areas of interest to LaRC, including acoustics and combustion;
- Experimental research in transition and turbulence and aerodynamics involving LaRC facilities and scientists;
- Computer science.

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 April 1, 1993 through September 30, 1993 is given in the Reports and Abstracts section which follows a brief description of the research in progress.

1Presently, ICASE is operated at NASA Langley Research Center, Hampton, VA, under the National Aeronautics and Space Administration, NASA Contract No. NAS1-19480. In the past, support has been provided by NASA Contract Nos. NAS1-19480, NAS1-18605, NAS1-18107, NAS1-17070, NAS1-17130, NAS1-15810, NAS1-16394, NAS1-14101, and NAS1-14472.
RESEARCH IN PROGRESS

APPLIED AND NUMERICAL MATHEMATICS

Saul Abarbanel

We have continued to explore issues connected with long time integration. One of these is the time advancement of systems of hyperbolic partial differential equations via high order Runge-Kutta algorithms. Typically if the R-K methods is of, say, fourth order accuracy then there will be four intermediate steps between time level \( t = n\delta \) and \( t + \delta = (n + 1)\delta \). We can designate those “mid-levels” by \( n + \alpha_i, 0 < \alpha_i < 1 \). Suppose the physical problem calls for a boundary condition on, say, \( x = 0 \) of the form \( u(0, t) = g(t) \). Clearly we impose at \( t = \delta \) the condition \( g = g(t) \) and at \( t = t + \delta \) we impose \( g = g(t + \delta) \). The question is what should we impose at \( t + \alpha_i\delta \), so that the overall accuracy of the scheme is preserved. (It is assumed that the approximation to the spatial derivative is at least of the same order of accuracy as the temporal one). The conventional (and natural) procedure is to impose at the \( \alpha_i \)th level the condition \( u(0, t + \alpha_i\delta) = g(t + \alpha_i\delta) \). Here our intuition fails us – this approach degrades the accuracy of the solution to 1st order on near-boundary points and to second order overall.

In an upcoming ICASE report (with D.Gottlieb and M.Carpenter) we delineate the correct, albeit counter-intuitive, procedure for R-K of arbitrary order for systems of linear p.d.e’s with constant coefficients. In the more relevant case of systems of non-linear conservation laws we know how to apply the procedure only up to 3rd order R-K algorithms. Thus for many cases of interest the question of the proper imposition of intermediate levels boundary conditions remains open.

Eyal Arian

A multigrid optimization method is being developed for the infinite dimensional optimal design problem. In this case, the number of parameters, which define the design space, is increasing with grid refinement. This is a flexible framework which allows for a general non smooth solution to the optimization problem. The optimization problem is represented on a set of nested grids with different scales. Each coarse grid problem acts as an approximation for the fine grid optimization problem, and is used to accelerate the fine grid iteration. Lagrange multipliers are introduced and the optimization problem is represented by three sets of equations, i.e. the analysis, adjoint, and design equations. All three equations must be fulfilled by the solution of the optimization problem.
Successful results have been obtained for the small disturbance case. The problem was to calculate Dirichlet values for the $2-D$ Poisson equation solved in a periodic geometry in the $x$-direction and bounded in the $y$-direction, such that the normal derivative of the solution on the boundary will match some desired values. A decrease by an order of magnitude in the residuals of the analysis, adjoint and design equations was achieved within $O(N)$ operations (where $N$ is the number of grid points on the fine grid).

Work is now continued on the aerodynamic shape design problem, in the subsonic regime. In this problem, the unknown is part of the boundary, which defines the physical domain. The problem is to find a shape of the boundary such that some condition on the boundary will be minimized. This work is being done in collaboration with Shlomo Ta'asan.

H. Thomas Banks

In collaboration with Yun Wang (N.C. State University) and D.J. Inman (VPISU) and W.Winfree (Instrument Research Division, LaRC), efforts on development of a nondestructive evaluation (NDE) methodology for testing of materials using piezoceramic sensors and actuators have been initiated. Preliminary results are most promising. An algorithm for reliably determining spatially varying material parameters (mass density, stiffness, internal damping) in elastic structures (beams, plates) from vibration data has been developed and tested on both simulation examples and experimental data. Results demonstrate that accumulated strain data (from piezoceramic patch sensors) can be used as effectively as accelerometer data in determining material parameters. Moreover, the algorithms perform quite well on experimental data obtained using the patches first as an actuator (to produce vibrations) and then as a sensor. Thus a self-exciting, self-sensing "smart" structure can be developed that is capable of NDE analysis. Continuing efforts involve use of these ideas to characterize how damage (cracks, holes, corrosion, delaminations, etc.) is reflected in changes in the material parameters, and how one detects the presence of damage and identifies its location with these methods.

Rama B. Bhat

Plate characteristic functions are obtained by reducing the plate partial differential equation and solving the resulting ordinary differential equation exactly. Iterating this reduction operation, using the Kantorovich method, yields very good estimates for the plate natural frequencies and provides the corresponding mode shapes.

Plate characteristic functions for a plate with all edges supported in some fashion have been obtained. Analysis of a plate with two opposite edges free and the other two edges
supported in some fashion is completed. Presently, plates with two adjacent edges free, thus introducing a corner reaction force at the free corner, are being studied.

The plate characteristic functions for a fully clamped plate are used to study the noise transmission into a rigid-walled rectangular cavity through one flexible face. Since the mode shapes are obtained in terms of products of simple functions, the response evaluation becomes quite easy, involving no huge summations. Results agree very well with those obtained using the Rayleigh-Ritz techniques to evaluate plate response.

Later on, sound emitted by plates will also be studied using plate characteristic functions.

Gerald Browning

In work done in collaboration with H.-O. Kreiss, we found that in previous two dimensional turbulence spindown studies, there was a period of time when the flow was maximal dissipative (spectrum decays as $K^{-3}$ where $K$ is the wave number) and then one where only vortex blobs remained (spectrum decays as $K^{-4}$ or faster). In these studies, the effects of the Coriolis parameter were neglected. The question has been raised as to what effect this parameter will have on the flow, e.g., can it alter the decay of the spectrum at later stages.

To answer the above question, the original turbulence code was rejuvenated and a Coriolis-type term added to the vorticity equation. The term clearly has a substantial impact on the topology of the flow (as it should because it is an $O(1)$ term for the larger scales of motion). These preliminary results will be investigated in a more quantitative manner in the near future.

Kurt Bryan

Work has continued with W.P. Winfree of the Nondestructive Sciences Evaluation Branch, LaRC, on methods for thermal nondestructive evaluation of materials. The recent focus has been on thermal modeling and methods for the testing of interfacial corrosion in composite materials, specifically silicon nitride with embedded silicon carbide fibers. Previous research suggests that the interfacial carbide/nitride thermal properties have a strong effect on the overall thermal behavior of the material, and that the condition of this interface (a thin carbon-rich layer) can be determined effectively by using thermal methods. A mathematical model of the situation has been formulated and a computer program has been developed to solve the resulting three-dimensional partial differential equations in the case for a single isolated fiber. In order to obtain reasonably rapid solutions we will use a boundary integral approach and solve the resulting integral equations by using a spectral Galerkin method. The ultimate goal is to derive an algorithm to solve the inverse problem of recovering an
estimate of interfacial contact resistance and apply the technique to real data. Also, a real
sample of the composite may contain hundreds or thousands of microscopic silicon carbide
fibers, and thus the sample may have a quite complicated internal structure. We are thus
investigating the techniques of homogenization for partial differential equations, which may
considerably simplify the resulting model. Moreover, the program to solve the single fiber
case should be useful in solving the so-called “cell” problem, which arises in homogenization
models. However, the underlying mathematical model of the composite does not fit the
usual assumptions under which one applies homogenization. Resolving this should give rise
to some interesting mathematics.

Work has also continued with Michael Vogelius of Rutgers University and Valdis Liepa
of the Radiation Laboratory at the University of Michigan, Ann Arbor. Previously, an
algorithm was developed for locating multiple cracks in electrical conductors. The algorithm
made use of adaptive applied current patterns in order to provide data which is maximally
sensitive to crack locations. Liepa and students built an apparatus to generate data for
testing the algorithm, and more generally, exploring the practicality of these techniques
and physical principles for nondestructive testing. We used the apparatus to collect data for
testing the algorithm and the sensitivity of this technique. Some forty different configurations
of cracks were tried, with great success. These results were presented at the SIAM annual
meeting and IEEE/URSI meeting in Ann Arbor in June. We are now looking at applying the
techniques of homogenization to the underlying partial differential equation which governs
the electrical conduction in order to simplify the model in the case in which many cracks are
present.

Work was also begun with Lester Caudill of the chemistry department at Princeton on
an approach to solving inverse problems which involve an unknown boundary; that is, part
of the domain on which the partial differential equation holds is unknown. The goal is to
determine this unknown boundary by taking measurements of the solution to the differential
equation on a known portion of the boundary. Our approach attempts to pose the inversion
problem for the unknown surface as a constrained optimization problem in whatever space
the unknown function describing the surface lies. However, the objective functional is not
of the usual fit-to-data least squares type. Instead, we minimize the norm of the function
describing the unknown surface, subject to the constraint that the function give rise to
solutions to the differential equation which agree with finitely many measurements on the
known surface. We are in the process of writing a program to test our ideas.
Wei Cai

We study multi-resolution numerical methods for the simulation of chemically reacting flows, especially the problem of deflagration to detonation (DDT). We have made progress in the following two areas:

First, to compute of cellular structures of 2-D detonation waves, we have constructed and implemented a hybrid high order method for the simulation of 2-D detonation waves. Detailed features of transverse wave structures of the detonation waves with simple one-step chemistry have been obtained for different cases of detonation and channel width parameters. The hybrid method consists of components of spectral element methods, high order ENO finite difference methods, and high order shock tracking methods, all integrated together using domain decomposition technique. The numerical results show the importance of resolving the detonation front without excessive numerical viscosity in order to obtain the correct cellular patterns. Current research is under way to include more realistic chemistry models so that meaningful comparison with experiment results on the cell size of detonation waves can be carried out.

Second, in order to simulate flame acceleration under the influence of turbulence, we have constructed a multi-resolution algorithm, jointly with De. J.Z. Wang, based on a newly developed wavelet collocation method for the initial value boundary problem of nonlinear PDE's. The key component in this collocation method is a so-called "Discrete Wavelet Transform," (DWT) which maps a solution between the physical space and the wavelet coefficient space. The DWT transformation takes only $O(N \log N)$ operations, where $N$ is the total number of unknowns. Thus the nonlinear terms in the PDE can be easily treated in the physical space, and the derivatives of these nonlinear terms then computed in the wavelet space. Wavelet collocation methods have the following advantages: (a) the capability of handling arbitrary non-periodic boundary conditions; (b) the capability of treating general nonlinearity through collocation of the PDE, instead of the Galerkin approximation; (c) flexibility of adaptive meshing in regions where high solution gradients occur, such as in shock waves and turbulent premixed flames; (c) the capability of parallel implementation. In collaboration with Steve Orszag at Princeton, we are applying the wavelet collocation method to simulate turbulent flames and study the effects of turbulence modeling.

Daniele Funaro

During my visit at ICASE in the last two weeks of August, I have been involved in discussions on my recent results concerning the approximation by the spectral collocation method of the incompressible Navier-Stokes equations. The idea is based on a new treatment of the pressure, which allows the elimination of spurious modes and requires no boundary
conditions. Meeting with ICASE visitors is usually very constructive, and I got several ideas for future improvements of the method.

Harry Gingold

We are concerned with the development of computational tools relevant to wave propagation in inhomogeneous media, with specialized applications to acoustics and hydrodynamic stability. A hierarchy of new approximations for solution of the one dimensional wave equation is being developed. In this hierarchy, the (L-G) WKB approximation may be considered as being at the low end, say at the first level of a new hierarchy of approximations. The WKB approximation breaks down at a turning point and at a regular singular point and is not efficient as a computational tool for the one dimensional wave equation with low frequencies, thus leading to many challenges. At the second level of this hierarchy, new asymptotic approximations are proposed which retain the physical significance of incident and reflected waves, and overcome the mentioned shortcomings of the WKB approximation. We are thus relieved from the burden, built in the traditional methods, of matching solutions away from a turning point with solutions at the turning point. In joint work with W.E. Zorumski, NASA acoustics division, the “second level” approximations are utilized to approximate quantities like wave phase and amplitude, reflection and transmission coefficients, intensity, admittance, and impedance. Extension of principles of wave propagation in inhomogeneous media, derived so far for high frequencies, is carried out for low frequencies. In joint work with F. Hu (Old Dominion University) computations of special functions of mathematical physics is carried out as a preliminary step to calculations of eigenfunctions and eigenvalues relevant to acoustics and hydrodynamic stability.

David Gottlieb

We continue to develop an efficient spectral code for numerically solving the time dependent two dimensional Navier-Stokes equations for the interaction of a shock wave with several jets. We also compare the results with a fourth order ENO scheme. In order to justify theoretically the order of accuracy, and to post process the results, we needed more theoretical tools for resolving the Gibbs phenomenon. Together with C.W. Shu, we have shown how to extract, from a given expansion by Fourier, Chebyshev or Legendre functions based on an interval $[-1, 1]$, an exponentially convergent point value of a function in any subinterval in which the original function is analytic. This is being used now to postprocess the spectral simulation of the above problem.

We have also been developing nonlinear Galerkin methods (NLG) for the Chebyshev spectral and pseudo-spectral cases, which are relevant to the analysis of turbulence in nonpe-
periodic domains. In the process, we have proved that the high order Chebyshev and Legendre polynomials are indeed small scale functions.

We have also shown that when one uses time marching techniques, e.g., Runge-Kutta schemes, the intermediate imposition of the inflow boundary conditions leads to the deterioration of the overall accuracy. A remedy has been found for the linear case, and for the nonlinear case up to third order accuracy.

Max Gunzburger

We have studied a variety of flow control and optimization problems. Objectives of the optimization include drag reduction, flow matching, and temperature matching. Controls include boundary value controls, e.g., injection and suction of flow through orifices and heating or cooling of the flow along bounding surfaces, and shape controls, e.g., shape design. We have considered different optimization approaches, including sensitivity derivative and adjoint equation based methods. Algorithmically, we have considered incompressible viscous and compressible inviscid flows. Numerous computational simulations have been carried out, both to test algorithms and to solve interesting problems. We have also carried out a complete analysis of flow optimization problems for the steady state Navier-Stokes equations of incompressible flow. This analysis includes existence theorems for optimal controls and states and for Lagrange multipliers and error estimates for finite element approximations to the optimal states and controls. An outgrowth of this analytical work is an abstract theory of approximation of a certain class of nonlinear optimization problems which may be applied to a variety of settings other than the optimization of flows.

Isaac Harari

In collaboration with Eli Turkel finite difference methods for solving problems of time-harmonic acoustics were developed and analyzed. Multi-dimensional inhomogeneous problems with variable work, possibly discontinuous coefficients were considered, accounting for the effects of employing nonuniform grids. A weighted-average representation was found to be less sensitive to the direction of propagation and transition in wave resolution than the familiar pointwise representation. Further enhancement in method performance was obtained by basing the stencils on a generalized definition of the derivative, reducing spurious dispersion, anisotropy and reflection, and by improving the representation of source terms. The resulting schemes have fourth-order accurate local truncation error on uniform grids and third order in the nonuniform grids. Guidelines for discretization pertaining to grid orientation and resolution were derived.
**Amiram Harten**

My recent work is on adaptive multiresolution schemes for the computation of discontinuous solutions of hyperbolic conservation laws. Starting with the given grid, we consider the cell-averages of the numerical solution for a hierarchy of nested grids which is obtained by diadic coarsening, and compute its equivalent multiresolution representation. This representation provides information about the local regularity of the solution, which is used to obtain data compression and to simplify the computation of the numerical fluxes. The numerical flux of the adaptive scheme is taken to be that of a standard centered scheme, unless it corresponds to an identified discontinuity, in which case it is taken to be that of an essentially non-oscillatory (ENO) scheme. We use the data compression of the solution in order to find out whether the solution is already well resolved at a certain level of refinement, in which case we approximate the local value of the numerical flux by interpolation from its values on the coarser grid. I am currently working on the extension of these adaptive multiresolution schemes to multidimensional problems.

**Graham Horton**

Markov systems generated by computer modeling tools, such as queueing networks, Petri nets, or reliability modeling packages may contain hundreds of thousands of states. The resulting sparse linear systems of equations have a correspondingly large number of unknowns, and must, in general, be solved numerically using an iterative scheme. Typical solvers are the Power, Gauss-Seidel, and SOR methods. All of these methods have the drawback that they may require many iterations to reach a solution, particularly if the system is large, as will often be the case in practice, or when a high degree of accuracy is required. This can lead to unacceptably long computation times.

We have developed a new multi-level solution algorithm for discrete or continuous time steady-state Markov chains which is loosely based on the classical multigrid algorithm for PDEs. The algorithm utilizes a set of recursively coarsened representations of the original Markov system to achieve accelerated convergence. Initial results of numerical experiments show significant reductions in computation time relative to the Gauss-Seidel and SOR algorithms for a variety of test problems. We intend to further develop the algorithm applying it to real-life problems, and incorporating techniques from the classical multigrid field, several of which have already proven to provide significant improvements in performance.

**Angelo Iollo**

A new method for aerodynamic design and optimization, based on the Euler equations, was investigated. The design of a Laval nozzle, assuming inviscid, quasi-one dimensional flow,
was considered, with special emphasis on flows with embedded shocks. The optimization problem consisted of finding a set of design variables, in this case shape parameters, that minimize some cost function; for example, a desired pressure or velocity distribution under some side constraints. The optimization problem was attacked using the adjoint method. The adjoint method introduces a new set of equations and dual variables which are solved together with the flow-field equations. Some properties of these equations were discussed.

These ideas are now applied to a two-dimensional shape optimization problem with moving boundaries. The costate equations for this case have been developed and will be applied to the optimization of an internal flow. This research has been conducted in collaboration with Manuel D. Salas (NASA-LaRC) and Shlomo Ta’asan (ICASE).

Leland Jameson

Research has been conducted in the area of wavelets as basis functions in numerical analysis. The following summarizes the results obtained:

- For periodic boundary conditions and an evenly-spaced grid, it has been proven that the differentiation matrix for a Daubechies-based wavelet basis is accurate to order \(2M\), even though the basis can exactly approximate only polynomials up to degree \(M - 1\). This phenomenon is referred to as superconvergence.

- When the boundary conditions are no longer periodic, the superconvergence is lost at the boundaries. This result holds for the currently available boundary constructions.

- For spline-based wavelet bases, again superconvergence has been proven when the boundary conditions are periodic. When the boundary conditions are no longer periodic, superconvergence is again lost at the boundaries.

- A new numerical method which utilizes the strength of wavelet methods, scale detection, and avoids the possibly insurmountable difficulties involving boundaries and nonlinear terms has been constructed. The method utilizes wavelets to define a grid for finite difference methods. The method differs from a Daubechies-based wavelet method only in the manner in which degrees-of-freedom are added and removed. One works with point values, eliminating a problem with nonlinear terms, and boundaries are treated in the same manner as for finite difference methods. The degrees-of-freedom are added only where needed: at locations where small-scale structure exists. The method has performed very well when applied to Burger’s equation.

The next step in the research is to see how well the new “Wavelet-Optimized, Adaptive Grid, Finite Difference” method works when applied to Euler’s equations.
A.Q.M. Khaliq

Numerical methods, known as "Parallel Time-stepping Methods,", were developed and implemented for parabolic equations in two and three space variables. These methods are based on rational approximations to the exponential function, which have real distinct poles. An attempt was made to have space-time parallelism in order to utilize a maximal number of processors, allowing scalability of the scheme on MIMD machine. The methods were applied on practical problems, e.g. in combustion and in computational fluid dynamics.

David Kopriva

Research continues on the development and application of spectral multidomain methods for the solution of compressible viscous flows. A conforming Chebyshev method in two space dimensions is already implemented. Here, basically, the grid lines must be continuous through interfaces and the subdomain boundaries must match at corners. The method uses a characteristic condition for the advective terms and a penalty method for the viscous terms. It has been applied to boundary layer, nozzle, and blunt body flows. Currently, the blunt body program is being benchmarked against finite difference viscous-shock-layer solutions.

Two extensions of the method are now being considered. The first is to extend the conforming method to three space dimensions. The interface conditions would be applied along planes in this case. The second extension is to allow for non-conforming approximations, where the sizes of the subdomains and the resolution within them are arbitrary. The first phase of this extension would be the development of interface conditions for the heat equation. Conditions for two cases have been derived: The first is the situation where the number of collocation points differs between subdomains. The second, the subdomain refinement case, is the situation where the solution where the subdomains are not required to match at corners.

Dimitri Mavriplis

Work is continuing on the use of unstructured meshes for solving computational fluid dynamics problems in two and three dimensions. A three dimensional unstructured turbulent Navier-Stokes solver has been developed. This has been achieved by adding viscous terms and a field equation turbulence model to the previously developed unstructured Euler solver. A multigrid method which operates on a sequence of non-nested coarse and fine meshes has also been incorporated to accelerate convergence. The code has been validated on a grid of 1.1 million grid points. The code has also been autotasked on the CRAY-YMP-C90, delivering speedups of 13 on 16 processors.
In conjunction with V. Venkatakrishnan, research has also been conducted on the use of agglomeration techniques for unstructured multigrid solvers. In contrast to the non-nested multigrid technique employed in the above work, agglomeration provides an automatic mechanism for generating coarse grid levels from a given fine unstructured grid. The links between agglomeration multigrid and algebraic multigrid are also being investigated. The methodology has been adapted to the solution of Euler and Navier-Stokes flows in two dimensions. This work has resulted in a paper at the 6th Copper Mountain Multigrid Conference in April 1993, entitled “Unstructured Multigrid through Agglomeration,” and a forthcoming paper at the AIAA 32nd Aerospace Sciences Meeting in Reno Nevada in January 1994 entitled “Agglomeration Multigrid for the 3-D Euler Equations.”

In conjunction with Eric Morano, a parallel implementation of a three dimensional unstructured grid Euler solver on the Thinking Machines Corporation CM-5 is being undertaken. A global CMF (Fortran 90-type language) version of the original code has been written, and vendor supplied support functions for data-partitioning and inter-processor communication were employed. This work will be presented at the AIAA 32nd Aerospace Sciences Meeting in Reno Nevada in January 1994.

**Eric Morano**

Computer technology has grown rapidly over the last several years, especially with regards to parallel architectures. Such machines are becoming useful for solving very large computational fluid dynamics problems, such as inviscid and viscous three dimensional flows about complex configurations, using upwards of one million grid points.

Since many different architectures have been developed and are available, efficient solution techniques and software are required which are adapted to the numerical problem and also to the particular machine. There are essentially two requirements: the software must be parallelizable, and in our case, also vectorizable, since each processor of the CM-5 contains vector units (e.g. Jacobi iteration is suitable, but Gauss-Seidel iteration would not be, since it is not inherently vectorizable). Therefore we need to use colored-type algorithms, which are traditionally used for vector architectures such as the CRAY-YMP. Moreover, the algorithm must also be efficient enough, that is must require a minimum number of operations (iterations) to obtain a converged solution. In the case of unstructured meshes, few algorithms satisfy these requirements, and the subject of this research will be to show how an efficient 3-D-Euler solver may be implemented on the CM-5 machine.

The CM-5 architecture can be used as a SIMD/MIMD computer. That means that the different processors (1024 - max) may be allocated to the same function but also to different functions. In the first case, only data are treated as parallel components, while in the
second case the data and functions are different on each processor. On the CM-5 computer, the programmer can access a set of libraries: CM Fortran Utility Library and Connection Machine Scientific Software Library (CMSSL) for CM-Fortran. The first library allows the programmer to "call" subroutines to use, or to produce CM-objects instead of writing lower-level software (CMF_FE_ARRAY_FROM/TO_CM). The second library is related to the use of scientific functions such as the manipulation of CM-arrays: L2 vector/matrix norms, or the gather/scatter operations for sparse matrices, for example, which are often required in unstructured grid computations. There also exist partitioning subroutines which provide a more optimal partition of the mesh, and corresponding gather/scatter routines which take advantage of the resulting data-locality, thus reducing the communication time between processors.

A parallel version (Message Passing) of the original serial software has already been implemented on the Intel iPSC/860 hypercube using the so-called PARTI primitives.

This work, done in collaboration with Dimitri Mavriplis, will result in a paper ("Implementation of a Parallel Unstructured Euler Solver on the CM-5") concerned with the comparison of the different ways to compute on the CM-5, and then with performance comparisons, to be presented at "AIAA 32nd Aerospace Sciences Conference," in Reno, NV, in January 1994.

Timothy Phillips

Research on the development of pseudospectral approximations to fourth order elliptic problems has proceeded. Theoretical error estimates have been derived for a multi-domain model problem. The algorithm has been applied to the Navier-Stokes equations in an L-shaped domain. The usual convergence rates associated with spectral methods are observed.

Work is in progress on the development of stable and efficient time splitting methods for solving transient problems in Newtonian and viscoelastic flow, when spectral methods are used in space. When the same approximation spaces for velocity and pressure are used the spurious modes in the pressure are removed using a singular value decomposition. The extension of this idea to the case of multi-domain problems is currently being investigated. A spectral element method for viscoelastic flows is also being developed at the present time.

Kenneth Powell

The governing equations for ideal magnetohydrodynamics are significantly more complicated than the equations of ideal hydrodynamics. Work has only recently been done on the development of Godunov-type schemes for solving the MHD equations. Previous work, how-
ever, has been on solving the one-dimensional equations, and there is a non-trivial problem in the extension to two or three dimensions, related to the divergence of the magnetic field.

Work carried out at ICASE this year included the derivation of source terms that modify the eigensystem such that two- and three-dimensional problems can be solved without an instability arising due to non-zero divergence of the magnetic field. A code based on this new flux-difference splitting scheme was developed and tested on a rotated shock-tube problem. The results were very promising.

Current work is addressing problems relating to eigenvector scaling issues and the development of a Roe average for the equations of MHD.

James Quirk

Work continued on the development of tools with which to perform large scale simulations of detonation phenomena. Previously, it had been recognized that despite the large computational savings gained from using a sophisticated Adaptive Mesh Refinement (AMR) algorithm it would be necessary to be able to exploit some form of parallel computing environment before realistic simulations could be performed on a regular basis. Working with Ulf R. Hanebutte a parallel AMR algorithm has now been developed, and this work has been written up as an ICASE report. Although this parallel algorithm lacks some of the advanced capabilities of the serial version, it is now used routinely for performing detailed simulations of the reflection process for a detonation wave impinging on a ramp. These simulations are part of a collaborative project with J.E. Shepherd (CALTECH) for predicting the transition: Regular Reflection $\rightarrow$ Mach Reflection. At present there is excellent qualitative agreement between the simulations and experiment. Specifically, numerical soot traces have been generated that reveal the same complex dynamical behaviour as their experimental counterparts. Further work is required to see if a quantitative agreement can also be obtained.

Looking to the future, work is planned to further improve the general capability of the parallel AMR algorithm. Also, it will be demonstrated that this algorithm has broader applications than just detonation flows. However, the existing detonation effort will be consolidated.

Rolf Radespiel

Previous work on the solution of the Euler and Navier-Stokes equations for a calorically perfect gas indicated that the combination of multigrid algorithms and explicit multistage time stepping schemes is effective for both upwind and central-difference spatial discretizations. The convergence rates obtained so far are in the range between 0.9 and 0.99 depending
on the computational mesh and flow conditions. Significant further improvements can only be expected if the stiffness in the discretized equations due to different wave speeds and cell aspect ratio is alleviated. In the high-speed flow regime, the overall robustness of the method becomes an additional issue, in particular, for strong interacting shocks and flows with strong expansions.

The work with R. C. Swanson (NASA) will expand the multigrid approach to high-speed reacting flows. Therefore, we concentrate on the following three focal points; (i) the selection of a suitable spatial discretization scheme, (ii) the treatment of large source terms within the multigrid algorithm used to advance the solution to the steady state, and (iii) preconditioning of the residuals to cluster the speeds of convective and acoustic waves.

The work to select a suitable spatial discretization covers two upwind schemes, as there is little hope that pure central-differencing would predict general shock interaction patterns and shear layers accurately. Starting from flux-difference splitting of the Roe-type, we have now included a flux-vector split scheme based on M.-S. Liou’s AUSM method in our investigations. It was found that flux-vector splitting appears to be more robust at strong shocks and strong expansions. The original AUSM scheme can be modified to yield nonoscillatory pressure distributions over strong shocks. Moreover, a special limiter is required for MUSCL-extrapolation of the velocity components to the cell faces in order to avoid oscillatory solutions where the flow is aligned with the mesh. Initial comparisons of Roe’s scheme and the new flux-vector splitting for high-Reynolds-number transonic flow over an airfoil show an amazing agreement in both accuracy and convergence rates.

The treatment of strong source terms within a multigrid algorithm is studied with a newly developed 1-D code for a reacting hydrogen-air mixture with nine species. Point-implicit treatment of the source terms is used, so that the time step is evaluated using only the fluid dynamics wave speeds. A series of computations are currently being performed.

Preconditioning of the residuals to equalize wave speeds shall be used to enhance wave propagation and to cluster eigenvalues of high-frequency Fourier modes. As a first step, preconditioning is implemented in our 1-D code. This exercise will address the behaviour of the preconditioned difference equations. In contrast to experience published elsewhere, we expect that the flux-difference and flux-vector split schemes should both perform well with preconditioning.

Philip Roe

During my summer visit this year I concentrated on developing the multidimensional version of an “upwind leapfrog” scheme for long range propagation of linear waves. The second-order version of the scheme has been successfully applied to the acoustic equations,
where waves are generated by a divergence operator, to Maxwells equations, where they are generated by a curl operator, and to the elastodynamic equations, where both types of wave arise. In all cases the waves are propagated without dissipation, and with acceptable phase errors on grids that provide about 8 points within the shortest waves of interest. The bicharacteristic form of the governing equations is used in each case, and a particular staggered storage of the variables is employed that matches the number of available equations to the number of unknowns. An empirically derived nonreflecting boundary condition has proved effective in experiments.

I have also worked on the genuinely multidimensional Euler code described in the last Semianual Report. Numerical production of spurious entropy and vorticity are reduced by an order of magnitude in comparison with conventional Euler codes, but convergence is very slow. To understand the problem better a comparison is being made with a related scheme developed by David Sidilkover at the Courant Institute.

Paul E. Saylor

(With Jeff Scroggs) A straightforward implementation of the transonic small disturbance equation is completed. It is a tool for experimenting with various numerical algorithms for the solution of time dependent problems. We have also conducted numerical experiments on physically motivated preconditioners for the diffusion convection equation, work in collaboration with S. Ashby of Lawrence Livermore National Lab. A report is under preparation.

There is recent work of S. Lee (The University of Illinois and Oak Ridge National Lab) on estimates of the departure of normality, a concept due to P. Henrici. This scalar quantity is important for many applications. One is in choosing a stepsize for the reliable use of an iterative method for the solution of the linear systems that arise in time dependent problems. (Lee’s results include this application.) Another use is in estimating the field of values of a matrix, which is a convex region containing the convex hull of the set of eigenvalues. The relation of the field of values to the convex hull is useful in the design of adaptive iterative methods and for estimating the usefulness of eigenvalues in predicting turbulence. The latter application is to be explored further.

Chi-Wang Shu

Jointly with Harold Atkins at NASA Langley, we are investigating stability of initial boundary value problems for high order conservative upwind schemes, which serve as prototypes of ENO schemes with biasing. Both GKS stability and eigenvalue stability are considered. It is found that the usual practice in implementing ENO schemes near the boundary, namely restricting the stencil to within the computational domain for evaluating
the numerical flux, is stable for third through fifth order cases, which are the cases used most often in practice.

Ralph Smith

In collaboration with H.T. Banks (North Carolina State University), work has continued on the development of modeling, parameter estimation and control techniques which can be used for the reduction of interior acoustic pressure levels in structural acoustic systems. In the systems of interest, an interior cavity is separated from an exterior noise field by a flexible structure (a beam, plate or shell). The exterior field causes structural vibrations, which through acoustic/structure interactions, lead to unwanted interior noise. Control is implemented via piezoceramic patches on the structure, which create pure bending moments and/or in-plane strains depending on the patch configuration and manner in which the exciting voltage is applied. The goal of the optimal control problem is to use a periodic LQR theory to determine voltages which affect the structural vibrations in a manner which leads to reduced interior acoustic pressure levels (the structural and acoustic dynamics are fully coupled through pressure and velocity conditions).

Since the last report, work has progressed on three fronts. The first consists of an extension of the linear 2-D techniques (reported earlier) to the nonlinear system which results when fully nonlinear coupling conditions are retained. In extending the control results, several numerical examples were developed which demonstrate the success of the scheme for reducing interior acoustic pressure levels in systems involving multiple frequency excitation (up to 20 frequencies excited), nonsymmetric system excitation, and excitation through periodic fields having modulating amplitudes. Through these examples, the effectiveness of this time domain method was demonstrated for structural acoustic applications, which are difficult if not impossible to treat using frequency domain control techniques. A comprehensive set of numerical examples demonstrating the estimation of physical parameters through data fitting techniques was also compiled, and effective strategies for parameter estimation in structural acoustic systems with experimental data were developed.

These strategies were then applied with structural data obtained in experiments performed in collaboration with Don Brown (Lockheed Engineering and Sciences Corp.), Vern Metcalf (U.S. Army Aviation Research and Technology Office) and Richard Silcox (Acoustics Division, LaRC). In these experiments, the structure consisted of a circular plate which was excited both with an impact hammer and through an applied voltage to the patches. By varying the points of impact, both symmetric and nonsymmetric responses were obtained with data in all cases consisting of accelerometer measurements. This provided an initial experimental verification of the modeling, numerical techniques and parameter esti-
mation methodology for an isolated structure. Currently, the experimental efforts are being extended to include control techniques for the plate as well as parameter estimation and control schemes for the 3-D structural acoustic system of interest.

As a prelude to obtaining experimental results for the 3-D system, the third component of our recent work has centered around the development of software which will be used in the estimation of parameters and calculation of control gains in the 3-D system. Initial numerical examples demonstrating the reduction of interior acoustic noise levels in the 3-D system through an applied optimal voltage have been run, and subsequent numerical tests of the parameter estimation and control methodologies are being developed.

Shlomo Ta'asan

The development of efficient multigrid solvers for constraint optimization problems governed by partial differential equations has continued with research in two directions. The first, which is well developed by now, deals with problems in which the parameter space on which optimization is performed is of finite dimension in the differential formulation of the problem. The methods use relaxation for the parameter space in a multilevel way. Parameters that have a non-smooth effect on the solution are relaxed on fine levels while those of smooth effect are solved for on coarse grids only. The methods use adjoint variables to define a descent direction for the minimization problem. The other direction focuses on problems in which the optimization is over an infinite dimensional parameter space (in the differential level). Similar ideas for the treatment of the different scales in the problems are being used here. Special attention is given to the numerical processes in the vicinity of the boundary, including a new type of analysis to predict the behaviour of different iterative techniques.

The above ideas have been applied in aerodynamics design problems where airfoils are to be calculated to meet certain design requirements; for example, to give the pressure distribution in flow conditions which are closest to a given pressure distribution. The present model for the flow is the transonic full potential equation with a body fitted grid. The shape of the airfoil in these calculations is expressed in terms of a finite number of given shape functions with amplitudes to be found by the design process. Currently, subsonic design problems are being investigated. The goal is to obtain a solution of the optimization problem in a computational cost which is just a few (2-3) times that of the flow solver. At this stage we have been able to show that the design can be done on coarse levels, with essentially optimal convergence rates for fine levels. An effort is being made to reduce the coarse grid work related to the optimization with the hope of getting the desired efficiency in total CPU time. This work is being done jointly with M. D. Salas (Fluid Dynamics Division, LaRC) and G. Kuruvila (Vigyan, Inc.).
In a second research direction, new multigrid solvers for inviscid flow problems have been developed in which the convergence rates are essentially the same as that of the full potential equation. These methods are based on canonical forms of the inviscid equations, in which elliptic and nonelliptic parts of the system are separated. Such representation allow an optimal treatment of the problem. New discretization methods based on these forms have been developed. These discretizations require numerical viscosity only for the non-elliptic part of the system. The resulting schemes are staggered and admit no spurious (or weakly spurious) solutions, even for very small Mach numbers. The schemes are formulated on general grids, structured as well as unstructured, in both two and three dimension. At present, we are focussing on the incompressible and compressible inviscid case, working with body fitted grids in two dimensions. Flow in a nozzle and flow around a cylinder are being studied both for the compressible and incompressible cases.

Another field of study is the efficient treatment of time dependent problems for long integration times. The grids needed for such problems are usually much finer than that needed for spatial resolution. A method for efficiently calculating the time evolution using mainly coarse grids (depending on the spatial resolution only), has been developed. Coarse grids use extra source terms to correct their evolution process, making the solution arbitrarily close to the fine grid solution. These source terms are shown to satisfy certain equations, in general, and are being solved for on the coarse grid along with the main solution. The method referred to as Large Discretization Step (LDS) method yields extremely efficient evolution processes. Experiments with hyperbolic equations with periodic boundary conditions have demonstrated typical efficiencies to be expected. Extensions to general boundary conditions and to the nonlinear case is under development.

Hillel Tal-ezer

Iterative solution for large scale, general linear systems is an intensive area of research. When the relevant matrix is symmetric positive definite, the state-of-the-art is to use pre-conditioned conjugate gradient iteration. The situation is more complicated in the general case. It is customary to develop an iterative algorithm based on spectrum analysis. Recently it was shown that for the general case, spectrum analysis is not enough and one has to consider a larger domain, namely, the pseudo-spectra. As a result of our research, we came to the conclusion that even the pseudo-spectra is not enough. It is possible to have matrices for which pseudo-spectra analysis does not show any fatality while a standard method (e.g. GMRES) stagnates. We show that one has to consider a larger domain which is included in the field of values of the matrix. Another conclusion of our research is that the standard definition of the condition number does not accurately reflect the difficulty of the problem.
It can happen that after transforming the original system to an equivalent one, such that the condition number is increased, the new system will converge much faster than the original one. Hence the term "preconditioning," which means reducing the condition number, is not appropriate. Based on these observations, we have developed a general, highly efficient iterative algorithm.

Saleh Tanveer

In incompressible Euler flows, we (Cowley & Tanveer) found that for a specific initial condition, initial singularities that are incompatible with the equation are transformed at \( t = 0^+ \), as surmised earlier by Tanveer & Speziale (ICASE Report No. 92-54). A numerical algorithm for direct complex plane calculation requiring only \( O(N^3 \log N) \) operation at each time step, where \( N \) is the number of discretization points in one space dimension, has been formulated. This is a generalization of an algorithm that works well for the Hele-Shaw flow (Baker, Siegel & Tanveer, under preparation). Efforts are underway to relate the statistical ensemble of complex singularities to dynamical aspects of cascading processes.

With regards to singularity formation in the 2-D Kelvin-Helmholtz interfacial instability, we (Cowley, Baker, Tanveer & Paige, under preparation) have completed work that shows singularities appearing in the physical domain after a finite time can be traced back to an initial formation of complex singularities at predictable points in the complex spatial plane.

In addition, we (Vasconcelos & Tanveer) have some preliminary results on surface tension driven Stokes flow with a free boundary and buoyancy driven convection in porous medium. We seriously revised and completed the earlier version of our earlier paper on steady convection effects in Bridgman Crystal Growth (ICASE report, to appear).

Eli Turkel

Work has continued on preconditioning methods for both the compressible and incompressible inviscid equations. A general three parameter preconditioning was developed for the incompressible equations that equalizes the wave speeds. It was shown that this preconditioning was equivalent to the pseudo-time method of Viviand. Computations were performed together with Andrea Arnonè. A paper appeared as an ICASE report and also in the Orlando AIAA CFD conference. In collaboration with Van Leer, additional theory was developed for the compressible case. In the past, preconditioning was used mainly to accelerate the convergence to a steady state. Instead we concentrated on using the preconditioning to improve the accuracy of the solution. In particular the convergence of a compressible code to an incompressible code as the Mach number goes to zero was analyzed. Necessary con-
ditions were developed for the preconditioning matrix to allow this convergence. An ICASE report was issued.

In addition work was begun with Rolf Radespiel on an explicit/implicit residual smoother. The original work of Jameson developed an implicit tridiagonal operator that allowed larger time steps with an explicit multi-stage code. This was later extended by Enander to a combination of an explicit and an implicit operator that was more robust than that of Jameson. However, in our tests this did not work that well and, in particular, was useful only for inviscid flows. We developed new parameters that depend on the aspect ratio to allow for extension to viscous flows. The work is still under development.

**Bram van Leer**

The effect of local preconditioning of the Euler equations on the accuracy of upwind difference approximations in the limit of incompressible flow was studied. Together with Eli Turkel he discovered that the preconditioned difference schemes, incorporating the preconditioning matrix in their artificial viscosity coefficients, are consistent with the incompressible Euler equations, and include non-vanishing artificial viscosity terms capable of stabilizing the schemes. The non-preconditioned scheme appears to lead to a central-difference approximation of the incompressible flow equations. This explains some, but not all of the inaccuracies found when computing (almost) incompressible flow with a non-preconditioned method.

**John Van Rosendale**

There are two basic approaches to computation of steady state compressible Euler flows, shock-capturing and shock-fitting. In shock-capturing, one applies a well chosen finite difference scheme everywhere in the flow field, including across the shocks. The alternative is shock-fitting, in which shocks are treated as internal boundaries in the flow field across which one applies the Rankine-Hugoniot jump conditions. Given accurate treatment of these internal boundaries, global solutions of arbitrarily high order of accuracy are possible. However, properly locating shocks can be quite difficult, especially for complex flows with embedded shocks.

In recent work we have developed a moving-mesh adaptive grid algorithm which aligns the mesh with shocks and other discontinuities in the flow field. This “floating shock-fitting” scheme uses triangular elements on an unstructured mesh, coupled with a MUSCL-style cell centered finite-volume discretization. To adapt the mesh, we reconstruct shocks along the edges of the mesh. The reconstructed shock locations are then use to attract neighboring mesh points to shocks. Once two vertices of a triangular element have been attracted to a
shock, the intervening edge lies along the shock as well, effectively fitting the shock on this element.

There are several advantages to this approach to shock fitting. First, no explicit imposition of jump conditions is required; when an edge is aligned with a shock, the finite-volume scheme automatically imposes the proper jump conditions. Second, unlike most shock-fitting schemes, we have a consistent and conservative shock-capturing approximation throughout the computation. Thus even if the shocks are improperly fit, one retains a perfectly adequate shock capturing scheme. Third, the additional cost of this refinement strategy is modest. The principal extra cost is the necessity to recompute the cell volumes and normals at every iteration.

Our focus at the moment is transonic airfoil calculations. Typical cases having only isolated shocks are fairly straightforward, though maintaining the mesh quality of the moving meshes can be complex. We plan eventually to look at multi-element airfoils and other cases where multiple intersecting shocks occur. In such cases, our moving-mesh scheme will properly fit shocks away from shock intersections, but will not resolve points of intersection. However, by combining the present scheme with a conventional mesh enrichment scheme, we should be able to effectively treat intersecting shocks as well.

V. Venkatakrishnan

In collaboration with D.J. Mavriplis, an agglomeration multigrid technique was investigated for the solution of the compressible Euler and Navier-Stokes equations on two- and three-dimensional unstructured grids. This approach is different from earlier approaches wherein a sequence of unnested grids of varying degrees of coarseness is constructed. However, for complex geometries, especially in three dimensions, constructing coarse grids that faithfully represent the complex geometries can be a difficult proposition. Thus it is often desirable to derive the coarse grids directly from a given fine grid.

The coarse grids for use in our multigrid procedure are derived directly from the fine grid through fusion (agglomeration) of control volumes. This agglomeration is accomplished by using a greedy-type frontal algorithm and is done in such a way that the load, which is proportional to the number of edges, goes down by nearly a constant factor (4 in 2-d and 8 in 3-d) when moving from a fine to a coarse grid. The algorithm maintains a priority queue of edges on the front, and the new starting point for the algorithm is picked as the first element in this queue. A variation of the agglomeration algorithm also attempts to control the aspect ratios of the coarse grid control volumes. This version is called the semi-coarsened version and produces more uniform coarse grids. It is expected to be beneficial especially in viscous calculations. The algorithm is a combination of breadth-first and depth-first searches and
is more expensive than the first version. Both the algorithms have been optimized and run in linear time. This has enabled us to agglomerate large three-dimensional grids with over 800,000 grid points in a very reasonable amount of time.

A number of modifications are made to the basic multigrid algorithm as well. For instance, injection is used as the prolongation operator. The boundary conditions for the coarse grids are derived from the fine grids as well. Convergence rates comparable to the original multigrid technique have been obtained. The coarse grids for the more complex configurations do not even have to conform topologically to the fine grid. In fact, the whole agglomeration procedure can be interpreted as merely summing different equations to derive a coarse grid discretization, and hence is very closely related to the algebraic multigrid procedure.

Work is also continuing on the design of a parallel implicit solver for the solution of the compressible Euler equations in two-dimensions. The approach taken here is to solve the linear system that arises at each time by iterative means. The GMRES procedure with a modified block-Jacobi preconditioner is used to solve the linear system. An incomplete LU factorization is used as a preconditioner within each processor and diagonal preconditioning is used for the points on the interface. Vertex-partitioned and a triangle-partitioned schemes are implemented on the Intel iPSC/860. With the above-mentioned choice of the preconditioner, good parallel performance has been obtained with some degradation in convergence as the number of processors increases. Work is in progress to improve the preconditioner at the interface by using a coarse grid to bring to bear some global influence on the preconditioner.

Technical papers on both the topics will be presented at the 32nd Aerospace Sciences Meeting in Reno, Nevada in January 1994.

Hong Zhang

The waveform relaxation method (WR) has been proposed and used as a parallel method for the solution of large ordinary differential systems and time-dependent partial differential equations. It has been proven that the WR iteration always converges superlinearly on any finite time interval. However, for many problems, it converges much faster on short intervals than on longer ones. Thus windowing is generally recommended in practice. In this approach the WR iteration is applied to a sequence of short intervals, called windows, consecutively.

Experimental results revealed that the efficiency of the windowing depends strongly on the problem, in particular, on the stiffness of the ODE solved. I have been investigating the effectiveness of the windowing in WR iterations. Using model problems, the computed estimates for a window of \( \omega \)-convergence have been developed for non-stiff problems. For stiff cases, it has been shown that the convergence rates of WR iteration on any finite interval
is almost identical to that of corresponding static iteration. The windowing does not have any computational advantage if machine features are disregarded. Experiments have been conducted, and the results match our analytic results surprisingly well. Thus this work provides useful guidance in the implementation of the WR method.

In collaboration with Shlomo Ta'asan, the work on the waveform multigrid method for certain type of time-dependent PDEs is continuing. The parallel implementation of the algorithm is also under investigation.
FLUID MECHANICS

Alvin Bayliss

In work done in collaboration with L. Maestrello and J.L. McGreevy, we are studying the role of jet noise in exciting a flexible surface, such as an aircraft panel. We solve the nonlinear Euler equations on both sides of the panel. On one side of the panel the flow field includes the jet flow exiting from a nozzle, while on the other side of the panel we solve the Euler equations without any imposed flow field. We have computed both the panel response and the resulting acoustic radiation into the far field. In addition we have computed instability waves in the jet and have studied the role of the instability waves in exciting the panel. An ICASE report on this work is in preparation.

In work done in collaboration with A. Frendi, L. Maestrello, and J. Robinson, we have studied the problem of plane wave excitation of a flexible panel at or near a resonant frequency. The problem is solved by coupling the nonlinear Euler equations describing the near and far field radiation to an equation for the evolution of the flexible surface. The pressure difference across the surface acts as a source term.

Results in two dimensions were included in ICASE Report No. 92-67. These results demonstrated both linear and nonlinear panel responses, as well as a relative increase in the harmonic content as the acoustic disturbance propagated into the far field. Results for three dimensions have been obtained, including the directivity of the resulting radiation field. An ICASE report describing these results is in preparation.

Stanley Berger

I am continuing my research on vortex breakdown. A recent ICASE report (No. 92-63) discussed reasons why previous numerical simulations of vortex breakdown often resulted in breakdowns which occurred very near or at the first computational cell, causing some critics to question the validity of all these numerical simulations of breakdown. We are now using a multi-grid finite-difference code developed by Kuruvila and Salas to explore breakdown. These simulations are being carried in the context of what we have learned about the sudden incipience of breakdown. We are also interested in using this code to investigate the relationship between spiral and bubble-type breakdowns. We have also been looking at the use of compact finite-difference schemes to carry out direct numerical simulations of breakdown in order to explore the turbulent region which usually appears in the wake of breakdowns, and which has never been modeled.
Fabio Bertolotti

A study of the properties of the equations leading to the PSE formulation was made in spring 93. The results were presented in the ICASE Short-course on Transition to Turbulence held in June 1993. In this work, it was demonstrated that the equations obtained using only the change of variable used in the PSE formulation, but without applying the assumption of slow variation, can capture both transmitted and reflected waves traveling through an inhomogeneous medium. In some cases, it is possible to obtain the complete solution to the boundary-value problem using a marching procedure which marches only once through the domain. To help the reader comprehend the PSE formulation, these equations were compared with those given by WKB theory and the related geometrical acoustics, and with those given by a modified method of variation of parameters. This work will be described in the Short-Course notes to be published by Springer-Verlag.

The study of boundary-layer transition due to detuned modes that was initiated last year in a collaborative effort with Tom Corke at IIT was continued. Runs made using the xPSE toolkit showed that the streamwise location of transition due to detuned modes can lie as close to the leading edge as that caused by subharmonic and fundamental resonances. This result agreed with Corke’s experiments, and further validated Corke’s belief of the importance of detuned modes in natural transition. The experimental result showing higher disturbance growth-rates in the detuned case than the tuned case, however, was show to be caused by the particular way in which detuning was introduced, and sub-harmonic resonances having equally high growth-rates were not considered in the experiment.

A study of transition over a plate having the surface corrugated in the streamwise direction has been completed. The corrugation introduces streamwise vortices into the boundary layer. If concave plate curvature is then applied, these vortices become Görtler vortices. Thus, this study is similar to that of J. Denier, P. Hall, and S. Seddougui (ICASE Report No. 90-31) involving the seeding of Görtler vortices by surface irregularities, but differs in the type of wall geometry: they used a single localized hump, while we used streamwise corrugations that extend from the leading edge to locations far downstream.

In addition, Tollmien-Schlichting waves were introduced using acoustic noise, following the model of J. Crouch. Curvature was shown to affect these waves at the low frequency limit, resulting in neutral-stability curves markedly different from those of the Blasius boundary-layer.
The wave and vortex parameters that led to weak or strong nonlinear interaction were studied. In some cases, the interaction between the vortex and a two-dimensional wave (Bertolotti, 1991 Thesis) was shown to be more energetic than that involving a vortex and two oblique TS-waves (studied by Hall and Smith (ICASE Report No. 89-82)). This work will be presented in an upcoming ICASE report.

Thomas M. Brown, III

Laminar flamelet models that describe combustion as stretched 1-D steady laminar flames are promising as sub-grid models of finite-rate chemistry in turbulent flames. Opposed jet flame burners producing 1-D steady laminar flames have been developed at the University of California San Diego and at NASA Langley Research Center. The UCSD burner developed by K. Seshadri has a high aspect ratio and can be run at extremely low strain rates. The LaRC burner developed by G. L. Pellett (FLMD-Experimental Methods Branch, NASA LaRC) has a low aspect ratio and can be run at higher strain rates. These well controlled laboratory flames are currently being used to validate 1-D flamelet models.

At Vanderbilt University a line Raman system has been developed, capable of instantaneously measuring species and temperature at multiple points through a flame sheet. This system has been used to measure complete temperature and species profiles of H\textsubscript{2}-Air flames in both the large (UCSD) and small (LaRC) aspect ratio opposed jet burners. Measured concentrations of H\textsubscript{2}, O\textsubscript{2}, N\textsubscript{2}, H\textsubscript{2}O and OH along with temperature profiles are currently being compared to flamelet calculations made at Yale University by M.D. Smooke and at University of Missouri, Rolla by K.M. Isaac.

William O. Criminale

Initial-value problems have been explored for a wide variety of prototypical basic flows. As opposed to stability investigations, initial-value problems are designed to answer questions such as (a) early period transient dynamics, (b) effects of arbitrary initial specifications, and (c) determining means whereby flows can be controlled. A means for making such assessments has been established by considering separately vorticity as well as the perturbation velocities. The particular flows that have been examined are (1) stagnation point flow, (2) jets and wakes, (3) vortices, (4) pipe flow, and (5) channel flow. The strength of the analysis allows for closed form solutions and is three dimensional. This work can further be extended to probing of mixing using Lagrangian fluid mechanics.
Andrew Dando

In joint work with N.D. Blackaby and Philip Hall (ICASE Report No. 93-36) we considered the nonlinear evolution of modes on unstable stratified shear layers. As was noted in this paper, the initial motivation for this study was the author's desire to develop a theory to describe the nonlinear evolution of the inviscid Görtler modes initially considered by Bassom and Hall (1991), (Journal of Fluid Mechanics, 232, 647-680), and Dando (1992), (Theoretical and Computational Fluid Dynamics, 3, 253-265). As was pointed out in Blackaby and Choudhari (1993), (Proceedings of the Royal Society London A, 440, 701-710), there is a close connection between the problem of nonlinear evolution of modes on unstable stratified shear layers and the nonlinear evolution of inviscid Görtler modes in three-dimensional boundary layers. It was this that led us to consider the 'model' stratified shear layer problem. We are currently extending the ideas we developed to the more complex Görtler problem, and expect to submit this for publication as an ICASE report in the near future.

Manhar Dhanak

The structure of the stagnation point flow in the presence of weak steady cross-stream vorticity in the external flow was investigated. A specific case of the two-dimensional basic forward stagnation point flow past a circular cylinder was considered with the external three-dimensional vortical disturbance taken to be periodic in the spanwise direction with a wavelength $\lambda^* \leq \lambda^* N = \pi D/(R_D)^{1/2}$, where $D$ is the diameter of the cylinder and $R_D$ is the flow Reynolds number. It was shown that the presence of weak but finite streamwise vorticity of certain preferred values of $\lambda^*$ in the external flow can be supported by the flow in the stagnation zone, leading to a substructure of counter-rotating streamwise eddies in the boundary layer. The magnitude of the streamwise vorticity in the boundary layer is found to be of the same order as that in the external flow if $\lambda^* = \lambda^* N$ but is of a smaller order in the flow Reynolds number if $\lambda^* < \lambda^* N$. The work will be reported in the proceedings of the ICASE workshop.

Peter Duck

The work on the interaction between a shock wave attached to a wedge and small amplitude, unsteady, freestream disturbances (with D. Glen Lasseigne and M. Yousuff Hussaini) has been complete, and is now the subject of an ICASE report which is shortly to be published. This work has now been extended to the case of a shock wave attached to a cone. Here the situation is a good deal more complicated, since the base flow (behind the shock) is much more complicated (the flow is no longer uniform in this region, but rather described by a conically similar solution due to Taylor, in which all flow quantities vary). A computer
code has been developed to compute the disturbed flow, and these solutions are now being used to develop asymptotic theories to describe the nature of the flow far from the cone apex.

Work on the nonlinear excitation of inviscid stationary vortex instabilities in a boundary-layer flow is currently under study (joint with Meelan Choudhari). In this study the main computational problem reduces to the solution of the three-dimensional boundary-layer equations with outer boundary conditions of the streamwise flow approaching a linear profile plus a (prescribed) displacement function. A system of skewed coordinates is being used, which greatly simplifies the computational procedure; a computer code has been developed to study this aspect of the flow.

**Gordon Erlebacher**

Work is still in progress with Chi-Wang Shu (Brown University) on the interaction of a shock with an impinging longitudinal vortex. This work has relevance for the stability of aircraft. The high sensitivity of pressure fluctuations to shock velocities has been established. We are now proceeding with a shock fitted code to better compare results against linear theory.

We recently initiated research into the physics of shock/turbulence interactions. A Von Karman spectrum has been computed and is being input upstream of the shock. This servers as a good validation procedures of the shock fitted code. The final goal of this work is to better understand the behaviour of turbulence as it is processed through a shock. Both algorithmic issues and physical mechanisms are being addressed.

We also participated in ICASE’s transition workshop during the month of June, 1993 and begun work on several projects. With Piomelli, we are performing direct numerical turbulence simulation of turbulent supersonic boundary layers using the temporal assumption. A novel technique is used to insure a quasi-stationary displacement thickness. With Ray Ristorcelli and S. Dinavahi (Analytical Services and Materials, Inc.), we have analyzed some databases of temporal DNS on cylinders and several homogeneous shear databases. The object is to assess the importance of the Reynolds average of the Favre fluctuations, terms which are often neglected in the current Reynolds stress models.

In another project, work with Man Rai and Gatski on the spatial DNS of turbulent supersonic boundary layers is proceeding well. The highest resolution simulations are about to begin. We have already obtained realistic skin friction plots as a function of streamwise distance which match well with experiment.

Finally, I participated in the ICASE Short Course on Transition and gave talks covering direct numerical simulation of transition. Notes are being written for the course.
Michael Gaster

The velocity perturbations induced by a small shallow bump on the surface over which a boundary layer develops has an important influence on the receptivity to additional sound fields present. The sound field couples with the flow distortion to act as sources of periodic excitation that then generate Tollmien-Schlichting waves. The approach used in this investigation is based on the solutions of the linearised perturbation equations appropriate to a parallel mean flow, as have been used to study the flow arising from a vibrating ribbon type of excitation (Gaster and Sen Gupta, 1993). The boundary conditions appropriate to a static bump are modelled by a streamwise velocity perturbation on the wall obtained by expanding the streamfunction close to the boundary. The solution to the problem then arises as a Fourier integral over wavenumber space. It turned out that inversion required a large number of steps of close spacing in wavenumber close to the origin. The calculations went through without any problem and the shapes of the contours of velocity perturbations obtained for a range of boundary layer Reynolds numbers. The results of these computations were found to be close to those for a very low frequency of excitation when the solutions are virtually quasi-steady. The low frequency work is important because the calculations can be verified by experiment. Good comparisons have been made with wind tunnel measurements for such a case. The theoretical work is being extended to cater to three-dimensional forms of excitation and further experimental comparisons are planned.

James F. Geer

Work is continuing on the problem of determining the acoustic field in an inviscid, isentropic fluid generated by a solid body whose surface executes prescribed vibrations in the presence of a prescribed external flow field. The problem is being formulated as a multiple scales perturbation problem involving two “small” parameters, namely, the Mach number $M$ based on the maximum surface velocity, and the Mach number $M_{\infty}$, based on the external, prescribed flow. Thus this work extends some previous work on this topic for the same problem with no mean flow present. Following the idea of multiple scales, new “slow” spatial scales are introduced. These scales are defined as the usual physical spatial scale multiplied by powers of $M$. The governing nonlinear differential equations lead to a sequence of linear problems for the perturbation coefficient functions. It appears that the higher order perturbation functions obtained in this manner will dominate the lower order solutions (as in the case of zero mean flow), unless their dependence on the slow spatial scales is chosen in a certain manner. In particular, it appears that the perturbation functions must satisfy an equation similar to a “convective” Burger’s equation with a slow spatial scale playing the role of the time-like variable. The method has been applied successfully to a simple
A three-step hybrid analysis technique, which successively uses the regular perturbation expansion method, the Padé expansion method, and then a type of Galerkin approximation, is being further developed and studied. Currently, it is being applied to several model problems which develop boundary layers as a certain parameter becomes large. These problems involve ODE's, PDE's, and integral equations. In particular, the technique appears to simulate these boundary layers by producing approximate solutions with singularities which lie just outside the domain of interest. Based on some preliminary results involving simple ODE's and PDE's (which will appear soon in an ICASE report), the technique appears to provide good approximations to the solution, even when the perturbation and Padé approximations fail to do so. Currently, the technique is also being applied to and studied in the context of some ODE's and elliptic PDE's which develop internal layers, as well as boundary layers, and also to two classes of integral equations of the first kind which arise in slender body theory.

Work is also continuing on another new technique, temporarily called the “flexible singularity expansion technique.” This technique is being developed to determine a family of approximate solutions, based on a small parameter ε, to certain classes of linear and nonlinear exterior boundary value problems. These solutions are expressed in terms of singular solutions to the governing differential equation, but with the singularities lying outside the region of interest. In general, the exact type, location, and strength of these “flexible” singularities are determined by the governing equation and shape of the domain of the problem. More specifically, the various parameters associated with these new singularities are determined by requiring that the “flexible singularity solution” agrees with the perturbation solution to the problem to within a prescribed order in ε as ε → 0. The technique is being applied to several classes of problems involving nonlinear PDE’s and to problems which are geometrically nonlinear.

Work is also continuing on understanding and further developing a new class of approximations $S[N, M]$ to a periodic function $f$ which uses the ideas of Padé approximations based on the Fourier series representation of $f$, rather than on the Taylor series representation of $f$. (Several fundamental results concerning this class of approximations will appear soon in an ICASE report.) Each approximation $S[N, M]$ is the quotient of a trigonometric polynomial of degree $N$ divided by a trigonometric polynomial of degree $M$. The coefficients in these polynomials are determined by requiring that an appropriate number of the Fourier coefficients of $S[N, M]$ agree with those of $f$. Explicit expressions have been derived for these coefficients in terms of the Fourier coefficients of $f$. It has been proven that these “Fourier-
Pade' approximations converge point-wise to \((f(x^+) + f(x^-))/2\) more rapidly (in some cases by a factor of \(1/k^{2M}\)) than the Fourier series partial sums on which they are based. The approximations are being applied to several model functions, and applications to the solution of a variety of initial, boundary-value problems for several classes of PDE's are being explored. In addition, several different ideas are being explored concerning the conjunction of these approximations with certain spectral methods to solve a variety of problems involving PDE's, especially time dependent problems which develop shocks as time increases. In particular, several robust and efficient recursive algorithms are being developed to determine the coefficients in the approximations.

**Sharath S. Girimaji**

Since joining ICASE in the beginning of July I have focussed on two projects. The first, research towards understanding and modeling turbulent reacting flows culminated in an ICASE report 'Simulations of diffusion reaction equations with implications to turbulent combustion modeling' (ICASE Report No. 93-69). In this work, it is first established that the diffusion-reaction system (DRS) has many features in common with the scalar and temperature evolution equations in a turbulent reacting flow. The data from DRS simulations are used to understand the effect of chemical conversion and also to evaluate mixing models.

The second project is an ongoing project (performed in collaboration with Y. Zhou of ICASE) is understand the energy transfer mechanism in Burger's turbulence. A pseudo-spectral code has been developed and high resolution studies are being conducted. The turbulence is maintained statistically stationary by forcing the small wavenumbers. The behavior of the spectrum, inverse energy cascade and triadic interactions are being examined.

**Chester E. Grosch**

During this period I have carried out calculations in order to model the experiments, done with Michael Gaster, of the boundary layer displacement modes. These calculations involve using boundary layer codes as well as a complete time dependent incompressible Navier-Stokes code. The experimental results were analyzed in detail and the results are now being written for publication. I also began a writeup of the theoretical calculations.

**Philip Hall**

Work continued on the receptivity problem for Görtler vortices with particular attention being given to the order one wavelength problem. Further progress on the unsteady critical layer problems for Görtler vortex disturbances in three-dimensional boundary layers was
made. Results on the instability of fluid layers in pipe flows were obtained. A new formulation of strongly nonlinear instabilities in slowly varying flows is being undertaken using a phase equation approach.

Fang Q. Hu

A numerical study on the acoustic and instability waves of a confined two-dimensional jet has been conducted. The confining walls are lined with acoustically treated liners. The application is in the noise reduction schemes for the High Speed Civil Transport (HSCT) project. Two major effects of the lined walls on the propagation properties of the linear waves have been identified. First, the growth rates of the linear instability waves could be reduced when the lined walls were used, as compared to the solid walls. Second, the upstream propagating neutral waves of a free supersonic jet could become attenuated when the jet was confined. This work is to be presented in the 15th AIAA Aeroacoustic Conference.

A second area of work is in the study of time integration methods for spectral discretizations, with applications in Computational Aeroacoustics. In particular, the family of Runge-Kutta schemes has been examined and a class of schemes optimized for low dissipation and dispersion is being proposed.

Thomas L. Jackson

Work continues on flame/vortex interactions, a fundamental problem for the understanding of small scale structures in turbulent reacting flows. We have recently investigated the ignition dynamics when a diffusion flame is embedded in the field of a vortex pair. The model consists of a constant-density, one-step, irreversible Arrhenius reaction between initially un-mixed species occupying adjacent half-planes, which are then allowed to mix and react in the presence of a vortex pair. The evolution in time of the temperature and mass-fraction fields is followed. Emphasis is placed on the ignition time and location as a function of vortex Reynolds number, spacing between the centers of the vortex pair, and initial temperature differences of the reacting species. The study brings out the influence of the vortex pair on the chemical reaction. This work will appear in the proceedings of the summer workshop on Transition, Turbulence and Combustion. In addition, the effect of shear in the streamwise direction on flame/vortex interactions is under investigation, with the velocity field now having a point vortex embedded in it. A combination of asymptotics and numerics will be used to isolate key physical effects for analysis. This work is in collaboration with M. Macaraeg (Fluid Mechanics Division, LaRC) and M.Yousuff Hussaini.

In collaboration with William Criminale (University of Washington) and D.Glenn Lasseigne (Old Dominion University), work is continuing on the evolution of disturbances in
a class of three dimensional flows. An initial value approach is undertaken to investigate
the effect of transients on the evolution of the disturbances. Flow fields of fundamental
importance considered thus far are stagnation flows, jet and wake flows, and vortex flows.

Daniel Joseph

John Nelson (Wright Patterson Air Force Base), Amy Alving (University of Minnesota)
and I worked out a boundary layer theory for the flow of a liquid film on a flat plate driven by
an air stream above. We found a solution that satisfies the Blasius equations in the air and
the water asymptotically for large $x$ values, far down the plate. The free surface ultimately
increases like $x^{1/4}$. We showed that this solution attracts many, possibly all, the nonsimilar
small $x$ solutions. The work was published in ICASE Report No. 93-57, “Boundary Layer
Flow of Air Over Water on a Flat Plate” by Nelson, Alving, and Joseph.

The solution we found is suitable for studying stability properties of water on aircraft in
flight. We are now engaged in such study using the parabolized stability equations (PSE),
with a finite element method, not used before, to solve the equations. Finite difference
approximations can be made to form second derivatives of quantities, but experience has
shown these approximations are poor. In the finite element method, all derivatives higher
than degree one are removed after integration by parts. We are also going to implement an
analysis of the energy of the PSE equations which has not been done before.

Ashwani Kapila

In collaboration with Tom Jackson and James Quirk, studies continue of the manner in
which introduction of small disturbances in an otherwise uniform, reacting environment can
lead to detonations. Through asymptotic analysis, early phases of the evolution process have
been identified and described. Later stages of the process, characterized by large changes in
the state variables, require accurate numerics for a description. However, asymptotics plays a
role there as well, suggesting features to look for in the numerical solution. Work to date has
dealt with small-amplitude pulse disturbances. Further work is planned on large-amplitude
pulses, and on disturbances of other types. Work on detonation failure in environments of
decreasing temperature has also been initiated.

Martin Landahl

The work concerned a new and uniform treatment of transition and turbulence in a
boundary layer. The problem of the fluctuations in a boundary layer was formulated by
considering the nonlinear terms (the “instantaneous Reynolds stresses”) as driving the shear
flow, which was treated as a linear system. The following new and important results came out of this treatment, namely:

- Treatment of the fluctuation field as a linear one, driven by its own nonlinearities, allows a unified treatment of instability, transition, and turbulence.
- The pressure fluctuations serve to communicate the outside flow disturbances down to the viscous wall layer.
- The viscous Stokes' wall layer gives a nonvanishing vertical velocity at large distances, producing coherence of the fluctuating velocities throughout the layer.
- The Reynolds stresses receive their major contribution from components of zero streamwise wave numbers due to algebraic-type instabilities.

The work was presented in a seminar entitled “Transition and turbulence in a boundary layer – a unified approach.” on June 18 to the participants in the transition workshop.

**D. Glenn Lasseigne**

The response of the flow field behind nonreacting and reacting oblique shock waves to rather general but finite disturbances upstream of the shock is being investigated in detail. This work is analytical in nature in that the disturbance fields are written as inverse Fourier Transforms, which are then computed numerically. A wide class of model disturbances are to be investigated and the vorticity, entropy, and pressure disturbances downstream of the shock are to be computed.

In collaboration with William Criminale (University of Washington) and Tom Jackson (ICASE), work is continuing on the evolution of disturbances in a class of three dimensional flows. An initial value approach is undertaken to investigate the effect of transients on the evolution of the disturbances. Flow fields of fundamental importance considered thus far are stagnation flows, jet and wake flows, and vortex flows.

**Anthony Leonard**

The possibility of developing a vortex-like method for compressible flows was considered. Vortex methods have well known advantages for incompressible flows but, heretofore, were not considered good candidates for compressible flows. For example, in one formulation, one must add a transport equation for velocity dilatation and retain the transport equation for density. However, recent advances in fast algorithms and the treatment of viscous effects
in incompressible methods have led us to reconsider what can be and what cannot be done efficiently. Further work is needed.

Geoffrey Lilley

My work at ICASE has continued to assist in the development of the newly created field of Computational Aeroacoustics, and in particular to exploit the growth during the past decade of computational fluid dynamics including the use of DNS (direct numerical simulations) and LES (large eddy simulations) in the modelling of turbulent flow. An essential aspect of my work has been to investigate methods to calibrate new aeroacoustic numerical codes, designed to simulate the radiated noise characteristics from compressible turbulent shear flows, against existing theoretical and semi-empirical models, and against good, reliable experimental data. I have collaborated with Jay Hardin and Lucio Maestrello of the Acoustics Division (LaRC), and many members of the ICASE scientific staff, in addition to the Director, including Stephen Otto, and Jay Webb, and summer visitors, Sutanu Sarkar and Thiery Dubois.

The simplest compressible turbulent flow that can be simulated in numerical calculations is that of a field of decaying isotropic turbulence within a given box in an infinitely periodic domain. Recently Sarkar and Hussaini (1993) completed a direct numerical simulation of this flow at low Mach numbers, and found many characteristics of the radiated sound field, including the total acoustic power output per unit volume of turbulence, the far-field noise spectrum, and the equivalent noise source distribution. An analytical treatment of this problem had previously been undertaken by Proudman (1952), and I undertook a reappraisal of this work during my work at ICASE in 1992, mainly as a result of the initial results of Sarkar and Hussaini (1992) showing surprisingly large differences when compared with Proudman's results. Proudman (1952) had made two main assumptions: (i) retarded time effects could be neglected since the turbulent Mach number was negligibly small, and (ii) the fourth-order space-time covariance of $T_{ij}$ in Lighthill's acoustic analogy could be reduced to the sum of products of corresponding second order covariances on the assumption that the velocity fluctuations obeyed Gaussian statistics. In the reappraisal of Proudman's work I retained the second assumption throughout, but I found that assumption (i) was not justified in the early stages of the complex analysis. I therefore retained retarded times up to a later stage in the analysis, where from that point onwards it was clear that their neglect could be justified. However the final numerical results showed only minor differences from Proudman's earlier results, and hence the large differences between these results and those of Sarkar and Hussaini (1992) remained.
To explore these differences further I developed an alternative theory based on the direct evaluation of the fourth-order space-time covariance of $T_{ij}$ using the Lighthill Relationship(1991) between a fourth-order covariance and a corresponding second-order covariance, without making any statistical assumptions. This alternative theory, just as in Proudman’s theory, required information on two quantities, namely the function $f(r,t)$, where $f(r,t)$ is the two-point longitudinal velocity correlation function, and the numerical value of the turbulent Strouhal number. Values of these two quantities became available for the first time from the DNS results obtained at ICASE by Sarkar and Hussaini(1993) for unforced decaying isotropic turbulence, and from the DNS results of Dubois(1993) for the case of forced isotropic turbulence. The results of Sarkar et al. and Dubois were also used to verify the Lighthill Relationship for the general case of the evaluation of a fourth-order space-time covariance for various space and time separations.

The results obtained by Sarkar and Hussaini(1993), using their improvements in time resolution as compared with their earlier results, were found to be in fair agreement with this new theory, although the theory was based on the assumption that the turbulent Reynolds number was large, whereas the DNS results were for low to moderate Reynolds numbers. Certain minor differences between the results from DNS and the analysis remain and are being further investigated, to ascertain whether they are simply the effect of the low Reynolds in the results from DNS or whether they have a deeper significance.

Hanasoge S. Mukunda

Considerable research has been reported in the last several years on various aspects of supersonic combustion. These are specifically mixing issues, experimental studies on model geometries, and developmental studies including the mission studies relevant to engine design. It appears that these various studies are generally being conducted with no significant impact on each other. Thus our present work is an attempt to examine these related issues on a common platform and draw inferences for future work. Our work in relation to spatially developing mixing layers and jets and other development studies has been discussed in this context. Yet the combustion counterpart has lagged behind, for what appears lack of focussed effort in simpler geometries, both experimentally and computationally. The experimental scheme used by Erdos et. al. (1992) is most eminently suited to the elucidation of the fundamental features. Experiments with more diagnostics for tests with heated hydrogen (to say 1000–1200 K) will be of great value. Computationally, studies on two-dimensional and three-dimensional mixing layers with boundary layer profiles as the initial conditions are vital to make progress on understanding flow features. Use of full chemistry has become a standard part of the simulation and should continue. The role of stretch caused by curvature
and unsteadiness in enhancing the disequilibrium of the mixing layer needs study and should be related to the results obtained on the thermal development of the mixing layer. Some work on this has been reported recently [Mukunda, 1992]. Use of asymptotic analysis in this area also seems possible.

Work on single jets along the lines adopted in Jarrett experiments, but including the effects of confinement, is another flow configuration which should receive attention, particularly in view of the fundamental differences in the development of the turbulence between mixing layers and jets. The features related to ignition, flame stability, and thermal development may be obtained. These must be well resolved simulations, perhaps three-dimensional, where the calculations should address extraction of stretch (local) and relate it to the thermal development.

Finally, it appears important to include stretching effects due to curvature and unsteadiness in the models for chemistry-turbulence interactions.

**Stephen R. Otto**

The bulk of my research during this period has concerned the evolution of vortices and their subsequent breakdown. The effect of crossflow on centrifugal instabilities has been considered theoretically (Otto and Bassom, (93-33), for narrow gap Taylor vortices) and numerically for the Görtler problem, in joint work with J. P. Denier from the University of New South Wales, Sydney, Australia. The equations have been solved numerically, and it has been shown that a small crossflow re-orientates the modes and induces a temporal periodicity. Work is underway to consider the effect of a hump at the plate on this situation, where it is thought that the crossflow will increase the receptivity coefficient. The secondary instability of a state comprised of the Falkner-Skan-Cooke profile and a finite amplitude vortex is considered by solving the three-dimensional Rayleigh equation. This kind of analysis is also being done for a nonlinear vortex state, derived in Otto and Bassom (92-45), a preliminary report on this work has appeared as Otto and Denier (93-46). These methods have been extended to a situation with a larger crossflow, where the dominant modes are of a crossflow type. Unfortunately this problem does not possess the disparity in scales exhibited by the Görtler problem. In this investigation with C. L. Streett (Theoretical Fluids Physics Branch, LaRC), the secondary stability of modes obtained from a linearised Navier-Stokes calculation is discussed. In a precursory report we have considered the secondary stability of steady crossflow modes derived from an Orr-Sommerfeld equation (Otto and Streett, to appear in the proceedings of the ICASE-LaRC workshop on Transition, Turbulence and Combustion). It is still an open question what effect imposing a spanwise structure on a inflectional profile has on the states stability. This is being investigated with Philip Hall
(University of Manchester, UK) for a variety of shear layers configurations: incompressible, compressible, and stratified fluids.

In work with Fang Hu (Old Dominion University, VA) and Tom Jackson the effect of curvature of the centreline of a mixing layer is being considered. It has been shown that the inviscid travelling waves present are virtually unaffected, however the curvature of the centreline promotes centrifugal instabilities. This has been shown in an inviscid framework (which corresponds to a high Görtler number), we hope to extend this to the order one Görtler number situation. As with the flow over a flat plate, it is not acceptable to use any kind of parallel flow approximation, so we shall have to march the parabolic governing equations forward, where we shall have linearised about a basic flow.

Time has been devoted to the study of the instabilities present within an unsteady boundary layer. A theoretical study using an Orr-Sommerfeld and triple deck approach has shown that the situation is unstable to viscous Tollmien-Schlichting waves. The physical problem that we are considering is the impulsive motion of an ‘infinite’ flat plate within its plane. The early work (Otto (93-76)) represents the first step in a series of articles which should eventually enable us to describe the sound generated by this situation. In theoretical work with M. Yousuff Hussaini, we shall describe the sound generated by this unsteady boundary layer, even though it may be small. So far all the modes considered have been situated on the lower branch of the neutral curve. It will be interesting to see if we can obtain agreement between the Orr-Sommerfeld results and the upper branch stability results. It is obviously interesting to extend this study to a compressible situation, and work with A. P. Bassom (University of Exeter, UK) is underway to study the structure of wave instabilities in this situation. This problem is far more complicated than its incompressible counterpart due to the possible influence of the inherent shock.

**J. Ray Ristorcelli**

Fundamental issues involving the Reynolds stress and $k - \varepsilon$ turbulence models of compressible turbulence in anisotropic and inhomogeneous situations are being explored. Our investigation is, at this point, focused in two areas: an understanding of the relevance and importance of the mass flux and also an investigation, using DNS, of the new statistical quantities due to compressibility appearing in the moment evolution equations of the turbulence.

The mass flux emerges as an important quantity relating time-averaged and Favre-averaged statistics and quantifying the effects of mean density gradients on the intensity and anisotropy of the turbulence. A general algebraic model for the mass flux has been derived. Key features of the model involve its dependence on the Reynolds stress, the mean
velocity gradients, the mean density gradient, and its coupling to other components of the mass flux. Current models are known to be very destabilizing and this problem has been resolved with the new mass flux model. The algebraic model for the density flux has been tested using the DNS data of S. Dinavahi (Analytical Services and Materials, Inc.) in an evolving wall bounded boundary layer at Mach 4.5. Comparisons of the model predictions with the DNS data is surprisingly good. Computations with the mass flux model in turbulence model calculations are being conducted in coordination with R. Abid (High Technology Corp., LaRC).

Work regarding the inadequacies and inconsistencies in the usual formulation of the mean and second-order equations used in the Reynolds stress and $k-\varepsilon$ turbulence models has been completed. The reformulation of the viscous terms in terms of the neglected mass flux in the mean momentum equations allows them to be carried without any modeling assumptions. A similar reformulation of the viscous and pressure work terms in the mean energy equation also allows them to be carried exactly. A post-processing code developed to analyze the DNS data of the relevant compressible statistics has been completed in collaboration with S. Dinavahi (Analytical Services and Materials, Inc.) and Gordon Erlebacher. The inadequacy of these modeling assumptions has been verified. In the second-order equations the proper formulation of the near wall problem requires a recognition of the fact that the dissipation-like terms are carried using the Reynolds decomposition while the problem is posed in Favre variables. This distinction, usually not acknowledged in the current literature, is a necessary prerequisite to the proper formulation of the near wall problem. It will be especially important when there are mean density gradients. Carrying the exact equations, without the usual neglect of the mass flux, for the mean flow and the second-order statistics will be important in complex compressible turbulent flows: these include flows in which there are mean density gradients due to large Mach number or combustion, separation or reattachment (inflection points), cold wall boundary conditions, mean dilatation, shocks, adverse pressure gradients, or strong streamwise accelerations.

In the area of incompressible turbulence a rapid-pressure model, frame-indifferent in the two-dimensional limit, referred to in the last semi annual report is nearing completion. The 2DMFI model, which is derived from first principles satisfying the mathematical constraints of realizability and geostrophy, insures that the modeled equations are consistent with the Taylor-Proudman theorem. This is an issue of substantial importance in the computation of any complex flows. The model was developed as part of the thesis of Ristorcelli (1991). The 2DMFI model, without any sacrifice of its rigorous mathematical underpinnings, has been calibrated to the asymptotic homogeneous shear.
Sutanu Sarkar

Our work in computational aeroacoustics is continuing. The hybrid DNS method for the computation of sound radiated from isotropic turbulence has been compared with the theoretical model developed by G. Lilley. Although the scaling laws for the acoustic power in the numerical and analytical studies are the same, the constant of proportionality in the simulation is somewhat smaller than in the analytical model.

The influence of compressibility in turbulent shear flow is also being investigated. The motivation is to develop turbulence models which are applicable to both the high-speed mixing layer and the wall boundary layer. A new series of DNS of homogeneous shear flow has been performed which distinguishes between the effects of the two relevant Mach numbers - the gradient Mach number, and the turbulent Mach number. The stabilizing effect of the gradient Mach number on the turbulence is due to the reduced Reynolds shear stress anisotropy. The reduced 'production efficiency' seen in the simulations may arise from major changes in the pressure field introduced by the additional acoustic mode in compressible turbulence.

Charles G. Speziale

A detailed theoretical and computational study of the realizability of Reynolds stress turbulence closures has been conducted in collaboration with R. Abid (High Technology Corp., LaRC) and P. A. Durbin (CTR, Stanford University). It was proven that a well known second-order closure model that was formulated to satisfy the strong realizability constraints of Lumley and Schumann is, in fact, not a realizable model. More importantly, it was shown that it is impossible to identically satisfy the strong form of realizability in any version of the current generation of second-order closure models. Only the weak form of realizability – wherein access to one or two component states of turbulence is avoided – leads to realizable models. The issue of realizability has been of real interest in turbulence modeling, since it has long been known that models which become unrealizable (yielding negative components of the turbulent kinetic energy) can give rise to unstable solutions. However, the results of this study indicate that this is not as severe a problem as first thought, and that traditional approaches in turbulence modeling which have been used to guarantee realizability, either fail to do so or give rise to ill-behaved solutions that are highly unphysical. An alternative and simple mathematical means for making any second-order closure model realizable – based on a stochastic analysis – was explored independently with P. A. Durbin. These results can have important applications in the future formulation of full Reynolds stress closures that are more physical and better behaved computationally.

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Siva Thangam

The development of two-equation turbulence models that have a wide range of predictive capability for separated flows was undertaken from analytical and computational point of view. This is the second phase of this collaborative effort involving M.Yousuff Hussaini and Ye Zhou of ICASE, Thomas Gatski of the Theoretical Flow Physics Branch, and George Vahala of William & Mary. During this period, a recursion renormalization group theory (r-RNG) based anisotropic two-equation model for incompressible turbulent flows was developed. The proposed model uses a finite wavenumber truncation scheme to account for the spectral distribution of energy. The model incorporates the effects of both local and nonlocal interactions. The nonlocal interaction are shown to be equivalent to that from small perturbation renormalization group theory (e-RNG), while the local interactions introduce higher order terms.

A formal analysis of the model was developed and was subsequently incorporated into a second-order accurate finite-volume algorithm. The model has been validated for the prediction of massively separated turbulent flows by considering the benchmark test case of turbulent separated flow past a backward-facing step. The results demonstrate that r-RNG based two-equation model can accurately predict the mean flow and turbulent stresses for separated flows. During the next phase, the model will be further refined to include near wall effects as well as flow parameter dependent model coefficients for the higher order terms. The model will then be validated by considering a variety of turbulent flows including wakes and flows with recirculation.

Lu Ting

In collaboration with Drs. L. Maestrello (Structural Acoustics Branch, LaRC) and A. Frendi (Analytical Services and Materials, Inc.) we continued our studies of the structural/acoustic interaction problem simulating the transmission of exterior incident waves through an airframe into the interior. The mathematical model simulates the experiments conducted at NASA. The airframe is modeled by a flexible panel mounted on a large rigid plate. In the first experimental setup, nearly planar waves originated from a stationary point source are incident normal to the plate at $t = 0$. In the second setup, the incident waves originate from a supersonic jet parallel to the panel. The sources are moving relative to the panel and the incident waves are not planar and not at normal incidence. In both experimental setups, the incident wave frequency is near a natural frequency of the panel so that nonlinear oscillation of the panel can be excited. The real time pressure variations on the incident and transmitted sides are measured.

Two mathematical models simulating the first experimental set up were described in
ICASE Report No. 93-18. One (the fully coupled model) solves numerically the three dimensional nonlinear Euler equations for the flow field coupled with the plate equations. Approximate boundary conditions on the finite computational domain of the flow field are employed for the Euler solver. The second model (the decoupled model) uses the linear wave equation for the acoustic field and expresses the load as a double integral involving the panel oscillation. The integral is an exact solution of the initial value problem for the acoustic field. The panel oscillation is then governed by a system of integro-differential equations and is solved numerically. The acoustic field is then defined by an explicit formula, the double integral. Numerical examples showing the efficiency and accuracy of the decoupled model versus the fully coupled model were presented in the ICASE report. Comparison of the numerical simulations with the real time experimental data from the first setup is in progress.

For the second experimental setup, the source distribution or the jet noise is moving relative to the panel. Experiments for steady, accelerating, and/or decelerating jets have been carried out. It is well known that a source initiated at $t = 0$ moving at a constant supersonic speed can reach a stationary point (on the panel) either twice or not at all. To formulate a theoretical model for the propagation of jet noise from an unsteady jet, we consider the acoustic field induced by an unsteady source distribution, $q(t, x)$, in a media moving with velocity $U(t)\hat{v}$ relative to the coordinate system $x$. Rules to determine how many times the signal issued from a point $S(x')$ will arrive at point $P(x)$ at time $t$, and the corresponding retarded time(s) $\tau$'s are being formulated. This part of the theoretical investigation has been carried out in collaboration with L. Maestrello of NASA LaRC with the help of Bruce Kruger who was in the ICASE summer student program.

Nick Verhaagen

The visit to ICASE was made in the frame of a cooperative research program between ICASE, NASA LaRC, NAWC and TUD. The program is meant to generate experimental and numerical data on the interaction process of vortices over double delta wing configurations. This data will help the further development of wing planforms useful for future high-speed aircraft.

The summer visit was used to carry out experimental research on a 76/40-degree swept double-delta wing wind-tunnel model provided by NAWC. The objective of this research was to gather experimental data on the characteristics of the subsonic vortex flow over this wing. The tests took place in the Basic Aerodynamics Research Tunnel of the Experimental Methods Branch of NASA LaRC. Extensive flowfield visualization tests, using oil and smoke-laserlight-sheet equipment, were performed to visualize the flow on and off the surface of the
double-delta wing model at angles of attack ranging from -10 to +22.5 degree and Reynolds numbers ranging from 0.5 to 1.5 million. The wind tunnel model is provided with a number of pressure orifices. These were used to measure the pressure on the surface of the model at the various test conditions. Quantitative data on the vortex flowfield was obtained by surveying the flowfield over the model at an angle of attack of 5 degrees using advanced five-hole probe flow surveying equipment. Time available for the wind tunnel measurements did not allow us to perform flowfield surveys at other angles of attack. To complete the experimental data set for this wing, flowfield surveys will also have to be carried out at other angles of attack outside the range considered here. Experimental data obtained thus far will be used to validate the Navier-Stokes solution for the flow over the double-delta wing computed and made available by NAWC.

The summer visit was also spent meeting with scientists of the Computational Aerodynamics Branch who use experimental data from vortex flow tests carried out at the Delft University of Technology to validate their numerical solutions.

Jay Webb

My research is primarily concerned with the direct numerical simulation of noise caused by instabilities in fluid flows. I am currently working with Stephen Otto on a numerical study of Tollmien-Schlichting waves generated in an unsteady boundary layer, caused by the impulsive motion of an infinite flat plate. The study will include a linearized Navier-Stokes solution to the incompressible problem, which will be compared with the Orr-Sommerfeld results. The corresponding nonlinear problem will also be considered. We also intend to effect a compressible simulation and compare the results with those of stability theory from a concurrent study (Otto and Bassom). Ultimately, it is hoped that the noise generated by these instabilities can be found.

It is well known that noise from supersonic, perfectly expanded jets is primarily due to unstable Kelvin-Helmholtz waves convecting supersonically relative to the free stream conditions. Because of this, and also the fact that the most unstable of these waves have wavelengths on the order of a few jet diameters, it is feasible to compute the noise from such a jet directly, without having to rely on the acoustic analogy. There are difficulties, however, in treating boundaries. In particular, it is not yet established how to properly treat the jet nozzle lip, or how to allow the jet outflow to transmit large vortices as well as acoustic waves. Also, it is unclear how to make the outer radiation boundaries transparent to acoustic waves, while also allowing a steady entrainment velocity into the domain. I am currently considering the third of these problems, with the hope of addressing all three and ultimately performing the noise simulation.
Robert Wilson

Numerical simulations of spatially developing, forced shear layers have been performed using a variety of inlet boundary conditions, numerical schemes, and subgrid-scale stress models. The effect of inlet boundary conditions on the spread rate and vortex dynamics of the shear layer are being investigated. Initial results show shear layer rollup, pairing, and development similar to that found in the literature for spatial and temporal simulations. In collaboration with A.O. Demuren, a study on near-wall elliptic relaxation models for two-equation and Reynolds-stress turbulence models was completed.

Sean Wu

While I was at ICASE this past summer, from May 17 to June 18, I concentrated on fluid-structure interaction between a finite plate and a supersonic turbulent flow. I developed several theoretical models for describing the dynamic response of a finite plate clamped to an infinitely extended rigid baffle under the excitation of a turbulent flow. In particular, the effect of full coupling between the radiated acoustic pressure field and an elastic plate was taken into account. The nonlinearities caused by stretching of in-plane forces were also considered. Since returning to Wayne State University, I continued the work initiated at ICASE, and obtained some numerical results of the plate response to turbulent boundary layer excitations. The predicted cross power spectrum of the plate response compared well with the experimental measurements obtained earlier.

In October, I developed a new method for the plate stability analysis, with the effects of fluid loading and nonlinearities due to stretching of in-plane forces taken into account. In this analysis, I was able to tell the exact causes of the structural instabilities. As an example, I demonstrated the stability of conditions for a linearized case, namely, the effects of nonlinearities due to stretching of in-plane force should be neglected. The analysis showed that structural instabilities can be caused by fluid loading resulting from acoustic radiation. Two unstable mechanisms were found to be attributable to the added damping and stiffness resulting from the radiated acoustic pressure field. In particular, the effects of the added damping and stiffness increase with the Mach number of the flow, the former increasing linearly while the latter increases quadratically.

These results have been summarized in an ICASE report and will be sent out for journal publications. The next step is to generate stability charts for both linear and nonlinear cases. These stability charts should tell us when, and under what condition, structural instabilities will happen.
Ye Zhou

To demonstrate the performance of a recently proposed recursive renormalization group based Reynolds stress model (Zhou, Vahala, and Thangam, ICASE Report No. 93-51), the flow past a backward facing step—a flow field characterized by the presence of separated shear layer straddling a massive recirculation zone, and the symmetric wake behind a flat plate—a flow field involving the evolution of a turbulent boundary layer into a free-shear layer down stream of the trailing edge, were considered (with Thangam). The results obtained demonstrate that the proposed recursive-RNG based model can yield very good predictions. As an example, the near wake region, which constitutes the initial segment of this transition, offers a substantial challenge for the predictive capabilities of most turbulence models. Our analysis indicates that the prediction of our model is in excellent agreement with the experimental findings.

In large-eddy simulations of high Reynolds number turbulent flows, a subgrid-scale closure model is necessary to represent the effect of the small unresolved scales on the large resolved scales. The subgrid-scale model based on classical closure theory is achieved by the introduction of a spectral eddy viscosity. Additionally, a backscatter term has also been found important, and some recent calculations have included a model of this term. The phenomenological renormalization group theory of Lam (S.H. Lam, Phys. Fluids, A 4, 1007 (1992)) directly recommends the choice of a turbulent eddy viscosity, and models the correlation of the backscatter term for the resolvable scales. We verify that the model used by Lam is indeed consistent with the classical theory.
David Banks

Recent work has focused on developing and applying feature-finding tools to CFD data. For 2-D data this involves ridge-detection algorithms which were originally designed for medical image processing. For 3-D data this requires new techniques, developed jointly with Bart Singer in the Fluid Mechanics Division.

In a second effort, an SGI's Explorer is being used to render images of vortex tubes whose skeletons have been extracted from numerical simulation. The goals of the reconstruction are to enhance the visual presentation of vortical motion in a static image, and to effectively decompress thinned data to produce an animation of the flow.

In a collaborative effort with D. Manocha (UNC-CH) and B. Tebbs (Numerical Design, LTD), we have been examining ways to decompose parametric surfaces into unobscuring patches. These patches can typically be rendered using the painter's algorithm, which is an attractive solution for device-independent 2-D image-generation.

Shahid Bokhari

Research is continuing on “Parametric Binary Dissection” in collaboration with Tom Crockett and David Nicol. An ICASE report on this research has been prepared. Our current focus is to evaluate this algorithm on a set of large (approximately 1 million edges) unstructured meshes obtained from colleagues at LaRC.

In another effort, research is continuing on “Multiphase Complete Exchange” on hypercube architectures. An ICASE report describing the properties of the hull of optimality of this family of algorithms has been prepared. This work is being extended (in collaboration with D. M. Nicol) to arbitrary dimensional meshes, with emphasis on 2-D and 3-D meshes and torii.

Gianfranco Ciardo

The development of a large-grain distributed algorithm for state space exploration in Stochastic Petri Nets has been started. This algorithm could exploit, for example, a local area network of workstations overnight when the workload is low, to solve models with at least one order of magnitude more states than feasible on a single workstation. Implementation work on this problem will follow.

In collaboration with Larry Leemis, another summer visitor at ICASE, we developed a discrete-event simulation validating an approximate numerical decomposition approach
which I had previously defined. With simulation, it is possible to quantify the approximation when the model scales up. This cannot be done analytically, since an exact numerical solution requires an exponential amount of memory and time.

Also with Larry Leemis, I started working on a comparison of the exponential and geometric distributions, when used to model the failure or service behavior of concurrent activities. An interesting result is that the discrete nature of the geometric distribution has an effect on the distribution of the time-to-first-failure. We plan to write a short paper on the findings.

**Tom Crockett**

PGL, our parallel graphics library, was ported to the Intel Paragon. A simple PGL-based geometry viewer was written to demonstrate the use of a workstation-based interactive interface to control a remote Paragon-based rendering application. Using a vortex tube dataset produced by David Banks from a CFD simulation by B. Singer (High Technology Corp., LaRC) and R. Joslin (Fluid Mechanics Division, LaRC), we were able to achieve rendering rates which compare favorably with our SGI Indigo Elan graphics systems. These rates can be expected to improve further as the PGL rendering algorithms become more efficient and network connections to the Langley Paragon are upgraded from Ethernet to FDDI. The vortex tube visualization is featured in the 1994 Intel User Group calendar, where it was judged to be the best of approximately twenty submissions.

We are continuing our performance experiments on the new span-based rendering algorithm used in PGL. The data obtained will improve our understanding of overheads in the parallel algorithm, which in turn should lead to improved performance models and better algorithms. Part of this effort involves developing appropriate visualization techniques to assess the complex multivariate data from our experiments.

**Phil Dickens**

We have made significant progress in our theoretical investigation of the benefits of blending aggressive and non-aggressive techniques for parallel discrete event simulation. This research is in collaboration with David Nicol (The college of William and Mary, currently on sabbatical at ICASE), Paul Reynolds (Department of Computer Science, University of Virginia) and Mark Duva (Department of Applied Mathematics, University of Virginia). We have shown that adding aggressive processing to a non-aggressive windowing protocol offers the potential for significant performance gains. Also, we have shown that the aggressive windowing protocol maintains the very important scalability properties of the non-aggressive version. A summary of this research is presented in “The Impact of Adding Aggressive Processing to a Non-Aggressive Windowing Protocol” to be published in the Proceedings of
the 1993 Winter Simulation Conference. The analysis and results are given in “Bounds
and Approximations for an Aggressive Windowing Protocol” which will be published as an
ICASE research report and submitted to the ACM Transactions on Modeling and Computer
Simulation.

In addition to our theoretical investigation of parallel simulation protocols, we are in
the process of developing a testbed for the study of synchronization and load balancing
issues in parallel simulation. This research is also in collaboration with David Nicol. We
are developing a multiprocessor version of CSIM, a widely used simulation package based
on the C programming language, to serve as the common platform for this research. We
have ported CSIM to a single processor of the Intel Paragon and are continuing with our
multiprocessor design.

Finally, we are in the initial stages of developing a methodology for predicting the perfor-
mance of parallel codes on a target parallel architecture, in collaboration with David Nicol
and Philip Heidelberger (IBM Watson, on sabbatical at ICASE). Assume a user has some
codes running on an Intel Paragon with 32 nodes (the host machine) and would like to predict
the performance of these codes on a 64 node Paragon (the target machine). One way to ob-
tain this estimate is to combine direct execution of the codes with parallel simulation. That
is, the host machine is used to execute the codes and the target machine is simulated using
the techniques of parallel simulation. Combining direct execution with parallel simulation
will allow accurate performance predictions to be obtained quickly.

Matthew Haines

In collaboration with Piyush Mehrotra, Brian Hess, and David Cronk, we are working on
the design and implementation of multi-threaded runtime support for scientific applications
on distributed memory multiprocessors. The current language support for various scientific
applications is deficient in areas of managing parallel tasks and distributed data structures
to obtain high performance. We are working on a runtime layer of software designed to
ameliorate these deficiencies. The goal is to achieve a higher level of abstraction for the
scientific programmer, without losing much performance.

Ulf Hanebutte

Work has centered around the development of a portable parallel Adaptive Mesh Re-
finement (AMR) algorithm geared towards large scale simulations of complex shock wave
phenomena. To ensure portability across a wide range of parallel computers a private mes-
sage passing interface has been designed, upon which all support routines were built. For
example, this strategy allowed the porting of the entire AMR code from a cluster of workstations to an INTEL iPSC/860 and its NX message passing library in less than one morning's work. Working with James Quirk, the author of the original AMR algorithm, it has been possible to merge the parallel machinery that has been developed over the last year with the original serial algorithm in a seamless fashion. Thus, parallel execution has become an integral part of the general AMR framework. Details of this work have been written up in ICASE Report No. 93-63.

To demonstrate the worth of the new parallel AMR algorithm, detonation flows through a straight duct and over a ramp have been simulated. For such simulations, a near perfect load balance can be guaranteed by means of simple heuristic load distribution functions. These large calculations, which require about 40 hours on 8 SUN Sparc 10's, obtained over 80% sustained efficiency, even with Ethernet communication between processors.

For the future, it is planned to improve the capability of the parallel AMR algorithm further and to embark on a study to analyze the associated load balance issues. This work should lead to effective load balance algorithms of broad interest.

Mark A. Holliday

I am developing a generic database simulation package to facilitate exploration of database research issues. Currently, the simulator emulates a single processor relational DBMS with any number of disks. The simulator includes buffer, disk, and CPU management routines and workload routines for short TPC-A type transactions and joins. Scott Leutenegger is developing a TPC-C workload routine. We are collaborating in using the simulator to investigate scheduling issues in the context of workloads similar to TPC-C.

David Keyes

Demands for massive memory and high speed typically accompany one another in scientific and engineering computations, linking space to time in algorithm design. Some degree of programmer control must be exerted over data layout in coding for scalable distributed memory machines. Fortunately, the laws of nature often cooperate with a basic scaling law of computer architecture: the magnitude of interaction between two degrees of freedom in a physical system decays with their spatial separation; therefore, the frequency and volume of data exchange between different points in the computational domain can be allowed to decay with distance in a trade-off of communication overhead with the precision required in a final result or the rate of convergence required in a preconditioner. For model problems, this trade-off has been formalized in convergence theorems. We have been exploring it ex-
perimentally, applying domain decomposition preconditioners to problems in computational fluid dynamics.

Modern iterative domain decomposition (or "substructuring") methods require predominantly local information. Nonlocal information is accessed hierarchically, through exchanges requiring only a small volume of data relative to the scale of the discretization. Hence, domain decomposition is an natural algorithmic bridge between application and architecture for elliptically dominated problems, such as inverting the full potential operator or the left-hand sides of deferred-correction methods for aerodynamic steady states. In a collaboration with Driss Tidriri, we have replaced conventional approximation solvers in compressible Euler codes with Schwarzian domain decomposition solvers, which permits large CFL numbers without time factorization error and defers the CFL barrier to the next higher limit of consistency between (lower-order) left- and (higher-order) right-hand side discretizations. This is a subject of current research interest to researchers at NASA and ICASE because it stands in the way of asymptotic Newton-like convergence to the steady-state solution. In a collaboration with Xiao-Chuan Cai, we have examined one- and two-level Schwarzian preconditioners for the full potential equation. In this setting, Newton’s method works well. The presence of a coarse grid significantly improves convergence, at the expense of solving a small global problem.

Larry Leemis

In collaboration with Kishor Trivedi, also visiting at ICASE, a technical note has been prepared to compare the accuracy of two approximate confidence interval estimators for the Bernoulli parameter $p$ for large sample sizes. As performance models (e.g., stochastic Petri nets) become larger and more complex, Monte Carlo simulation will be relied on more often to approximate solutions to intractable models. When the probability of failure is small and the number of replications is large, this technical note will help a modeler determine whether the normal or Poisson approximation to the binomial is more appropriate for placing confidence intervals on the probability of failure. Charts are given to indicate which approximation is appropriate for certain sample sizes and point estimators.

In collaboration with Gianfranco Ciardo, also visiting at ICASE, a discrete-event simulation program has been written that estimates the completion rate for a stochastic Petri net of an Ada rendezvous between one callee and multiple callers. The purpose of the code is to determine the accuracy of an approximation technique that is appropriate when there is a large number of callers.
In collaboration with Adrian Filipi-Martin, a student at the College of William and Mary, we are conducting research in providing database support for scientific visualization. Currently, solution sets are saved as files, and then the entire file read into a visualization package (such as FAST or AVS). The user can then visualize regions of the data. The goal of our research is to study efficient indexing and clustering methods of objects to enable quick retrieval of subsets of the data set. We are implementing indexing methods and building a prototype capable of visualizing subsets of large scientific data sets. The system is an extension of the Exodus system, an existing public domain Client-Server Object Oriented Database Management System. Our work is driven by real data sets obtained from computational fluid dynamics researchers and LaRC (ICASE). Initially, we are implementing three alternative multi-attribute indexing techniques and comparing them by using them to retrieve subsets of two and three dimensional computational fluid dynamics solution sets. We consider both block structured and unstructured grids.

In collaboration with Mark Holliday from Duke University, we are investigating scheduling of mixed workloads for database systems. We are using a generic database simulator implemented by Mark Holliday to simulate the system. We are using the TPC-C benchmark as the workload of our study. We have chosen this benchmark since it represents a consensus among industry and academia on a typical workload. We then intend to modify the workload with additional transactions to see how more complex queries affect system performance. Our scheduling work is focusing on buffer allocation, load control, and cpu/disk scheduling.

In collaboration with David Nicol from the College of William and Mary, we are investigating bulk loading algorithms for grid files. Our goal is to develop an algorithm that maximizes the bucket (disk) utilization of the grid file and also minimizes the number of disk accesses needed to retrieve data when indexing on two and three attributes. To aid in the second objective, we have developed a new extension to the grid file that allows retrieval for partially specified queries to proceed without returning to the grid directory after locating the first bucket. The technique results in a lower disk utilization. We are currently developing simulations to evaluate both our algorithm, and the tradeoffs of our new retrieval technique.

Finally, in collaboration with Graham Horton from the University of Erlangen-Nurnberg, we have developed a multi-level solution technique for the solution of Markov chains. This research project is described in more detail elsewhere in the semi-annual report under the work by Graham Horton.
Kwan-Liu Ma

In collaboration with Jamie Painter (University of Utah), Charles Hansen and Michael F. Krogh (Los Alamos National Laboratory), we have designed a data-distributed parallel algorithm for ray-traced volume rendering, to perform high-quality rendering of high-resolution data. The algorithm has been implemented on both the Connection Machine CM-5 and a network of workstations. The volume data, once distributed, is left intact. The processing nodes perform local ray-tracing of their subvolume concurrently. No communication between processing units is needed during this local ray-tracing process. A subimage is generated by each processing unit, and the final image is obtained by compositing subimages in the proper order, which can be determined a priori. The algorithm, along with tests results which demonstrate the practicality of our rendering algorithm and compositing method, will be presented at the Parallel Rendering Symposium. The next step is to port this algorithm to the Intel Paragon and to investigate machine-dependent modifications to the algorithm to achieve optimal performance.

In collaboration with Philip Smith (University of Utah), work is continuing on the development of computer graphics techniques for visualization of the mixing of fluid elements as well as the mixing of inertial particles in a convection-diffusion system. A technique that we have developed allows a computational fluid dynamics user to visualize the basic physical processes of dispersion and mixing rather than just the vector and scalar values computed by the simulation. This technique is based on transforming the vector field from a traditionally Eulerian (fixed) reference frame into a Lagrangian (moving) reference frame. Fluid elements are traced through the computed vector field along the mean path. At the same time, the statistical dispersion of the fluid elements about the mean position is computed by using added scalar information of the root mean square value of the vector field and its Lagrangian time scale. We have used the technique to visualize the simulation of an industrial incinerator to help identify mechanisms causing poor mixing and will report the results at the Visualization '93 conference. Extension to visualization of the mixing of inertial particles is underway and will be presented at the AIAA 32nd Aerospace Sciences Meeting.

Piyush Mehrotra

High Performance Fortran (HPF) is a set of extensions to Fortran designed to exploit data parallelism on a wide variety of parallel architectures. Since HPF is becoming an industry-standard language for data parallel algorithms, we have been evaluating the expressiveness of HPF for complex codes. In collaboration with John Van Rosendale, Mike Cokus, Brian Hess, Jean Mayo, and Dave Middleton, we are currently examining several NASA codes, including a single version of ISAAC, the multi-block code, TLNS3D, a Monte Carlo code, DSMC, and
a Finite Element structural analysis code from the Lamps benchmark. We have been using the Vienna Fortran Compiler System (VFCS) and the HPF compiler from Applied Parallel Research for our evaluation.

In the multi-block code, the fundamental issue is the exploitation of both intra-block and inter-block parallelism. This requires the distribution of grid blocks over subsets of processors, a capability not provided by HPF. We have designed extensions to HPF which give the user finer control over the distributions of the blocks in such codes. Preliminary results using the VFCS give good speedups on the intra-block code but have problems in the inter-block communication. We have been studying ways of improving this performance using a combination of aggressive interprocedural analysis and user specified directives.

Analysis of the DSMC code shows that it can be expressed in HPF but would not achieve good performance, since HPF code is generally written independent of the distributions. We are exploring several alternatives which take into account processor boundaries, and thus are as efficient as hand-written code in both overall performance and memory usage.

Another area of research has been multidisciplinary design optimization codes, which exhibit both functional and data parallelism. In a joint effort with John Van Rosendale, Hans Zima, and Barbara Chapman of the University of Vienna, we have designed a tasking layer to exploit the functional parallelism in the HPF. This extension of HPF allows users to express both the coarse grained parallelism across disciplines and the inter-disciplinary sharing of data. At the same time, parallelism within each discipline can still be expressed via HPF, since the tasking layer is well integrated with HPF. Preliminary work on the programming environment using this tasking layer has begun, along with a runtime system which will support this approach in an heterogeneous environment.

David Nicol

In collaboration with Kishor Trivedi (Duke University) I began investigating the notion of Fluid Stochastic Petri Nets, and their application to joint performance/reliability analysis.

In collaboration with Shahid Bokhari (ICASE) I analyzed the Multiphase Direct Exchange algorithm, and its extensions to One-to-all broadcast, All-to-all broadcast, and One-to-all personalized communication.

In collaboration with Bhgaraith Narahari, I developed algorithms that optimally remap parallel computations subject to a constraint on the volume of communication permissible.

In collaboration with Phil Dickens (ICASE), and Phil Heidelberger (ICASE, visiting scientist) I began examining the problem of using parallel simulation to emulate a numerical
code running on many more processors than are used in the simulation. The numerical code runs directly on the architecture, and the simulator engages only to simulate the underlying communication network.

Daniel Reed

The ICASE Parallel Short Course brought together researchers in programming languages, tools, and numerical analysis to present an overview of the current state of the art in these areas. I was a speaker at this workshop. My task at ICASE was to organize the text describing this work and begin writing a paper (some of this is joint work with David Nicol).

My work at Illinois focuses on parallel computing. To benefit from parallel computers, programs must be partitioned into units that work in parallel. Once partitioned, these units, called processes, tasks or threads, must be assigned to specific processors for execution. Using program task creation traces, we compared the performance of a large number of possible task placement policies. We found that policies based on measured system load were often inefficient because they could not quickly track changes in network load (i.e., they were using information that was in error). To characterize the penalty for this information error, we developed a simple analytic model of task placement that reflects the performance of random task placement, the limiting case of minimal network state information.

Joel Saltz

We have developed two new ideas by which an HPF compiler can deal with irregular computations effectively. The first mechanism invokes a user specified mapping procedure via a set of compiler directives. The directives allow the user to use program arrays to describe graph connectivity, spatial location of array elements and computational load. The second is a simple conservative method that, in many cases, enables a compiler to recognize that it is possible to reuse previously computed results from inspectors (e.g. communication schedules, loop iteration partitions, information that associates off-processor data copies with on-processor buffer locations). This work was implemented in the context of the Syracuse Fortran90D compiler and benchmarked using code templates from unstructured mesh CFD codes and from computational combustion codes. This work was carried out in collaboration with Ravi Ponnusamy (Maryland, Syracuse), Alok Choudhary (Syracuse) and with the generous assistance of Geoffrey Fox's group at Syracuse. In an ICASE report, to be submitted October 1993, we present performance results for these mechanisms.
Arun K. Somani

Most reliability analysis techniques and tools assume that a system is used for a single mission consisting of a single phase. However, multiple phases are natural in many missions. The failure rates of components, system configuration, and success criteria may vary from phase to phase. In addition, the duration of a phase may be deterministic or random. Recently, several researchers have addressed the problem of reliability analysis of such systems using a variety of methods. We describe a new technique for phased-mission system reliability analysis based on Boolean algebraic methods. Our technique is computationally efficient and is applicable to a large class of systems for which the failure criterion in each phase can be expressed as a fault tree (or an equivalent representation). Our technique avoids the state space explosion commonly seen in Markov chain-based analysis. We develop a phase algebra to account for the effects of variable configurations and success criteria from phase to phase. Our technique yields exact (as opposed to approximate) results. We demonstrate the use of our technique by means of an example and present numerical results to show the effects of mission phases on the system reliability.

Xian-He Sun

Research has continued in two directions: design of highly parallel matrix algorithms for scientific applications, and on performance evaluation for parallel algorithms and architectures.

In algorithm design, the Reduced Parallel Diagonal Dominant (PDD) algorithm (ICASE Report No. 93-6) has been modified to reduce the arithmetic operations. We took the approach of providing approximate solutions based on an accuracy analyses. Exploiting partitioning and truncation, the Reduced PDD algorithm has a smaller arithmetic operations count than the conventional sequential algorithm for periodic problems. For instance, to achieve $O(10^{-4})$ accuracy, the Reduced PDD algorithm only needs $5n/p + 41$ operations, where $n$ is the order of the matrix and $p$ is the number of processors; to achieve $O(10^{-8})$ accuracy, the Reduced PDD needs $5n/p + 62$ operations. The conventional sequential algorithm, Thomas Mgorithm, requires $7n - 1$ operations for periodic problems. The approach taken, of introducing bounded numerical errors in order to obtain greatly improved parallel performance, seems to be widely applicable.

In related work, the Simple Parallel Prefix (SPP) algorithm (ICASE Report No. 93-16) has been modified to solve periodic systems. The modified SPP algorithm has the same parallel operation count for solving periodic systems as the SPP algorithm for solving nonperiodic systems, and for hypercube architecture, it has the same communication cost for solving periodic systems as the SPP algorithm has for solving nonperiodic systems.
The communication pattern, however, has been changed from prefix communication to shift communication for solving periodic systems.

In performance evaluation, in collaboration with Jianping Zhu (Mississippi State University), we investigated the performance evaluation of Shared Virtual Memory machines. From the viewpoint of processes, there are two basic process synchronization and communication models. One is the shared memory model, in which processes communicate through shared variables. The other is the message passing model, in which processes communicate through explicit message-passing. With its shared virtual address space, the shared memory model supports shared virtual memory, but requires sophisticated hardware and system support. Traditionally, the message passing model is limited by the small local memories of the processor elements. With recent technology advances, the message passing model has been extended to support shared virtual memory. Shared virtual memory simplifies the software development and porting process. It is becoming a standard feature of modern parallel computers. However, the memory access of shared virtual memory is highly nonuniform, which can lead to poor performance.

Using the generalized speedup metric proposed by John Gustafson and myself, the performance evaluation of shared virtual memory machines and parallel computers in general has been investigated. It has been shown that the main difference between generalized speedup and traditional speedup is how one defines the uniprocessor efficiency. When uniprocessor speed is fixed, these two speedups are virtually the same. Extending these results to the scalability study, we have found that the difference between isospeed scalability and isoefficiency scalability is also due to uniprocessor efficiency. As part of our performance study, we have shown that an algorithm-machine combination achieves perfect scalability if and only if it achieves perfect speedup. Eight possible reasons for superlinear speedup have also been discussed. A scientific application has been implemented on the 128 node Kendall Square KSR-1 shared virtual memory machine at the Cornell Theory Center. Experimental results show that uniprocessor efficiency is an important issue for virtual memory machines, and the generalized speedup provides a reasonable way to define the uniprocessor efficiency. Therefore, it is a more reasonable metric than traditional speedup.

**Alan Sussman**

I have made several improvements to the multiblock Parti library. The library now supports regular section moves between distributed arrays that do not have the same number of dimensions (by fixing indexes in the array with more dimensions). I have also redesigned
the exch-sched primitive to allow filling in “corner” internal ghost cells, but the implementation is not yet complete. This functionality is required to properly implement the parallel version of TLNS3D.

We have enhanced the library so that it is now easily ported between different distributed memory architectures (done with Jim Humphries, a University of Maryland undergraduate). The TLNS3D template has been run on the Intel iPSC/860, TMC CM-5, and on a network of workstations under PVM. The template has also been rewritten in Fortran 90D and run through the Syracuse F90D compiler, as modified by our graduate student Gagan Agrawal, to generate parallel code that uses the library primitives. The performance of both the compiler parallelized code and my hand parallelized version has been documented in a paper to appear in Supercomputing '93 and in a paper we have submitted to IEEE Transactions on Parallel and Distributed Computing. This work shows that the overhead introduced by using the library is small, compared to an optimal, essentially unrealizable, hand implementation.

The implementation of the complete TLNS3D code is continuing. When it is completed, I will run the code on several distributed memory machines (Intel iPSC/860 and Paragon, TMC CM-5, IBM SP-1) and compare the performance with that on a Cray vector supercomputer.

Kishor S. Trivedi

Four papers were begun during my stay at ICASE in July 1993. One paper entitled, "Dependability and Performability Analysis" co-authored with Gianfranco Ciardo, Manish Malhotra and Robin Sahner has been finished and has appeared in a Springer-Verlag book. This was an invited tutorial at the IFIP symposium, PERFORMANCE '93 held in Rome during September 1993.

The second paper with Larry Leemis, entitled, "A Comparison of Approximate Interval Estimators for the Bernoulli Parameter," has been submitted for publication to the American Statistician.

The third paper with Arun Somani entitled, "Phased-Mission Analysis Using Boolean Algebra Methods," is nearly completed and will be submitted to IEEE Transactions on Computers.

The fourth paper with David Nicol dealing with Fluid Stochastic Petri Nets is still pending. Such fluid models are likely to be extremely useful in modeling the dynamic behavior of ATM networks and process control systems. We expect to finish the paper within the next couple of months.
REPORTS AND ABSTRACTS


Over recent years, a variety of shock-capturing schemes have been developed for the Euler equations of gas dynamics. During this period, it has emerged that one of the more successful strategies is to follow Godunov’s lead and utilize a nonlinear building block known as a Riemann problem. Now, although Riemann solver technology is often thought of as being mature, there are in fact several circumstances for which Godunov-type schemes are found wanting. Indeed, one inherent deficiency is so severe that if left unaddressed, it could preclude such schemes from being used to capture detonation fronts in simulations of complex flow phenomena. In this paper, we highlight this particular deficiency along with some other little known weaknesses of Godunov-type schemes, and we outline one strategy that we have used to good effect in order to produce reliable high resolution simulations of both reactive and nonreactive shock wave phenomena. In particular, we present results for simulations of so-called galloping instabilities and detonation cell phenomena.


A compact scheme is a discretization scheme that is advantageous in obtaining highly accurate solutions. However, the resulting systems from compact schemes are tridiagonal systems that are difficult to solve efficiently on parallel computers. Considering the almost symmetric Toeplitz structure, a parallel algorithm, simple parallel prefix (SPP), is proposed. The SPP algorithm requires less memory than the conventional LU decomposition and is highly efficient on parallel machines. It consists of a prefix communication pattern and AXPY operations. Both the computation and the communication can be truncated without degrading the accuracy when the system is diagonally dominant. A formal accuracy study has been conducted to provide a simple truncation formula. Experimental results have been measured on a MasPar MP-1 SIMD machine and on a Cray 2 vector machine. Experimental results show that the simple parallel prefix algorithm is a good algorithm for the compact scheme on high-performance computers.


Language extensions of Fortran are being developed which permit the user to map data structures to the individual processors of distributed memory machines. These languages allow a programming style in which global data references are used. Current efforts are
focussed on designing a common basis for such languages, the result of which is known as High Performance Fortran (HPF). One of the central debates in the HPF effort revolves around the concept of templates, introduced as an abstract index space to which data could be aligned. In this paper, we present a model for the mapping of data which provides the functionality of High Performance Fortran distributions without the use of templates.


We study the scattering of an incident wave by a flexible panel. The panel vibration is governed by the nonlinear plate equations while the loading on the panel, which is the pressure difference across the panel, depends on the reflected and transmitted waves. Two models are used to calculate this structural-acoustic interaction problem. One solves the three dimensional nonlinear Euler equations for the flow-field coupled with the plate equations (the fully coupled model). The second uses the linear wave equation for the acoustic field and expresses the load as a double integral involving the panel oscillation (the decoupled model). The panel oscillation governed by a system of integro-differential equations is solved numerically and the acoustic field is then defined by an explicit formula. Numerical results are obtained using the two models for linear and nonlinear panel vibrations. The predictions given by these two models are in good agreement but the computational time needed for the "fully coupled model" is 60 times longer than that for "the decoupled model".


In this paper we consider the problem of using reduced order dynamic compensators to control a class of nonlinear parabolic distributed parameter systems. We concentrate on a system with unbounded input and output operators governed by Burgers' equation. We use a linearized model to compute low-order-finite-dimensional control laws by minimizing certain energy functionals. We then apply these laws to the nonlinear model. Standard approaches to this problem employ model/controller reduction techniques in conjunction with LQG theory. The approach used here is based on the finite-dimensional Bernstein/Hyland optimal projection theory which yields a fixed-finite-order controller.


The Lecture begins by sketching some of the background to contemporary jet aeroacoustics. Then it reviews scaling laws for noise generation by low-Mach-number airflows and by turbulence convected at "not so low" Mach number. These laws take into account the influence of Doppler effects associated with the convection of aeroacoustic sources.
Next, a uniformly valid Doppler-effect approximation exhibits the transition, with increasing Mach number of convection, from compact-source radiation at low Mach numbers to a statistical assemblage of conical shock waves radiated by eddies convected at supersonic speed. In jets, for example, supersonic eddy convection is typically found for jet exit speeds exceeding twice the atmospheric speed of sound.

The Lecture continues by describing a new dynamical theory of the nonlinear propagation of such statistically random assemblages of conical shock waves. It is shown, both by a general theoretical analysis and by an illustrative computational study, how their propagation is dominated by a characteristic “bunching” process. That process – associated with a tendency for shock waves that have already formed unions with other shock waves to acquire an increased proneness to form further unions – acts so as to enhance the high-frequency part of the spectrum of noise emission from jets at these high exit speeds.


Waveform multigrid method is an efficient method for solving certain classes of time-dependent PDEs. This paper studies the relationship between this method and the analogous multigrid method for steady-state problems. Using a Fourier-Laplace analysis, practical convergence rate estimates of the waveform multigrid iterations are obtained. Experimental results show that the analysis yields accurate performance prediction.


We present an approach for reducing the number of variables and constraints, which is combined with System Analysis Equations (SAE), for multiobjective optimization-based design. In order to develop a simplified analysis model, the SAE is computed outside an optimization loop and then approximated for use by an optimizer. Two examples are presented to demonstrate the approach.


Many CFD (computational fluid dynamics) and other scientific applications can be partitioned into subproblems. However, in general the partitioned subproblems are very large. They demand high performance computing power themselves, and the solutions of the subproblems have to be combined at each time step. In this paper, the cube-connect cube (CCCube) architecture is studied. The CCCube architecture is an extended hypercube structure with each node represented as a cube. It requires fewer physical links between nodes than the hypercube, and provides the same communication support as the hypercube does on many applications. The reduced physical links can be used to enhance the bandwidth of the remaining links and, therefore, enhance the overall performance. The concept
and the method to obtain optimal CCCubes, which are the CCCubes with a minimum number of links under a given total number of nodes, are proposed. The superiority of optimal CCCubes over standard hypercubes has also been shown in terms of the link usage in the embedding of a binomial tree. A useful computation structure based on a semi-binomial tree for divide-and-conquer type of parallel algorithms has been identified. We have shown that this structure can be implemented in optimal CCCubes without performance degradation compared with regular hypercubes. The result presented in this paper should provide a useful approach to design of scientific parallel computers.


The convergence rate of standard multigrid algorithms degenerates on problems with stretched grids or anisotropic operators. The usual cure for this is the use of line or plane relaxation. However, multigrid algorithms based on line and plane relaxation have limited and awkward parallelism and are quite difficult to map effectively to highly parallel architectures. Newer multigrid algorithms that overcome anisotropy through the use of multiple coarse grids rather than line relaxation are better suited to massively parallel architectures because they require only simple point-relaxation smoothers.

In this paper, we look at the parallel implementation of a V-cycle multiple semicoarsened grid (MSG) algorithm on distributed-memory architectures such as the Intel iPSC/860 and Paragon computers. The MSG algorithms provide two levels of parallelism: parallelism within the relaxation or interpolation on each grid and across the grids on each multigrid level. Both levels of parallelism must be exploited to map these algorithms effectively to parallel architectures. This paper describes a mapping of an MSG algorithm to distributed-memory architectures that demonstrates how both levels of parallelism can be exploited. The result is a robust and effective multigrid algorithm for distributed-memory machines.


Finite difference schemes for the evaluation of first and second derivatives are presented. These second order compact schemes for long-time integration of evolution equations by solving a quadratic constrained minimization problem. The quadratic cost function measures the global truncation error while taking into account the initial data. The resulting schemes are applicable for integration times fourfold, or more, longer than similar previously studied schemes. A similar approach was used to obtain improved integration schemes.


Multigrid methods are good candidates for the resolution of the system arising in Numerical Fluid Dynamics. However, the question is to know if those algorithms which are
efficient for the Poisson equation on structured meshes will still apply well to the Euler and Navier-Stokes equations on unstructured meshes. The study of elliptic problems leads us to define the conditions where a Full Multigrid strategy has $O(N)$ complexity. The aim of this paper is to build a comparison between the elliptic theory and practical CFD problems.

First, as an introduction, we will recall some basic definitions and theorems applied to a model problem. The goal of this section is to point out the different properties that we need to produce an FMG algorithm with $O(N)$ complexity. Then, we will show how we can apply this theory to the fluid dynamics equations such as Euler and Navier-Stokes equations. At last, we present some results which are 2nd-order accurate and some explanations about the behaviour of the FMG process.


The finite-volume and finite-difference implementations of high-order accurate essentially non-oscillatory shock-capturing schemes are discussed and compared. Results obtained with fourth-order accurate algorithms based on both formulations are examined for accuracy, sensitivity to grid irregularities, resolution of waves that are oblique to the mesh, and computational efficiency. Some algorithm modifications that may be required for a given application are suggested. Conclusions that pertain to the relative merits of both formulations are drawn, and some circumstances for which each might be useful are noted.


The dependence of the energy transfer process on the disparity of the interacting scales is investigated in the inertial and far-dissipation ranges of isotropic turbulence. The strategy for generating the simulated flow fields and the choice of a disparity parameter to characterize the scaling of the interactions is discussed. The inertial range is found to be dominated by relatively local interactions, in agreement with the Kolmogorov assumption. The far-dissipation range is found to be dominated by relatively non-local interactions, supporting the classical notion that the far-dissipation range is slaved to the Kolmogorov scales. The measured energy transfer is compared with the classical models of Heisenberg [Z. Physik, *124*, 628, (1948)], Obukhov [Isv. Geogr. Geophys. Ser., *13*, 58, (1949)] and the more detailed analysis of Tennekes and Lumley [*The First Course of Turbulence*, MIT press, (1972)]. The energy transfer statistics measured in the numerically simulated flows are found to be nearly self-similar for wavenumbers in the inertial range. Using the self-similar form measured within the limited scale range of the simulation, we construct an 'ideal' energy transfer function and the corresponding energy flux rate for an inertial range of infinite extent. From this flux rate we calculate the Kolmogorov constant to be 1.5, in excellent agreement with experiments [A.S. Monin and A.M. Yaglom, *Statistical Fluid Mechanics*, Vol. 2, MIT Press, (1975)].

The goal of the research described in this paper is to develop flexible language constructs for writing large data parallel numerical programs for distributed memory (MIMD) multiprocessors. Previously, several models have been developed to support synchronization and communication. Models for global synchronization include SIMD (Single Instruction Multiple Data), SPMD (Single Program Multiple Data), and sequential programs annotated with data distribution statements. The two primary models for communication include implicit communication based on shared memory and explicit communication based on messages. None of these models by themselves seem sufficient to permit the natural and efficient expression of the variety of algorithms that occur in large scientific computations. In this paper, we give an overview of a new language that combines many of these programming models in a clean manner. This is done in a modular fashion such that different models can be combined to support large programs. Within a module, the selection of a model depends on the algorithm and its efficiency requirements. In this paper, we give an overview of the language and discuss some of the critical implementation details.


This paper describes many of the issues in developing an efficient interface for communication on distributed memory machines and proposes a portable interface. Although the hardware component of message latency is less than one microsecond on many distributed memory machines, the software latency associated with sending and receiving typed messages is on the order of 50 microseconds. The reason for this imbalance is that the software interface does not match the hardware. By changing the interface to match the hardware more closely, applications with fine grained communication can be put on these machines. Based on several tests that we have run on the iPSC/860, we propose an interface that will better match current distributed memory machines. The model used in the proposed interface consists of a computation processor and a communication processor on each node. Communication between these processors and other nodes in the system is done through a buffered network. Information that is transmitted is either data or procedures to be executed on the remote processor. The dual processor system is better suited for efficiently handling asynchronous communications compared to a single processor system. The ability to send data or procedure invocations is very flexible for minimizing message latency, based on the type of communication being performed. This paper describes the tests performed and the proposed interface.


An overview describing the use of piezoceramic patches in reducing noise in a structural acoustics setting is presented. The passive and active contributions due to patches which
are bonded to an Euler-Bernoulli beam or thin shell are briefly discussed and the results are incorporated into a 2-D structural acoustics model. In this model, an exterior noise source causes structural vibrations which in turn lead to interior noise as a result of nonlinear fluid/structure coupling mechanisms. Interior sound pressure levels are reduced via patches bonded to the flexible boundary (a beam in this case) which generate pure bending moments when an out-of-phase voltage is applied. Well-posedness results for the infinite dimensional system are discussed and a Galerkin scheme for approximating the system dynamics is outlined. Control is implemented by using LQR optimal control theory to calculate gains for the linearized system and then feeding these gains back into the nonlinear system of interest. The effectiveness of this strategy for this problem is illustrated in an example.


Simplified equations for slender jets are derived for a circular jet of one fluid flowing into an ambient second fluid, the flow being confined in a circular tank. Inviscid flows are studied which include both surface tension effects and Kelvin-Helmholtz instability. For slender jets a coupled nonlinear system of equations is found for the jet shape and the axial velocity jump across it. The equations can break down after a finite time and similarity solutions are constructed, and studied analytically and numerically. The break-ups found pertain to the jet pinching after a finite time, without violation of the slender jet ansatz. The system is conservative and admissible singular solutions are those which conserve the total energy, mass and momentum. Such solutions are constructed analytically and numerically, and in the case of vortex sheets with no surface tension certain solutions are given in closed form.


A number of practically relevant problems involving the impulsive motion or the rapid rotation of bodies immersed in fluid are susceptible to vortex-like instability modes. Depending upon the configuration of any particular problem the stability properties of any high-wavenumber vortices can take on one of two distinct forms. One of these is akin to the structure of Görtler vortices in boundary layer flows whilst the other is similar to the situation for classical Taylor vortices.

Both the Görtler and Taylor problems have been extensively studied when crossflow effects are excluded from the underlying base flows. Recently, studies have been made concerning the influence of crossflow on Görtler modes and here we use a linearised stability analysis to examine crossflow properties for the Taylor mode. This work allows us to identify the most unstable vortex as the crossflow component increases and we show how, like the Görtler case, only a very small crossflow component is required in order to completely stabilise the flow. Our investigation forms the basis for an extension to the nonlinear problem and is of potential applicability to a range of pertinent flows.
Canonical forms and canonical variables for inviscid flow problems are derived. In these forms the components of the system governed by different types of operators (elliptic and hyperbolic) are separated. Both the incompressible and the compressible cases are analyzed and their similarities and differences are discussed. The canonical forms obtained are block upper triangular operator form in which the elliptic and non-elliptic parts reside in different blocks. The full nonlinear equations are treated without using any linearization process. This form enables a better analysis of the equations as well as better numerical treatment. These forms are the analog of the decomposition of the one dimensional Euler equations into characteristic directions and Riemann invariants.

Multilevel (ML) algorithms for eigenvalue problems are often faced with several types of difficulties such as: the mixing of approximated eigenvectors by the solution process, the approximation of incomplete clusters of eigenvectors, the poor representation of solution on coarse levels and the existence of close or equal eigenvalues. Algorithms that do not treat appropriately these difficulties usually fail, or their performance degrades when facing them. These issues motivated the development of a robust adaptive ML algorithm which treats these difficulties, for the calculation of a few eigenvectors and their corresponding eigenvalues, presented in this paper. The main techniques used in the new algorithm include: the adaptive completion and separation of the relevant clusters on different levels, the simultaneous treatment of solutions within each cluster, and the robustness tests which monitor the algorithm's efficiency and convergence. The eigenvectors' separation efficiency is based on a new ML projection technique generalizing the Rayleigh Ritz projection, combined with a novel technique, the backrotations. These separation techniques, when combined with an FMG formulation, in many cases lead to algorithms of $O(qN)$ complexity, for $q$ eigenvectors of size $N$ on the finest level. Previously developed ML algorithms are less focused on the mentioned difficulties. Moreover, algorithms which employ fine level separation techniques are of $O(q^2N)$ complexity and usually do not overcome all these difficulties. Computational examples are presented where Schrödinger type eigenvalue problems in 2-D and 3-D, having equal and closely clustered eigenvalues, are solved with the efficiency of the Poisson multigrid solver. A second order approximation is obtained in $O(qN)$ work, where the total computational work is equivalent to only a few fine level relaxations per eigenvector.

The nonlinear development of disturbances in stratified shear flows (having a local Richardson number of value less than one quarter) is considered. Such modes are initially fast growing but, like related studies, we assume that the viscous, non-parallel spreading of the shear layer results in them evolving in a linear fashion until they reach a position where their
amplitudes are large enough and their growth rates have diminished sufficiently so that amplitude equations can be derived using weakly nonlinear and non-equilibrium critical-layer theories. Four different basic integro-differential amplitude equations are possible, including one due to a novel mechanism; the relevant choice of amplitude equation, at a particular instance, being dependent on the relative sizes of the disturbance amplitude, the growth rate of the disturbance, its wavenumber and the viscosity of the fluid. This richness of choice of possible nonlinearities arises mathematically from the indicial Frobenius roots of the governing linear inviscid equation (the Taylor–Goldstein equation) not, in general, differing by an integer. The initial nonlinear evolution of a mode will be governed by an integro-differential amplitude equations with a cubic nonlinearity but the resulting significant increase in the size of the disturbance’s amplitude leads on to the next stage of the evolution process where the evolution of the mode is governed by an integro–differential amplitude equations with a quintic nonlinearity. Continued growth of the disturbance amplitude is expected during this stage, resulting in the effects of nonlinearity spreading to outside the critical level, by which time the flow has become fully nonlinear.


We prove a cell entropy inequality for a class of high order discontinuous Galerkin finite element methods approximating conservation laws, which implies convergence for the one dimensional scalar convex case.


A three-step hybrid analysis technique, which successively uses the regular perturbation expansion method, the Padé expansion method, and then a Galerkin approximation, is presented and applied to some model boundary value problems. In the first step of the method, the regular perturbation method is used to construct an approximation to the solution in the form of a finite power series in a small parameter ε associated with the problem. In the second step of the method, the series approximation obtained in step one is used to construct a Padé approximation in the form of a rational function in the parameter ε. In the third step, the various powers of ε which appear in the Padé approximation are replaced by new (unknown) parameters {δ_j}. These new parameters are determined by requiring that the residual formed by substituting the new approximation into the governing differential equation is orthogonal to each of the perturbation coordinate functions used in step one. The technique is applied to model problems involving ordinary or partial differential equations. In general, the technique appears to provide good approximations to the solution even when the perturbation and Padé approximations fail to do so. The method is discussed and topics for future investigations are indicated.
Binary dissection is widely used to partition non-uniform domains over parallel computers. This algorithm does not consider the perimeter, surface area, or aspect ratio of the regions being generated and can yield decompositions that have poor communication to computation ratio.

Parametric Binary Dissection (PBD) is a new algorithm in which each cut is chosen to minimize load + \( \lambda \times (\text{shape}) \). In a 2 (or 3) dimensional problem, load is the amount of computation to be performed in a subregion and shape could refer to the perimeter (respectively surface) of that subregion. Shape is a measure of communication overhead and the parameter \( \lambda \) permits us to trade off load imbalance against communication overhead. When \( \lambda \) is zero, the algorithm reduces to plain binary dissection.

This algorithm can be used to partition graphs embedded in 2 or 3-d. Here load is the number of nodes in a subregion, shapes the number of edges that leave that subregion, and \( \lambda \) the ratio of time to communicate over an edge to the time to compute at a node. We present an algorithm that finds the depth \( d \) parametric dissection of an embedded graph with \( n \) vertices and \( e \) edges in \( O(\max[n \log n, de]) \) time, which is an improvement over the \( O(dn \log n) \) time of plain binary dissection. We also present parallel versions of this algorithm; the best of these requires \( O((n/p) \log^3 p) \) time on a \( p \) processor hypercube, assuming graphs of bounded degree.

We describe how PBD is applied to 3-d unstructured meshes and yields partitions that are better than those obtained by plain dissection. We also discuss its application to the color image quantization problem, in which samples in a high-resolution color space are mapped onto a lower resolution space in a way that minimizes the color error.


We present a new collocation method for the numerical solution of partial differential equations. This method uses the Chebyshev collocation points, but because of the way the boundary conditions are implemented, has all the advantages of the Legendre methods. In particular \( L_2 \) estimates can be obtained easily for hyperbolic and parabolic problems.


When surfaces intersect, one may desire to highlight the intersection curve in order to make the shape of the penetrating surfaces more visible. Highlighting the intersection is especially helpful when the surfaces become transparent, because transparency makes the intersections less evident. This paper discusses a technique for locating intersections in screen space using only the information locally available to a pixel. The technique is designed to exploit parallelism at the pixel level and has been implemented on the Pixel-Planes 5 graphics supercomputer.

We consider the use of preconditioning methods to accelerate the convergence to a steady state for both the incompressible and compressible fluid dynamic equations. We also consider the relation between them for both the continuous problem and the finite difference approximation. The analysis relies on the inviscid equations. The preconditioning consists of a matrix multiplying the time derivatives. Hence, the steady state of the preconditioning can change and improve the steady state solutions. An application to flow around an airfoil is presented.


We investigate the stability of two phase Couette flow of different liquids bounded between plane parallel plates. One of the plates has a time dependent velocity in its own plane, which is composed of a constant steady part and a time harmonic component. In the absence of time harmonic modulations the flow can be unstable to an interfacial instability if the viscosities are different and the more viscous fluid occupies the thinner of the two layers. Using Floquet theory, we show analytically in the limit of long waves, that time periodic modulations in the basic flow can have a significant influence on flow stability. In particular, flows which are otherwise unstable for extensive ranges of viscosity ratios, can be stabilized completely by the inclusion of background modulations, a finding that can have useful consequences in many practical applications.


We study the long-wave, modulational, stability of steady periodic solutions of the Kuramoto-Sivashinsky equation. The analysis is fully nonlinear at first, and can in principle be carried out to all orders in the small parameter, which is the ratio of the spatial period to a characteristic length of the envelope perturbations. In the linearized regime we recover a high-order version of the results of Frisch, She and Thual, [1], which shows that the periodic waves are much more stable than previously expected.


A viscous or inviscid cylindrical jet with surface tension in a vacuum tends to pinch due to the mechanism of capillary instability. We construct similarity solutions which describe this phenomenon as a critical time is encountered, for two physically distinct cases: (i) Inviscid jets governed by the Euler equations, (ii) highly viscous jets governed by the Stokes
equations. In both cases the only assumption imposed is that at the time of pinching the jet shape has a radial length scale which is smaller than the axial length scale. For the inviscid case, we show that our solution corresponds exactly to one member of the one-parameter family of solutions obtained from slender jet theories and the shape of the jet is locally concave at breakup. For highly viscous jets our theory predicts local shapes which are monotonic increasing or decreasing indicating the formation of a mother drop connected to the jet by a thin fluid tube. This qualitative behavior is in complete agreement with both direct numerical simulations and experimental observations.


Recent studies have demonstrated the most unstable Görtler vortex mode is found in flows, both two and three-dimensional, with regions of (moderately) large body curvature and these modes reside within a thin layer situated at the base of the conventional boundary layer. Further work concerning the nonlinear development of the most dangerous mode demonstrates that the flow results in a self induced flow reversal. However, prior to the point at which flow reversal is encountered the total streamwise velocity profile is found to be highly inflectional in nature. Previous work then suggests that the nonlinear vortex state will become unstable to secondary, inviscid, Rayleigh wave instabilities prior to the point of flow reversal. Our concern is with the secondary instability of the nonlinear vortex states, which result from the streamwise evolution of the most unstable Görtler vortex mode, with the aim of determining whether such modes can induce a transition to a fully turbulent state before separation is encountered.


In order to study multi-dimensional unstable detonation waves, we have developed a high order numerical scheme suitable for calculating the detailed transverse wave structures of multidimensional detonation waves. The numerical algorithm uses a multi-domain approach so different numerical techniques can be applied for different components of detonation waves. The detonation waves are assumed to undergo an irreversible, unimolecular reaction \( A \rightarrow B \). Several cases of unstable two dimensional detonation waves are simulated and detailed transverse wave interactions are documented. The numerical results show the importance of resolving the detonation front without excessive numerical viscosity in order to obtain the correct cellular patterns.


We have designed a cubic spline wavelet decomposition for the Sobolev space \( H^2(I) \) where \( I \) is a bounded interval. Based on a special "point-wise orthogonality" of the wavelet basis
functions, a fast Discrete Wavelet Transform (DWT) is constructed. This DWT transform will map discrete samples of a function to its wavelet expansion coefficients in \( O(N \log N) \) operations. Using this transform, we propose a collocation method for the initial value boundary problem of nonlinear PDE's. Then, we test the efficiency of the DWT transform and apply the collocation method to solve linear and nonlinear PDE's.


A numerical study of the long-time evolution of a number of cases of inviscid, isotropic, incompressible, three-dimensional fluid and magneto-fluid turbulence has been completed. The results confirm that ideal magnetohydrodynamic turbulence is non-ergodic if there is no external magnetic field present. This is due essentially to a canonical symmetry being broken in an arbitrary dynamical representation. The broken symmetry manifests itself as a coherent structure, i.e., a non-zero time-averaged part of the turbulent magnetic field. The coherent structure is observed, in one case, to contain about eighteen percent of the total energy.


Although the advent of fast and inexpensive parallel computers has rendered numerous previously intractable calculations feasible, many numerical simulations remain too resource-intensive to be directly inserted in engineering optimization efforts. An attractive alternative to direct insertion considers models for computational systems: the expensive simulation is evoked only to construct and validate a simplified input-output model; this simplified input-output model then serves as a simulation surrogate in subsequent engineering optimization studies. We present here a simple "Bayesian-validated" statistical framework for the construction, validation, and purposive application of static computer simulation surrogates. As an example, we consider dissipation-transport optimization of laminar-flow eddy-promoter heat exchangers: parallel spectral element Navier-Stokes calculations serve to construct and validate surrogates for the flowrate and Nusselt number; these surrogates then represent the originating Navier-Stokes equations in the ensuing design process.


Reynolds stress closure models based on the recursion renormalization group theory are developed for the prediction of turbulent separated flows. The proposed model uses a finite wavenumber truncation scheme to account for the spectral distribution of energy. In particular, the model incorporates effects of both local and nonlocal interactions. The nonlocal interactions are shown to yield a contribution identical to that from the \( \epsilon \)-RNG, while the local interactions introduce higher order dispersive effects. A formal analysis of the model is
presented and its ability to accurately predict separated flows is analyzed from a combined theoretical and computational standpoint. Turbulent flow past a backward facing step is chosen as a test case and the results obtained based on detailed computations demonstrate that the proposed recursion-RNG model with finite cut-off wavenumber can yield very good predictions for the backstep problem.


The high Reynolds number (Re) flow past a rapidly rotating circular cylinder is investigated. The rotation rate of the cylinder is allowed to vary (slightly) along the axis of the cylinder, thereby provoking three-dimensional flow disturbances, which are shown to involve relatively massive \(O(Re)\) velocity perturbations to the flow away from the cylinder surface. Additionally, three integral conditions, analogous to the single condition determined in two dimensions by Batchelor (1), are derived, based on the condition of periodicity in the azimuthal direction.


The implementation and performance of a parallel spatial direct numerical simulation (PSDNS) approach on the Intel iPSC/860 hypercube is documented. The direct numerical simulation approach is used to compute spatially evolving disturbances associated with the laminar-to-turbulent transition in boundary-layer flows. The feasibility of using the PSDNS on the hypercube to perform transition studies is examined. The results indicate that the DNS approach can effectively be parallelized on a distributed-memory parallel machine. By increasing the number of processors, nearly ideal linear speedups are achieved with nonoptimized routines; slower than linear speedups are achieved with optimized (machine-dependent library) routines. This slower than linear speedup results because the FFT routine dominates the computational cost and because the FFT routine indicates less than ideal speedups. However, with the machine-dependent routines, the total computational cost decreases by a factor of 4 to 5 compared with standard Fortran routines. The computational cost increases linearly with spanwise, wall-normal, and streamwise grid refinements. The hypercube with 32 processors was estimated to require approximately twice the amount of Cray supercomputer single processor time to complete a comparable simulation; however, it is estimated that a subgrid-scale model, which reduces the required number of grid points and becomes a large-eddy simulation (PSLES), would reduce the computational cost and memory requirements by a factor of 10 over the PSDNS. This PSLES implementation would enable transition simulations on the hypercube at a reasonable computational cost.

Linear stability of the incompressible flow along a streamwise corner is studied by solving the two-dimensional eigenvalue problem governed by partial differential equations. It is found that this fully three-dimensional flow is subject to inviscid instability due to the inflectional nature of the streamwise velocity profile. The higher growth rates for the inviscid instability mode, which is symmetric about the corner bisector, as compared to the viscous Tollmien-Schlichting instability operative away from the corner is consistent with the experimental findings that the corner flow transitions to turbulence earlier than the two-dimensional Blasius flow away from the corner.


The weakly nonlinear interaction of oblique Tollmien-Schlichting waves and longitudinal vortices in compressible, high Reynolds number, boundary-layer flow over a flat plate is considered for all ranges of the Mach number. The interaction equations comprise of equations for the vortex which is indirectly forced by the waves via a boundary condition, whereas a vortex term appears in the amplitude equation for the wave pressure. The downstream solution properties of interaction equations are found to depend on the sign of an interaction coefficient. Compressibility is found to have a significant effect on the interaction properties; principally through its impact on the waves and their governing mechanism, the triple-deck structure. It is found that, in general, the flow quantities will grow slowly with increasing downstream co-ordinate; i.e. in general, solutions do not terminate in abrupt, finite-distance 'break-ups'.


The evolution of three-dimensional disturbances in an incompressible three-dimensional stagnation-point flow in an inviscid fluid is investigated. Since it is not possible to apply classical normal mode analysis to the disturbance equations for the fully three-dimensional stagnation-point flow to obtain solutions, an initial-value problem is solved instead. The evolution of the disturbances provide the necessary information to determine stability and indeed the complete transient as well. It is found that when considering the disturbance energy, the planar stagnation-point flow, which is independent of one of the transverse coordinates, represents a neutrally stable flow whereas the fully three-dimensional flow is either stable of unstable, depending on whether the flow is away from or towards the stagnation point in the transverse direction that is neglected in the planar stagnation point.

A non-similar boundary layer theory for air blowing over a water layer on a flat plate is formulated and studied as a two-fluid problem in which the position of the interface is unknown. The problem is considered at large Reynolds number (based on $x$), away from the leading edge. We derive a simple non-similar analytic solution of the problem for which the interface height is proportional to $x^{1/4}$ and the water and air flow satisfy the Blasius boundary layer equations, with a linear profile in the water and a Blasius profile in the air. Numerical studies of the initial value problem suggests that this asymptotic, non-similar air-water boundary layer solution is a global attractor for all initial conditions.


In this paper we make an investigation of the receptivity of boundary layer flows to Görtler vortex modes. A study by Denier, Hall & Seddougui (1991) of the generation of vortices by wall roughness elements concluded that such elements are extremely poor as mechanisms to stimulate short wavelength modes. That work also examined the equivalent problem pertaining to $O(1)$ wavelength modes but that analysis was in error. We re-examine this problem here and demonstrate how the form of the wall roughness is crucial in determining the vortex stability characteristics downstream of the roughness. In particular we investigate the cases of both isolated and distributed forcing functions and show that in general a distributed function is much more important in generating vortices than are either isolated roughness or free-stream disturbances.


This paper presents a divide-and-conquer ray-traced volume rendering algorithm and a parallel image compositing method, along with their implementation and performance on the Connection Machine CM-5, and networked workstations. This algorithm distributes both the data and the computations to individual processing units to achieve fast, high-quality rendering of high-resolution data. The volume data, once distributed, is left intact. The processing nodes perform local raytracing of their subvolume concurrently. No communication between processing units is needed during this locally ray-tracing process. A subimage is generated by each processing unit and the final image is obtained by compositing subimages in the proper order, which can be determined a priori. Test results on both the CM-5 and a group of networked workstations demonstrate the practicality of our rendering algorithm and compositing method.
The three-dimensional flow of a self-gravitating fluid is numerically simulated using a Fourier pseudospectral method with a logarithmic variable formulation. Two cases with zero total angular momentum are studied in detail, \(32^3\) simulation (Run A) and a \(64^3\) simulation (Run B). Other than the grid size, the primary differences between the two cases are that Run A modelled atomic hydrogen and had considerably more compressible motion initially than Run B, which modelled molecular hydrogen. The numerical results indicate that gravitational collapse can proceed in a variety of ways. In the Run A, collapse led to an elongated tube-like structure, while in the Run B, collapse led to a flatter, disk-like structure.


We present a study of the interaction of small amplitude, unsteady, freestream disturbances with a shock wave induced by a wedge in supersonic flow. These disturbances may be acoustic waves, vorticity waves, or entropy waves (or indeed a combination of all three). Their interactions then generate behind the shock disturbances of all three classes, an aspect that is investigated in some detail, our motivation here being to investigate possible mechanisms for boundary-layer receptivity, caused through the amplification and modification of freestream turbulence through the shock-body coupling. Also, the possibility of enhanced mixing owing to additional vorticity produced by the shock-body coupling is investigated.


This paper describes a highly interactive method for computer visualization of the basic physical process of dispersion and mixing of fluid elements in convection-diffusion systems. It is based on transforming the vector field from a traditionally Eulerian reference frame into a Lagrangian reference frame. Fluid elements are traced through the vector field for the mean path as well as the statistical dispersion of the fluid elements about the mean position by using added scalar information about the root mean square value of the vector field and its Lagrangian time scale. In this way, clouds of fluid elements are traced not just mean paths. We have used this method to visualize the simulation of an industrial incinerator to help identify mechanisms for poor mixing.
Over recent years, Adaptive Mesh Refinement (AMR) algorithms which dynamically match the local resolution of the computational grid to the numerical solution being sought have emerged as powerful tools for solving problems that contain disparate length and time scales. In particular, several workers have demonstrated the effectiveness of employing an adaptive, block-structured hierarchical grid system for simulations of complex shock wave phenomena. Unfortunately, from the parallel algorithm developer's viewpoint, this class of scheme is quite involved; these schemes cannot be distilled down to a small kernel upon which various parallelizing strategies may be tested. However, because of their block-structured nature such schemes are inherently parallel, so all is not lost. In this paper we describe the method by which Quirk's AMR algorithm has been parallelized. This method is built upon just a few simple message passing routines and so it may be implemented across a broad class of MIMD machines. Moreover, the method of parallelization is such that the original serial code is left virtually intact, and so we are left with just a single product to support. The importance of this fact should not be underestimated given the size and complexity of the original algorithm.

While the parallel version currently lacks some of the advanced features of the serial version, it is sufficiently mature that it can be used routinely to perform very large scale simulations of detonation phenomena using workstation clusters. Hence the parallel algorithm has progressed beyond the level of being solely an exercise in computer science to become a powerful research tool for investigating fluid phenomena. Finally, although it will be seen that we have produced a fair amount of paraphernalia to parallelize just a single algorithm, it should be appreciated that the AMR algorithm is itself sufficiently general to be applicable to a large class of problems. And so the method described here could be legitimately construed as being a template for parallelizing block-structured, adaptive grid algorithms.

Complete Exchange requires each of $N$ processors to send a unique message to each of the remaining $N - 1$ processors. For a circuit switched hypercube with $N = 2^d$ processors, the Direct and Standard algorithms for Complete Exchange are optimal for very large and very small message sizes, respectively. For intermediate sizes, a hybrid Multiphase algorithm is better. This carries out Direct exchanges on a set of subcubes whose dimensions are a partition of the integer $d$. The best such algorithm for a given message size $m$ could hitherto only be found by enumerating all partitions of $d$.

The Multiphase algorithm is analyzed assuming a high performance communication network. It is proved that only algorithms corresponding to equipartitions of $d$ (partitions in which the maximum and minimum elements differ by at most 1) can possibly be optimal. The run times of these algorithms plotted against $m$ form a hull of optimality. It is proved that, although there is an exponential number of partitions, (1) the number of faces on this hull is $\Theta(\sqrt{d})$, (2) the hull can be found in $\Theta(\sqrt{d})$ time, and (3) once it has been found, the optimal algorithm for any given $m$ can be found in $\Theta(\log d)$ time.

These results provide a very fast technique for minimizing communication overhead in many important applications, such as matrix transpose, Fast Fourier transform and ADI.

The low cost and availability of clusters of workstations have lead researchers to re-explore distributed computing using independent workstations. This approach may provide better cost/performance than tightly coupled multiprocessors. In practice, this approach often utilizes wasted cycles to run parallel jobs. In this paper we address the feasibility of such a non-dedicated parallel processing environment assuming workstation processes have preemptive priority over parallel tasks. We develop an analytical model to predict parallel job response times. Our model provides insight into how significantly workstation owner interference degrades parallel program performance. A new term \textit{task ratio}, which relates the parallel task demand to the mean service demand of non parallel workstation processes, is introduced. We propose that \textit{task ratio} is a useful metric for determining how large the demand of a parallel applications must be in order to make efficient use of a non-dedicated distributed system.


We consider preconditioning methods to accelerate convergence to a steady state for the incompressible fluid dynamic equations. The analysis relies on the inviscid equations. The preconditioning consists of a matrix multiplying the time derivatives. Thus the steady state of the preconditioned system is the same as the steady state of the original system. We compare our method to other types of pseudo-compressibility. For finite difference methods preconditioning can change and improve the steady state solutions. An application to viscous flow around a cascade with a non-periodic mesh is presented.


We consider positivity preserving property of first and higher order finite volume schemes for one and two dimensional compressible Euler equations of gas dynamics. A general framework is established which shows the positivity of density and pressure whenever the underlying one dimensional first order building block based on an exact or approximate Riemann solver and the reconstruction are both positivity preserving. Appropriate limitation to achieve high order positivity preserving reconstruction is described.
A class of approximations \( \{ S_{N,M} \} \) to a periodic function \( f \) which uses the ideas of Padé, or rational function, approximations based on the Fourier series representation of \( f \), rather than on the Taylor series representation of \( f \), is introduced and studied. Each approximation \( S_{N,M} \) is the quotient of a trigonometric polynomial of degree \( N \) and a trigonometric polynomial of degree \( M \). The coefficients in these polynomials are determined by requiring that an appropriate number of the Fourier coefficients of \( S_{N,M} \) agree with those of \( f \). Explicit expressions are derived for these coefficients in terms of the Fourier coefficients of \( f \). It is proven that these “Fourier-Padé” approximations converge point-wise to \( (f(x^+) + f(x^-))/2 \) more rapidly (in some cases by a factor of \( 1/k^{2M} \)) than the Fourier series partial sums on which they are based. The approximations are illustrated by several examples and an application to the solution of an initial, boundary value problem for the simple heat equation is presented.

An enhanced diffusion-reaction reaction system (DRS) is proposed as a statistical model for the evolution of multiple scalars undergoing mixing and reaction in an isotropic turbulence field. The DRS model is close enough to the scalar equations in a reacting flow that other statistical models of turbulent mixing that decouple the velocity field from scalar mixing and reaction (e.g. mapping closure model, assumed-pdf models) cannot distinguish the model equations from the original equations. Numerical simulations of DRS are performed for three scalars evolving from non-premixed initial conditions. A simple one-step reversible reaction is considered. The data from the simulations are used (i) to study the effect of chemical conversion on the evolution of scalar statistics, and (ii) to evaluate other models (mapping-closure model, assumed multivariate \( \beta \)-pdf model).

Compressible stability of growing boundary layers is studied by numerically solving the partial differential equations under a parabolizing approximation. The resulting parabolized stability equations (PSE) account for non-parallel as well as nonlinear effects. Evolution of disturbances in compressible flat-plate boundary layers are studied for freestream Mach numbers ranging from 0 to 4.5. Results indicate that the effect of boundary-layer growth is important for linear disturbances. Nonlinear calculations are performed for various Mach numbers. Two-dimensional nonlinear results using the PSE approach agree very well with those from direct numerical simulations using the full Navier-Stokes equations while the required computational time is less by an order of magnitude. Spatial simulations using PSE have been carried out for both the fundamental and subharmonic type breakdown for a Mach 1.6 boundary layer. The promising results obtained in this study show that the
PSE method is a powerful tool for studying boundary-layer instabilities and for predicting transition over a wide range of Mach numbers.


Subspace iteration is a reliable and cost effective method for solving positive definite banded symmetric generalized eigenproblems, especially in the case of large scale problems. This paper discusses an algorithm that makes use of two parallel banded solvers in subspace iteration. A shift is introduced to decompose the banded linear systems into relatively independent subsystems and to accelerate the iterations. With this shift, an eigenproblem is mapped efficiently into the memories of a multiprocessor and a high speed-up is obtained for parallel implementations. An optimal shift is a shift that balances total computation and communication costs. Under certain conditions, we show how to estimate an optimal shift analytically using the decay rate for the inverse of a banded matrix, and how to improve this estimate. Computational results on iPSC/2 and iPSC/860 multiprocessors are presented.


We analytically study the influence of convection caused by horizontal heat transfer through the sides of a vertical Bridgman apparatus. We consider the case when the heat transfer across the side walls is small so that the resulting interfacial deformation and fluid velocities are also small. This allows us to linearize the Navier-Stokes equations and express the interfacial conditions about a planar interface through a Taylor expansion. Using no tangential stress conditions on the side walls, asymptotic expressions for both the interfacial slope and radial segregation at the crystal-melt interface are obtained in closed form in the limit of large thermal Rayleigh number. It is suggested that these can be reduced by appropriately controlling a specific heat transfer property at the edge of the insulation zone in the solid side.


The aim of this article is to determine the stability characteristics of a Rayleigh layer, which is known to occur when the fluid above a flat plate has a velocity imparted to it (parallel to the plate). This situation is intrinsically unsteady, however as a first approximation we consider the instantaneous stability of the flow. The Orr-Sommerfeld equation is found to govern fixed downstream wavelength linear perturbations to the basic flow profile. By the solution of this equation we can determine the Reynolds numbers at which the flow is neutrally stable; this quasi-steady approach is only formally applicable for infinite Reynolds
numbers. We shall consider the large Reynolds number limit of the original problem and use a three deck mentality to determine the form of the modes. The results of the two calculations are compared, and the linear large Reynolds number analysis is extended to consider the effect of weak nonlinearity in order to determine whether the system is sub or super critical.
### ICASE COLLOQUIA
**April 1, 1993 - September 30, 1993**

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| Sanjeev Setia, University of Maryland  
“Scheduling Policies for Multiprogrammed Distributed Memory Parallel Computers” | April 5 |
| Thomas M. Eidson, High Technology Corporation  
“A Parallel/Distributed Memory Programming Strategy for a Periodic Tridiagonal Solver” | April 7 |
| Vinh That Ton, University of California  
“A Numerical Method for Mixing/Chemically Reacting Compressible Flow with Finite Rate Chemistry” | April 12 |
| Murshed Hossain, University of Delaware  
“Boundary Conditions for the Simulation of Compressible Convection” | April 13 |
| David G. Crighton, University of Cambridge  
“Nonlinear Theory of the Broadbent-Moore Compressible Vortex Instability” | April 14 |
| Sir James Lighthill, University College London  
“An Active Mechanism for Drag Reduction by Herring” | April 20 |
| Shlomo Ta’asan, ICASE  
“Canonical Forms for Inviscid Flow Problems” | April 21 |
| Maurizio Pandolfi, Politecnico di Torino  
“Non Equilibrium Phenomena in Compressible Flows” | April 22 |
| Samuel Temkin, Rutgers University  
“Acoustics Agglomeration of Aerosols” | April 26 |
| C. David Pruett, Analytical Services and Materials, Inc.  
“Spatial DNS for High-Speed Flows – The Devil is in the Details” | April 28 |
| Don Burgess, Los Alamos National Laboratory  
“Modeling Turbulence in Flows with a Strong Rotating Component” | May 3 |
| David Banks, ICASE  
“Technology and Applications for Virtual Environments” | May 4 |
| Xian-He Sun, ICASE  
“Scalability of Parallel Algorithm-Machine Combinations” | May 5 |
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<td>&quot;Numerical Calculations of Weak Shock Reflections Near Grazing Incidence&quot;</td>
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<td>&quot;Encounters with Turning Points&quot;</td>
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<td>&quot;Cyclo-difference Techniques for Hyperbolic Systems&quot;</td>
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<td>James Geer, State University of New York</td>
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<td>&quot;Rational Trigonometric Approximations using Fourier Series Partial Sums&quot;</td>
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<td>&quot;Vorticity-Creation/Reaction on a Solid Wall and Applications to Aeroacoustics,</td>
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<td>Vortex Controls and Vorticity-Based Numerical Methods&quot;</td>
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<td>Lionel M. Ni, Michigan State University</td>
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<td>&quot;Issues in Scalable Library Design for Massively Parallel Computers&quot;</td>
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<td>&quot;A Spectral Approach for Partitioning and Ordering Finite Element Systems&quot;</td>
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<td>Sesh Venugopal, Rutgers University</td>
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<td>&quot;Parallelizing Unstructured Sparse Computations on Large-Scale Multiprocessors&quot;</td>
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<td>Philip Roe, University of Michigan</td>
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<td>&quot;Very Accurate Long Range Integration of Multidimensional Wave Phenomena&quot;</td>
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<td>Theodore Johnson, University of Florida</td>
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<td>&quot;Issues in Performance Modeling of Mass Storage Systems&quot;</td>
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<td>David Kopriva, Florida State University</td>
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<td>&quot;A Multidomain Spectral Method for Viscous Compressible Flows&quot;</td>
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| Graham Horton, Erlangen University, Germany  
  “A Parallel Space-Time Multigrid Method for Parabolic PDE’s” | August 18  |
| Hillel Tal-Ezer, Tel-Aviv University, Israel  
  “GIS - General Iterative Solver” | August 23  |
| David Banks, ICASE  
  “The Best of SIGGRAPH 93: Highlights of the Technical Session” | August 23  |
| Roddam Narasimha, National Aeronautical Laboratory, Bangalore, India  
  “Stability Theory in Spatially Developing Flows” | August 27  |
| Daniele Funaro, Pavia University, Italy  
  “An Alternative Approach to the Analysis and the Approximation of the Incompressible Navier-Stokes Equations” | August 30  |
| Amiram Harten, Tel-Aviv University, Israel  
  “Multiresolution Representation of Data and Applications, Part I” | September 7 |
| Amiram Harten, Tel-Aviv University, Israel  
  “Multiresolution Representation of Data and Applications, Part II” | September 9 |
| Anastasios M. Lappas, California Institute of Technology  
  “Riemann Invariant Manifolds for the Compressible Euler Equations” | September 10 |
| Amiram Harten, Tel-Aviv University, Israel  
  “Multiresolution Representation of Data and Applications, Part III” | September 15 |
| Saleh Tanveer, Ohio State University  
  “Singularities of the Euler Equation and Hydrodynamic Stability” | September 16 |
| Craig Wittenbrink, University of Washington  
  “Designing Optimal Parallel Volume Rendering Algorithms” | September 20 |
| Saul Abarbanel, Tel-Aviv University, Israel  
  “Issues in Long Time Integration” | September 21 |
| Gerald L. Browning and Heinz-Otto Kreiss, Collins, Colorado, 80523, USA  
  “The Impact of Rough Forcing on Systems with Multiple Time Scales” | September 24 |
| Katepalli R. Sreenivasan, Yale University  
  “Scaling in Turbulence” | September 30 |
ICASE SUMMER ACTIVITIES

The summer program for 1993 included the following visitors:

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<td>Abarbanel, Saul</td>
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<td>Harten, Amiram</td>
<td>9/06 – 10/1</td>
<td>Applied &amp; Numerical Mathematics</td>
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<td>Hemker, Pieter W.</td>
<td>7/26 – 8/06</td>
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<td>Holliday, Mark A.</td>
<td>7/12 – 7/23</td>
<td>Computer Science</td>
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<td>Horton, Graham</td>
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<td>Jamieson, Lee</td>
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<td>Applied &amp; Numerical Mathematics</td>
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<td>Jordan, Harry F.</td>
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<td>University of Colorado, Boulder</td>
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<td>Kapila, Ashwani K.</td>
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<td>Karpel, Mordechay</td>
<td>8/16 – 9/17</td>
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<td>Israel Institute of Technology</td>
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<td>Keyes, David Yale University</td>
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<td>Kopriva, David Florida State University</td>
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<td>Kozusko, Frank Old Dominion University</td>
<td>6/07 - 7/02</td>
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<td>Kruger, Bruce L. New York University</td>
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<td>Landahl, Marten Massachusetts Institute of Technology</td>
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<td>Leemis, Larry College of William &amp; Mary</td>
<td>7/05 - 7/30</td>
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<td>Liandrat, Jacques I.M.S.T., Marseille, France</td>
<td>8/09 - 9/03</td>
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<td>Liandrat, Marie I.M.S.T., Marseille, France</td>
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<td>Lilley, Geoffrey University of Southampton, England</td>
<td>7/01 - 12/31</td>
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<td>Mukunda, Hanasoge S. Indian Institute of Science, India</td>
<td>5/24 - 6/25</td>
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<td>Narahari, Bhagir George Washington University</td>
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<td>Nicol, David M.</td>
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<td>College of William &amp; Mary</td>
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<td>Parameswaran, Siva</td>
<td>6/07 – 7/02</td>
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<td>Powell, Kenneth</td>
<td>6/21 – 7/02</td>
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<td>Radespiel, Rolf</td>
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<td>DLR, Institute for Design Aerodynamics, Germany</td>
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<td>Reed, Daniel A.</td>
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<td>University of Michigan, Ann Arbor</td>
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<td>Ting, Lu Courant Institute of Technology</td>
<td>6/07 - 6/11, 7/12 - 7/16, 8/08 - 8/15</td>
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<td>van Leer, Bram University of Michigan, Ann Arbor</td>
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OTHER ACTIVITIES

On April 19, 1993, Sir James Lighthill, University College London, inaugurated the Theodorsen Lectureship Award with a lecture at the H.J.E. Reid Conference Center entitled “Some Aspects of the Aeroacoustics of High-Speed Jets.” This award is sponsored biennially by ICASE and NASA Langley Research Center to recognize individuals who have distinguished themselves by making significant theoretical contributions in the field of aeronautical sciences and engineering.

A program celebrating the 20th anniversary of ICASE was held on May 25, 1993 at the H.J.E. Reid Conference Center at Langley Research Center. Speaking at the program were the past and present ICASE and NASA personnel, as well as university researchers having close associations with ICASE. A twenty-year anniversary volume was prepared and given to all in attendance.

On June 1-5, 1993, ICASE and NASA LaRC co-sponsored a Short Course on Transition at the OMNI Hotel in Newport News, VA. The objective of this course was to provide scientists and engineers with a broad view of experimental, computational and theoretical methods applied to the study of mechanisms leading to transition to turbulence. There were 40 attendees. A proceedings from the course will be forthcoming.

ICASE and NASA LaRC also co-sponsored a Workshop on Software Tools and Techniques for Performance and Reliability Estimation on June 17-18, 1993. The Workshop was held at ICASE and brought together researchers and users of software tools to understand and predict their “behavior” which can mean performance, reliability, and correctness. There were 42 researchers in attendance at the workshop.

Scientists and doctoral students from around the world participated in the ICASE/LaRC Workshop on Transition, Turbulence, and Combustion, held at NASA Langley Research Center during June 7 - July 2. Subjects covered at this highly successful workshop, the third in its series, included:

**Transition:** Receptivity, linear stability, nonlinear stability, direct and large-eddy simulation, and phenomenological modeling of the transition zone.
**Turbulence:** Development of closures for heat and mass flux correlations, second-order closures for high Reynolds number flows, the modeling of compressibility effects, and RNG theory.

**Combustion:** The structure of strained, laminar hydrogen-air counterflow diffusion flames, and novel mixing enhancement techniques.

There were 96 participants, with numerous specialized talks and panel discussions throughout the workshop. A formal proceedings is forthcoming.

The ICASE/LaRC Short Course on Parallel Computation was held July 26-30, 1993 at the Radisson Hotel in Hampton, VA. The objective of this course provided an overview of parallel computing and the issues that affect the performance of parallel programs. There were 76 attendees and a formal proceedings will be published.

The ICASE/LaRC Short Course on Parallel Computation was held the last week of July at the Hampton Radisson Hotel. This week-long course, attracting 76 scientists and engineers from around the world, provided an overview of parallel computing and the issues that affect the performance of parallel programs. Topics and speakers were:

**Parallel Architectures:** G. Fox and D. Nicol

**Languages and Tools:** D. Walker, A. Geist, P. Mehrotra, D. Reed, K. Kennedy, and J. Saltz

**Parallel Numerical Methods:** A. Sameh, J. Van Rosendale, and D. Keyes

A formal proceedings will be published.
ICASE STAFF

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Rachel A. Lomas, Payroll and Accounting Clerk

Rosa H. Milby, Executive Secretary/Visitor Coordinator

Shelly D. Millen, Technical Publications Secretary

Emily N. Todd, Conference Manager

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James P. Kendall, Jet Propulsion Laboratory.

Heinz-Otto Kreiss, Professor, Department of Mathematics, University of California at Los Angeles.

Sanjoy Mitter, Professor of Electrical Engineering, Massachusetts Institute of Technology.
Robert O'Malley, Jr., Chairman, Department of Applied Mathematics, University of Washington.

Steven A. Orszag, Professor, Program in Applied & Computational Mathematics, Princeton University.

Eli Reshotko, Department of Mechanical and Aerospace Engineering, Case Western University.

John Rice, Head, Department of Computer Science, Purdue University.

Ahmed Sameh, Professor, Center for Supercomputing Research and Development, University of Illinois at Urbana.

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Sutanu Sarkar - Ph.D., Mechanical and Aerospace Engineering, Cornell University, 1988. Professor, Department of AMES, University of California, San Diego. Fluid Mechanics [Turbulence in High-Speed Compressible Fluid Dynamics]

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This report summarizes research conducted at the Institute for Computer Applications in Science and Engineering in applied mathematics, fluid mechanics, and computer science during the period April 1, 1993 through September 30, 1993.