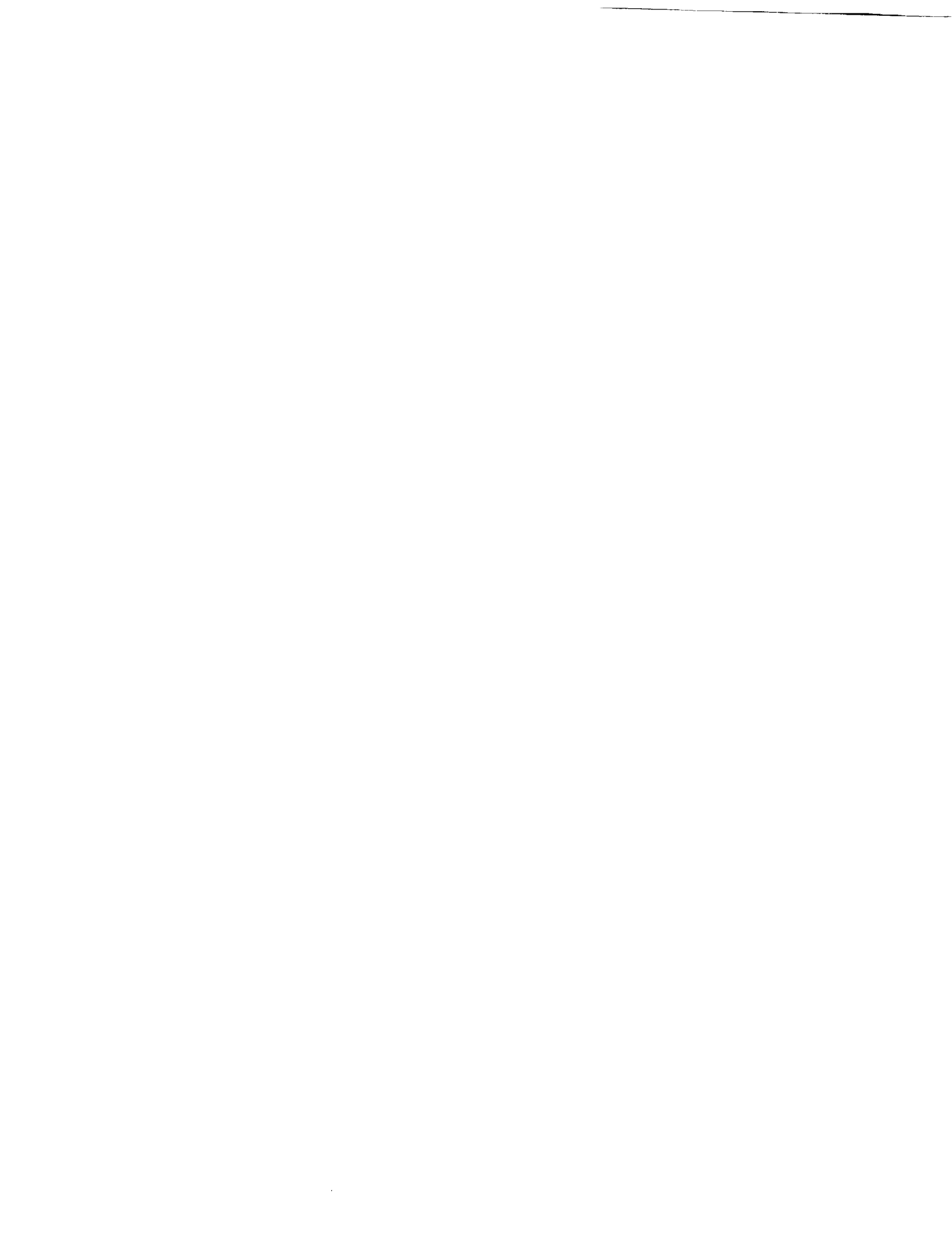


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## INTRODUCTION

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

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

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

The major categories of the current ICASE research program are:

- Numerical methods, with particular emphasis on the development and analysis of basic numerical algorithms;
- Control and parameter identification problems, with emphasis on effective numerical methods;
- Computational problems in engineering and the physical sciences, particularly fluid dynamics, acoustics, and structural analysis;
- Computer systems and software for parallel computers.

ICASE reports are considered to be primarily preprints of manuscripts that have been submitted to appropriate research journals or that are to appear in conference proceedings. A list of these reports for the period October 1, 1989 through March 31, 1990 is given in the Reports and Abstracts section which follows a brief description of the research in progress.

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## RESEARCH IN PROGRESS

### Saul Abarbanel

The work on "spurious" oscillations due to non-characteristic imposition of boundary conditions, reported in ICASE Report No. 90-16, has now branched out to become an investigation on possible interaction of inflow and outflow boundary conditions to produce oscillatory results with more than a single "spurious" frequency. This work, together with D. Gottlieb, is in progress and some of the new results will be reported on in the Third International Conference on Hyperbolic Problems to be held June 11-15, 1990 in Uppsala, Sweden.

A new approach to accelerating convergence to steady state is also being studied together with D. Gottlieb. The idea is to generalize the concept of local-time stepping by minimizing the resulting residual (in a suitable norm that accounts also for boundary conditions). One then gets, even for linear problems, a distribution of Courant numbers that depends on the solution at the previous "time-step". The method was tried on a model one-dimensional Burgers problem (with a stiff source term and a highly stretched mesh). The convergence rate, in terms of the number of iterations required to reduce the residual by 5 orders of magnitude, showed an order of magnitude improvement (typically 4 vs. 55 iterations) in comparison to standard local-time stepping methods wherein the local Courant number is determined a priori from linear stability theory. This work will also be presented at the Uppsala conference.

### H. T. Banks and Fumio Kojima

We are continuing our investigations (in collaboration with W. Winfree of the Instrument Research Division, LaRC) on inverse problems arising in thermal testing of materials in space transportation systems and passenger airplanes. A spline-based parameter estimation technique has been developed using techniques and ideas related to the 'method of mapping'. The ideas developed were successfully tested with the experimental data from IRD laboratories at NASA Langley. We are currently pursuing investigations to further refine our methods with regard to ease and accuracy in detection and characterization of flaws with thermal based methods. Furthermore, our results are now extended to the case of more complicated structures such as might occur in airplanes. The domain decomposition technique as well as the 'method of mapping' plays an important role in our approach.

**H. Scott Berryman, Charles Koelbel, Piyush Mehrotra, and Joel Saltz**

We are developing techniques which allow a nonshared memory multiprocessor (such as ICASE's iPSC/860) to be programmed at a higher level than is currently possible. Our research explores the efficient implementation, on distributed machines, of programs involving accesses to globally defined data structures. It is natural to use operations on globally defined data structures to express data parallel algorithms typically used in scientific applications. We have placed particular emphasis on examining optimizations that are suited to parallel loops over distributed globally defined arrays.

Our work can be broken down into four interrelated areas: handling regular problems, handling irregular problems, run-time support, and compiler implementation.

In all cases, our approach is to transform parallel do loops over globally defined data structures into code that executes on each processor. The code actually executed by each processor in a distributed memory machine can directly reference elements of global data structures that are stored on that processor. Data elements that are stored on other processors must first be communicated by message passing. For efficiency, these nonlocal elements must be prefetched before the actual computation and stored in local memory. Two techniques are needed to deal with this prefetching: one for regular problems and one for irregular problems.

In regular problems, such as solving PDEs on regular meshes and dense linear algebra applications, the pattern of nonlocal data accesses can be specified analytically at compile time, based on analysis of the program. In this case, it is possible to produce very efficient code by using this specification to generate the appropriate send and receive statements. We are pursuing this aspect of the work by deriving the necessary analytical formulas and by incorporating them into a compiler.

In irregular problems, such as solving PDEs on unstructured meshes and sparse matrix algorithms, the communications pattern depends on the input data. This typically arises due to some level of indirection in the code. In this case, it is not possible to predict what data must be prefetched. We deal with this lack of information by transforming the original parallel loop into two constructs which we call the **inspector** and **executor**. During program execution, the **inspector** examines the data references made by a processor and calculates what off-processor data needs to be fetched and where that data will be stored once it is received. The **executor** loop then uses the information from the **inspector** to implement the actual computation. We are pursuing this aspect of the work by supplying user subroutines to implement **inspector/executor** pairs in existing languages and by generating the **inspector/executor** code in a compiler. We have described some of the facets of this work in "A Scheme for Supporting Automatic Data Migration on Multicomputers"

by Mirchandaney, Saltz, Mehrotra, and Berryman and in "Parallel Loops on Distributed Machines" by Koelbel, Mehrotra, Saltz, and Berryman. Both of these papers will appear in "Proceedings of the Fifth Distributed Memory Conference," Charleston, South Carolina, April 1990.

For run-time support we are developing a set of primitives (PARTI - Parallel Automated Runtime Toolkit at ICASE) which will be callable from FORTRAN or other languages. The PARTI system is a set of primitives that can be used to implement a wide range of scientific algorithms on distributed memory machines. These primitives support various run-time operations required by programs that need to make use of an embedded shared name space on a distributed machine. In addition, the primitives are used to study compile-time techniques that can be incorporated into a compiler for distributed memory architectures.

The PARTI primitives are initialized by specifying a mapping into distributed memory for each globally defined multidimensional array. The primitives include procedures that allow one to scatter and gather array elements to the distributed memory. Primitives also are implemented that support several different methods of caching and retrieving copies of off-processor data.

The PARTI system is organized into two levels. The lower level supports memory operations such as scatters and gathers across processors. The higher level binds mapping information to distributed arrays and uses this information to call the lower level primitives. The primitives allow the storage of information about memory access patterns so that memory operations with the same address calculations need not repeat these calculations. Send/receive schedules are generated for memory operations. The schedules may be stored and reused as well. This is particularly important in iterative codes. A preliminary description of these primitives can be found in "Execution Time Support for Scientific Programs on Distributed Memory Machines" by Berryman, Saltz, and Scroggs; this will appear in the Proceedings of the SIAM Conference on Parallel Processing for Scientific Computing, Chicago, Illinois, December 1989.

In the compiler implementation area, we have designed the Kali language as a testbed for implementing these techniques. The analysis for both regular and irregular problems is incorporated into the compiler. We are currently testing and enhancing the compiler and expect to eventually use it for realistic problems.

### **Shahid Bokhari**

The multigrid method, an efficient procedure for solving partial differential equations, has very poor utilization when implemented on a massively parallel processor. We are exploring techniques for pipelining several parallel multigrid algorithms. By carefully organizing our

computations, we are able to achieve very significant increases in utilization. An ICASE report describing this work will be completed soon.

A second effort is focused on the development of a network flow model for load balancing in circuit-switched multicomputers. In multicomputers that utilize circuit switching or wormhole routing, communication overhead depends largely on link contention – the variation due to distance between nodes is negligible. This has a major impact on the load balancing problem. In this case, there are some nodes with excess load (sources) and others with a deficit of load (sinks), and it is required to find which sources should transmit to which sinks so as to avoid contention. The problem is made complex by the fact that routing on currently available machines is hardwired. (On the Intel iPSC-2 and iPSC/860, the ‘e-cube’ algorithm is used; the Symult 2100 employs a ‘row-column’ strategy.) Thus the user can control only which nodes communicate but not how the messages are routed.

Network flow models of message flow in the mesh and the hypercube have been developed to solve this problem. The crucial property of these models is the correspondence between minimum cost flows and correctly routed messages. To solve a given load balancing problem, a minimum cost flow algorithm is applied to the network. This permits us to determine efficiently a maximum contention free matching of sources to sinks which, in turn, tells us how much of the given imbalance can be eliminated without contention. An ICASE report describing this research is nearing completion.

Experiments have been conducted on the Intel IPSC/860 hypercube in order to evaluate the overhead of interprocessor communication. It is demonstrated that (1) contrary to popular belief, the distance between two communicating processors has a significant impact on communication time, (2) edge contention can increase communication time by a factor of more than 7, and (3) node contention has no measurable impact.

### **John Burns**

We are completing an ICASE report on the application of linear quadratic regulator theory to the problem of stability enhancement for the Burgers’ equation. In particular, optimal feedback gain operators were computed by minimizing an energy functional based on a linearization of the nonlinear model. These linear feedback control laws were then applied to the nonlinear Burgers’ equation and several theoretical and numerical results were obtained for the nonlinear closed-loop system. A computational scheme was developed to compute the optimal functional gains and several numerical experiments were performed. The following important observations were made:

1. The functional gains strongly depend on the location of the “sensors” used in the cost



functional. In the case where the cost functional contained "averaged gradients", the functional gains were discontinuous at those points where the gradients were measured.

2. The closed-loop system does decay at a faster rate than the open-loop (Burger's equation) and for large Reynolds number the steep gradients were smoothed by full linear state feedback.
3. The LQR gains computed on low Reynolds number linearized models also enhanced stability for the nonlinear problem over a wide range of Reynolds numbers. Although the large gradients were still smoothed, performance was decreased. However, the closed-loop system was more stable than the open-loop.

These results provide some insight into the more complex problem of fluid flow control. We are continuing our efforts on active control of several fluid/structure problems.

### **Richard Carter**

The interaction of structural design with control law formulation is an important topic in the construction of large scale, flexible space structures. By formulating the design process as a numerical optimization problem using engineering design goals as merit functions and constraints, improved structures and control laws can be determined simultaneously. The optimization problems arising from this approach are typically very computationally intensive, and are often highly nonlinear, nonconvex, and poorly conditioned, so that robust and efficient solution algorithms are imperative. In conjunction with the Control-Structures Interaction (CSI) group at LaRC, simulated model structures are being examined to develop methodology and to investigate features of optimization problems of this type. A variety of solution techniques are being applied to an Earth Pointing System (EPS) simulation model in order to identify the most promising approaches. Early difficulties associated with jump discontinuities and discontinuous gradients in some proposed design constraints/goals have been alleviated by substituting carefully selected, smooth merit functions provided by Peiman Maghami of the CSI-ADM team. Several new approaches for self-scaling the perturbation level in finite difference gradient calculations are also being pursued.

Another topic under investigation involves the robustness of optimization algorithms when gradient computations are inexact. Trust region methods and linesearch methods are the two major approaches to creating robust algorithms. Previous theoretical work and extensive numerical testing have shown algorithms based on the trust region methodology to be exceptionally robust with respect to gradient errors, while simple examples exist to suggest that linesearch algorithms are potentially very fragile with respect to even small errors.

Nevertheless, a recent software study at Cornell found two implementations of the linesearch approach that were competitive when finite difference gradients were used. I am currently examining these results to determine whether they are an artifact of the experimental design of the study (which compared different finite difference routines rather than specifically addressing trust region versus linesearch methodologies), or whether they reveal unknown principles about the behavior of linesearch methods.

### **Leon M. Clancy**

ICASE has begun the process of converting its Sun network to SPARC based workstations running the 4.1 version of the operating system. In addition, two Silicon Graphics Personal Iris workstations have been integrated into the network. Other equipment upgrades include the installation of additional memory for SPARCstations and the file servers.

### **Thomas W. Crockett**

The iPSC/2 hypercube computer was upgraded to an iPSC/860, with additional I/O capacity added. The system was checked out and made available to users. Accounting procedures were established to monitor processor and disk utilization. Benchmarks show that the upgraded system ranges from 5 to 35 times faster for double-precision floating-point computations. Substantial improvements are expected as the compilers mature. New releases of the X Window System and Andrew were installed on the ICASE Suns. A set of default configuration files were built to make it easier for novice users to get started with X and Andrew.

### **Naomi Decker**

Research is proceeding along two paths with a common goal: an efficient and robust parallel multigrid algorithm for solving transonic and hypersonic compressible flow problems. The first path is the development of a good sequential multigrid code using semicoarsened multigrid algorithms with implicit relaxations. Past research in robust multigrid algorithms with J. VanRosendale showed that the coarsening of the grid in only one direction, and using an implicit method in the orthogonal direction(s), is an effective and efficient strategy for solving elliptic partial differential equations. The insensitivity of these methods to grids with high aspect ratio and to directionally-biased data dependencies has lead us to extend these methods to solve the non-elliptic systems arising in computational fluid dynamics. We wish to compare the efficiency of these new multigrid methods with easily parallelizable, explicit

Runge-Kutta, fully coarsened, multigrid algorithms. The Runge-Kutta multigrid algorithms, developed by A. Jameson for transonic calculations, can also be used for hypersonic problems, as shown in work with E. Turkel.

For the Euler or Navier-Stokes equations, the use of implicit time stepping requires the inversion of block tridiagonal systems, which can be efficiently solved using the block version of the Thomas algorithm for Gaussian elimination. However, since the implicit methods involve global data dependencies, their efficient parallel implementation is considerably more difficult and non-intuitive than for the explicit methods. Despite the extra effort involved, the potential for increased robustness justifies a careful examination of the implicit methods for parallel architectures. Thus, the other path is the parallelization of implicit schemes. We have considered various partitioning and scheduling schemes for alleviating the effects of the global data dependencies. The communication and the computation aspects of these methods have been analyzed in the overall context of the solution process, including, for example, the effects of the various other data dependencies resulting from the boundary condition and residual computations. Performance of the proposed methods are being verified on the Victor multiprocessor system, a message passing architecture developed at the IBM, T. J. Watson Research Center. A report summarizing these results is in preparation.

### Peter Duck

Work following on from ICASE Report Nos. 89-19 and 90-14 continues on the temporal stability of axisymmetric supersonic boundary layers. Most recently the effect of wall surface cooling (and heating) has been investigated. This indicates that, just as in the planar case (which has been the subject of much investigation over the years), cooling generally (i) stabilizes the so-called "first mode" of instability, but (ii) de-stabilizes the "second mode" of instability. Curvature is found to generally play a stabilizing role on the inviscid stability of the flow. In connection with this work, a number of computations are being carried out jointly with Dr. M. G. Macaraeg (Fluid Mechanics Division, LaRC) involving the full (small disturbance) equations, with a view to comparing with a number of asymptotic theories, including those in ICASE Report Nos. 89-19 and 90-14.

Work is also continuing with R. Bodonyi on 2D receptivity problems, in particular investigating the interaction between a suction slot and a small amplitude unsteady freestream disturbance. These computations lead to a prediction of the amplitude of resulting Tollmien-Schlichting waves.

Very recently, this type of work has been extended to three-dimensions. In particular the effect of a three-dimensional surface distortion inside a boundary layer on a small amplitude, unsteady, freestream disturbance is currently being computed.

## **Thomas Eidson**

In collaboration with M. Y. Hussaini and T. A. Zang (Fluid Mechanics Division, LaRC), the filtering analysis of a direct simulation (DNS) of the turbulent Rayleigh-Benard problem has been completed and a paper is currently being written. Briefly, a large eddy simulation (LES) type filter was used to split the velocity and temperature fields calculated in the DNS into a larger scale or filtered part and a smaller scale or fluctuation part. By varying the filter width, information for a wide range of flow scales can be ascertained. The components of kinetic energy equations for the filtered and fluctuation velocity fields were computed and studied. One of the important results from this study was to quantify the magnitude of the thermal and "cascading" production of kinetic energy at different flow scales. Also the calculation of the diffusion, particularly for the small velocity scales, provided new information about turbulent flows. In addition, two LES models were evaluated by determining how well they predicted "cascading" production as compared to the direct calculation of the production from the simulation results. The scale similarity model gave much better predictions than the Smagorinsky model.

A three-dimensional, incompressible, homogeneous shear flow code developed by T. A. Zang (Fluid Mechanics Division, LaRC) was studied for possible parallel optimization. This is a typical pseudo-spectral flow simulation code used at NASA and ICASE. Several parallel versions of the code were developed:

1. small granularity, micro-tasking,
2. large granularity, micro-tasking,
3. large granularity, macro-tasking,
4. large granularity, macro-tasking, minimum tasks.

Granularity is defined as the amount of code that is executed in parallel at one time (before returning to the sequential controlling code). The small granularity version was over 10% faster than the other versions. This is possible due to the fact that the large granularity codes can have more code that is executed (redundantly) in each parallel process. The average speedup was 3.7 for the small granularity code and averaged 3.2 for the other versions. The study was done on a 4 processor CRAY-2.

## **Gordon Erlebacher**

Work begun on compressible turbulence in collaboration with S. Sarkar, H. Kreiss, and M. Hussaini has been completed and reported in ICASE Reports 89-79 and 90-15. The objective

of this work was to understand the different types of turbulent structures as a function of initial conditions in compressible turbulent flows when the fluctuating Mach number is small. Several regimes were identified and explained for homogeneous isotropic turbulence when the fluctuating Mach number is small: a quasi incompressible regime, an acoustic regime, dominated by acoustic waves, and a regime where shocks are present. Studies are currently underway to study homogeneous compressible shear flow.

Expertise was developed in the use of the new symbolic manipulation language, Mathematica. Mathematica was then applied to compute the characteristics of several stability problems in incompressible and compressible flows. These problems include primary instability, secondary instability, and weakly non-linear stability theory. The work related to weakly non-linear wave interaction in incompressible flows was done in collaboration with Bart Singer (High Technology Corporation, LaRC). New symbolic algorithms were developed which generate all the matrix coefficients of the discrete problem, along with over 8000 lines of fortran code in under 15 minutes on a personal Iris workstation. This execution time is at least two orders of magnitude faster than the brute force approach previously adopted with Macsyma. These symbolic manipulation programs, along with sophisticated linear stability programs allow users to quickly perform stability experiments using different sets of partial differential equations and different coordinate systems in a matter of hours instead of days.

Side by side with the previous item, Herbert's linear stability code `linear.x` was modified to provide a nice graphic interface. `Linear.x` allows users to quickly test out the stability properties of various problems with very little effort. Mathematica code has been written to interface directly with `linear.x`. The user inputs into Mathematica a set of differential equations, and in a matter of minutes, matrix coefficients have been computed and properly included into the code. To complement this effort, I have written a visual interface which allows `linear.x` to run on a Cray supercomputer, and display spectra and eigenfunctions on a local Iris workstation. The graphic interface permits the user to interactively pick eigenvalues off the screen, which are then sent back to the Cray. Then, in quasi real-time, the eigenfunction is computed via local procedure and returned to the Iris to be plotted. In this way, the user is freed from the burden of manipulating data files to ultimately visualize results.

### David Gottlieb

Together with W. S. Don (Brown University) and J. Crawford (Brown University), we continue our research on flows past circular cylinders. We use the 2D code to study some fundamental features of the flow such as the critical Reynolds number and the effect of the actual body shape on the behavior of the flow. A 3D code is in its completion stages.

Together with S. Abarbanel we are studying the role of boundary conditions in creating numerical spurious frequencies. This problem has its origin in the study of flow past bluff bodies. We have shown that both the inflow and the outflow boundary conditions can create this type of frequency and we are studying the interaction between the inflow and outflow boundary conditions.

We are developing essentially non-oscillatory spectral schemes for shockwaves calculations. We have developed one side filters, e.g., filters that yield spectral accuracy in one side of the shock even at the shock itself. These filters are being tested and applied to two flows. We have shown that these methods can be applied successfully to interactions of shocks and density waves. We are trying to simulate shock-vortex interactions (with W. S. Don and A. Solomonoff (Brown University)). We continue our study in parallel spectral methods. The main idea here is to use domain decomposition techniques and to use known conserved quantities in order to completely decouple the sub-domain. The runs are done on a hypercube architecture.

Together with C. L. Streett (Fluid Mechanics Division, LaRC), we have developed accurate quadrature formula to substitute for the classical Clanshaw-Curtiss formula. We have shown that our formula is more robust when applied to spectral simulations of incompressible flows.

### **M. Yousuff Hussaini**

The research program deals with instability, transition and turbulence in simple canonical flows. Specifically, the linear stability of supersonic/hypersonic wedge and conical flows is being studied taking into account the presence of shocks. This study involves the assumption of parallel flow. It is planned in the next step to use parabolized stability equations which will include the nonparallel effects. The linear stability of compressible attachment-line boundary layer is also under study. The point of interest is the comparison of results from the two different approaches – the classical linear parallel flow stability theory and the triple-deck theory. In another study, the evolution of the compressible Couette flow from laminar to fully developed turbulent state is being investigated. The focus is the direct numerical simulation. Even so some aspects of the problem amenable to mathematical analysis are being studied. This research program is carried out in collaboration with G. Erlebacher and M. R. Malik (High Technology Corporation, LaRC).

### **Thomas L. Jackson and Chester E. Grosch**

Our work focuses on the hydrodynamic stability of compressible high speed reacting free

shear flows, directly applicable to the study of supersonic diffusion flames in the context of scramjet engines. Our current work in this area includes the study of both near and far wakes, three-dimensional mean flows, and more realistic kinetics using quasi-global models for the chemistry. In tackling problems in this area, we have employed a combination of asymptotics and numerics to reduce the complex problems to model problems, thus isolating key physical effects for analysis.

### **Peter A. Jacobs**

In recent years, shock-tunnels and expansion-tubes have been used to obtain experimental data at hypersonic flight speeds ( $3 < v < 7\text{km/s}$ ) for the National Aero-Space Plane project. The chemistry of the air is important at these speeds and much of the physical and numerical modelling used in Computational Fluid Dynamic (CFD) simulations has not been fully validated. We have been involved with the experimental side of this work, and now we are becoming involved with CFD simulations of the pulse facilities themselves and the generic scramjet models that have been tested in these facilities.

We have also been studying the powder flow problems in the manufacturing process of Dynamic Powder Consolidation (DPC). In this process, a metal powder is compacted into a solid component by the passage of a strong shock wave. DPC has the ability to achieve compacts with close to theoretical densities and can do so without affecting the microstructure of the bulk of the metal grains. We are modelling the powder as a compressible fluid with a nonstandard equation of state, and we are using a second-order Godunov method to compute the powder flow.

### **Charles R. Johnson**

Among primary research projects completed during the period were a complete sparsity analysis of the QR factorization with D. Olesky and P. van den Driessche (University of Victoria, British Columbia) and a refined Gersgorin-type lower bound for the smallest singular value with A. Hoffman (IBM Watson Research Center). In the former, given only the sparsity pattern of a matrix with independent columns, the zero patterns of both factors Q and R are predicted with algorithms that can be cheaply implemented. The results are exact in the sense that every position predicted to be nonzero will be nonzero for some (in fact, almost every) matrix with the original pattern, and every zero is necessary. This refines and completes work by several authors interested in algorithm design and storage allocation. Necessary zeros in Q or R can occur in a variety of subtle ways.

In addition, a lengthy survey of matrix completion problems was completed for a volume

published by the IMA at Minnesota.

### **Fumio Kojima**

Work is continuing on the development of parameter estimation techniques based on the boundary integral equation approach. Domain identification problems related to an electrical impedance tomography has been studied. Those are formulated as a parameter estimation problem for an integral equation of the second kind. We developed a spline based technique using the collocation method. Numerical experiments indicate the method is attractive and convergence arguments for the proposed algorithm are currently under study.

### **Jacques Liandrat and Thomas W. Eidson**

Work is continuing on the definition and implementation of numerical algorithms for the resolution of partial differential equations based on a spatial wavelet approximation. Numerical results have been obtained in the case of the 1D regularized Burgers equation with periodic boundary conditions. They show that algorithms based on the multiscale and local approach provided by the wavelet decomposition can be very efficient when a solution of a partial differential equation exhibits local behavior (rapid variations for instance) that requires locally very fine resolution. Different fields are now under investigation: the numerical analysis of such methods and their generalisation to non-periodic and multi-dimensional problems. Close to this numerical program is the use of wavelets as a tool to extract substantial physical information from turbulence data. The study of the results of different numerical direct simulations of turbulence or transition is currently underway. The combination of these two approaches should lead to numerical simulations of turbulence on a wavelet basis.

### **Dimitri Mavriplis**

Work is continuing on the use of unstructured triangular meshes for solving turbulent viscous flow problems about arbitrary configurations in two dimensions. In previous work, a method for generating highly stretched triangular meshes for accurate shear-layer resolution (ICASE Report No. 88-47) has been developed, and a finite-element Navier-Stokes solver has been devised and validated (ICASE Report No. 89-11). Hence, the present work has concentrated on refining the basic mesh generation and flow solution algorithms, as well as on the implementation of a suitable turbulence model, and the incorporation of adaptive meshing techniques in order to enhance the accuracy and efficiency of the method.



An algebraic turbulence model has been developed for use on unstructured meshes. Based on the Baldwin-Lomax model, this algebraic model makes use of background structured mesh lines. A local structured mesh is constructed in the vicinity of each solid wall boundary and wake line. At each time step within the solution of the flow on the global unstructured mesh, the current flow variables are interpolated onto these background structured meshes. The turbulence model is then executed on these meshes, and the resulting eddy viscosities are interpolated back onto the global unstructured mesh where they interact with the flow field solution. When adaptive meshing is invoked, the global unstructured mesh is refined by adding new points in regions of high flow gradients and performing local retriangulation. The turbulence background meshes are also refined by adding new normal mesh lines corresponding to each newly inserted unstructured mesh boundary point, and by increasing the resolution of the existing mesh lines in regions of high flow gradients. After each mesh adaptation stage, the coefficients for interpolation between the new unstructured mesh and the refined background turbulence meshes must be recomputed prior to resuming time-stepping on the flow-field equations. This method has been employed to compute the turbulent flow over a 4-element airfoil configuration. Good comparison between computed and experimental wind tunnel (surface pressure) measurements has been observed. Such problems are of particular importance to the aircraft industry, with regards to the design and development of high-lift airfoil-flap systems for take-off and landing conditions.

Further work is aimed at investigating different turbulence models and extending this methodology to three dimensions.

### **Kirsten Morris**

Robustness of controllers designed using Galerkin approximations has been shown for bounded semigroup control systems. The extension to "Pritchard-Salamon" systems is straightforward. However, accelerometers, which are becoming increasingly important in the study of flexible structures, do not fall within this framework. Under certain conditions of regularity, we have shown that control systems with accelerometers are "well-defined" in a certain sense, and that an equivalence exists between frequency domain and time domain definitions of stability. This last result is critical for modern controller design methods, such as  $H_\infty$  techniques, which depend upon frequency domain criteria. This work is continuing with H. T. Banks. The eventual goal is to establish conditions under which the use of Galerkin techniques is justified in control of systems with these sensors.

Research is being conducted with J. Juang (Spacecraft Dynamics Division, LaRC) into control of large scale space structures using  $H_\infty$  methods. Second-order systems with collocated actuators and sensors can be stabilized by any controller with a frequency response

in the right-half plane. We are trying to establish a design technique for more general configurations which is robust with respect to damping errors. A preliminary design for active control of acoustic plane waves has been obtained. This design will be implemented by R. Silcox (Acoustics Division, LaRC).

### **David M. Nicol**

While the parallelization of discrete-event simulations has been a topic of interest for at least ten years, few formal performance analyses of such systems have been developed. We have developed stochastic models of parallel discrete event simulations that help to answer a number of fundamental questions: what is the optimal performance one can achieve?, how well can so-called "conservative" methods perform?, and under what circumstances can a conservative method achieve better performance than an "optimistic" method?

In another effort, we have been developing new algorithms for mapping highly irregular grids onto parallel machines and have been developing graphical tools to aid the user in viewing the partitioning of these grids.

### **Yuh Rong Ou**

Research continued on control of fluid-structure interaction problems. The basic approach is to formulate the problem by coupling various control laws with theories of the Navier-Stokes equations.

Our current effort is devoted to simulating the problem of controlling unsteady flow around a circular cylinder. The initial focus of our investigation is on the computational aspects of the cylinder undergoing a constant speed of rotation. The development of flow patterns and histories of lift and drag on the cylinder are computed. The good agreement between these computational results and the experimental results of Coutanceau and Ménard confirm their respective validity. Subsequent work will remove the restriction of constant speed of rotation and extend our development to model large variations in rotation. The main objective of this study is to achieve the desired lift enhancement by varying the rotation rate. In particular, we want to incorporate control theory to explore the various theoretical aspects of our research.

The ultimate goal of this project is to develop both computational and theoretical methods for modeling the interaction of control and fluid dynamics. The tools developed here will be used to investigate fundamental questions regarding control of separated flows by using different boundary control mechanisms.

## Merrell L. Patrick and Mark Jones

Development of algorithms for solving the generalized eigenvalue problem is continuing. An eigensolver, LANZ, based on the Lanczos method has been implemented and tested on the Convex, Cray Y-MP, and Cray 2 computers. The performance of a uni-processor version of LANZ has been compared with that of the eigensolver module, EIG, in the NASA Langley structural analysis testbed system running on the Convex and Cray 2 systems. For all problems tested the performance of LANZ is substantially superior to that of EIG.

Our approach required the development of a routine for solving indefinite linear systems of equations. Such systems arise because shifting is required to improve convergence rates of the Lanczos iterations. A shifting strategy was developed for improving the performance of the algorithm and tested for robustness. A routine based on the Bunch-Kaufman algorithm for solving indefinite systems was implemented and shown to perform better than a LINPACK algorithm based on LU factorization. Three new algorithms, based on Bunch-Kaufman factorization, that take advantage of high performance architectures have been developed.

A multiprocessor version of LANZ has been implemented and tested using the Force language on the Cray Y-MP computer. Preliminary results suggest three important activities for the future for obtaining a more efficient implementation, particularly for very large problems. They are:

1. The factorization phase of the Lanczos process should be as efficient as possible. We intend to add the option of sparse factorization to LANZ which currently uses variable band factorization.
2. Since backsolving will not parallelize well, we need to reduce the number of backsolves in the Lanczos process. This can be accomplished by reducing the number of Lanczos iterations which calls for intelligent dynamic shifting.
3. Iterative methods require less storage and parallelize more easily than direct elimination methods. The option of iterative methods will be added to LANZ if they prove to offer advantages over elimination methods.

We will also begin to make an assessment on the appropriateness of other parallel architectures for implementing LANZ.

This work is being done in collaboration with the NASA Langley CSM group.

### **Merrell L. Patrick and Terrence W. Pratt**

Methods for porting existing FORTRAN based applications codes to new parallel architectures are the focus of this study. The NASA LAURA code (Langley Aerothermodynamic Upwind Relaxation Algorithm), developed by Peter Gnoffo (Space Systems Division, LaRC), is being studied as a test case. We are looking at both spatial and temporal partitioning methods for parallel execution of this code on various architectures, including the Intel iPSC/860. An execution time profile of the code has been obtained and an analysis of data partitioning and data flow from subroutine to subroutine is being carried out.

### **Ugo Piomelli**

Further studies on the applicability of the large-eddy simulation approach to transitional wall-bounded flows have been performed. In large-eddy simulations (LES) of the Navier-Stokes equations, the large, energy-carrying scales of motion are accurately captured while the effect of the small scales is modeled. Thus, LES provides an attractive alternative to both the direct simulation, in which all scales of motion are resolved, and which require very massive computational efforts, and to the solution of the Reynolds averaged equations of motion, which require modeling of all scales of motion. The models used to parameterize the effect of the subgrid scales (known as residual stress models or subgrid-scale stress models) are simpler and more universal than the turbulence models used for the Reynolds-averaged Navier-Stokes equations, since the subgrid scales tend to be more isotropic and homogeneous than the large ones, and less affected by the boundary conditions. This technique has been successfully applied to many turbulent flows, but only recently have efforts been made to study transition to turbulence using LES. While during the linear stages, very little subgrid scale activity occurs, and subgrid-scale models should contribute little to the Reynolds stress, during laminar breakdown, significant amounts of small scales are generated, and inclusion of a model greatly improves the accuracy with which statistical quantities of engineering interest can be predicted. Since standard subgrid-scale stress models damp the growth of the velocity perturbation at the early stages of transition, modifications were developed to obviate this difficulty. The results of the calculation of transition to turbulence in a plane channel indicate that such models allow one to predict the entire development of the perturbations from the linear stage through laminar breakdown into fully-developed turbulent flow. Current efforts are directed towards the development of more general models that better incorporate the flow physics.

## Peter Protzel

Work continued on the investigation of the fault-tolerance characteristics of artificial neural networks (ANNs) and their applications in the area of Reliable Computing. Together with D. Palumbo (Information Systems Division, LaRC), we studied the application of an ANN to control the allocation of tasks to processors in a distributed multiprocessor system. The architecture of the multiprocessor system is based on the Software Implemented Fault-Tolerance (SIFT) Computer, which was developed by NASA as a highly reliable, reconfigurable computer system for flight control applications. In SIFT, the failure of a processor requires the isolation of this processor and a reconfiguration of the system with a reallocation of all tasks among the remaining processors. The reallocation has to observe hard real-time constraints and should be performed in a way that balances the load of the processors. A certain type of ANN that solves constraint optimization problems in real-time can be used to generate these new allocations. With the ANN being a critical component in this application, the fault-tolerance of the ANN itself becomes an important characteristic. By studying the performance of the ANN in the presence of simulated hardware faults, we could demonstrate the extreme fault-tolerance with a hardly discernible degradation even after multiple faults. These characteristics of high speed, fault-tolerance, and low weight and power consumption make a hardware implemented ANN interesting for this and similar applications in the area of real-time control.

Another project in collaboration with C. Jeffries from Clemson University investigates a novel architecture of a high order ANN that functions as an auto-associative memory. The main feature of this high order model is the absence of spurious attractors and the guaranteed convergence to one of the stored memories. One application for this ANN is the decoding and error-correction of block codes transmitted over a noisy channel. Since the ANN converges to the closest attractor (code word) stored in memory given an arbitrary analog vector as its initial input, it is possible to perform soft-decision decoding on block codes with the corresponding increase in performance. In computer simulations, we studied the performance of the ANN in terms of post-decoding bit error rate versus signal-to-noise ratio for two exemplary block codes. The results in comparison with a conventional decoding algorithm show, for example, that the bit error rate for a (15,5) block code at 7dB signal-to-noise ratio can be decreased by two orders of magnitude. A hardware implementation could produce different integrated circuits for different block codes to be employed as real-time, soft-decision decoders in potentially many different communication systems.

## Joel Saltz and Ravi Mirchandaney

Dependencies between loop iterations cannot always be characterized during program

compilation. *Doacross* loops typically make use of a priori knowledge of inter-iteration dependencies to carry out required synchronizations. We propose a type of *doacross* loop that allows us to partition iterations of a loop between processors without advance knowledge of inter-iteration dependencies. The method proposed for partitioning loop iterations requires us to carry out parallelizable stages of preprocessing and post-processing during program execution. We have performed experimental studies using this construct and will report our results in an upcoming ICASE Report.

### **Joel Saltz and V. Venkatakrishnan**

A fully implicit scheme is used to solve the compressible Euler equations for transonic flows. An approximate Riemann solver is used to compute the numerical fluxes to second order accuracy in space. The large linear system arising at each time step from the linearization of a fully implicit scheme is solved by iterative means using a preconditioned conjugate gradient-like algorithm. Incomplete LU (ILU) factorization with no fill-in is used to precondition the system followed by the use of the Generalized Minimum Residual technique (GMRES). Two ways to achieve parallelism are tested: one which makes use of parallelism inherent in triangular solves and the other which employs domain decomposition techniques. The vectorization/parallelism in triangular solves is realized by the use of a reordering technique (called wavefront ordering) wherein the triangular matrix is interpreted as a directed graph and the data dependencies are analyzed. The graph is analyzed once using the connectivity of the grid points and all the matrix operations are done in the context of  $4 \times 4$  blocks since we have four unknowns to a grid point. The factorization can also be done in parallel with the wavefront ordering. In the domain decomposition case, the wave front ordering is used for getting vectorization within each sub-domain and, since the sub-domains are disjoint, the factorization and triangular solves are done in parallel. The domain decomposition does introduce a sequential overhead. We compare the performances of two ways of partitioning the domain, viz. strips and slabs. Results on a Cray Y-MP are reported for an inviscid transonic test case. The performances of the linear algebra kernels are also reported. This work is reported in "Domain Decomposition in Aerodynamics" in the Proceedings of SIAM Conference on Parallel Processing for Scientific Computing, Chicago, Illinois, December 1989.

### **Sutanu Sarkar**

We are engaged in the direct simulation and Reynolds stress modeling of turbulent flows. Most of this research addresses compressibility effects in high-speed turbulence. In collabo-

ration with G. Erlebacher and M. Y. Hussaini, we have performed simulations of isotropic turbulence at various Mach numbers and are presently engaged in the simulation of homogeneous shear turbulence with a spectral collocation method. These simulations and an asymptotic theory (developed by H. O. Kreiss in association with G. Erlebacher, M. Y. Hussaini and myself) are being used to assist in the generation of turbulence models. We have obtained an interesting result that compressibility leads to enhanced dissipation, and a model parameterizing this phenomenon has been developed and successfully applied to the supersonic shear layer. We are continuing the application of second-order closures to other high-speed flows in collaboration with L. Balakrishnan (Research Associate, Old Dominion University).

### Paul Saylor

An ICASE report on iterative methods and initial value problems, written with R. Skeel of the University of Illinois, is nearing completion. Analysis in the paper suggests that if the linear systems in a stiff initial value problem are to be solved iteratively, then the Chebyshev iterative method would be appropriate. This method is implemented in the package Chebycode of Ashby and Manteuffel. The differential algebraic system solver (DASSL) package of Petzold has been modified (at the University of Illinois and Lawrence Livermore National Lab) to call Chebycode. The resulting package will be applied to a discretization of the low frequency approximation of the transonic small disturbance equation.

Another effort is focused on separating eigenvalues. The small interior eigenvalues for a generalized eigenvalue problem are difficult to compute. It is an unresolved question whether using a polynomial to separate the eigenvalues in conjunction with a Lanczos-style algorithm would be a good idea. If it is, then there exist algorithms and software, due to S. F. Ashby, for computing a polynomial of given degree that separates eigenvalues optimally. To explain, suppose that the interval  $[\lambda_b, \lambda_c]$  is contained in a cluster of eigenvalues. Let  $\mu \in [\lambda_b, \lambda_c]$ . Ashby's algorithms, based on the Remez algorithm, compute a polynomial,  $\omega_k$ , of given degree,  $k$ , such that (i)  $\omega_k$  is the minimax polynomial on the complement of  $[\lambda_b, \lambda_c]$ ; and (ii)  $\omega_k(\mu) = 1$ . The peak at  $\mu$  separates the eigenvalues clustered around  $\mu$  from all other eigenvalues. Some technical details are omitted; for example, the complement of  $[\lambda_b, \lambda_c]$  means the complement within the spectrum. A careful definition of the complement makes  $\omega_k$  unique.

Polynomial  $\omega_k$  is the polynomial approximation of the delta function on the complement of  $[\lambda_b, \lambda_c]$ . Polynomial approximations to the delta function may also be computed using orthogonal polynomials in which case they are called kernel polynomials. I have previously discussed using kernel polynomials to separate eigenvalues. Aside from questions about the

superiority of the minimax norm, the advantages to the minimax polynomial approach is the existence of algorithms and their Fortran implementation.

Ashby's application was to the iterative solution of symmetric indefinite linear algebraic equations. In that case, the objective is to find a polynomial,  $\omega_k$ , that is small on the positive and negative eigenvalues and takes on the value 1 at  $\mu = 0$ . The particular value  $\mu = 0$  is easily generalized in the algorithm. A description of the algorithms and the application is in the December, 1989, special issue of BIT on preconditioning.

### **Paul Saylor and Jeffrey Scroggs**

This is a preliminary investigation into combining asymptotic analysis and waveform relaxation to form a numerical method with both high accuracy and parallel capability. Since waveform methods easily exploit medium-grain to small-grain parallelism, the focus will be on obtaining accuracy.

In its application to CFD, the method of lines yields a system of ordinary differential equations by discretizing the spatial derivatives. The waveform technique is to decouple the ODEs, solve each equation, then employ functional iteration to obtain a solution to the system. Waveform relaxation has the advantages that different time steps can be used for different components, and that decoupling makes it trivial to distribute the system among multi-processors for a parallel solution.

The role of asymptotic analysis is to adapt waveform relaxation to the special requirements of CFD. As an example, asymptotic analysis may be used to formulate a conservative scheme in the presence of shocks. In addition, asymptotic analysis may be used to resolve the physically relevant and diverse scales that arise when simulating flow with smooth regions interspersed with boundary layers and shocks.

The first phase of this project is to demonstrate the waveform technique on a conservative finite difference approximation to the fluid dynamic equations representing conservation of mass and conservation of momentum. We are implementing the technique using DASSL, the differential algebraic system solver of L. Petzold. This work is being done in collaboration with Fen-Lien Juang of the University of Illinois.

### **Jeffrey Scroggs and Marc Garbey**

This research is the symbiosis of asymptotics and numerical analysis to generate domain decomposition methods that are both accurate and computationally efficient.

We are developing a method that consists of multiple-stages. The first stage of the method is to obtain a first approximation by a standard conservative numerical method (e.g., the



Godunov method). Subsequent stages of the method consist of corrections. The correction differs depending on whether the problem is inviscid (hyperbolic) or viscous (parabolic). A shock-layer correction which minimize the effect of the viscosity is used for the inviscid case; whereas, the viscous profile of the shock is computed when the problem is viscous. The method is derived and justified via asymptotic analysis that treats the order of accuracy  $\epsilon = O(\Delta t^p, \Delta x^q)$  of the standard numerical method as a small parameter in an asymptotic expansion.

A residual correction based on asymptotic analysis is utilized outside the zone of strong singularities. For inviscid problems, this residual correction can be understood as an antidiffusion correction. For example, this correction is able to improve the Godunov scheme in the neighborhood of a weak singularity such as a jump of the first derivatives of the solution (corner-layers).

The method has been implemented for a system of equations arising in fluid dynamic equations representing conservation of mass and conservation of momentum, and has demonstrated that capturing the shock-layer profile (for a slowly varying profile) can be performed in an efficient manner.

### **Sharon S. Seddougui**

The spatial inviscid instability problem for Görtler vortices is being investigated jointly with Philip Hall. The aim of this work is to determine the fastest growing spatial mode for large Görtler numbers. For an incompressible fluid, it is found that these modes are localized in an asymptotically thin layer at the wall. The receptivity problem has also been addressed showing that  $O(1)$  coupling coefficients between a surface perturbation and the induced vortex field are possible. The extension of this work to include the effects of compressibility is currently being studied.

### **Chi-Wang Shu**

We are continuing our investigations of ENO (essentially non-oscillatory) finite difference schemes. One project is to obtain a user-oriented two-dimensional Navier-Stokes code which handles generalized coordinates via transformations and various boundary conditions and to use it to test problems including direct turbulence simulation and acoustic related phenomena. This project is coordinated with the Theoretical Flow Physics Branch of LaRC. Another project is to analyze the accuracy of ENO schemes and how to effectively use centered schemes in the smooth part of the flow and use ENO in the rapid transition regions.

## **Charles G. Speziale**

Research has continued on the development of a compressible second-order closure model for high-speed turbulent flows in collaboration with S. Sarkar. This latest research has concentrated on the development of models which are asymptotically consistent near walls and computationally robust. Some preliminary boundary layer calculations conducted with R. Abid (Vigyan, LaRC) have indicated that none of the existing second-order closure models have both of these desired properties. In order to properly account for anisotropies in the turbulent dissipation rate, a modeled tensor dissipation rate transport equation was recently developed in collaboration with T. B. Gatski (Fluid Mechanics Division, LaRC). A more simple algebraic model will be extracted from this transport model based on a local homogeneous equilibrium hypothesis. Unlike the older models, this new algebraic model will account for nonlinear effects arising from the mean velocity gradients. The compressible dissipation model recently developed by Sarkar, Erlebacher, Hussaini, and Kreiss (ICASE Report No. 89-79) will then be incorporated into this algebraic model to account for compressible effects.

Research continues on the large-eddy simulation of transitional flows with U. Piomelli and T. A. Zang (Fluid Mechanics Division, LaRC). The most recent discussions have centered around the development of a one-equation subgrid-scale model to account for history effects. Results obtained previously were based on a rescaled Smagorinsky model which does not directly account for these effects which are known to be important in most transitional flows. New work on the large-eddy simulation of compressible turbulent flows – conducted in collaboration with G. Erlebacher, T. A. Zang, and M. Y. Hussaini – has also begun recently.

## **Shlomo Ta'asan**

The development of efficient multigrid solvers for constraint optimization problems governed by partial differential equations has continued. A new method for treatment of control problems governed by elliptic PDE's has been developed. The case of finite dimensional control has been considered so far. In that case, solution for the full optimization problem was reached with the same cost as solving the constraint equations about 2-3 times. Research is continuing in applying the techniques developed for identification problems in which the parameter space is finite dimensional (and not too large), e.g., impedance tomography.

The same ideas are being considered in the context of aerodynamics design problems where airfoils are to be calculated so as to meet certain design requirements. For example, to give pressure distribution in some flow conditions which are closest to a given pressure distribution. In the course of developing these ideas new Euler solvers are being developed which uses DGS relaxation schemes and perform equally well for all Mach numbers.

Another area of research is the development of new computational techniques in elastic-plastic problems. Here a set of non-linear equations which involve also weak dependence of the history of the loading are to be calculated. Our effort is focused on trying to perform most of the computation on coarse levels. Different continuation techniques (in the load parameters) are being tested to obtain ones which are best suited for multigrid algorithms.

A new method for the calculation of several eigenfunctions of elliptic problems has been developed. Its computational complexity is  $O(qN)$  where  $q$  is the number of eigenfunctions involved and  $N$  is the number of unknowns for each eigenfunction. Previously developed algorithms had complexity of  $O(q^2N)$ , because of the Ritz projection that is needed for such problems. Our new algorithm also uses a Ritz projection but it is done on the coarsest level so its cost is negligible, reducing the cost of the algorithm to a minimum.

### Eitan Tadmor

We study the convergence rate of approximate solutions to the possibly discontinuous entropy solutions  $u(x, t)$  of scalar nonlinear conservation laws. In [ICASE Report No. 89-80] we have shown that by post-processing the small viscosity approximations  $u_\epsilon$ , we can recover pointwise values of  $u$  and its derivatives with an error as close to  $\epsilon$  as desired.

Our approach does not 'follow the characteristics' and, therefore, applies *mutatis mutandis* to other approximate solutions such as E-difference schemes. Together with H. Nessyahu we extend these results to E-stable approximations, Glimm-type schemes and we are working on the convergence rate of certain kinetic approximations discussed below.

Together with B. Perthame (Université de Mathématiques, France) we study the construction of multi-dimensional entropy solutions for nonlinear scalar conservation laws. To this end we employ kinetic solutions depending on the microscopic scale  $\epsilon > 0$  which were constructed in ICASE Report No. 90-11. We show that the phase averages (as well as higher moments) of these kinetic solutions, form a compact family of approximate solutions which are strongly convergent to the 'macroscopic' quantities associated with the multi-dimensional conservation laws (e.g., fluxes, entropy, etc.), as the microscopic scale,  $\epsilon \downarrow 0$ .

Moreover, we precisely identify the governing evolution model of the kinetic limit solution, as  $\epsilon \downarrow 0$ . The governing model is shown to consist of linear transport equations with a phase space gradient of the sink terms which are responsible for the loss of entropy at the kinetic level. Using this we conclude that for multi-dimensional scalar conservation laws which satisfy a rather weak nonlinearity assumption, then the corresponding macroscopic solution operator is compact.

Finally, together with D. Gottlieb, we study the stability of spectral approximations to scalar hyperbolic initial-boundary value problems with variable coefficients. Time is dis-

cretized by explicit multi-level or Runge Kutta methods of order  $\leq 3$  (forward Euler time differencing is included), and we study spatial discretizations by spectral and pseudospectral approximations associated with the general family of Jacobi polynomials. We prove that these fully explicit  $N$ -degree spectral approximations are stable provided their time-step,  $\Delta t$ , is restricted by the CFL-like condition,  $\Delta t < \text{Const.}N^{-2}$ . We give two independent proofs of this result, depending on two different choices of appropriate  $L^2$ -weighted norms. Our result confirms the commonly held belief that the above CFL stability restriction, which is extensively used in practical implementations, guarantees the stability (and hence the convergence) of fully-explicit spectral approximations in the non-periodic case. An ICASE report describing this research is nearing completion.

### **Bram van Leer**

The work on the multi-dimensional Riemann Solver, in collaboration with C. Rumsey (Fluid Mechanics Division, LaRC), has led to a robust algorithm that treats shocks and shears in the proper frame and thereby considerably reduces their numerical spread. After implementation in a 2-D Euler airfoil code, the next step is incorporation of the new flux function in a Navier-Stokes code. The results of the Euler calculations have been summarized in an extended abstract submitted to the next AIAA Aerospace Sciences Meeting, January 1991, Reno, Nevada.

### **John Van Rosendale and Naomi Decker**

In recent work, we have been looking at the design of iterative methods for the linear systems arising in implicit spectral calculations. Our first target is the variable coefficient Helmholtz equation, a problem arising in the Ozawa formulation of the Navier-Stokes equations and in stream-function/vorticity ocean circulation models.

Deville and Mund have explored the idea of using finite elements as preconditioners for spectral methods. They found that standard trilinear finite elements in three dimensions lead to a preconditioned spectral system having condition number 1.44, a major improvement over finite difference preconditioned spectral methods. We have improved this condition number to 1.25. The new discretization is formed by using linear finite elements in one dimension with a partially lumped mass matrix. One then tensors this discretization appropriately to yield the optimal 9-point discretization in two dimensions, and optimal 27-point discretization in three dimensions. The new discretization induces no extra work and retains the standard tensor product structure, allowing efficient treatment of variable coefficient problems without storage of multiple coefficient arrays.

We have also designed a Petrov-Galerkin discretization based on quintic splines, leading to a preconditioned system having condition number 1.001, for smoothly varying coefficients. To exploit this low condition number, we constructed a two level algorithm with the spectral method preconditioned by this spline discretization, and the latter, in turn, preconditioned by a 27-point finite element discretization. The resulting algorithm reduces the spectral residual by a factor of a million, through six solves of the finite element linear system, but requires only one spectral residual calculation.

To solve the finite element systems occurring, we use, ZOOM, a fast semicoarsening based multigrid algorithm. ZOOM has a spectral radius of .003 per v-cycle on the positive definite Helmholtz equation on a uniform grid. It's convergence rate degenerates to about .05 on Chebyshev grids, but this is still fast enough that one v-cycle suffices for each solution of the finite element linear system above.

### **John Van Rosendale and Piyush Mehrotra**

In the last year, we have been designing a programming environment, called Kali, which provides a software layer supporting a global name space on distributed memory architectures. In Kali, the computation is specified via a set of parallel loops, which act on values in this global name space. The user provides annotations to specify distribution of arrays across the distributed memory, and to assign work to processors. In this way, the user controls aspects of the program critical to performance, such as data distribution and load balance, while relegating the details of message-passing to the compiler.

We are currently studying the efficacy of this approach using a Fortran-like language, KF1 (Kali Fortran 1). KF1 contains most of standard Fortran, plus Kali-style constructs for expressing parallel algorithms for distributed execution. While no KF1 compiler exists yet, we have been studying the efficacy of KF1 constructs using an existing compiler for a Pascal-like version of Kali.

Preliminary results suggest that KF1 constructs are quite effective for expressing regular algorithms, such as tensor product array computations, relying on static load balancing. Work on several large numerical applications programs, including a multigrid algorithm and an ADI algorithm, suggests that programs written in KF1 will obtain efficiency comparable to that of analogous programs expressed in lower level message-passing languages. We have also recently added constructs to the language for problems requiring dynamic load balancing, and have begun looking at irregular problems requiring run-time analysis.

## REPORTS AND ABSTRACTS

Kosloff, Dan and Hillel Tal-Ezer: *Modified Chebyshev pseudospectral method with  $O(N^{-1})$  time step restriction.* ICASE Report No. 89-71, December 5, 1989, 27 pages. Submitted to Journal of Computational Physics.

The extreme eigenvalues of the Chebyshev pseudospectral differentiation operator are  $O(N^2)$  where  $N$  is the number of grid points [4]. As a result of this, the allowable time step in an explicit time marching algorithm is  $O(N^{-2})$  which, in many cases, is much below the time step dictated by the physics of the P.D.E. In this paper we introduce a new set of interpolating points such that the eigenvalues of the differentiation operator are  $O(N)$  and the allowable time step is  $O(N^{-1})$ . The properties of the new algorithm are similar to those of the Fourier method but in addition it provides highly accurate solution for nonperiodic boundary value problems.

Funaro, Daniele: *Computational aspects of pseudospectral Laguerre approximations.* ICASE Report No. 89-72, November 27, 1989, 17 pages. Applied Mathematics Computation.

Pseudospectral approximations in unbounded domains by Laguerre polynomials lead to ill-conditioned algorithms. We introduce a scaling function and appropriate numerical procedures in order to limit these unpleasant phenomena.

Freeman, T. L.: *Parallel projected variable metric algorithms for unconstrained optimization.* ICASE Report No. 89-73, November 27, 1989, 13 pages. To be submitted to Mathematical Programming.

We review the parallel variable metric optimization algorithms of Straeter (1973) and van Laarhoven (1985) and point out the possible drawbacks of these algorithms. By including Davidon (1975) projections in the variable metric updating we can generalize Straeter's algorithm to a family of parallel projected variable metric algorithms which do not suffer the above drawbacks and which retain quadratic termination. Finally we consider the numerical performance of one member of the family on several standard example problems and illustrate how the choice of the displacement vectors affects the performance of the algorithm.

Maestrello, L., A. Bayliss, and R. Krishnan: *Numerical study of three-dimensional spatial instability of a supersonic flat plate boundary layer.* ICASE Report No. 89-74, October 6, 1989, 19 pages. Submitted to Physics of Fluids.

The behavior of spatially growing three-dimensional waves in a supersonic boundary layer is studied. The objectives are to validate our computer code by comparing with experiments and parallel and non-parallel linear stability theories for  $M_\infty = 4.5$ ,  $\sqrt{\text{Re}/ft} = 1550$  and at

$T_{t,\infty} = 100^\circ\text{F}$  and then use the program to study nonlinear effects. The three-dimensional unsteady Navier-Stokes equations are solved by a finite difference method which is fourth-order and second-order accurate in the convection and viscous terms respectively, and second-order accurate in time. Spanwise periodicity is assumed. The inflow disturbance is composed of eigenfunctions from linear stability theory. Computed results for small amplitudes of this disturbance agree well with linear theory and experiment for several frequencies. By increasing the amplitude of the inflow disturbance, nonlinear effects in the form of a relaxation type oscillation of the time signal of  $\rho u$  are observed.

Brewer, Dennis W., John A. Burns, and Eugene M. Cliff: *Parameter identification for an abstract Cauchy problem by quasilinearization*. ICASE Report No. 89-75, October 13, 1989, 35 pages. Submitted to the Quarterly Journal of Applied Mathematics.

A parameter identification problem is considered in the context of a linear abstract Cauchy problem with a parameter-dependent evolution operator. Conditions are investigated under which the gradient of the state to a parameter possesses smoothness properties which lead to local convergence of an estimation algorithm based on quasilinearization. Numerical results are presented concerning estimation of unknown parameters in delay-differential equations.

Nicolaides, R. A.: *Direct discretization of planar div-curl problems*. ICASE Report No. 89-76, October 23, 1989, 31 pages. Submitted to SIAM Journal.

A control volume method is proposed for planar div-curl systems. The method is independent of potential and least squares formulations, and works directly with the div-curl system. The novelty of the technique lies in its use of a single local vector field component and two control volumes rather than the other way round. A discrete vector field theory comes quite naturally from this idea and is developed in the paper. Error estimates are proved for the method, and other ramifications investigated.

Bassom, Andrew P. and Sharon O. Seddougui: *A note concerning the onset of three dimensionality and time dependence in Görtler vortices*. ICASE Report No. 89-77, October 31, 1989, 28 pages. Submitted to Journal of Fluid Mechanics.

Recently Hall & Seddougui (1989) considered the secondary instability of large amplitude Görtler vortices in a growing boundary layer into a three-dimensional flow with wavy vortex boundaries. They obtained a pair of coupled, linear ordinary differential equations for this instability which constituted an eigenproblem for the wavelength and frequency of this wavy mode. Investigations into the nonlinear version of this problem by Seddougui & Bassom have revealed several omissions in the numerical work of Hall & Seddougui; these issues are addressed in this note. In particular, we find that many neutrally stable modes are possible; we derive the properties of such modes in a high wavenumber limit and show that the combination of the results of Hall & Seddougui and our modifications lead to conclusions which are consistent with the available experimental observations.

Zang, Thomas A. and M. Yousuff Hussaini: *Multiple paths to subharmonic laminar breakdown in a boundary layer*. ICASE Report No. 89-78, October 31, 1989, 14 pages. Physics Review Letters, in press.

Numerical simulations demonstrate that laminar breakdown in a boundary layer induced by the secondary instability of two-dimensional Tollmien-Schlichting waves to three-dimensional subharmonic disturbances need not take the conventional lambda vortex/high-shear layer path.

Sarkar, S., G. Erlebacher, M. Y. Hussaini, and H. O. Kreiss: *The analysis and modeling of dilatational terms in compressible turbulence*. ICASE Report No. 89-79, December 6, 1989, 33 pages. Submitted to Journal of Fluid Mechanics.

It is shown that the dilatational terms that need to be modeled in compressible turbulence include not only the pressure-dilatation term - the compressible dissipation. The nature of these dilatational terms in homogeneous turbulence is explored by asymptotic analysis of the compressible Navier-Stokes equations. A non-dimensional parameter which characterizes some compressible effects in moderate Mach number, homogeneous turbulence is identified. Direct numerical simulations (DNS) of isotropic, compressible turbulence are performed, and their results are found to be in agreement with the theoretical analysis. A model for the compressible dissipation is proposed; the model is based on the asymptotic analysis and the direct numerical simulations. This model is calibrated with reference to the DNS results regarding the influence of compressibility on the decay rate of isotropic turbulence. An application of the proposed model to the compressible mixing layer has shown that the model is able to predict the dramatically reduced growth rate of the compressible layer.

Tadmor, Eitan: *Local error estimates for discontinuous solutions of nonlinear hyperbolic equations*. ICASE Report No. 89-80, December 6, 1989, 21 pages. Submitted to Communications on Pure & Applied Mathematics.

Let  $u(x, t)$  be the possibly discontinuous entropy solution of a nonlinear scalar conservation law with smooth initial data. Suppose  $u_\varepsilon(x, t)$  is the solution of an approximate viscosity regularization, where  $\varepsilon > 0$  is the small viscosity amplitude. We show that by post-processing the small viscosity approximation  $u_\varepsilon$ , we can recover pointwise values of  $u$  and its derivatives with an error as close to  $\varepsilon$  as desired.

The analysis relies on the adjoint problem of the forward error equation, which in this case amounts to a backward linear transport equation with discontinuous coefficients. The novelty of our approach is to use a (generalized) E-condition of the forward problem in order to deduce a  $W^{1,\infty}$  energy estimate for the discontinuous backward transport equation; this, in turn, leads us to  $\varepsilon$ -uniform estimate on moments of the error  $u_\varepsilon - u$ .

Our approach does not 'follow the characteristics' and, therefore, applies mutatis mutandis to other approximate solutions such as E-difference schemes.



Hall, Philip: *Görtler vortices in growing boundary layers: The leading edge receptivity problem, linear growth, and the nonlinear breakdown stage.* ICASE Report No. 89-81, December 14, 1989, 74 pages. To appear in *Mathematica*.

Görtler vortices are thought to be the cause of transition in many fluid flows of practical importance. In this paper a review of the different stages of vortex growth is given. In the linear regime nonparallel effects completely govern this growth and parallel flow theories do not capture the essential features of the development of the vortices. A detailed comparison between the parallel and nonparallel theories is given and it is shown that at small vortex wavelengths the parallel flow theories have some validity; otherwise nonparallel effects are dominant. New results for the receptivity problem for Görtler vortices are given; in particular vortices induced by free-stream perturbations impinging on the leading edge of the wall are considered. It is found that the most dangerous mode of this type can be isolated and its neutral curve is determined. This curve agrees very closely with the available experimental data. A discussion of the different regimes of growth of nonlinear vortices is also given. Again it is shown that, unless the vortex wavelength is small, nonparallel effects are dominant. Some new results for nonlinear vortices of  $O(1)$  wavelengths are given and compared to experimental observations. The agreement between theory and experiment is shown to be excellent up to the point where unsteady effects become important. For small wavelength vortices the nonlinear regime is of particular interest since there a strongly nonlinear theory can be developed. Here the vortices can be large enough to drive the mean state which then adjusts itself to make all modes neutral. The breakdown of this nonlinear state into a three-dimensional time dependent flow is also discussed.

Hall, Philip and Frank T. Smith: *On strongly nonlinear vortex/wave interaction in boundary-layer transition.* ICASE Report No. 89-82, December 20, 1989, 36 pages. Submitted to *Journal of Fluid Mechanics*.

The interactions between longitudinal vortices and accompanying waves considered here are strongly nonlinear, in the sense that the mean-flow profile throughout the boundary layer is completely altered from its original undisturbed state. Nonlinear interactions between vortex flow and Tollmien-Schlichting waves are addressed first, and some analytical and computational properties are described. These include the possibility in the spatial-development case of a finite-distance break-up, inducing a singularity in the displacement thickness. Second, vortex/Rayleigh-wave nonlinear interactions are considered for the compressible boundary-layer, along with certain special cases of interest and some possible solution properties. Both types, vortex/Tollmien-Schlichting and vortex/Rayleigh, are short-scale/long-scale interactions and they have potential applications to many flows at high Reynolds numbers. Their strongly nonlinear nature is believed to make them very relevant to fully fledged transition to turbulence.

Seddougui, S. O. and Andrew P. Bassom: *On the instability of Görtler vortices to nonlinear travelling waves.* ICASE Report No. 90-1, January 31, 1990, 44 pages. Submitted to *IMA Journal of Mechanics and Applied Mathematics*.

Recent theoretical work by Hall & Seddougui (1989) has shown that strongly nonlinear, high wavenumber Görtler vortices developing within a boundary layer flow are susceptible

to a secondary instability which takes the form of travelling waves confined to a thin region centered at the outer edge of the vortex. This work considered the case in which the secondary mode could be satisfactorily described by a linear stability theory and in the current paper our objective is to extend this investigation of Hall & Seddougui (1989) into the nonlinear regime. We find that at this stage not only does the secondary mode become nonlinear but it also interacts with itself so as to modify the governing equations for the primary Görtler vortex. In this case then, the vortex and the travelling wave drive each other and, indeed, the whole flow structure is described by an infinite set of coupled, nonlinear differential equations. We undertake a Stuart-Watson type of weakly nonlinear analysis of these equations and conclude, in particular, that on this basis there exist stable flow configurations in which the travelling mode is of finite amplitude. Implications of our findings for practical situations are discussed and it is shown that the theoretical conclusions drawn here are in good qualitative agreement with available experimental observations.

Ou, Yuh-Roung and S. S. Sritharan: *Upper semicontinuous global attractors for viscous flow*. ICASE Report No. 90-2, January 2, 1990, 28 pages. Submitted to Quarterly of Applied Mathematics.

A particular form of regularization of the Navier-Stokes equations is studied. It has been shown that as the regularization parameter goes to zero, the global attractor for the regularized system converges to the global attractor for the conventional Navier-Stokes system.

Mavriplis, D. J.: *Euler and Navier-Stokes computations for two-dimensional geometries using unstructured meshes*. ICASE Report No. 90-3, January 2, 1990, 30 pages. Submitted to the Canadian Aeronautics.

A general purpose unstructured mesh solver for steady-state two-dimensional inviscid and viscous flows is described. The efficiency and accuracy of the method are enhanced by the simultaneous use of adaptive meshing and an unstructured multigrid technique. A method for generating highly stretched triangulations in regions of viscous flow is outlined, and a procedure for implementing an algebraic turbulence model on unstructured meshes is described. Results are shown for external and internal inviscid flows and for turbulent viscous flow over a multi-element airfoil configuration.

Nicol, David M. and Joel H. Saltz: *An analysis of scatter decomposition*. ICASE Report No. 90-4, January 3, 1990, 20 pages. Submitted to IEEE Transactions on Computers.

This paper provides a formal analysis of a powerful technique known as scatter decomposition. Scatter decomposition divides an irregular computational domain into a large number of equal sized pieces, and distributes them modularly among processors. We use a probabilistic model of workload in one dimension to formally explain why, and when scatter decomposition works. Our first result is that if correlation in workload is a convex function of distance, then scattering a more finely decomposed domain yields a lower average processor workload variance. Our second result shows that if the workload process is stationary Gaussian and the correlation function decreases linearly in distance until becoming zero and then

remains zero, scattering a more finely decomposed domain yields a lower expected maximum processor workload. Finally we show that if the correlation function decreases linearly across the entire domain, then among all mappings that assign an equal number of domain pieces to each processor, scatter decomposition minimizes the average processor workload variance. The dependence of these results on the assumption of decreasing correlation is illustrated with situations where a coarser granularity actually achieves better load balance.

Speziale, Charles G., Sutanu Sarkar, and Thomas B. Gatski: *Modeling the pressure-strain correlation of turbulence - An invariant dynamical systems approach*. ICASE Report No. 90-5, January 2, 1990, 52 pages. To be submitted to the Journal of Fluid Mechanics.

The modeling of the pressure-strain correlation of turbulence is examined from a basic theoretical standpoint with a view toward developing improved second-order closure models. Invariance considerations along with elementary dynamical systems theory are used in the analysis of the standard hierarchy of closure models. In these commonly used models, the pressure-strain correlation is assumed to be a linear function of the mean velocity gradients with coefficients that depend algebraically on the anisotropy tensor. It is proven that for plane homogeneous turbulent flows the equilibrium structure of this hierarchy of models is encapsulated by a relatively simple model which is only quadratically nonlinear in the anisotropy tensor. This new quadratic model - the SSG model - is shown to outperform the Launder, Reece, and Rodi model (as well as more recent models that have a considerably more complex nonlinear structure) in a variety of homogeneous turbulent flows. However, some deficiencies still remain for the description of rotating turbulent shear flows that are intrinsic to this general hierarchy of models and, hence, cannot be overcome by the mere introduction of more complex nonlinearities. It is thus argued that the recent trend of adding substantially more complex nonlinear terms containing the anisotropy tensor may be of questionable value in the modeling of the pressure-strain correlation. Possible alternative approaches are discussed briefly.

Iqbal, M. Ashraf: *Efficient algorithms for dilated mappings of binary trees*. ICASE Report No. 90-6, January 9, 1990, 41 pages. Submitted to IEEE Trans. Parallel & Distributed Computing.

We address the problem of finding a 1-1 mapping of the vertices of a binary tree onto those of a target binary tree such that the son of a node on the first binary tree is mapped onto a descendent of the image of the cost of this mapping, namely the *dilation cost* i.e. the maximum distance in the target binary tree between the images of vertices that are adjacent in the original tree. The other measure, *expansion cost*, is defined as the number of extra nodes/edges to be added to the target binary tree in order to ensure a 1-1 mapping. We describe an efficient algorithm to find a mapping of one binary tree onto another. We show that it is possible to minimize one cost of mapping at the expense of the other.

This problem arises when designing pipelined Arithmetic Logic Units for special purpose computers. The pipeline is composed of ALU chips connected in the form of a binary tree. The operands to the pipeline can be supplied to the leaf nodes of the binary tree which then process and pass the results up to their parents. The final result is available at the root. As each new application may require a distinct nesting of operations, it is useful to be able to find a good mapping of a new binary tree over existing ALU tree. Another problem arises

if every distinct required binary tree is known beforehand. Here it is useful to hardwire the pipeline in the form of a minimal supertree that contains all required binary trees.

Koelbel, Charles, Piyush Mehrotra, and John Van Rosendale: *Supporting shared data structures on distributed memory architectures*. ICASE Report No. 90-7, January 9, 1990, 19 pages. To appear in the Proceedings of the 2nd SIGPLAN Symposium on Principles and Practice of Parallel Programming, March 1990.

Programming nonshared memory systems is more difficult than programming shared memory systems, since there is no support for shared data structures. Current programming languages for distributed memory architectures force the user to decompose all data structures into separate pieces, with each piece "owned" by one of the processors in the machine, and with all communication explicitly specified by low-level message-passing primitives. This paper presents a new programming environment for distributed memory architectures, providing a global name space and allowing direct access to remote parts of data values. We describe the analysis and program transformations required to implement this environment, and present the efficiency of the resulting code on the NCUBE/7 and IPSC/2 hypercubes.

Jones, Mark T. and Merrell L. Patrick: *Factoring symmetric indefinite matrices on high-performance architectures*. ICASE Report No. 90-8, January 9, 1990, 15 pages. Submitted to SIAM Journal for Matrix Analysis and Application.

The Bunch-Kaufman algorithm is the method of choice for factoring symmetric indefinite matrices in many applications. However, the Bunch-Kaufman algorithm does not take advantage of high-performance architectures such as the Cray Y-MP. Three new algorithms, based on Bunch-Kaufman factorization, that take advantage of such architectures are described. Results from an implementation of the third algorithm are presented.

Singer, Bart A., Thomas A. Zang, and Gordon Erlebacher: *TS - Dean interactions in curved channel flow*. ICASE Report No. 90-9, January 18, 1990, 44 pages. Submitted to Journal of Fluid Mechanics.

A weakly nonlinear theory is developed to study the interaction of TS waves and Dean vortices in curved channel flow. The predictions obtained from the theory agree well with results obtained from direct numerical simulations of curved channel flow, especially for low amplitude disturbances. At low Reynolds numbers the wave interaction is generally stabilizing to both disturbances, though as the Reynolds number increases, many linearly unstable TS waves are further destabilized by the presence of Dean vortices.

Durlofsky, Louis J., Stanley Osher, and Bjorn Engquist: *Triangle based TVD schemes for hyperbolic conservation laws*. ICASE Report No. 90-10, January 19, 1990, 30 pages. Submitted to Journal of Computational Physics.

A triangle based TVD (total variation diminishing) scheme for the numerical approximation of hyperbolic conservation laws in two space dimensions is constructed. The novelty of the scheme lies in the nature of the preprocessing of the cell averaged data, which is accomplished via a nearest neighbor linear interpolation followed by a slope limiting procedure. Two such limiting procedures are suggested. The resulting method is considerably more simple than other triangle based non-oscillatory approximations which, like this scheme, approximate the flux up to second order accuracy. Numerical results for linear advection and Burgers' equation are presented.

Perthame, Benoit and Eitan Tadmor: *A kinetic equation with kinetic entropy functions for scalar conservation laws*. ICASE Report No. 90-11, January 19, 1990, 20 pages. Submitted to SIAM Journal on Applied Mathematics.

We construct a nonlinear kinetic equation and prove that it is well-adapted to describe general multidimensional scalar conservation laws. In particular we prove that it is well-posed (uniformly in  $\varepsilon$  - the microscopic scale). We also show that the proposed kinetic equation is equipped with a family of kinetic entropy functions - analogous to Boltzmann's microscopic  $H$ -function, such that they recover Krushkov-type entropy inequality on the macroscopic scale. Finally, we prove by both - BV compactness arguments in the multidimensional case and by compensated compactness arguments in the one-dimensional case, that the local density of kinetic particles admits a 'continuum' limit, as it converges strongly with  $\varepsilon \downarrow 0$  to the unique entropy solution of the corresponding conservation law.

Morris, K. A.: *Robustness of controllers designed using Galerkin type approximations*. ICASE Report No. 90-12, January 24, 1990, 20 pages. Submitted to SIAM Journal on Control and Optimization.

One of the difficulties in designing controllers for infinite-dimensional systems arises from attempting to calculate a state for the system. In this paper it is shown that Galerkin type approximations can be used to design controllers which will perform as designed when implemented on the original infinite-dimensional system. No assumptions, other than those typically employed in numerical analysis, are made on the approximating scheme.

Osher, Stanley and Chi-Wang Shu: *High order essentially non-oscillatory schemes for Hamilton-Jacobi equations*. ICASE Report No. 90-13, February 5, 1990, 27 pages. Submitted to SIAM Journal of Numerical Analysis.

Hamilton-Jacobi (H-J) equations are frequently encountered in applications, e.g. in control theory and differential games. H-J equations are closely related to hyperbolic conservation laws - in one space dimension the former is simply the integrated version of the latter.

Similarity also exists for the multi-dimensional case, and this is helpful in the design of difference approximations. In this paper we investigate high order essentially non-oscillatory (ENO) schemes for H-J equations, which yield uniform high order accuracy in smooth regions and resolve discontinuities in the derivatives sharply. The ENO scheme construction procedure is adapted from that for hyperbolic conservation laws. We numerically test the schemes on a variety of one-dimensional and two-dimensional problems, including a problem related to control-optimization, and observe high order accuracy in smooth regions, good resolution of discontinuities in the derivatives, and convergence to viscosity solutions.

Duck, Peter W. and Stephen J. Shaw: *The inviscid stability of supersonic flow past a sharp cone*. ICASE Report No. 90-14, February 7, 1990, 60 pages. Submitted to Theoretical & Computational Fluid Dynamics.

In this paper we consider the laminar boundary layer which forms on a sharp cone in a supersonic freestream, where lateral curvature plays a key role in the physics of the problem.

This flow is then analysed from the point of view of linear, temporal, inviscid stability. Indeed, the basic, non-axisymmetric disturbance equations are derived for general flows of this class, and a so called "triply generalised" inflexion condition is found for the existence of "subsonic" neutral modes of instability. This condition is analogous to the well-known generalised inflexion condition found in planar flows, although in the present case the condition depends on both axial and aximuthal wavenumbers.

Extensive numerical results are presented for the stability problem at a freestream Mach number of 3.8, for a range of streamwise locations. These results reveal that a new mode of instability may occur, peculiar to flows of this type involving lateral curvature.

Additionally, asymptotic analyses valid close to the tip of the cone / far downstream of the cone are presented, and these give a partial (asymptotic) description of this additional mode of instability.

Erlebacher, Gordon, M. Y. Hussaini, H. O. Kreiss, and S. Sarkar: *The analysis and simulation of compressible turbulence*. ICASE Report No. 90-15, February 8, 1990, 29 pages. Submitted to Theoretical and Computational Fluid Dynamics.

This paper considers compressible turbulent flows at low turbulent Mach numbers. Contrary to the general belief that such flows are almost incompressible, (i.e. the divergence of the velocity field remains small for all times), it is shown that even if the divergence of the initial velocity field is negligibly small, it can grow rapidly on a non-dimensional time scale which is the inverse of the fluctuating Mach number. An asymptotic theory which enables one to obtain a description of the flow in terms of its divergence-free and vorticity-free components has been developed to solve the initial-value problem. As a result, the various types of low Mach number turbulent regimes have been classified with respect to the initial conditions. Formulae are derived that accurately predict the level of compressibility after the initial transients have disappeared. These results are verified by extensive direct numerical simulations of isotropic turbulence.

Abarbanel, Saul S., Wai Sun Don, David Gottlieb, David H. Rudy, and James C. Townsend: *Secondary frequencies in the wake of a circular cylinder with vortex shedding*. ICASE Report No. 90-16, February 9, 1990, 26 pages. Submitted to Journal of Fluid Mechanics.

A detailed numerical study of two-dimensional flow past a circular cylinder at moderately low Reynolds numbers has been conducted using three different numerical algorithms for solving the time-dependent compressible Navier-Stokes equations. It was found that if the algorithm and associated boundary conditions were consistent and stable, then the major features of the unsteady wake were well-predicted. However, it was also found that even stable and consistent boundary conditions could introduce additional periodic phenomena reminiscent of the type seen in previous wind-tunnel experiments. However, these additional frequencies were eliminated by formulating the boundary conditions in terms of the characteristic variables. An analysis based on a simplified model provides an explanation for this behavior.

Decker, Naomi H.: *On the parallel efficiency of the Frederickson-McBryan multigrid algorithm*. ICASE Report No. 90-17, February 9, 1990, 10 pages. Submitted to SIAM Journal on Scientific and Statistical Computing.

To take full advantage of the parallelism in a standard multigrid algorithm requires as many processors as points. However, since coarse grids contain fewer points, most processors are idle during the coarse grid iterations. Frederickson and McBryan claim that retaining all points on all grid levels (using all processors) can lead to a 'superconvergent' algorithm. Has the 'parallel superconvergent' multigrid algorithm, PSMG, of Frederickson and McBryan solved the problem of implementing multigrid on a massively parallel SIMD architecture? How much can be gained by retaining all points on all grid levels, keeping all processors busy?

The purpose of this work is to show that the PSMG algorithm, though it achieves perfect processor utilization, is no more efficient than a parallel implementation of standard multigrid methods. PSMG is simply a new and perhaps simpler way of achieving the same results.

Sarkar, S. and L. Balakrishnan: *Application of a Reynolds stress turbulence model to the compressible shear layer*. ICASE Report No. 90-18, February 28, 1990, 29 pages. Submitted to AIAA Journal.

Theoretically based turbulence models have had success in predicting many features of incompressible, free shear layers. However, attempts to extend these models to the high-speed, compressible shear layer have been less effective. In the present work, the compressible shear layer was studied with a second-order turbulence closure, which initially used only variable density extensions of incompressible models for the Reynolds stress transport equation and the dissipation rate transport equation. The quasi-incompressible closure was unsuccessful; the predicted effect of the convective Mach number on the shear layer growth rate was significantly smaller than that observed in experiments. Having thus confirmed that compressibility effects have to be explicitly considered, a new model for the compressible dissipation was introduced into the closure. This model is based on a low Mach number, asymptotic analysis of the Navier-Stokes equations, and on direct numerical simulations of compressible, isotropic turbulence. The use of the new model for the compressible dissipation

led to good agreement of the computed growth rates with the experimental data. Both the computations and the experiments indicate a dramatic reduction in the growth rate when the convective Mach number is increased. Experimental data on the normalized maximum turbulence intensities and shear stress also show a reduction with increasing Mach number. The computed values are in accord with this trend.

Seddougui, S. O., R. I. Bowles, and F. T. Smith: *Surface - Cooling effects on compressible boundary-layer instability*. ICASE Report No. 90-19, February 28, 1990, 51 pages. Submitted to European Journal of Mechanics.

The influence of surface cooling on compressible boundary-layer instability is discussed theoretically for both viscous and inviscid modes, at high Reynolds numbers. The cooling enhances the surface heat transfer and shear stress, creating a high-heat-transfer sublayer. This has the effect of distorting and accentuating the viscous Tollmien-Schlichting modes to such an extent that their spatial growth rates become comparable with, and can even *exceed*, the growth rates of inviscid modes, including those found previously. This is for moderate cooling, and it applies at any Mach number. In addition, the moderate cooling destabilizes otherwise stable viscous or inviscid modes, in particular triggering outward-traveling waves at the edge of the boundary layer in the supersonic regime. Severe cooling is also discussed as it brings compressible dynamics directly into play within the viscous sublayer. All the new cooled modes found involve the heat-transfer sublayer quite actively, and they are often multi-structured in form and may be distinct from those observed in previous computational and experimental investigations. The corresponding nonlinear processes are also pointed out with regard to transition in the cooled compressible boundary layer. Finally, comparisons with Lysenko and Maslov's (1984) experiments on surface cooling are presented.

Nicol, David M.: *The cost of conservative synchronization in parallel discrete event simulations*. ICASE Report No. 90-20, May 9, 1990, 31 pages. Submitted to the Journal of the ACM.

This paper analytically studies the performance of a synchronous conservative parallel discrete-event simulation protocol. The class of simulation models considered are oriented around a physical domain, and possess a limited ability to predict future behavior. Using a stochastic model we show that as the volume of simulation activity in the model increases relative to a fixed architecture, the complexity of the average per-event overhead due to synchronization, event list manipulation, lookahead calculations, and processor idle time approaches the complexity of the average per-event overhead of a serial simulation. The method is therefore within a constant factor of optimal. Our analysis demonstrates that on large problems—those for which parallel processing is ideally suited—there is often enough parallel workload so that processors are not usually idle. We also demonstrate the viability of the method empirically, showing how good performance is achieved on large problems using a thirty-two node Intel iPSC/2 distributed memory multiprocessor.



Nicol, David M.: *Performance bounds on parallel self-initiating discrete-event*. ICASE Report No. 90-21, March 2, 1990, 29 pages. Submitted to ACM Transactions on Modelling and Computer Simulations.

This paper considers the use of massively parallel architectures to execute discrete-event simulations of what we term "self-initiating" models. A logical process in a self-initiating model schedules its own state re-evaluation times, independently of any other logical process, and sends its new state to other logical processes following the re-evaluation. Our interest is in the effects of that communication on synchronization. We consider the performance of various synchronization protocols by deriving upper and lower bounds on optimal performance, upper bounds on Time Warp's performance, and lower bounds on the performance of a new conservative protocol. Our analysis of Time Warp includes the overhead costs of state-saving and rollback. The analysis points out sufficient conditions for the conservative protocol to outperform Time Warp. The analysis also quantifies the sensitivity of performance to message fan-out, lookahead ability, and the probability distributions underlying the simulation.

Karageorghis, Andreas and Timothy N. Phillips: *Conforming Chebyshev spectral collocation methods for the solution of laminar flow in a constricted channel*. ICASE Report No. 90-22, March 2, 1990, 45 pages. Submitted to IMA Journal of Numerical Analysis.

The numerical simulation of steady planar two-dimensional, laminar flow of an incompressible fluid through an abruptly contracting channel using spectral domain decomposition methods is described. The key features of the method are the decomposition of the flow region into a number of rectangular subregions and spectral approximations which are pointwise  $C^1$  continuous across subregion interfaces. Spectral approximations to the solution are obtained for Reynolds numbers in the range  $[0, 500]$ . The size of the salient corner vortex decreases as the Reynolds number increases from 0 to around 45. As the Reynolds number is increased further the vortex grows slowly. A vortex is detected downstream of the contraction at a Reynolds number of around 175 that continues to grow as the Reynolds number is increased further.

Rosen, I. G. and C. Wang: *On the continuous dependence with respect to sampling of the linear quadratic regulator problem for distributed parameter systems*. ICASE Report No. 90-23, March 6, 1990, 42 pages. Submitted to SIAM Journal on Control and Optimization.

The convergence of solutions to the discrete or sampled time linear quadratic regulator problem and associated Riccati equation for infinite dimensional systems to the solutions to the corresponding continuous time problem and equation, as the length of the sampling interval (the sampling rate) tends toward zero (infinity) is established. Both the finite and infinite time horizon problems are studied. In the finite time horizon case, strong continuity of the operators which define the control system and performance index together with a stability and consistency condition on the sampling scheme are required. For the infinite time horizon problem, in addition, the sampled systems must be stabilizable and detectable, uniformly with respect to the sampling rate. Classes of systems for which this condition can be verified are discussed. Results of numerical studies involving the control of a heat/diffusion equation, a hereditary of delay system, and a flexible beam are presented and discussed.

Rosen, I. G. and Chien-Hua Frank Su: *An approximation theory for the identification of linear thermoelastic systems*. ICASE Report No. 90-24, March 7, 1990, 31 pages. Submitted to *Differential and Integral Equations*.

An abstract approximation framework and convergence theory for the identification of thermoelastic systems is developed. Starting from an abstract operator formulation consisting of a coupled second order hyperbolic equation of elasticity and first order parabolic equation for heat conduction, well-posedness is established using linear semigroup theory in Hilbert space, and a class of parameter estimation problems is then defined involving mild solutions. The approximation framework is based upon generic Galerkin approximation of the mild solutions, and convergence of solutions of the resulting sequence of approximating finite dimensional parameter identification problems to a solution of the original infinite dimensional inverse problem is established using approximation results for operator semigroups. An example involving the basic equations of one dimensional linear thermoelasticity and a linear spline based scheme is discussed and numerical results indicating how our approach might be used in a study of damping mechanisms in flexible structures are presented.

Lafon, F. and S. Osher: *High order methods for approximating hyperbolic systems of conservation laws*. ICASE Report No. 90-25, March 9, 1990, 36 pages. Submitted to *Journal of Computational Physics*.

In the computation of discontinuous solutions of hyperbolic systems of conservation laws, the recently developed ENO (Essentially Non-Oscillatory) schemes appear to be very useful. However, they are computationally costly compared to simple central difference methods. In this paper we develop a filtering method which uses simple central differencing of arbitrarily high order accuracy, except when a novel local test indicates the development of spurious oscillations. At these points, generally few in number, we use the full ENO apparatus, maintaining the high order of accuracy, but removing spurious oscillations. Numerical results indicate the success of the method. We obtain high order of accuracy in regions of smooth flow without spurious oscillations for a wide range of problems and a significant speed up of generally a factor of almost three over the full ENO method.

Speziale, Charles G.: *Analytical methods for the development of Reynolds stress closures in turbulence*. ICASE Report No. 90-26, March 21, 1990, 61 pages. To appear in the *Annual Review of Fluid Mechanics*, January 1991.

Analytical methods for the development of Reynolds stress models in turbulence are reviewed in detail. Zero, one and two equation models are discussed along with second-order closures. A strong case is made for the superior predictive capabilities of second-order closure models in comparison to the simpler models. The central points of the paper are illustrated by examples from both homogeneous and inhomogeneous turbulence. A discussion of the author's views concerning the progress made in Reynolds stress modeling is also provided along with a brief history of the subject.

Cai, Wei, David Gottlieb, and Ami Harten: *Cell averaging Chebyshev methods for hyperbolic problems*. ICASE Report No. 90-27, March 28, 1990, 22 pages. To appear in *Computer and Math with Application*, special issue: Advance in P.D.E.

This paper describes a cell averaging method for the Chebyshev approximations of first order hyperbolic equations in conservation form. We present formulas for transforming between pointwise data at the collocation points and cell averaged quantities, and vice-versa. This step, trivial for the finite difference and Fourier methods, is nontrivial for the global polynomials used in spectral methods. We then prove that the cell averaging methods presented are stable for linear scalar hyperbolic equations and present numerical simulations of shock-density wave interaction using the new cell averaging Chebyshev methods.

Karni, S.: *Viscous shock profiles and primitive formulations*. ICASE Report No. 90-28, March 29, 1990, 24 pages. Submitted to *SIAM Journal of Numerical Analysis*.

We consider weak solutions of hyperbolic systems in primitive (non-conservation) form for which a consistent conservation form exists. We show that for primitive formulations, shock relations are not uniquely defined by the states to either side of the shock but also depend on the viscous path connecting the two. Scheme-dependent high order correction terms are derived that enforce consistent viscous shock profiles. The resulting primitive algorithm is conservative to the order of the approximation. One dimensional Euler calculations of flows containing strong shocks clearly show that conservation errors in primitive calculations are reduced to truncation levels and that both conservative and primitive flow calculations are of comparable quality.

## ICASE INTERIM REPORTS

Hiranandani, Seema, Joel Saltz, Harry Berryman, and Piyush Mehrotra: *A scheme for supporting distributed data structures on multicomputers*. Interim Report No. 9, January 4, 1990, 14 pages. To appear in Proceedings of the Fifth Distributed Memory Computing Conference, Charleston, South Carolina, April 1990.

We propose a data migration mechanism that allows an explicit and controlled mapping of data to memory. While read or write copies of each data element is assigned to a specific location in the memory of a particular processor. Our proposed integration of a data migration scheme with a compiler is able to eliminate the migration of unneeded data that can occur in multiprocessor paging or caching. The overhead of adjudicating multiple concurrent writes to the same page or cache line is also eliminated. We present data that suggests that the scheme we suggest may be a practical method for efficiently supporting data migration.

## ICASE COLLOQUIA

October 1, 1989 through March 31, 1990

Name/Affiliation/Title	Date
Mr. Patrick Queutey, Laboratoire d'hydrodynamique Navale, France "Three-Dimensional Incompressible Navier-Stokes Solutions over Bodies at Incidence"	October 6
Professor J. Walker, Lehigh University "Dynamics of Turbulent Wall Layers"	October 13
Professor Max Gunzburger, Virginia Polytechnic Institute and State University "Numerical Algorithms for the Boundary Control of Flows with Applications to Viscous Drag Minimization"	October 16
Dr. Nahil A. Sobh, Old Dominion University "Finite Element Computations on the Connection Machine"	October 18
Dr. Tobias Orloff, Institute for Computer Applications in Science and Engineering "A Parallel 3D Triangle Renderer"	October 19
Dr. Serge Petition, Yale University "Subspace Methods as a Methodology to Solve Eigenproblems on Massively Parallel Architectures; Example of Arnoldi's Method on the CM2"	October 20
Professor Anthony Leonard, Rutgers University "Dynamical Systems and Mixing in Fluid Mechanics"	October 30
Professor Helen Reed, Arizona State University "Receptivity of the Boundary Layer on a Semi-Infinite Flat Plate with an Elliptic Leading Edge"	October 31
Professor Helen Reed, Arizona State University "Stability of High-Speed Chemically Reacting and Three-Dimensional Boundary Layers"	October 31
Dr. Andrew Neish, University College London "Internal Hypersonic Nozzle Flow"	November 6

Name/Affiliation/Title	Date
Dr. Gerald Hedstrom, Lawrence Livermore National Laboratory "The Behavior of Waves in Grids"	November 8
Professor Swami Manohar, University of North Carolina, Charlotte "Large Parallel Architectures for Multigrid"	November 20
Dr. Takashi Abe, The Institute of Space and Astronomical Science, Japan "Direct Simulation Monte Carlo Method in Rarefied Gas Flow Simulations"	November 28
Dr. Naomi Decker, Institute for Computer Applications in Science and Engineering "On the Efficiency of the Frederickson-McBryan Multigrid Algorithm"	November 29
Dr. John Goodrich, NASA Lewis Research Center "Hopf Bifurcation in the Driven Cavity"	December 5
Professor Paul Reynolds, University of Virginia "Atomic Operations Without Locking"	December 14
Professor Thomas F. Balsa, University of Arizona "The Evolution of Nonlinear Disturbances in a Supersonic Mixing Layer"	December 18
Professor K. R. Rajagopal, University of Pittsburgh "Swirling Flows of Newtonian and Non-Newtonian Fluids and Some Related Problems"	January 12
Dr. Abdelkader Frendi, Northeastern University "A Numerical Study of Ignition Limits for Methane-Air Mixtures"	January 19
Professor Steven Orszag, Princeton University "Organization and Structure in Turbulent Flows"	January 23
Mr. Kurt Bryan, University of Washington "An Inverse Problem in Impedance Tomography"	February 1
Professor Bernard Grossman, VPI&SU "Anomalous Wave Speeds in Non-Equilibrium Flows with Multiple Translational Temperatures"	February 5

Name/Affiliation/Title	Date
Professor George Karniadakis, Princeton University "Computation of Transitional and Turbulent Flows in Complex Geometries"	February 6
Mr. Charles Koelbel, Purdue University "Compiling Programs for Nonshared Memory Machines"	February 8
Bracy Elton, University of California, Davis "Stability and Convergence Results for Lattice Gas and Lattice Boltzmann Methods for Solving PDEs"	February 9
Mr. Steve Lee, University of Illinois at Urbana "Large Krylov Methods in the Solution of Nonlinear Initial Value Problems in ODEs and DAEs"	February 12
Professor Bernard Grossman, VPI&SU "Integrated Aerodynamics/Structural Design Optimization"	February 13
Professor Otto Zeman, Stanford University "Recent Developments in Modeling Compressible Turbulence"	February 14
Dr. Peter Jacobs, University of Queensland, Australia "Hypervelocity Flow in Axisymmetric Nozzles"	March 7
Mr. Gregory Byrd, Stanford University "Streamline: Cache-Based Message Passing in Scalable Shared Memory Multiprocessors"	March 8
Professor Biswa Datta, Northern Illinois University "Large-Scale and Parallel Computations in Control"	March 9
Dr. Mark Morkovin, Professor Emeritus, Illinois Institute of Technology "On the Physics of Vorticity and Turbulence at Supersonic Speeds—Informal Ruminations"	March 12
Professor W. O. Criminale, University of Washington "The Evolution of Linearized Perturbations of Parallel Flows"	March 13
Professor Thomas C. Corke, Illinois Institute of Technology "Three Dimensional Mode Resonance in Boundary Layers and Wakes"	March 19

Name/Affiliation/Title	Date
Dr. Shahid H. Bokhari, University of Engineering & Technology, Lahore, Pakistan "Pipelined Parallel Multigrid"	March 20
Professor Joel Ferziger, Stanford University "Direct Simulation of Turbulent Combusting Flows"	March 21
Dr. Shahid H. Bokhari, University of Engineering & Technology, Lahore, Pakistan "A Network Flow Model for Analyzing Link Contention in Circuit-Switched Multicomputers"	March 27



## OTHER ACTIVITIES

The Combustion Workshop co-sponsored by ICASE and NASA Langley Research Center was held October 2-4, 1989, at the Omni Hotel, Newport News, VA. Fifty-five people attended this workshop. The objectives of the workshop were to review the current status of knowledge on flame structure, flame stability, flame holding/extinction, ignition, chemical kinetics, turbulence/kinetic interaction, transition to detonation, and reacting free shear layers. Invited speakers and their topics are listed below:

### **Flame Structure:**

M. Smooke, Yale University  
B. Rogg, University of California, San Diego  
S. M. Correa, General Electric Corporate R and D Center

### **Flame Stability:**

J. Buckmaster, University of Illinois  
T. Jackson, ICASE and Old Dominion University  
A. Kapila, Rensselaer Polytechnic Institute  
M. Matalon, Tech. Institute Engineering Science & Applied Mathematics

### **Mechanisms of Ignition, Extinction and Flame Stabilization in Subsonic and Supersonic Flows:**

C. K. Law, Princeton University  
A. Karagozian, University of California, Los Angeles  
I. Shepherd, Lawrence Berkeley Laboratory

### **Mixing Power Concepts in Scramjet Combustor Design:**

J. R. Swithenbank, Sheffield University  
P. Givi, SUNY at Buffalo  
J. Riley, University of Washington

### **Chemical Kinetics of Combustion Processes:**

R. W. Walker, Hull University  
F. L. Dryer, Princeton University  
R. Yetter, Princeton University  
C. J. Jachimowski, NASA Langley Research Center  
D. M. Golden, SRI International

**The Interaction of Turbulence and Chemical Kinetics:**

W. Kollman, University of California, Davis

D. R. Ballal, University of Dayton

P. A. Libby, University of California, San Diego

**On the Transition from Deflagration to Detonation:**

J. Shepherd, Rensselaer Polytechnic Institute

D. Pratt, University of Washington

M. Sichel, University of Michigan

A volume of the proceedings from this conference will be published by Springer-Verlag in the near future.

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