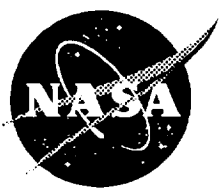


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INTRODUCTION

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

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

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

The major categories of the current ICASE research program are:

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

ICASE reports are considered to be primarily preprints of manuscripts that have been submitted to appropriate research journals or that are to appear in conference proceedings. A list of these reports for the period October 1, 1993 through March 31, 1994 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

APPLIED AND NUMERICAL MATHEMATICS

SAUL ABARBANEL

Issues in Long-time Integration

It is known that long-time integration of systems of PDEs (such as the Euler or the Navier-Stokes Equations) may lead to errors with exponential temporal growth. Previous work with D. Gottlieb and M. Carpenter has led to a new method of treating the boundary conditions, especially in the case of high order spatial accuracy.

The results above apply to the semi-discrete setting. When the temporal integration is considered new difficulties are encountered. For example, the boundary condition specification at the intermediate levels of a Runge-Kutta integration turns out to be counter-intuitive. If the “physical” boundary condition is $g(t)$, and one specifies at an intermediate level of $t + a\delta t$, ($0 < a < 1$), $g = g(t + a\delta t)$ then the spatial accuracy near the boundary deteriorates to first order. ICASE Report 93-83 deals with this issue.

Future work will deal with the long-time interaction between the advection and diffusion terms in the Navier-Stokes Equations. This interaction is responsible for a cell-Reynolds-number-like restriction on the mesh size, and hopefully methods can be derived to ameliorate this situation.

EYAL ARIAN

Multigrid One Shot Methods for Optimal Shape Design of Elliptic Systems

The objective is to continue development of efficient multigrid one shot methods for infinite dimensional optimization problems. In these problems the number of design variables grows with the grid refinement. One class of problems that was investigated was the aerodynamic shape design problem in the subsonic regime. In this problem the unknown is part of the boundary which defines the physical domain. The problem is to find a shape of the boundary such that some condition on the boundary will be minimized.

Numerical results have been obtained for an optimal shape design of a two-dimensional nozzle with a finite element discretization. A cost function was defined on the design boundary and measured the distance (in L^2 norm) of the normal derivative of the constraint PDE solution from a desired given function. The state, costate and design variables were smoothed at each relaxation sweep, which was accelerated using coarse grids on all levels, leading to a very efficiently converging algorithm. With this one shot full multigrid algorithm, a mesh size independent of convergence rate has been achieved for meshes ranging between $2^2 \times 2^2$ to $2^7 \times 2^7$ grid points. The computer time for solving the optimization problem, up to the discretization error, for 128 design parameters, was of the same order of magnitude as solving just a few times the constraint PDE.

In the small disturbance case, a two level analysis has been developed to approximate the convergence rate of the one shot algorithm. In some ill-posed problems the analysis shows how to overcome the ill posedness with the use of a high pass filter. Preliminary numerical tests have confirmed the predictions of the analysis. This work is being done in collaboration with S. Ta'asan.

RICHARD BALLING

Problem Formulation Approaches for Multidisciplinary Design Optimization

The increased demands of economic competition and the complexity of engineering systems have led to the rapid growth of the field of multidisciplinary design optimization (MDO) over the past decade. Several approaches to problem formulation for coupled systems have emerged in a rather *ad hoc* fashion. Some of these approaches still need further development, and the factors governing choice of approach are not well understood.

A unified classification of approaches has been developed. Six fundamental approaches have been identified. A compact notation has been devised to uniquely distinguish between the infinite number of variations which are possible. Some of the fundamental approaches are new, and others which were previously thought to be limited to hierarchic systems (systems in which children disciplines are coupled only to parent disciplines and not to each other) have been shown to apply to nonhierarchic systems. The approaches have been compared from both computational and managerial viewpoints. A new algorithm has also been developed to solve the system-level optimization problem in multilevel approaches. The system-level problem was shown to be a non-smooth optimization problem. The new algorithm is based on a cutting plane approach.

Further work is needed to verify and compare the approaches on a realistic engineering example. Work is also needed to develop the approaches further to accommodate large-scale problems and problems involving discrete and topological variables within disciplines.

H.T. BANKS

Damage Detection in Structures

This work is motivated by the need to test structures (such as aircraft walls, airfoil, etc.) for damage such as corrosion, cracks, delamination, etc., with nondestructive, noninvasive techniques. Our efforts here are in the spirit of earlier joint efforts with Bill Winfree (IRD, NASA Langley Research Center) and Fumio Kojima (ICASE) on a thermal tomography for nondestructive evaluation.

Our current approach, which is joint work primarily with Dr. Yun Wang (N.C. State University and Brooks AFB), entails the use of piezoceramics in self-excitation, self-sensing "smart material" configurations. Using distributed parameter models for piezoceramic loaded structures, we have developed a theoretical and computational methodology for detecting damage via changes in material parameters (mass density, stiffness, damping) during periodic vibration testing. Simulation studies are most promising, as are early use of these methods with experiments designed and carried out in collaboration with Dr. D.J. Inman and Don Leo in the Mechanical Systems Lab at VPISU.

Our early efforts focus on the detection and location of holes and corrosion type defects. Future plans involve development of these techniques for detection and characterization of cracks and disbonds/delaminations in composite material structures.

JOHN A. BURNS

Optimal Design and Sensor Location for Control of Partial Differential Equations

The development of feedback controllers for nonlinear partial differential equations holds considerable promise as a practical method for modifying continuous systems in order to achieve a desired behavior. A fundamental problem is the development of techniques for optimally locating sensors and actuators in distributed parameter systems. The objective of this work is to develop a mathematical framework and computational methods for attacking this problem and to apply the results to problems in fluid flow control.

Although this problem has been considered by several people over the past ten years, the approach we consider makes no prior assumptions regarding the form of the controls/actuators in an effort to make decisions about where actuators and sensors are best placed. In particular, we assume that the input operator is as general as possible and consider the problem of constructing kernels for integral representations of feedback control laws obtained by solving LQR and MinMax control problems. These kernels can be used to shape, design and locate sensors. However, this approach requires the existence of integral representations for feedback control laws and practical computational methods to “approximate” these kernels. In most existing papers, fundamental questions concerning the existence of these integral representations and the smoothness of the corresponding integral kernels are not considered. These issues are important in the development and analysis of rigorous numerical approximations. Also, the ability to accurately compute these kernels is an essential component in the study of actuator/sensor placement. We have established high order regularity of solutions of algebraic Riccati equations arising from certain infinite dimensional LQR and MinMax control problems. We show that distributed parameter systems described by parabolic partial differential equations often have a special structure that smoothes solutions of the corresponding Riccati equations. This analysis allows us to find specific integral representations for Riccati operators and can be used in the development of computational schemes for problems many boundary control problems and in other distributed control problems associated with optimal sensor/actuator placement.

These results will be combined with robust control designs and numerical approximations in order to study the effects of replacing distributed controllers with a set of discrete controls that reflect a physically realizable controlled system. The goal is to apply the method to determine the “best” type, size, number, and placement of sensors for PDE control problems of the type that occur in fluid flows.

WEI CAI

Wavelet Multi-Resolution Schemes

The purpose of the study is to apply wavelet multi-resolution schemes for the purpose of studying the deflagration to detonation (DDT) problem.

The numerical algorithm is based on a special wavelet collocation method for the initial boundary value problem of nonlinear PDE's. The key component in this collocation method is a so-called “Discrete Wavelet Transform” (DWT) which maps a solution between the physical space and the wavelet coefficient space. The fact that the wavelet basis forms a hierarchical basis for the Sobolev

space $H_0^2([-1, 1])$ implies that the DWT transformation only takes $O(\log N)$ operations where N is the total number of unknowns. The boundary condition treatment is similar to the techniques developed by Carpenter, Gottlieb and Abarbanel for compact schemes. Therefore, the adaptive wavelet collocation method effectively produces an adaptive compact scheme.

Current work is concentrated on the development of multi-grid methods for the algebraic systems from the time implicit discretization of evolution PDE's. An efficient solver for such system is important to overcome the CFL restriction on time steps. Another important issue under consideration is the development of efficient data structure associated with the adaptive wavelet collocation method for multidimensional problems.

SORIN COSTINER

Multigrid Techniques for Eigenvalue and Finite-Dimensional Parameter Space Optimization Problems

The main objective of our research is the development of efficient techniques for electromagnetism and for large scale eigenvalue problems.

The following multigrid (MG) techniques have been developed: the MG separation technique, the MG stable subspace technique, and an MG optimization technique (for finding the global minimum or several relevant local minima). These techniques have been used successfully for linear and nonlinear Schrödinger eigenvalue problems (in 2-D and 3-D), for bifurcation problems, and for design of resonant cavities. Compared with previous methods, the new techniques offer the following advantages: 1) they reduce significantly the large number of problem solutions needed for nonlinear, bifurcation, optimization, and design problems; 2) they improve the convergence rates and reduce the computational work of MG cycles; 3) they are robust; and 4) they can overcome central computational difficulties related to ill posedness, local minima, close and equal eigenvalues (for eigenvalue problems), and poor coarse level representations. A general, adaptive MG software, (for problems in 2-D and 3-D), which incorporates these techniques has been developed. The methods and part of the applications have been presented in a paper in print at IEEE-MTT, at two conferences and in several reports. Two patent applications have been filed.

Further directions of research include applying the new methods to flutter computations, to optimization for electromagnetism problems, as well as to parallel implementation of the algorithms.

This work was done in collaboration with Shlomo Ta'asan.

DAVID GOTTLIEB

Interactions of Shocks and Hydrogen Jets

The objective of this work is to study combustion and mixing induced by the interaction of a shock in air with a hydrogen jet. This model problem is of interest for the design of air-breathing scramjet engines, as it provides a mechanism for inducing millisecond combustion times. Extremely rapid combustion is a necessity in an engine where the reactants are escaping from the reaction chamber at supersonic speeds.

We have constructed (with W.S. Don and C. Quillen) a spectral shock capturing scheme as well as a third-order ENO scheme to simulate this problem. The spectral method provides a high order

of accuracy needed for the resolution of the details of the flow inside the jet. The ENO scheme is serving to check the spectral results. We need many more points in the ENO scheme to get the quality of the results obtained by the spectral code.

We plan to continue this work to more complicated interactions as well as to optimize the position of the jets relative to the shock waves.

Basic Research in Spectral Methods

The objective is to extend spectral methods to include arbitrary grids.

We have found ways to apply the Legendre Collocation methods on Chebyshev (and also arbitrary grids); recently we have found ways to apply the Legendre Galerkin method on an arbitrary grids. This task is being done in collaboration with M. Carpenter and W.S. Don.

We hope to find a way, using these ideas, to do spectral methods on nonregular domains.

MAX GUNZBURGER

Control of Transitional Flows

Control of fluid flows is a subject of considerable practical and scientific interest. A major goal of the present work is to investigate methods for controlling transitional flows. In this context we have been working on techniques for the identification and cancellation of unstable modes for delaying or avoiding transition to turbulence.

Our initial efforts have been directed towards stabilizing channel flows using feedback control, primarily injection, and suction at fixed locations on the channel wall. Early attempts made use of analytical results for the amplitude and phase of the TS wave and used these results to determine the amplitude and phase of the control necessary to diminish the growth rate of the unstable mode. Subsequently, efforts were directed towards determining the amplitude and phase of the TS wave from an FFT analysis of sensed pressure data at other locations along the wall. This computed data was then used to obtain the required amplitude and phases. While not as effective as using the analytical TS data this has turned out to be a satisfactory approach for reducing the growth rate of the unstable mode. Currently we are developing more direct feedback relations between the control and the sensed data with the goal of removing the need for an FFT analysis of the sensed data.

Future plans call for the use and implementation of other controls including shape and heating controls. This will necessitate the development of codes which are capable of handling time-varying domains. In addition we plan to develop appropriate linear and nonlinear feedback mechanisms. Beyond this, our ultimate goal is to formulate and apply optimal control strategies for aerodynamic control and design. For example, for transitional channel flow one could seek controls which maintain the flow close to the laminar parabolic profile (where closeness is measured in some appropriate norm). We will provide rigorous analysis of our techniques where this is possible.

This work is joint with Roy Nicolaides, Ron Joslin (NASA LaRC) and Gordon Erlebacher and Yousuff Hussaini (ICASE).

ISAAC HARARI

Computational Acoustics and Fluid-Solid Interaction

The interaction of an elastic or viscoelastic structure with a fluid involves many disciplines including solid mechanics, fluid dynamics, and wave propagation. This problem, particularly when the fluid is exterior to the structure, poses considerable challenges to computation. The objective of this work is to develop finite difference and finite element methods to numerically solve fluid-solid interaction problems.

In collaboration with Eli Turkel, finite difference methods for solving time-harmonic problems of wave propagation were developed and analyzed. Multi-dimensional inhomogeneous problems with variable, possibly discontinuous, coefficients were considered, accounting for the effects of employing non-uniform grids. A weighted-average representation, based on concepts of consistent representation that arise in Galerkin finite element formulations, was found to be less sensitive to transition in wave resolution (due to variable wave numbers or non-uniform grids) than the standard pointwise representation. Further enhancement in method performance was obtained by basing the stencils on generalizations of Padé approximation, or generalized definitions of the derivative, reducing spurious dispersion, anisotropy and reflection, and by improving the representation of source terms. The resulting schemes have fourth-order accurate local truncation error on uniform grids and third order in the non-uniform case. Guidelines for discretization pertaining to grid orientation and resolution were derived.

Numerical testing of these methods will be performed in future work. The enhancement of finite difference representations, particularly generalizations of Padé approximation, may be employed to improve finite element formulations. These methods will be useful for coupling to finite element structural models to compute problems of fluid-solid interaction.

LELAND JAMESON

Wavelet-based Numerical Methods

Often the solution to the partial differential equations which model physics will contain information at many different scales and in various regions of the domain. The goal of this research program has been to develop numerical methods which will do only the necessary work. That is, if one region of the domain contains most of the small-scale information then this region will contain the majority of the available degree-of-freedom regardless of the basis used.

Our approach is based on a wavelet basis. Wavelets provide a very convenient structure within which one can place degrees-of-freedom, or simply wavelet bases functions, at whatever scale and location is necessary to resolve the solution, to a given a tolerance. Previous work illustrated the efficacy of the new method, named the 'Wavelet Optimized Finite Difference Method' or WOFD, when applied to Burgers' equation in one dimension. Recently, the method has been upgraded to two dimensions and preliminary testing on simple combustion problems appears promising. Also, a method similar to WOFD designed for conservation laws has been developed jointly with R. B. Bauer. Cells are defined to be 'small' only where the data contains small scale structure and the numerical fluxes are evaluated on this arbitrary set of cells. The method appears to be working well when applied to the one-dimensional Euler equations. In both of the methods mentioned the

grid, or cells, are essentially arbitrary and the spatial accuracy can be set as high as desired by the user.

Future work will consist of thoroughly testing the above two methods in higher dimensions and on a variety of applications.

DAVID A. KOPRIVA

Spectral Domain Decomposition Optimization

Spectral domain decomposition methods are being developed as techniques for solving problems in complex geometries and/or where internal layers require local refinement. The objectives of this work are to develop methods applicable to the solution of steady and unsteady viscous and inviscid compressible fluid flows.

A two-dimensional multidomain Chebyshev collocation method has been developed for the compressible Navier-Stokes equations that is suitable for steady-state computations. The method has been applied to the solution of steady, viscous hypersonic flows over blunt cones and wedges. Comparisons with experimental data have been made, and are being prepared for publication. Several possible modifications are now being considered to make the method suitable for wave-propagation problems, such as in aeroacoustics. Application of a multidomain method to model problems describing flame ignition have also begun recently.

Future plans include an assessment of the suitability of spectral multidomain methods to the solution of wave-propagation problems such as those in aeroacoustics, including an assessment of boundary and radiation conditions. The solution of ignition problems using the full Navier-Stokes equations will also be considered.

DIMITRI MAVRIPLIS

Efficient Three-Dimensional Navier-Stokes Solvers for Unstructured Meshes

The objective of this work is the development of efficient solution techniques for the Navier-Stokes equations using unstructured meshes. This is motivated by the need to compute turbulent viscous flows over complex configurations.

A three-dimensional unstructured turbulent Navier-Stokes solver has been developed. This has been achieved by adding viscous terms and a field equation turbulence model to the previously developed unstructured Euler solver. A multigrid method which operates on a sequence of non-nested coarse and fine meshes has also been incorporated to accelerate convergence. The code has been validated on grids of up to 2 million points demonstrating consistent multigrid convergence rates and good accuracy. The code has also been parallelized on the CRAY-YMP-C90 delivering speedups of 13 on 16 processors. Parallelization on the CM-5 architecture has been undertaken in collaboration with Eric Morano.

In conjunction with V. Venkatakrishnan, research has also been conducted on the use of agglomeration techniques for unstructured multigrid solvers. In contrast to the non-nested multigrid technique employed in the above work, agglomeration provides an automatic mechanism for generating coarse grid levels from a given fine unstructured grid. While this methodology has previously been applied to the Euler equations in two and three dimensions, the present effort is

concerned with the Navier-Stokes equations. Agglomeration multigrid, however, does not extend in a straight-forward manner to the Navier-Stokes equations. Thus, the present research is concerned with devising extensions to the agglomeration strategy for diffusion dominated problems. In this context, the links between agglomeration multigrid and algebraic multigrid are also being investigated. Optimal coarsening strategies for both the agglomeration multigrid and the overlapping mesh multigrid algorithms are being investigated in conjunction with Eric Morano.

Future plans include the development of an agglomeration/algebraic multigrid strategy suitable for the Navier-Stokes equations, as well as the incorporation of optimal coarsening strategies. The results thus demonstrated in two-dimensions will then be extended to three dimensions.

ERIC MORANO

Unstructured Solvers for the Euler and Navier-Stokes Equations: Multigrid Techniques and Parallel Implementation

Multigrid algorithms and parallel computing are among the most effective techniques for reducing the costs of solving the fluid dynamics equations. The purpose of this work is to improve or to develop these technologies through the use of new kinds of solvers, smoothers, grid generators, and computers.

A 3D Euler solver has been implemented on the CM-5 architecture. In this work, done in collaboration with D. Mavriplis, the equations were discretized on the unstructured mesh using a Galerkin finite-element formulation. The flow variables are stored at the vertices of the mesh, and piecewise linear flux functions are assumed over the individual tetrahedra of the mesh. The scheme is a so-called central differencing scheme. The main data-structure of this code is edge-based. Residuals are constructed by executing loops over the edges of the mesh. At mesh boundaries, an additional loop over the triangular faces which form the boundary is then performed. Since such a scheme is not stable, we add artificial dissipation constructed as a blend of a Laplacian and a biharmonic operator. Then, the resulting spatially discretized equations must be integrated in time to obtain the steady-state solution. This is achieved using a 5-stage Runge-Kutta scheme. The whole implementation was done in CM-Fortran language, allowing use of the SIMD capability of the computer. We have demonstrated that partitioning the mesh, through the use of a parallel recursive spectral bisection (RSB) implemented in CMF by Johan et al., dramatically improves the performance. The solver requires a large amount of communication which results in a low overall performance. We have also shown that the communication time rates are strongly related to the value of $edge_ratio = \frac{cut_edges_part}{max_edges}$, where cut_edges_part is the number of cut edges between two partitions, divided by the number of partitions, and max_edges the maximum number of edges strictly included in a processor.

A Message Passing version of the code is currently being developed, using the PARTI Runtime Library, lately renamed CHAOS, proposed by Saltz et al. Another important feature in reaching good performance, is an efficient multigrid solver. The emphasis here is the generation of the multilevel grids. This can be done through a coarsening algorithm (see the work of Guillard at INRIA, France), or an agglomeration technique (see Lallemand at INRIA, France and, lately, Mavriplis and Venkatakrishnan at ICASE). Although both groups have produced good results for the resolution of the Euler equations, difficulties remain in the case of the Navier-Stokes equations where it is not

clear on how to produce the coarse grids. A multigrid code solving the Poisson equation, through a finite-volume formulation, on unstructured quadrilateral meshes has been developed in order to understand what is the “best” semi-coarsening strategy for the production of coarse meshes. Another version is currently being developed in which the implementation relies on a Galerkin finite-element formulation on unstructured triangulation.

CHI-WANG SHU

High-order Methods for CFD

High-order methods are important even for problems with discontinuities or sharp gradients. We study such methods both theoretically and computationally.

Jointly with Harold Atkins at NASA Langley, we are investigating stability of initial boundary value problems for high-order conservative upwind schemes which serve as prototypes of ENO schemes with biasing. Both GKS stability and eigenvalue stability are considered. Jointly with David Gottlieb, we are continuing our investigation of overcoming Gibbs phenomena when using spectral approximation for discontinuous but piecewise analytic functions.

Research will continue for high-order methods in finite difference, finite elements and spectral schemes. Application of ENO schemes to shock vortex interaction, and comparison with linear analysis and with shock fitted results (for small vortex) will be pursued.

RALPH SMITH

Noise Control in Structural Acoustic Systems

The problem of controlling noise in structural acoustic systems arises in applications ranging from the attenuation of interior sound pressure levels inside aircraft fuselages to the reduction of far-field noise generated by a transformer. In all such applications, the unwanted noise is generated by a vibrating structure which, through structural acoustic coupling, transfers energy to an acoustic field. One technique for controlling this structure-borne noise is through the use of piezoceramic patches bonded to the structure which generate in-plane forces and/or bending moments in response to an applied voltage. The modeling, development and implementation of control methods using this technology in structural acoustic systems is being investigated in collaboration with H.T. Banks (North Carolina State University), D.E. Brown, V.L. Metcalf, R.J. Silcox (Acoustics Division, LaRC) and Y. Wang (North Carolina State University).

Initial work on this problem started with the investigation of a 2-D slice from the actual 3-D systems of interest. Modeling and parameter estimation techniques were studied and an LQR time domain, state feedback control methodology was developed and numerically tested. Current efforts have centered around the extension of these techniques to three physical systems for which validation experiments can be performed. A structural system involving a circular plate with surface-mounted piezoceramic patches was considered first when developing techniques for estimating physical parameters and experimentally implementing the feedback control methodology. Initial experiments performed in the acoustics laboratory have demonstrated a reduction in vibration levels in response to the controlling voltage and we are currently working to refine these

results and extend the techniques to the case involving persistent excitation of the plate. The other two physical problems currently being studied are 3-D structural acoustic systems; one consists of a hardwalled cylinder with a flexible plate at one end while the other is a vibrating shell enclosing a cylindrical acoustic field. Numerical techniques for approximating the dynamics of the first system have been developed and numerical simulations demonstrating significant reductions in interior sound pressure levels, when full state measurements are available, have been performed.

Once the experiments involving the isolated circular plate are completed, we will begin experiments with the hardwalled structural acoustic system. An initial step in this process will involve the construction of a state estimator since measurements will be available only at isolated locations in the cavity and on the plate (this will extend state estimator techniques currently being used with the isolated plate). We will also continue analysis on the acoustic/shell system and will begin developing numerical techniques for approximating system dynamics, estimating parameters and implementing control.

SHLOMO TA'ASAN

One-Shot Methods for Optimization Problems

The objective of this research is to develop multigrid solvers for constraint optimization problems governed by partial differential equations. The PDE's to be studied are of elliptic and hyperbolic types and the optimizations are boundary related.

Research has been developed in two main directions: finite-dimensional parameter space and infinite-dimensional parameter space. In both directions the methods are already mature and have been demonstrated on several different examples (for more on the infinite-dimensional case see the work with Eyal Arian). The above ideas have been applied in aerodynamics design problems where airfoils are to be calculated to meet certain design requirements; for example, to give the pressure distribution in flow conditions that are closest to a given pressure distribution. The present model for the flow is the transonic full potential equation with a body fitted grid. The shape of the airfoil in these calculations is expressed in terms of a finite number of given shape functions with amplitudes to be found by the design process. Currently, subsonic design problems are being investigated. Solutions are obtained in just a few times the cost of the analysis problem. This work is being done jointly with M. D. Salas (Fluid Dynamics Division, LaRC) and G. Kuruvila (Vigyan, Inc.).

Optimal Multigrid Solvers for Inviscid Flow Problems

The objective of this research is to develop optimal solvers for Euler equations in all ranges of Mach numbers. Convergence rates similar to that of the full potential equation are anticipated.

New multigrid methods that are based on canonical forms of the inviscid equations, in which elliptic and nonelliptic parts of the system are separated have been developed. Such representation allow an optimal treatment of the problem. Discretization and solution methods based on these forms have been developed. These discretizations require numerical viscosity only for the non-elliptic part of the system. The resulting schemes are staggered and admit no spurious (or weakly spurious) solutions, even for very small Mach numbers. The schemes are formulated on general grids, structured as well as unstructured, in both two and three dimension. At present, we are

focusing on the incompressible and compressible inviscid case, working with body fitted grids in two dimensions. Flow in a nozzle and flow around a cylinder are being studied both for the compressible and incompressible cases. Convergence rates of 0.1 for nozzles and 0.2 for exterior problems have been obtained for subsonic cases, even as the Mach number approaches zero.

Future work will extend the ideas to transonic flows. This include the construction of appropriate schemes for the supersonic regions as well as an appropriate solver for the mixed problem.

Efficient Techniques for Time-Dependent Problems

The efficient solution of long-time integration problems is the subject of this research. The goal is to develop new discretization techniques and new efficient marching techniques for such problems.

Discretizations which are based on the energy content of the initial conditions have been developed. These discretizations enable marching tenfold times more than high order methods of the same complexity. The methods have been implemented for a variety of hyperbolic equations.

A method for efficiently calculating the time evolution using mainly coarse grids (depending on the spatial resolution only), has been developed. Coarse grids use extra source terms to correct their evolution process, making the solution arbitrarily close to the fine grid solution. These source terms are shown to satisfy certain equations, in general, and are being solved for on the coarse grid along with the main solution. The method referred to as Large Discretization Step (LDS) method yields extremely efficient evolution processes. Experiments with hyperbolic equations including linearized and nonlinear Euler equations have been performed. Efficiency is improved using this methods by a factor of 15 for two dimensional problems and by a factor of 30 for three dimensional problems.

Future work will involve the development of boundary conditions that are best suited for long-time integration problems. This will be done using a new theory for boundary conditions that enable the design of asymptotically stable boundary conditions using local analysis.

This work was done with Zigo Haras.

JAMES C. TURNER, JR.

Control of Magnetohydrodynamic Flows

The goal of the ongoing work is to develop mathematical theories and numerical algorithms for control of electrically conducting flows. Our initial investigation (in collaboration with L. Steven Hou) has concentrated on a simplified model that involves the velocity, pressure and electrical potential fields. This model is valid in a variety of applications, e.g., in the modeling of a two-dimensional magnetic pump with electrodes on the bounding surface, in the modeling of liquid lithium blanket in fusion technology and in metal melt cooling processes.

In the isothermal case we have obtained mathematical results such as the existence of optimal solutions and justification of the use of Lagrange multiplier rules to derive an optimality system of equations. We have also developed effective numerical algorithms and implemented these algorithms in simple geometries.

Our future research in this direction consists of the following: extend the mathematical results to the nonisothermal case; develop efficient algorithms suitable for large scale simulations and complicated geometries; and devise, implement and assess massively parallel and vector computer algorithms.

V. VENKATAKRISHNAN

Convergence Acceleration Techniques for Unstructured Grids

The purpose of this study is to develop an agglomeration strategy to accelerate convergence for unstructured grids. The solution of the compressible Navier-Stokes equations for flows over complex geometries poses some challenges, among which are the generation of coarse grids for a multigrid procedure and development of efficient parallel algorithms. An agglomeration multigrid strategy has been devised which generates the coarse grids automatically. A parallel implicit solver has also been developed for use on distributed-memory parallel computers. The agglomeration multigrid work was done in collaboration with D.J. Mavriplis of ICASE. The generation of coarse grids is accomplished by agglomerating or fusing fine grid control volumes. An efficient algorithm has been developed for this purpose. The coarse grids thus have arbitrary polyhedral control volumes. The multigrid algorithm that makes use of these grids has been shown to be quite efficient. We have been able to compute flows over complex geometries as a result of using this approach. An implicit scheme that allows large time steps to be taken has been developed for distributed-memory parallel computers. Preconditioned conjugate gradient-like methods have been implemented. A preconditioner that is implicit within a processor has been found to work well. The implicit scheme offers adequate parallelism at the expense of minimal sequential overhead. The use of a global coarse grid to further minimize this overhead has also been investigated. Work is in progress to study time-dependent flows with moving control surfaces. The ideas from the agglomeration multigrid procedure will be incorporated, enabling us to study unsteady flows over complex geometries in an efficient manner.

HONG ZHANG

A Scalable Parallel Algorithm for Multiple Objective Linear Programs

Multiple objective linear programming is becoming more prevalent; almost every important real world problem involves more than one objective. However, a multiple objective linear program (MOLP) often has a large number of solutions in the form of extreme efficient points and unbounded efficient edges. The process of finding all of them is very space and time consuming. The growing importance and enormous computational expense of MOLPs, as well as the structure of the solution set and the availability of high performance computers, motivated us to design an algorithm that is capable of solving very large size problems in a reasonable time.

In collaboration with M. M. Wiecek of Clemson University, the work was started from a well established sequential software ADBASE. Due to the nature of the problem, a straightforward parallelization of ADBASE suffered from severe job imbalance and other disadvantages. Therefore we proposed several strategies, such as generating multiple initial efficient extreme points and a recrash technique for activating idle processors. Incorporating these strategies to the basic parallelization of ADBASE, a parallel algorithm for solving MOLPs has been developed. Job balance, speedup and scalability are of primary interest in evaluating efficiency of this algorithm. Experimental results on an Intel iPSC/2 and Paragon multiprocessors show that the algorithm significantly speeds up the process of solving MOLPs and is scalable.

Several elements of this algorithm can be improved in near future. For instance, since ADBASE does not keep track of infeasible or inefficient bases, currently in the parallel algorithm multiple processors repeatedly check the same infeasible or inefficient bases, which generates redundant computations. If bookkeeping of inefficient bases was maintained, the communication between processors could be set up for transmitting the additional information about efficient and inefficient bases.

FLUID MECHANICS

ALVIN BAYLISS

Numerical Study of a Flexible Surface Excited by Jet Noise

The aim is to study the role of jet noise in exciting a flexible surface such as an aircraft panel.

We consider a panel-stringer assembly, so that there are two flexible panels rigidly connected. We solve the nonlinear Euler equations on both sides of the panel. On one side of the panel the flow field includes the jet flow exiting from a nozzle while on the other side of the panel we solve the Euler equations without any imposed flow field. Within the jet there are instability waves which act as sources of sound and which serve to excite the panels. We have computed both the panel response and the resulting acoustic radiation into the far field.

This work is in collaboration with J. L. McGreevy and L. Maestrello.

Numerical Study of Acoustic Radiation from a Flexible Surface

We have studied the problem of plane wave excitation of a flexible panel at or near a resonant frequency.

The problem is solved by coupling the nonlinear Euler equations describing the near and far field radiation to an equation for the evolution of the flexible surface. The pressure difference across the surface acts as a source term. The far field acoustic pressure can exhibit nonlinear effects.

Comparisons with experiments are in progress.

This work is in collaboration with A. Frendi, L. Maestrello and J. Robinson.

A.O. DEMUREN

On Elliptic Near-Wall Reynolds Stress Models

Reynolds stress models are required for calculating turbulent flows in which body forces are important or the anisotropy of the turbulence field plays a dominant role, such as flow in streamwise corners. In the development of Reynolds stress models the assumption of homogeneity is made, but very close to a wall the turbulence is highly inhomogeneous, so that such models are not valid. The objective of the present work is to develop and validate models based on the elliptic relaxation concept which will allow Reynolds stress models to be integrated all the way down to the wall in many practical flows.

A near-wall model based on the elliptic relaxation concept has been successfully implemented with the SSG Pressure strain model and applied to the plane channel flow, and the fully developed square duct flow. Computations show quite good agreement with DNS data, except in the viscous sublayer where the transition from nearly one-component turbulence to two-component turbulence is not reproduced. This shows a limitation of the elliptic relaxation concept which is based on the rapid distortion theory and can therefore not account for viscous effects. This method is now being generalized to complex three-dimensional flow so that the flow in a circular-to-rectangular transition duct can be computed. The results will then be compared to experimental data and those obtained in computations with the SSG model in which wall functions are used to bridge the near wall region.

Methods for optimizing the solution of the elliptic equations will be investigated, along with ideas for improving the results in the viscous sublayer. Applicability of the elliptic relaxation concept to free-shear flows will also be investigated.

GORDON ERLEBACHER

Two-dimensional Shock-Vortex Interaction

Shock/turbulence interaction is an ubiquitous phenomenon present in many high-speed aerodynamic flows of practical importance. The objective of the present work is to develop a direct numerical simulation capability to study basic mechanisms of turbulence enhancement in such situations and to create databases for testing turbulence closure models.

A 2-D multi-domain domain shock-fitted code has been written and tested. The tests ranged from the solution to 1-D Euler's equation without shocks to the solution of the nonlinear Euler equations in the presence of a fitted shock. Particular attention was given to comparisons with linear theory. A new buffer domain technique developed in house permits downstream boundary conditions to be removed, while very sharply reducing spurious wave reflections which permits long-time integrations. We established that by integrating for a long enough period (i.e. sound waves cross the physical domain 3 to 10 times), we can come within 1% of linear predictions. The code is based on a 6th order compact spatial discretization of the derivative operators. The previous work on the passage of turbulence through the shock was delayed while a host of numerical issues were resolved. An axisymmetric version of the code is also available.

The shock-turbulence code will be applied to the passage of 2-D turbulence through a planar shock. Results from these simulations will be useful for the development of more realistic turbulence closures.

JAMES GEER

Discontinuous Periodic Basis Functions and a Hybrid Pade-Galerkin Technique

Series expansions of functions, such as Fourier series, perturbation series, etc., are often useful in developing numerical or semi-numerical, semi-analytical algorithms for the solution of differential equations. However, when only a partial sum of such a series is used, some "undesirable" effects (such as Gibbs' phenomena) may be present, or the partial sum may have "difficulty" approximating certain features of the solution, such as boundary layers or internal layers.

A three-step hybrid analysis technique, which successively uses the regular perturbation expansion method, the Pade expansion method, and then a type of Galerkin approximation, is being developed and studied. Currently, it is being applied to several model problems which develop boundary layers as a certain parameter becomes large. These problems involve ODE's, PDE's, and integral equations. In particular, the technique appears to simulate these boundary layers by producing approximate solutions with real or complex singularities which lie just outside the domain of interest. In addition, work is also continuing on understanding and further developing a class of approximations to a periodic function f which uses the ideas of Pade approximations based on the Fourier series representation of f , rather than on the Taylor series representation of f . The

approximations are being applied to several model functions, and applications to the solution of a variety of initial, boundary-value problems for several classes of PDE's are being explored.

The hybrid Pade Galerkin technique will be applied to and studied in the context of some ODE's and elliptic PDE's which develop internal layers, as well as boundary layers, and also to two classes of integral equations of the first kind. Also, several different ideas will be explored concerning the conjunction of the Fourier-Pade approximations with certain spectral methods to solve a variety of problems involving PDE's, especially time-dependent problems which develop shocks as time increases. In particular, robust and efficient recursive algorithms will be developed to determine the coefficients in the approximations. In addition, the conjunction of several new periodic basis functions which have "built-in" singularities with Fourier series will be explored in order to more effectively approximate periodic functions with jump discontinuities.

SHARATH GIRIMAJI

Small Scale Processes in Turbulence

Large-eddy simulation (LES) of turbulent combustion is under consideration. The model for the reaction term again requires that the pdf (probability density function) of the scalar concentration be known; either presumed or solved from an evolution equation. Either approach entails the solution of the scalar variance equation. One of the major terms that needs closure modeling in the variance equation is the scalar dissipation. A model for this term is developed using the successive grid elimination procedure (work in collaboration with Ye Zhou).

Modified Restructured Euler Equation

This work is expected to shed light on the geometry of small scales in turbulence, the knowledge of which is important for understanding the material-element deformation and mixing characteristics of turbulence. The ongoing project deals with the analysis of velocity gradient tensor invariants in turbulent flow. A new restricted Euler equation, which accounts for the effect of the mean velocity gradient, is being considered. An existing stochastic velocity gradient model is also being modified to account for mean velocity gradients.

A paper entitled 'Energy transfer in Burgers equation' (with Y. Zhou) has been completed and submitted for publication.

CHESTER E. GROSCH

Multilevel Modeling of Transition

Transitional flows include a very wide variety of both spatial and temporal scales. These include the very slow variation in the mean flow, the relatively long wavelength, slowly changing instability waves, and the relatively short period, small wavelength weak turbulent fluctuations. The object of this research is to develop a computationally efficient scheme which can handle these multiple scales approximately with minimum computational cost.

The transitional flow is modeled as a a three level flow. The "fine" level contains the model of the turbulent fluctuations with the frozen mean flow and the slowly varying instability waves. The "medium" level contains the instability waves with a frozen mean flow and an effectively frozen

Reynolds stress from the “fine” level. Finally, the “coarse” level” contains the slowly varying mean flow and frozen Reynolds stresses from both the “medium” and ”fine” levels. The intent is to calculate for a short time on the “fine” level, a moderate time on the ”medium” level, and a long time on the “coarse” level; then return to the ”medium” and ”fine” levels and repeat the cycle. Currently we are experimenting with a Navier-Stokes code which can be used for the “coarse” and ”medium” level computations.

In the future, it is intended to continue these calculations. In particular, the transfer of information between the various levels will be studied. In addition, a suitable transitional turbulence model for the “fine” grid must be chosen and implemented.

PHILIP HALL

Hydrodynamic Instability and Transition

We aim to understand the nonlinear stages of boundary layer transition. In particular we are concerned with the later stages of transition when several different modes of instability are present. We wish to understand how the wavenumber of a Tollmien-Schlichting wave or vortex evolves in a strongly nonlinear situation. We also wish to understand the effect of thin liquid surface layers on transition.

We have used a combination of asymptotic and numerical methods to investigate the problems discussed below. A new phase-equation based approach to boundary layer instability theory has been developed. The approach can be used to derive new results concerning the breakdown of Tollmien-Schlichting waves in boundary layers. In addition it can be used to describe vortex splitting and merging in boundary layers. Work on the instability of layered fluids was carried out with application to airflow over a thin layer of water on a wing. Work on the instability of heated fluid layers was carried out.

Future work will include extending the sum of the phase equation approach to 3D disturbances, understanding unsteady critical layer behavior for inviscid Görtler vortices, and investigating theoretical methods for the control of TS or Görtler vortices in growing boundary layers.

FANG Q. HU

Computational Methods for Aeroacoustics

Far field noise propagation can be studied by the wave equation (or the convective wave equation). Thus numerical methods for the wave equation will be considered. The objective is to develop accurate numerical solutions for the noise propagation.

In our approach, the wave equation is reduced to the Helmholtz equation in the frequency domain, which is in turn reformulated into a boundary integral equation. A spectral method for the resulting integral equation has been developed for 2-D geometries. In the area of time integration schemes, the study of optimized Runge-Kutta schemes continues. Currently the effectiveness of the optimized schemes is being assessed in the proposed Benchmark Problems.

Future work is to develop time-domain wave equation solutions and use it to calculate noise in the far field from near field simulations.

T.L. JACKSON

Mathematical Combustion

Work continues in the general area of combustible flows at both subsonic and supersonic speeds. The objective of the work is to model complex physical problems with simple model problems which isolate certain fundamental physics of interest for study. Once the simple model problems are thoroughly understood, they can then be used as building blocks to generate increasingly complex model problems. The current problems of investigation include mixing layers, jets, vortex flows, stagnation point flows, and detonations.

In all of the work the basic kinetic model consists of a one-step, irreversible Arrhenius reaction. A combination of asymptotics and numerics are then used to solve each model problem.

Each simple model problem broadens our basic understanding of key physical effects. In the course of time we shall (i) develop more simple model problems while (ii) extending the present ones to include more realistic physics.

DANIEL D. JOSEPH

Suspension of Particles

We have been studying the motions of a few particles in a viscous fluid by direct numerical simulation at moderate values of the Reynolds number in the 100's. From these simulations, we find the mechanisms which give rise to lateral migration of particles and turn the broad side of long bodies perpendicular to the stream.

We find that a viscous "stagnation" point is a point on the body where the shear stress vanishes and the pressure is nearly a maximum. We show how the migration is controlled by stagnation and separation points and go further than before in the discussion of Segré-Silberberg effects of cross-streamline migration in two dimensions. We have analyzed the lift off and steady flight of solid capsules in Poiseuille flows. We do a three-dimensional simulation of steady flow at slow speeds and show that the extensional stresses in a viscoelastic flow change the sign of the normal stress which would exist at points of stagnation in a Newtonian fluid, causing the long side of the body to line up with the stream. CFD approaches to problems of two-phase flows which have been developed by my colleagues and ex-students, H. Hu and P. Singh, my present students, J. Feng, T. Hesla and Y. Huang, and my colleagues, M. Crochet, R. Glowinski and T. Pan. Our goal is to obtain exact results in which the nonlinear hydrodynamic mechanisms inducing flow microstructure are fully revealed. We have determined the motion of a few interacting particles in a variety of flows at Reynolds numbers up to the hundreds. Most, but not all, of our simulations have been restricted to two dimensions. Direct simulations of the motion of many particles, even in two dimensions, have not yet been done. Stokesian dynamics is an approximate and not direct numerical method of handling the motion of many particles when inertia of the fluid and inertia of the particle are neglected. By interrogating our simulations, we are able to identify the nonlinear mechanisms which produce microstructures through particle-particle and wall-particle interactions. Microstructural properties of fluidized suspensions in Newtonian fluids are associated with wake interactions and turning couples on long bodies in a scenario, which I have described as drafting, kissing and tumbling. Kissing particles are sucked together in wakes and the long body, which

kissing spheres momentarily form, is unstable when the axis of the long body is along the stream. The kissing spheres tumble into across-the-stream arrangements basically for the same reason that a long body will put its broadside perpendicular to the stream. These microstructural elements endow a fluidized suspension with anisotropic structure in which spherical particles on the average line up across the stream. The anisotropy, which is readily observed in experiments, is due to nonlinear mechanisms revealed in simulations that could not be predicted by any of the continuum models of two-phase flows or even by perturbation methods which were promoted in the 1980's. Other features of particle-fluid, particle-particle and particle-wall interactions which can be illuminated by intelligent interrogation of direct simulations are related to the effects of the shear and pressure distributions exerted by the fluid on the particle surface on the motion of the particle. These forces are responsible for lateral drift and rotation of particles in sedimenting and shear flows. We can determine the effects of the walls on the equilibrium position of the particles away from the wall. We can also study the evolution of systems of particles as dynamical systems by looking at the bifurcations of steady solutions. We have developed two types of direct finite-element simulations in which the forces exerted by the fluid on the body are computed. The first type of Calculation can be called a force calculation and the second is a motion calculation. In a force calculation, the position and velocity of the bodies are prescribed and the fluid motion is computed by a Navier-Stokes solver. We have used three kinds of solvers and they all work well. After having computed the fluid motion, we can compute the forces and moments that are exerted by the fluid on the objects in the flow. The forces tell us how the body would move thereafter if it could. In a motion calculation, we actually move the body with those forces and carry out a motion simulation iteratively. Of course, we like motion calculations better because they go further.

It is our intention to develop numerical methods for direct simulations of particles in flows of viscoelastic fluids and in three dimensions. The force calculation of Feng, Joseph, Glowinski and Pan [1993] is our first effort in this direction. The motion of particles in viscoelastic fluids is not at all like the motions of particles in Newtonian fluids. In general, particles aggregate in viscoelastic fluids in situations in which they would disperse in Newtonian fluids. Long bodies which turn broadside-on in Newtonian fluids put their broadside parallel to the stream in viscoelastic fluids. One of the mechanisms which appears to work in producing these maximal differences between Newtonian and viscoelastic flows is a reversal of the pressure (actually, the normal stress) at a point of stagnation. However, this mechanism does not explain all of the observed features and more needs to be done.

D. GLENN LASSEIGNE

Interaction of Reacting and Non-reacting Oblique Shock Waves with Freestream Disturbances

The response of the flow field behind nonreacting and reacting oblique shock waves to rather general but finite disturbances upstream of the shock is being investigated in detail. Currently, the ability to use existing and powerful numerical algorithms such as Quirk's Adaptive Mesh Refinement on such problems is being pursued. The comparison of numerical with analytical solutions in which the disturbance fields can be written as inverse Fourier Transforms is desired. A wide class of model disturbances are to be investigated and the vorticity, entropy, and pressure disturbances downstream of the shock are to be computed.

The Generalized Lees-Lin Regularity Condition for Mixing Layers – The Significant Effects of Non-trivial Reaction Mechanisms and Non-Uniform Molecular Weights

The temperature profile through external heating or cooling, internal viscous heating as well as exothermic chemical reactions significantly alters the regularity conditions sufficiently so that an additional pair of unstable modes exist. In the absence of reaction, viscous heating which is a function of Mach number significantly raises the temperature so that at a large enough Mach number, there are three neutral modes instead of one. The purpose of this study is to analyze how the stability characteristics of the mixing layer as they manifest themselves in the Lees and Lin regularity condition are affected by non-trivial chemical reactions. In particular, we will be concerned with the various reduced mechanisms that have been proposed as a model of the hydrogen-oxygen system. We will also consider the effects of differing molecular weights (as is the case in the hydrogen-oxygen system) on the stability characteristics.

This work is in collaboration with T.L. Jackson, C.E. Grosch and F.P. Kozusko.

GEOFFREY LILLEY

Radiated Noise from Isotropic Turbulence

The subject of Aircraft Noise prediction and its reduction remain one of the major challenges in the design of the power plants for all types of Civil Aircraft Transports and in certain problems concerning Military Aircraft. One important problem concerns the noise generated by turbulent flow in the jet engine exhaust. Methods for predicting the noise radiated from turbulent flow were pioneered by Sir James Lighthill in the early 1950's but the application of this methodology to practical exhaust systems relied heavily on experimental data measured both within the turbulent mixing region of the engine exhaust flow and in the far field of the aircraft. With the advent of supercomputers it was realized that this new tool could be harnessed to provide a major part of the input information required in the prediction of noise from turbulence. Thus the challenge was exposed to find how this could be achieved and the accuracy that could be placed on the results obtained from Computational Aeroacoustics (CAA).

It was decided that a first step was to compare the results obtained by an improved version of Proudman's work on the noise radiated from unit volume of isotropic turbulence at high Reynolds numbers and low Mach numbers with the numerical results obtained from direct Numerical Simulation(DNS) of the same problem as obtained by Sarkar and Hussaini (1993). The improvements to Proudman's work involved the use of a relationship proposed by Lighthill (1992) whereby the fourth-order covariance of the Lighthill stress tensor can be evaluated from products of corresponding second-order covariances, which are assumed known, and do not depend on the assumption of Gaussian statistics. The Lighthill relationship was checked independently from results obtained in decaying isotropic turbulence by Sarkar and Hussaini (1993) and Dubois (1993). The overall agreement between the results for the acoustic power output and its spectrum as obtained from analysis and DNS were satisfactory even though the DNS results were for a relatively low Reynolds number. However there remained differences in the noise source distribution which were not fully resolved although it was suggestive that the space resolution in the DNS computation needed improvement. It was hoped this could be achieved by repeating the calculations using Large Eddy Simulation(LES) and so providing data at higher Reynolds numbers. Further work needs to be con-

sidered at other Mach numbers and when homogeneous turbulence is in the presence of a uniform shear.

The extension of this work to mixing region noise involving the influence of a mean velocity gradient has also been considered. Some necessary preliminary work was completed on the self-preserving properties of compressible flow mixing regions covering a wide range of velocity and temperature ratios and Mach numbers. Further work was commenced on the structure of unsteady shear layers. These studies were made in cooperation with Drs. S. Otto and J.C. Webb.

JAMES E. MARTIN

The Nonlinear Evolution of Swirling Jets

Swirling jets are of importance in a variety of technical applications involving mixing and combustion processes. Furthermore, they are of interest from a more fundamental point of view, as they allow for the investigation of two competing and interacting instability mechanisms in the form of a classical shear-layer instability and a centrifugal instability. Our objective is to explore the nonlinear regime of the flow by means of inviscid vortex filament simulations.

To study this flow, we employ a fully three-dimensional helical vortex filament model involving both azimuthal as well as axial vorticity. This technique extends the ring-vortex description used in our previous studies of the non-swirling jet. The accuracy of the model was verified by comparing the numerical growth rates for the purely swirling situation with the analytical growth rates for the Rayleigh instability. In preliminary calculations for jets of very large swirl number under axisymmetric perturbation, we observed the swirl modifying the traditional dynamics of non-swirling jets through the creation of dominant counter rotating vortex rings. These in turn favor a pinch-off mechanism which leads to a dramatic decrease in the local jet diameter. Moreover, we find that the swirl renders the vortex ring circulation time dependent.

A more detailed quantitative study of these effects is clearly necessary. Furthermore, the effect of helical rather than axisymmetric perturbations needs to be investigated, along with the dynamics of additional azimuthal perturbations. It is hoped that such a study might also provide insight into the mechanisms governing vortex breakdown in swirling jets.

STEPHEN OTTO

The Fate of Longitudinal Instabilities in a Variety of Physical Situations

Many real fluid situations are susceptible to longitudinal vortex instabilities, it is our aim to determine how a variety of physical phenomenon will effect their structure and stability. The effect of a crossflow on the stability of Görtler vortices is of interest, and we wish to determine whether this will destroy the centrifugal mechanism. As the crossflow increases, which corresponds to a larger angle of sweep, the dominant mode of instability becomes a crossflow vortex. The structure of this mode can be determined using a linearized Navier-Stokes approach, and the question is; how does this mode break down? It is conjectured that the breakdown will be initiated by an inviscid mechanism due to the highly inflectional form of the flow. The centrifugal mechanism is operable due to a fluid flow over a curved interface. It is also known that if the centerline of a mixing layer

is curved then this produces a centrifugal force, but is this sufficient to maintain a longitudinal vortex?

The problems are approached using a combination of methods and numerical techniques to solve the resulting reduced equations. In a paper with J. P. Denier (UNSW, Australia) we have shown that a small crossflow may modify the Görtler instability rather than completely destroying it when the parabolic equations were solved. It was also found that a pressure gradient has a significant effect on the onset of the instability. In work with C. L. Streett (TFPB, NASA Langley RC), we are currently solving the three dimensional Rayleigh equation modified for the presence of a significant crossflow in order to determine the fate of crossflow modes. This analysis, although not totally asymptotically rigorous, is hoped to provide salient features of the modes' breakdown. Our results will be compared with previous work concerning the secondary stability of rotating disk flow. In work with Tom Jackson and F. Q. Hu (ODU) we are extending an earlier article (Hu, Otto & Jackson, Transition, Turbulence and Combustion Workshop 1993), to include the numerical calculation of the evolution of the Görtler modes within a curved mixing layer, specifically using the evolving Lock profile.

In the near future the problem of nonlinear receptivity of Görtler vortices is to be tackled with Andrew Bassom (University of Exeter, UK), and the effect of crossflow of receptivity will also be discussed with J. P. Denier. It will also be interesting to determine how the presence of a vortex will influence an already inviscid unstable situation, namely a shear layer, in work with P. Hall.

JAMES QUIRK

Large Realistic Simulations of Shock Wave Phenomena

Two detailed computational studies were conducted so as to shed light on fundamental shock wave phenomena that are not fully understood. One study examined the interaction of a planar shock wave with an isolated gas inhomogeneity that took the form of a cylindrical bubble (work with S. Karni, NYU), while the other looked at the reflection of a detonation wave from a ramp (work with J.E. Shepherd and R. Akbar, CALTECH).

The shock-bubble interaction is representative of a mechanism that has been proposed to ensure rapid mixing of air and fuel in supersonic combustion systems. The present numerical results reveal several subtleties of the interaction process that were not apparent from earlier experimental work. It also exposes flaws in recently proposed analytic models for the amount of vorticity produced by a shock-bubble interaction. This study has been written up and will appear as an ICASE report.

The numerical study for the reflection of a detonation wave highlights the phenomenological complexity of reactive fronts and thus far it has raised more questions than it has answered. However, progress is being made and soon it is hoped that this study will bridge the gap between current theories and experimental observations.

Both of the present numerical studies faithfully reproduce the complex mechanisms that have been observed experimentally. Given the disparate physical scales involved, this would not have been possible without the use of a sophisticated adaptive mesh refinement algorithm. Previous simulations in the literature were under-resolved and so prone to misinterpretation. The resolution of the present fully-resolved simulations has, however, exposed slight weaknesses in modern shock-capturing schemes and so work is planned to see if these weaknesses can be removed.

J. R. RISTORCELLI

Compressible Turbulence Modeling

Fundamental issues involving the Reynolds stress and $k - \epsilon$ turbulence models at speeds in which the compressibility of the fluid is important are being studied. Our primary concern is with producing suitable models for the effects of compressibility; the idea being that most of the terms requiring modeling in turbulence closures can be accounted for using incompressible turbulence models and that terms specifically related to compressible effects can be identified and treated independently of the terms already modeled using incompressible turbulence models.

The focus of our investigation in compressible turbulence has expanded to include theoretical developments as well as numerical experiment and modeling. In the area of numerical experiment a Mach 4.5 temporal DNS of wall bounded flow, by Dinavahi and Pruett (*AS&M*) is being used to understand the importance of various terms appearing in the first and second moment equations. Amongst the many terms in the moment equations evaluated it has been found, unexpectedly, that the mass flux emerges as a quantity of relative importance in a number of flow situations. The mass flux relates Reynolds-averaged and Favre-averaged statistics and quantifies the effects of mean density gradients on the intensity and anisotropy of the turbulence. This has suggested the work in modeling in which a general algebraic model for the mass flux has been derived. Key features of the model involves its dependence on the Reynolds stress, the mean velocity gradients as well as the mean density gradients. As the expression of the mass fluxes are coupled to other components of the mass flux a model that predicts countergradient transport as well as mass fluxes in which there are no mean density gradients is obtained. The algebraic model for the density flux has been tested using the temporal DNS data of Dinavahi (*AS&M*) in an evolving wall bounded boundary layer at Mach 4.5. Comparisons of the model predictions with the DNS data is unexpectedly good: the near wall peak in the mass flux due to the large velocity and density gradients is captured.

In the category of theoretical work an evolution equation for the fluctuating quantities associated with the compressible portions of the flow is being derived. The uniqueness and novelty of this approach lies in the fact that the fluctuating compressible portion of the flow can be closed in terms of the vortical motions: the effects of compressibility can be related, *analytically*, to quantities for which equations are already carried. Additional work has also been conducted on the effects of compressibility on the dissipation for which the theoretical development just described will be relevant.

Additional data bases for wall bounded flows, (Pruett at $Ma = 8$ and Mohan Rai $Ma = 2T$) still now in the computational stages, are expected to be used to verify and expand some of the findings of the numerical data base presently being used. The work on the mass flux, reported in the previous semi-annual brief is nearing completion. It remains to obtain additional data of flows with different mean deformations to further test the model. Our primary focus is on the theoretical work from which it is expected to obtain an expression for the compressible portions of the flow field. As the impact of this latter theoretical work is potentially substantial most of our effort will be directed towards formulating a general theory for the effects of compressibility on the turbulence of the flow.

Incompressible Turbulence Modeling

A rapid-pressure model frame-indifferent in the two-dimensional limit referred to in the last semi-annual report has been completed. The 2DMFI model, incorporating all the known mathematical and physical constraints insures that the modeled equations are consistent with the Taylor-Proudman theorem. This is a an issue of substantial importance in the computation of any complex flow and particularly those in which rotation is important. The 2DMFI model, without any sacrifice of its mathematically rigorous underpinnings, has been calibrated to the asymptotic homogeneous shear. Future plans include obtaining an algebraic stress Reynolds stress model using this representation for the pressure-velocity covariance.

CHARLES G. SPEZIALE

Full Second-Order Closures in Compressible Turbulent Flow

This study concerns the performance of full second-order closures in compressible homogeneous shear flow.

Consistent with previous studies, it was found that with the addition of the dilatational dissipation and pressure dilatation models of Sarkar and Zeman, the newest second-order closures are able to accurately predict the reduced growth rate of the turbulent kinetic energy that arises from compressibility effects. In addition, excellent predictions for the turbulence Mach number are obtained. However, a close examination of the equilibrium structural stress anisotropic are underpredicted by nearly 100% and the Reynolds shear stress anisotropy is overpredicted by 25%. The physical origin of these poor predictions was traced to the neglect of compressible terms in the modeling of the pressure-strain correlation. Research was conducted in collaboration with R. Abid (High Technology Corporation, LaRC) and N.N. Mansour (Ames RC).

Future research will be directed to eliminating this deficiency. Research with R. Abid has also continued on the development of improved methods for the direct integration of Reynolds stress closures to solid boundaries without the use of ad-hoc wall damping functions. Some promising results have been obtained.

SIVA THANGAM

Modeling and Prediction of Turbulent Separated Flows

Turbulent separated flows are of common occurrence in a variety of of physical systems of considerable scientific and engineering relevance. The aim of the present study is to develop and validate efficient two-equation turbulence models based on the recursion renormalization group theory that have the capability to accurately predict turbulent separated flows of practical importance.

While the physical aspects of turbulent flows are best described by the equations of motion, limitations in computer capacity and speed preclude their direct solution for complex flows of relevance to technical applications. The current practice for high Reynolds number flows of practical interest involves some type of modeling for the turbulence stress. In this context, the development of two-equation turbulence models that have wide range of predictive capability for separated flows was undertaken from analytical and computational point of view. This is a collaborative work involving Drs. Ye Zhou of ICASE, Dr. George Vahala of William & Mary and Dr. T.B. Gatski

of NASA. The work is currently in its second phase during which a recursion renormalization group theory (r-RNG) based anisotropic two-equation model for incompressible turbulent flows was developed and validated for the benchmark test case of separated flow past a backward-facing step. The proposed model uses a finite wavenumber truncation scheme to account for the spectral distribution of energy. The model incorporates the effects of both local and nonlocal interactions. The model has recently been applied for the analysis and prediction of turbulent wake flow past flat plates with considerable success.

During the next phase, the model will be refined to include near wall effects as well as flow parameter dependent model coefficients for the higher order terms. The model will then be applied for additional test cases including more complex wake flows as well as flows with recirculation.

L. TING

Structural Acoustic Interaction

The structural/acoustic interaction problem is essential for the prediction and control of the transmission of external acoustic waves through a panel or panels of an airframe into the interior. The problem becomes more critical when the incident wave is nearly in resonance with oscillations. The object of this work is to formulate theoretical models and carry out numerical simulation of the problems.

In collaboration with Drs. L. Maestrello and A. Frendi of NASA we are studying the structural/acoustic interaction problem simulating the experiments conducted at NASA. In the experimental setup, nearly planar waves originated from a stationary source distribution are incident to a panel mounted on a rigid plate. Two mathematical models were described in ICASE Report No. 93-18. One solves numerically the three-dimensional nonlinear Euler equations for the flow field coupled with the nonlinear plate equations (the *fully coupled* model). Approximate boundary conditions on the finite computational domain of the flow field are employed for the Euler solver. The second model uses the linear wave equation for the acoustic field and expresses the load as a double integral involving the panel oscillation (the *decoupled* model). The integral is an exact solution of the initial value problem for the acoustic field. The panel oscillation is then governed by a system of nonlinear integro-differential equations and is solved numerically. The acoustic field is then defined by an explicit formula; the double integral. Numerical examples showing the efficiency and accuracy of the *decoupled* model versus the *fully coupled* model were presented in the ICASE report. An updated version of this report with additional examples is accepted for publication in the *Journal of Sound and Vibration*.

We are extending our theoretical models to simulate the experimental setup, in which the source distribution or the jet noise is moving relative to the panel. The first step is to study the interaction problems for sources moving at a constant subsonic or supersonic speed. The next step is to study the interaction problems for sources moving at unsteady speed.

J. C. WEBB

Nonlinear Stability of an Unsteady Boundary Layer

Computational Aeroacoustics is a relatively new field which has recently become an important topic due, in part, to the necessity to reduce noise levels near commercial airports, and the ongoing interest in supersonic civil transport. There are many numerical issues to be resolved, and some of these will be addressed in the Workshop on Benchmark Problems in Computational Acoustics to be held at ICASE in late October of 1994.

With S.R. Otto, work is continuing concerning Tollmien-Schlichting instabilities in an unsteady boundary layer due to the impulsive motion of an infinite flat plate. A numerical study of the incompressible case has been completed. In this work, we developed numerical machinery whereby the effects of the shear layer growth on the developing instabilities could be determined. Spectral discretization was used and a period-fitting technique analogous to PSE was employed to reduce computational costs.

We are now considering the compressible case with the goal of ultimately being able to compute the noise generated when the plate speed is supersonic.

ROBERT V. WILSON

Simulation of Complex, Three-Dimensional Turbulent Jets

Three-dimensional, turbulent jets issuing from elliptic or rectangular nozzles exhibit many complex phenomena including strong azimuthal instabilities, switching of major and minor axes, and increased entrainment rates leading to increased mixing. The objective of the present work is to develop numerical methods to study such phenomena simulation.

The study will include 3-D Reynolds-averaged computations with closure at the Reynolds stress level, Large-Eddy Simulations, and Direct Numerical Simulations of rectangular and elliptic jets. Both finite volume and spectral methods are being investigated for such simulations.

Three-dimensional simulations of planar mixing layers will be performed followed by simulations of elliptic and rectangular jets.

YE ZHOU

Scalar Dissipation Model Using Successive Subgrid Scale Elimination Method for use in LES of Turbulent Scalar Mixing

Large-Eddy simulation (LES) of turbulent mixing and reaction is a possible means of calculating complex flows not amenable to full direct numerical simulations (DNS). In performing the LES of combustion, one is faced with a modeling problem not present in the LES of Navier-Stokes equation. The molecular mixing of scalars. Many combustion problems of practical interest are of the non-premixed type. In non-premixed combustion, scalar mixing, to a large extent, controls the rate of reactant conversion. The scalar mixing is predominantly a small-scale phenomenon occurring in scales not resolved in the LES calculations. Adequate modeling of the subgrid scale mixing process is hence crucial to the success of LES of reacting flows.

In collaboration with S. Girimaji, a subgrid model is developed using the recursive renormalization group (RNG) of Rose and Zhou & Vahala. A special feature of this model is that it takes into account the interaction between the smallest subgrid scales and the largest subgrid scales. One of the terms in the model, which represents the distant interactions, has the familiar form used routinely in most engineering calculation at present.

The recursive RNG method will be applied to modeling the dissipation tensor for the velocity field. Work has continued on near-wall turbulence modeling using the recursive RNG theory.

APPLIED COMPUTER SCIENCE

GIANFRANCO CIARDO

Numerical Solution of Discrete-Time Stochastic Models

A common modeling approach, especially in the area of reliability and availability estimation, is to use a high-level description formalism which is automatically translated into a continuous-time Markov chain (CTMC) and solved numerically. Unfortunately, detailed models often require the ability to model discrete-time synchronous activities which can only be approximated by the exponential distribution.

We have been exploring a new formalism based on Stochastic Petri Nets, where the activities can have a “D²-distributed” duration, including a geometric, constant, or discrete uniform distribution. The resulting formalism can be automatically translated into a discrete-time Markov chain (DTMC), but it is richer than the corresponding continuous-time one, and also greatly simplifies the description of systems with contemporary events. The formal definition of D²-SPNs includes, as special cases, several SPN-based formalisms previously defined in the literature. A related joint effort with Larry Leemis and David Nicol, initiated during our summer visit at ICASE, resulted in the article “On the minimum of independent geometrically distributed random variables,” which has now been accepted for publication in the journal *Statistics and Probability Letters*.

Next, we plan to work in two directions. An implementation of a basic D²-SPN solution algorithm is needed to gain experience in modeling real problems. At the same time, though, it appears clear that the size of the DTMC seriously limits the scalability of any modeling approach based on complete state-space generation, and even more so in the presence of discrete distributions. Hence, we plan to investigate approximate analysis algorithms for this class of models.

THOMAS W. CROCKETT

Visualization and Graphics for Parallel Applications

Computations which run on large-scale parallel supercomputers are often characterized by massive datasets. Due to their size, moving these datasets across the network for postprocessing and analysis can be cumbersome if not impossible. We are investigating techniques for exploiting the available parallelism to perform graphics and visualization operations in place. The size of the resulting image stream is bounded at a few megabytes per frame, and image compression techniques can often reduce this significantly. By integrating the graphics with the parallel computation, users can also obtain live visual feedback, which is useful for debugging, execution monitoring, and interactive steering.

Our research is focussed on two main goals: (1) development of efficient, scalable parallel rendering algorithms, and (2) incorporation of these algorithms into a parallel graphics library which can be called from application programs. Our recent work has concentrated on the second item. We have integrated our prototype parallel graphics library (PGL) into a Direct Simulation Monte Carlo (DSMC) code which is being used in Langley’s Aerothermodynamics Branch to study rarefied

flowfields. Integration of the graphics with the simulation was remarkably straightforward, requiring changes to only a few lines of code. The results of this exercise provided valuable feedback about additional functionality required in PGL, and will help to guide future algorithmic developments.

Near-term algorithmic studies will attempt to improve the load-balancing and scalability characteristics of the rendering algorithms through inexpensive static techniques. We also plan to work on strategies for reducing I/O bottlenecks in the image display phase. Improvements to PGL will include the addition of point and particle primitives, and anti-aliasing and color quantization capabilities. The latter will be based on a “Fast Adaptive Dissection” technique developed in previous work with S. Bokhari and D. Nicol.

PHILLIP DICKENS

Analytic Modeling of Parallel Simulations

The application of parallel processing to discrete-event simulation has proven to be a challenging problem, owing to the highly irregular and asynchronous interactions between submodels on different processors. Our objective is to better understand some of the tradeoffs between synchronization methods and their costs, using analytic modeling.

The work we’ve completed analyzes two forms of synchronization (conservative, optimistic) based on windows in simulation time. The model used is of a fully connected queueing network simulation, under high load. We find accurate approximations to the arrival time distributions of various messages that drive the synchronization mechanism, and in doing so address the question of whether there exists an optimal window size. We answer the question affirmatively, and also show that asymptotically the optimistic method achieves better performance for very sparse problems (on small submodel per processor) whereas the conservative method achieves better performance for a fixed sized architecture, as the number of submodels handled on each processor increases.

Our future plans are to extend the analysis to determine whether completely asynchronous or window-based protocols are better, and to compare the performance of synchronous relaxation and window-based Time Warp.

The project was in collaboration with David Nicol.

MATTHEW HAINES

Thread-based Runtime Systems

Integrating task and data parallelism requires sophisticated runtime support to handle issues of communication and synchronization among parallel tasks in an application, each of which may execute in a data parallel manner. Additionally, mapping these tasks onto a limited set of physical resources may require sharing resources among several tasks, which may or may not be related. Our objective is to design and implement a thread-based runtime system that can provide an efficient solution to the problems of integrating task and data parallelism. This work is being done in collaboration with Piyush Mehrotra, David Cronk, and Bryan Hess.

We have divided the runtime project into two layers, a lower layer for supporting language-independent, lightweight threads capable of communication in a distributed memory environment, and a higher layer for providing the support required by our task and data parallel integration

language, Opus. The lower layer, called Chant, has been defined as an extension to the POSIX pthread standard for lightweight threads, and is currently being implemented atop threads and p4 for Sun workstations and the Paragon multiprocessor. The higher layer is being prototyped to test our ideas for distributed data management and conditional method invocation.

We plan to continue development of these two layers of the runtime system, integrating them at some point in the near future. We also plan to use the Chant layer as a vehicle for studying issues related to load balancing, irregular scientific problems, and thread-based performance prediction and evaluation.

ULF HANEBUTTE

Parallel Performance of Large-Scale Simulations in CFD

Parallel computing environments have finally reached a level of performance and robustness which allows the computational scientist to consider these machines for large scale simulations. Vast differences exist between the tidy coupled MPP's, such as the INTEL Paragon, and clusters of workstations that enable parallel processing through a common software layer on top of an ordinary local area network. However, all systems support message-passing as the rudimentary parallel programming paradigm. In this light, the objective of the present work is: to continue developing new parallel algorithms and adapting existing ones based on the message passing model, and to build up an experience base for parallel performance for large-scale simulations in CFD.

Porting the fully functional parallel version of Quirk's Adaptive Mesh Refinement (AMR) algorithm to a large INTEL iPSC/860, a 144-node INTEL Paragon, a Thinking Machines CM-5 and various workstation cluster environments (P4, APPL, PVM) concluded the collaborative research project with J.J. Quirk of ICASE. As an exemplary result, we mention here the 128-node Paragon computation of a shock wave diffracting around a 90-degree corner, where 75 % parallel efficiency during the later stages of the simulation has been observed. While a single Sun Sparc 10 workstation requires one-and-a-half days for this simulation the 128-node Paragon delivers the result in under 30 minutes. This simulation was presented at the High Performance Computing 94 Conference in La Jolla, Ca, April 11-15, 1994.

The IBM SP1 belongs to a new and promising class of parallel architectures that combines the strength of a fast RISC workstation containing large core memory and secondary storage with a scalable high bandwidth network. To evaluate its potential work has started in collaboration with Ron Joslin from NASA and M. Zubair from Old Dominion University and IBM to port a parallel direct numerical simulation code to the SP1. We are planning to perform large-scale three-dimensional boundary-layer flow transition simulations.

We have also embarked on a project in collaboration with David Keyes of ICASE and Old Dominion University and Gary Warren of NASA to reformulate an existing serial Euler-solver into a parallel Newton-Krylov-Schwarz scheme.

DAVID E. KEYES

Newton-Krylov-Schwarz Algorithms for Parallel Computational Mechanics

Many parallel algorithms for large, irreducibly coupled systems iteratively solve concurrent problems within different subspaces of a Hilbert space, or within different subdomains of a physical region, which may correspond to the same thing with a proper choice of basis. Operators typically encountered are of the form $R_i^T A_i^{-1} R_i$, where R_i ($n_i \times n$) gathers selected global degrees of freedom (or weighted averages thereof) out of a vector of size n into a vector of size n_i local to subspace i (or subdomain i), and R_i^T scatters the result back after treatment with the lower dimensional inverse. Major computational kernels of both Schwarz methods and Schur complement methods contain such triple products. The operator A_i may itself come from such a form with reverse order of the factors: $A_i = R_i A R_i^T$, or an approximation thereto. The parallelism of the method is related to the communication inherent in the R_i operators, while operations with A_i are usually local by construction. The convergence of the method is also critically related to the R_i . Block Jacobi is a trivial, but well motivated, limiting choice. For general problems, there is more art than theory in the choices of partitioning, ordering, and segregation of scales that are inherent in the R_i .

Over the past reporting period, we have been collaboratively investigating domain-decomposed additive Schwarz preconditioners consisting of sums of the triple-products above on a variety of problems of one or multiple components, in two or three dimensions, on serial, tightly-coupled parallel, and loosely-coupled parallel (i.e., workstation network) computers. Application areas include Euler problems (with Driss Tidriri of ICASE), full potential problems (with Xiao-Chuan Cai of the University of Colorado-Boulder CS Department), and shallow water equation systems (with Julia Chefter of the Columbia University Applied Physics Department). The crux is to identify an operator with positive-definite symmetric part to which the elliptic theory will apply. This may come from an artificially diffusive low-order implicit operator or from an operator splitting (in the case of the shallow water equations) that handles the hyperbolic part by a modified method of characteristics, leaving an elliptic system to be solved implicitly. GMRES is typically used to accelerate convergence. When the original system is nonlinear, a matrix-free Newton method is the outer loop and the resulting algorithm is called “Newton-Krylov-Schwarz” (NKS). NKS solvers permit high CFL numbers. So far, only the full potential equation application has seen effective use of a two-level coarse-grid preconditioner.

We will continue to develop parallel implicit solvers for high CFL number applications (mainly steady state problems), but also plan to develop moderate CFL applications, such as to the fluid solver in transient aeroelasticity, in which the first-order time-factorization error left behind by conventional approximate factorization methods is unacceptable.

SCOTT T. LEUTENEGGER

Database Support for Scientific Data and Visualization

Visualization of scientific data is limited by the size of the data set that can be considered, yet scientist are producing increasingly larger data sets that they would like to visualize. Currently, solution sets are saved as files and then the entire file read into a visualization package (such as

FAST or AVS). Often scientists are only interested in visualizing a subset of the data set. The objective of our project is to provide database support for retrieval of subsets of the scientific data. The data we wish to consider is either structured or unstructured grids, i.e. a collection of points in 2 or 3 dimensions along with a vector of values associated with each point.

The current focus of the project is implementation and comparison of existing indexing techniques to determine which are most appropriate for storing and retrieving two dimensional scientific data. We are implementing indexing methods and building a prototype capable of retrieving subsets of large scientific data sets. The system is an extension of the *Exodus* system, an existing public domain Client-Server Object Oriented Database Management System. This work has been done in collaboration with Adrian Filipi-Martin, a student at the College of William and Mary.

We plan to extend our studies to include three dimensional data sets and then create and interface between FAST and our database server to allow exploration of large data sets. We also intend to investigate bulk loading algorithms for these indexing techniques. In collaboration with David Nicol from the College of William and Mary, we are developing an algorithm for bulk loading of the grid file that maximizes the bucket (disk) utilization.

Database Scheduling

A second project considers relational database scheduling. Although relational databases have been in use for a long time, little work has been done on how to schedule mixed workloads of transactions and queries. In collaboration with Mark Holliday from Western Carolina University, we are investigating scheduling of mixed workloads for database systems.

We are currently using a generic database simulator implemented by Mark Holliday to simulate a single workstation relational database. We are using the TPC-C benchmark as the workload of our study. We have chosen this benchmark since it represents a consensus among industry and academia on a typical workload. We intend to modify the workload with additional transactions to see how more complex queries affect system performance. Our scheduling work is focusing on buffer allocation, load control, and cpu/disk scheduling.

Multi-level Solution Techniques for Solving Markov Chains

In collaboration with Graham Horton from the University of Erlangen-Nurnberg, we have continued development of, and experimentation with, a multi-level solution technique for the solution of steady state Markov chains. Many scientific fields use Markov models requiring the numerical solution of large steady state Markov chains, thus this work has a significant impact on science in general. The technique delivers solution times up to two orders of magnitude faster than the current state of the art (SOR) method.

We are currently considering refinement of the aggregation strategy, and the application of the technique to nearly completely decomposable Markov chains. We plan to determine whether the technique can be developed into a general solver or whether it will be limited to special cases of Markov chains.

KWAN-LIU MA

3D Visualization of Unsteady 2D Airplane Wake Vortices

Air flowing around the wing tips of an airplane forms horizontal tornado-like vortices that can be dangerous to following aircraft. The dynamics of such vortices, including ground effects and

the effect of atmospheric stratification, can be predicted and monitored by numerical simulation, allowing the safety and capacity of airports to be improved. Proper visualization methods are needed to examine and verify the predicted flow field. One example is the ability of visualizing the history of the vortices. However, general-purpose visualization packages, like FAST and Tecplot, cannot be directly applied to data from a time-dependent, two-dimensional simulation.

In collaboration with Dr. Z. C. Zheng of the Department of Aerospace Engineering, Old Dominion University, a tracing algorithm for locating vortex cores as well as three-dimensional computer graphics techniques have been developed for visualization of time-dependent, two-dimensional wake vortex computations. In addition, an important quantity that may indicate vortex hazards is the induced rolling moment on the following airplane. Rolling moment can be calculated using the unsteady two-dimensional predicted flow fields. A novel approach has been introduced to comprehend the hazard strength near the vortices with direct, three-dimensional visualization of the induced rolling moment. The techniques we have developed and the visualization results we have obtained help verify and understand the predicted flow field.

The visualization techniques, implemented with an interactive user interface, can be used not only for researchers to tune their numerical models, but also for flight control at airports. Our future work will include developing interactive visualization of vortex hazards and integrating the visualization techniques into the numerical simulation for real-time monitoring.

PIYUSH MEHROTRA

Evaluation of HPF for Data Parallel Codes

High Performance Fortran (HPF) is a set of extensions to Fortran designed to exploit data parallelism on a wide variety of parallel architectures. Since HPF is becoming an industry-standard language for data parallel algorithms, we have been evaluating the expressiveness of HPF for codes of interest to NASA. This work is being done in collaboration with John Van Rosendale, Mike Cokus, Dave Middleton, and Kyle Winn.

The current focus is on the following codes: a single grid version of ISAAC, TLNS3D a multi-block code, and DSMC a Monte Carlo code. We have analyzed the codes to understand the parallelism and allowing us to insert appropriate HPF directives to specify the required data distributions. HPF seems to be adequate for the first code and for some versions of the distributions required for TLNS3D. However, the DSMC code requires more support than is currently available through HPF. We have been attempting to use Applied Parallel Research's HPF compiler and University of Vienna's Vienna Fortran Compiler to evaluate the performance of the HPF code. However, both these systems have proved to be too unstable to obtain useful performance results.

We plan to suggest extensions for HPF based on our experiences with these codes. We also plan to study other codes, including a Finite Element structural analysis code, and an eigenvalue code. The availability of stable HPF compilers will also enable us to evaluate the different versions of the HPF codes.

Integration of Task and Data Parallelism

High Performance Fortran has targeted data parallel algorithms. However, many scientific applications such as multidisciplinary optimization codes, exhibit a coarser grained task parallelism

at the outer level while being data parallel at the inner level. The objective of this project is to develop language extensions designed to address both the “programming in the large” issues, and the parallel performance issues arising in complex multidisciplinary applications.

In the language that we have designed, called Opus, a program executes as a system of tasks which interact by sharing access to a set of Shared Data Abstractions (SDAs). Tasks themselves may embody nested parallelism, for example, by executing a data parallel HPF program. SDAs generalize Fortran 90 modules by including features from both objects in object-oriented data bases and monitors in shared memory languages. The idea is to provide persistent shared “objects” for communication and synchronization between large grained parallel tasks, at a much higher level than simple communication channels transferring bytes between tasks.

Language design is an evolving process. As we gain more experience with the design we will include new features or modify old ones where appropriate. We have also started the design and implementation of a thread based runtime support system which will allow Opus programs to run in a parallel and distributed heterogeneous environment. This work has been done in collaboration with Hans Zima and Barbara Chapman of University of Vienna and John Van Rosendale.

DAVID MIDDLETON

An Executable Specification for a Simple Combining Network

While most parallel computer networks are designed just to deliver messages, enabling the message system to perform, in addition, some simple operations on the data as they proceed can yield a significant reduction in overall work. However, experience with the IBM RP3 computer, along with other proposed designs, has led to the conclusion that combining networks, while very powerful, consume too large a fraction of the hardware resource budget to be justifiable. The combining network proposed for the FFP Machine is extremely simple, but through appropriate choices of the operators and actions specified for the communication system, several subtle and useful operations can be accomplished. However, while the network is physically simple in construction, it is conceptually complex, with many interrelated design dependencies. The goal is to generate a complete specification of the network.

To define the network behavior, a simulator has been developed which serves three purposes. First, it provides a complete and concrete specification of the behavior of the network nodes. This specification can be tested and the possible behaviors can be verified. Second, it allows algorithms that would use the network to be designed and debugged in a more flexible environment than physical hardware would provide. Several algorithms have been developed and implemented with the system. Third, it provides the foundation for designing efficient network interfaces for the processing elements. The algorithms implemented so far illustrate that a very simple receiving scheme is adequate for processors to extract intended data from incoming message streams.

The system will be used to implement the communication for more complicated algorithms, such as matrix multiplication, and certain graph algorithms that might support database or logic programming systems. These communication algorithms will likely require more complex abilities in the message receivers, and such examples may help designers decide what levels of complexity are appropriate.

DAVID NICOL

Parallel Simulation of Message Passing Codes

As massively parallel computers become increasingly available, users' interest in the scalability of their parallel codes is growing. However, such computers are in high demand, and access to them is restricted. We are developing a system called LAPSE (Large Application Parallel Simulation Environment) that allows one to use a small number of parallel processors to simulate the behavior of a message-passing code running on a large number of processors of a "target" machine. With LAPSE, a user could performance tune a code for massive parallelism before actually using large numbers of processors.

The approach taken in LAPSE is to actually run the application using a separate process (called a Virtual Processor, or VP) for each simulated physical processor. The VPs are multitasked onto the available physical nodes. Application message-passing calls are trapped by LAPSE and redirected to the appropriate VP. In addition, the number of instructions executed by the application between message passing calls is determined and passed to a timing simulator. The timing simulator, which is also parallelized, models delays in the target machine's interconnection network and operating system, as well as certain message-passing overheads and delays in the target machine's operating system. The target machine currently supported by LAPSE is the Intel Paragon, and LAPSE runs on the Paragon. Several applications have been run under LAPSE. The timings predicted by LAPSE are typically within 5% of the actual application's execution time, but have ranged up to 15% errors for highly communications intensive applications. We are currently studying how application characteristics affect the execution speed of LAPSE. On the codes tested so far, LAPSE is from 1.5 to 15 times slower than the native application running on the same number of processors, depending on the computation to communication ratio. The primary limitation in using LAPSE is the ability to support a large number of VPs per physical node; this limitation is due to the limited amount of physical memory per Paragon node and the ability of the Paragon's software to efficiently support a large number of processes per processor. However, LAPSE has been used to predict the performance of a 512 node application running on only 64 nodes of the Paragon.

Our future plans are to broaden the number the applications run under LAPSE, for the purposes of both validating LAPSE timing predictions and understanding LAPSE execution speeds. We will also port LAPSE to run on a network of workstations.

The project was in collaboration with Phillip Dickens and Philip Heidelberger.

Partitioning of Irregular Meshes for Parallel Processing

Parallel processing of workloads related to highly irregular meshes creates the important problem of partitioning the mesh into submeshes where the induced communication cost is low, and the workload is balanced. Several methods have received much attention (e.g., recursive bisection, spectral partitioning, geometric partitioning), but have drawbacks. Our objective is to find a partitioning method whose computational cost is low, but which identifies good partitions.

The approach taken is to partition continuous field approximations of workload and communication. Description of these fields typically requires only $O(\log N)$ space for a grid with N points. One important aspect is whether the approximation is good. We have determined that it often is. Another aspect is whether regions of extremely high workload (frequently observed in highly irregular meshes) can be automatically isolated for special partitioning—this is desirable in

order to keep communication costs low. We have developed an algorithm for isolating such regions, and have found on example grids that over 50% of a grid may reside in a small number of separable regions.

Our future plans are to find ways of partitioning the high intensity workload regions, and the low intensity workload regions.

Parallel Simulation of Communication Networks

Simulation of large-scale communication networks is a taxing computational task for which parallelized simulation offers distinct performance advantages. We are especially motivated to find ways of applying SIMD architectures to such simulations, as such architectures are highly cost-effective on problems amenable to SIMD solution.

Together with researchers at AT&T Bell Labs (Boris Lubachevsky, Albert Greenberg) we have developed algorithms for simulating call-by-call models of wireless communication networks. The constraints of the model, that no frequency be reused within some radius r imposes extremely high synchronization demands on the intuitive (but naive) approach where one radio tower (assumed here to be the entire workload of one PE) blocks until its own next-event-time is less than those of all towers within radius r . We have identified methods for predicting towers' future behavior sufficiently well so that this constraint may be relaxed considerably. The effect of our optimizations are to simulate (using a 16K PE MasPar MP-1) a 128×128 tower domain 120 times faster than an optimized serial simulation running on a high-end workstation. The PE utilizations are in excess of 50%, as opposed to the 3% utilizations of the naive approach.

Our future plans are to develop uniformization-based algorithms for handling mobility of calls between radio towers, and to study simulations of more complex frequency allocation algorithms.

ALEX POTHEN

Spectral Algorithms for Partitioning and Ordering

Solving linear systems resulting from finite element discretizations of partial differential equations on parallel computers requires the partition of the computational domain into subdomains (if domain decomposition is used), or a nested dissection ordering that permits high concurrency to factor the coefficient matrix (if a direct factorization is employed). In both these cases and in many other computations involving irregular meshes, a mesh needs to be partitioned into a given number of submeshes with roughly equal computational costs such that few edges join different submeshes.

In joint work with Horst Simon (NASA Ames) and my former PhD student Lie Wang (IBM Toronto), I have developed spectral algorithms employing eigenvectors of the Laplacian matrix of the mesh to solve the partitioning problem. Extensive experiments show that recursive spectral bisection is capable of providing high quality partitions in comparison with other combinatorial, geometric, and inertial algorithms that have been proposed. This partitioning algorithm has been used in the solution of fluid flow problems (among others) on the iPSC/860 and the Thinking Machines CM-2. Similarly, spectral nested dissection orderings outperform other ordering algorithms by a wide margin in the computation of the Cholesky factorization on the Intel Paragon; for many large problems, spectral nested dissection makes this computation-intensive factorization tractable for the first time. We have extended a mathematical programming formulation of the partitioning

problem due to Franz Rendl (Graz, Austria) and Henry Wolkowicz (Waterloo, Canada) to explain the success of the spectral algorithm.

In future work we will consider extending the partitioning algorithm to convective, anisotropic, and heterogeneous problems, where there are preferred directions for partitioning the problem. The computation of profile-reducing orderings for incomplete factorization preconditioners will be studied. Comparisons with other partitioning algorithms and developing techniques to speed up the spectral algorithm will also be priorities.

JAMES QUIRK

Parallelization of AMR Algorithm for Euler Equations

The goal is to develop portable parallel adaptive mesh refinement algorithm for the shocked solutions of Euler equations. In the last six months I finished parallelizing the sophisticated mesh refinement algorithm which forms the basis of my computational machinery (ICASE Report No. 93-63). The parallelization was done in an abstracted fashion, using a message passing paradigm, and so the resultant parallel algorithm is highly portable. Indeed, while I devised and tested the algorithm on clusters of work stations, a colleague has subsequently demonstrated the ease with which it may be ported to dedicated parallel computing engines.

I now routinely use this parallel, mesh refinement scheme for serious investigations of several important shock wave phenomena. For example, working in collaborations with S. Karni, I have just finished a detailed study of shock refraction at a cylindrical interface. For this work, my colleague provided me with a novel shock-capturing scheme designed for multi-component flows. This scheme was straightforwardly amalgamated with the mesh refinement machinery to produce a powerful numerical tool which is capable of reproducing all the intricate mechanism that have been observed experimentally. This work is almost written up and will appear in an ICASE report.

Now that my computational machinery has reached a fairly mature state, I envisage spending more time investigating specific shock wave phenomena that are not well understood, and less time on basic algorithm development. For example, in the near future I hope to finish off a numerical study of the Mach reflection of detonation waves. This work will benefit from a parallel experimental and theoretical study by J.E. Shepherd and his colleagues.

MOULAY DRISS TIDRIRI

Newton-Krylov-Schwarz Methods in CFD

Newton-Krylov methods are potentially well suited for the implicit solution of nonlinear problems whenever it is unreasonable to compute or store a true Jacobian. Krylov-Schwarz iterative methods are well suited for the parallel implicit solution of PDE's that arise in CFD. They provide good data locality so that even a high-latency workstation network can be employed as a parallel machine.

In collaboration with David Keyes from ICASE and Old Dominion University we have investigated some algorithmic and implementation aspects: the use of mixed discretization schemes in

the (implicitly defined) Jacobian and its preconditioner, the selection of the differencing parameter in the formation of the action of the Jacobian, and workstation network implementation. An in-depth study performed on the convection-diffusion model problem gave sufficient conditions on the size of the differencing parameter and the consistency between (lower-order) left-hand side and (higher-order) right hand-side discretizations. The use of these techniques to solve compressible Euler equations shows that a large CFL number can be allowed. However, transition to a full Newton method (CFL number approaching infinity) is currently precluded by explicit boundary conditions. Preliminary experience with the Unix workstations connected only by a single ethernet is encouraging in that even for a modest fixed-size problem, wall clock execution time per iteration improves on up to sixteen workstations. When parallelism is exploited in its more advantageous scaling of fixed subdomain size per processor, we expect more encouraging results.

In the future we are considering replacing the explicit boundary conditions in the compressible Euler code by fully implicit boundary conditions. The application of Newton-Krylov-Schwarz method to a 3D Euler code is underway, and application of mixed-discretization domain-decomposed preconditioners to 3D Navier-Stokes will also be considered.

HANS P. ZIMA

Extending HPF for Advanced Data Parallel Applications

One major result of our activity was the development of a detailed proposal for extending the **data distribution** facilities of HPF. The stated goal of High Performance Fortran (HPF) was to “address the problems of writing data parallel programs where the distribution of data affects performance”. The current version of the language has not fully achieved this goal. While the basic distribution functions offered by the language – regular block, cyclic, and block cyclic distributions – can support regular numerical algorithms, advanced applications such as particle-in-cell codes or unstructured mesh solvers cannot be expressed adequately. Our proposal addresses this problem and develops a range of new language features which provide the required functionality, including

- distribution to processor subsets
- processor views
- general block distributions
- indirect distributions
- user-defined distribution functions and
- on-clauses for the control of the work distribution in an **INDEPENDENT** loop.

Some of these extensions have already been implemented in the Vienna Fortran Compilation System being developed at the University of Vienna. We intend to implement the others to show the feasibility of the approach and the performance achieved on various codes. This work is being done in collaboration with Barbara Chapman of University of Vienna and Piyush Mehrotra of ICASE.

REPORTS AND ABSTRACTS

Sarkar, S., and M. Y. Hussaini: *Computation of the sound generated by isotropic turbulence*. ICASE Report No. 93-74, October 6, 1993, 30 pages. Submitted to Journal of Fluid Mechanics.

The acoustic radiation from isotropic turbulence is computed numerically. A hybrid direct numerical simulation approach which combines direct numerical simulation (DNS) of the turbulent flow with the Lighthill acoustic analogy is utilized. It is demonstrated that the hybrid DNS method is a feasible approach to the computation of sound generated by turbulent flows. The acoustic efficiency in the simulation of isotropic turbulence appears to be substantially less than that in subsonic jet experiments. The dominant frequency of the computed acoustic pressure is found to be somewhat larger than the dominant frequency of the energy-containing scales of motion. The acoustic power in the simulations is proportional to ϵM_t^5 where ϵ is the turbulent dissipation rate and M_t is the turbulent Mach number. This is in agreement with the analytical result of Proudman (1952), but the constant of proportionality is smaller than the analytical result. Two different methods of computing the acoustic power from the DNS data bases yielded consistent results.

Lilley, Geoffrey M.: *The radiated noise from isotropic turbulence revisited*. ICASE Report No. 93-75, December 14, 1993, 58 pages. Submitted to Theoretical and Computational Fluid Dynamics (TCFD).

The noise radiated from isotropic turbulence at low Mach numbers and high Reynolds numbers, as derived by Proudman (1952), was the first application of Lighthill's *Theory of Aerodynamic Noise* to a complete flow field. The theory presented by Proudman involves the assumption of the neglect of retarded time differences and so replaces the second-order retarded-time and space covariance of Lighthill's stress tensor, T_{ij} , and in particular its second time derivative, by the equivalent simultaneous covariance. This assumption is a valid approximation in the derivation of the $\partial^2 T_{ij}/\partial t^2$ covariance at low Mach numbers, but is not justified when that covariance is reduced to the sum of products of the time derivatives of equivalent second-order velocity covariances as required when Gaussian statistics are assumed. The present paper removes these assumptions and finds that although the changes in the analysis are substantial, the change in the numerical result for the total acoustic power is small.

The present paper also considers an alternative analysis which does not neglect retarded times. It makes use of the Lighthill relationship, whereby the fourth-order T_{ij} retarded-time covariance is evaluated from the square of similar second-order covariance, which is assumed known. In this derivation no statistical assumptions are involved. This result, using distributions for the second-order space-time velocity squared covariance based on the Direct Numerical Simulation (DNS) results of both Sarkar and Hussaini (1993) and Dubois (1993), is compared with the re-evaluation of Proudman's original model. These results are then compared with the sound power derived from a phenomenological model based on simple approximations to the retarded-time/space covariance

of T_{xx} . Finally the recent numerical solutions of Sarkar and Hussaini(1993) for the acoustic power are compared with the results obtained from the analytic solutions.

Speziale, Charles G., Ridha Abid, and Paul A. Durbin: *New results on the realizability of Reynolds stress turbulence closures*. ICASE Report No. 93-76, October 12, 1993, 51 pages. To be submitted to Journal of Fluid Mechanics.

The realizability of Reynolds stress models in homogeneous turbulence is critically assessed from a theoretical standpoint. It is proven that a well known second-order closure formulated by Shih and Lumley using the strong realizability constraints of Schumann is, in fact, not a realizable model. The problem arises from the failure to properly satisfy the necessary positive second time derivative constraint when a principal Reynolds stress vanishes – a fatal flaw that becomes apparent when the non-analytic terms in their model are made single-valued as required on physical grounds. It is furthermore shown that the centrifugal acceleration generated by rotations of the principal axes of the Reynolds stress tensor can make the second derivative singular at the most extreme limits of realizable turbulence. This previously overlooked effect appears to make it impossible to identically satisfy the strong form of realizability in any version of the present generation of second-order closures. On the other hand, models properly formulated to satisfy the weak form of realizability – wherein states of one or two component turbulence are not accessible in finite time – are found to be realizable. However, unlike the simpler and more commonly used second-order closures, these models can be ill-behaved near the extreme limits of realizable turbulence due to the way that higher-degree nonlinearities are often unnecessarily introduced to satisfy realizability. Illustrative computations of homogeneous shear flows are presented to demonstrate these points which can have important implications for turbulence modeling.

Agrawal, Gagan, Alan Sussman, and Joel Saltz: *An integrated runtime and compile-time approach for parallelizing structured and block structured applications*. ICASE Report No. 93-77, October 22, 1993, 32 pages. Submitted to IEEE Transactions on Parallel and Distributed Systems.

Scientific and engineering applications often involve structured meshes. These meshes may be nested (for multigrid codes) and/or irregularly coupled (called multiblock or irregularly coupled regular mesh problems). In this paper, we present a combined runtime and compile-time approach for parallelizing these applications on distributed memory parallel machines in an efficient and machine-independent fashion. We have designed and implemented a runtime library which can be used to port these applications on distributed memory machines. The library is currently implemented on several different systems. To further ease the task of application programmers, we have developed methods for integrating this runtime library with compilers for HPF-like parallel programming languages. We discuss how we have integrated this runtime library with the Fortran 90D compiler being developed at Syracuse University. We present experimental results to demonstrate the efficacy of our approach. We have experimented with a multiblock Navier-Stokes solver template and a multigrid code. Our experimental results show that our primitives have low

runtime communication overheads. Further, the compiler parallelized codes perform within 20% of the code parallelized by manually inserting calls to the runtime library.

Iollo, Angelo, Manuel D. Salas, and Shlomo Ta'asan: *Shape optimization governed by the Euler equations using an adjoint method*. ICASE Report No. 93-78, November 4, 1993, 20 pages. To be submitted to the "14th International Conference on Numerical Methods in Fluid Dynamics," July 11-15, 1994, Bangalore, India.

In this paper we discuss a numerical approach for the treatment of optimal shape problems governed by the Euler equations. In particular, we focus on flows with embedded shocks. We consider a very simple problem: the design of a quasi-one-dimensional Laval nozzle. We introduce a cost function and a set of Lagrange multipliers to achieve the minimum. The nature of the resulting costate equations is discussed. A theoretical difficulty that arises for cases with embedded shocks is pointed out and solved. Finally, some results are given to illustrate the effectiveness of the method.

Chang, Cheng-Shang, Philip Heidelberger, and Perwez Shahabuddin: *Fast simulation of packet loss rates in a shared buffer communication switch*. ICASE Report No. 93-79, November 4, 1993, 22 pages. Submitted to the ECM Sigmetrics Conference.

This paper describes an efficient technique for estimating, via simulation, the probability of buffer overflows in a queueing model that arises in the analysis of ATM (Asynchronous Transfer Mode) communication switches. There are multiple streams of (autocorrelated) traffic feeding the switch that has a buffer of finite capacity. Each stream is designated as either being of high or low priority. When the queue length reaches a certain threshold, only high priority packets are admitted to the switch's buffer. The problem is to estimate the loss rate of high priority packets. An asymptotically optimal importance sampling approach is developed for this rare event simulation problem. In this approach, the importance sampling is done in two distinct phases. In the first phase, an importance sampling change of measure is used to bring the queue length up to the threshold at which low priority packets get rejected. In the second phase, a different importance sampling change of measure is used to move the queue length from the threshold to the buffer capacity.

Jameson, Leland: *On the spline-based wavelet differentiation matrix*. ICASE Report No. 93-80, November 5, 1993, 37 pages. To be submitted to SIAM Journal on Numerical Analysis.

The differentiation matrix for a spline-based wavelet basis will be constructed. Given an n -th order spline basis it will be proven that the differentiation matrix is accurate of order $2n + 2$ when periodic boundary conditions are assumed. This high accuracy, or superconvergence, is lost when the boundary conditions are no longer periodic. Furthermore, it will be shown that spline-based bases generate a class of compact finite difference schemes.

Horton, Graham, and Scott T. Leutenegger: *A multi-level solution algorithm for steady-state Markov chains*. ICASE Report No. 93-81, November 5, 1993, 31 pages. Submitted to *Sigmetrics '94*.

A new iterative algorithm, the *multi-level* algorithm, for the numerical solution of steady state Markov chains is presented. The method utilizes a set of recursively coarsened representations of the original system to achieve accelerated convergence. It is motivated by multigrid methods, which are widely used for fast solution of partial differential equations. Initial results of numerical experiments are reported, showing significant reductions in computation time, often an order of magnitude or more, relative to the Gauss-Seidel and optimal SOR algorithms for a variety of test problems. The paper also contrasts and compares the multi-level method with the iterative aggregation-disaggregation algorithm of Takahashi.

Gottlieb, David, and Chi-Wang Shu: *On the Gibbs phenomenon III: Recovering exponential accuracy in a sub-interval from a spectral partial sum of a piecewise analytic function*. ICASE Report No. 93-82, November 5, 1993, 19 pages. Submitted to *SIAM Journal on Numerical Analysis*.

We continue the investigation of overcoming Gibbs phenomenon, i.e., obtaining exponential accuracy at all points including at the discontinuities themselves, from the knowledge of a spectral partial sum of a discontinuous but piecewise analytic function.

We show that if we are given the first N expansion coefficients of an L_2 function $f(x)$ in terms of either the trigonometrical polynomials or the Chebyshev or Legendre polynomials, we can construct an **exponentially convergent approximation** to the point values of $f(x)$ in any sub-interval in which it is analytic.

Carpenter, Mark H., David Gottlieb, Saul Abarbanel, and Wai-Sun Don: *The theoretical accuracy of Runge-Kutta time discretizations for the initial boundary value problem: A careful study of the boundary error*. ICASE Report No. 93-83, November 5, 1993, 15 pages. To be submitted to *SIAM Journal on Scientific Computing*.

The conventional method of imposing time dependent boundary conditions for Runge-Kutta (RK) time advancement reduces the formal accuracy of the space-time method to first order locally, and second order globally, independently of the spatial operator. This counter intuitive result is analyzed in this paper.

Two methods of eliminating this problem are proposed for the linear constant coefficient case: 1) impose the exact boundary condition only at the end of the complete RK cycle, 2) impose consistent intermediate boundary conditions derived from the physical boundary condition and its derivatives. The first method, while retaining the RK accuracy in *all cases*, results in a scheme with much reduced CFL condition, rendering the RK scheme less attractive. The second method retains the same allowable time step as the periodic problem. However it is a general remedy only for the linear case. For non-linear hyperbolic equations the second method is effective only for RK schemes of third order accuracy or less. Numerical studies are presented to verify the efficacy of each approach.

Somani, Arun K., and Kishor S. Trivedi: *Phased-mission system analysis using Boolean algebraic methods*. ICASE Report No. 93-84, November 9, 1993, 20 pages. Submitted to Sigmetrics '94.

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

Trivedi, Kishor S., Gianfranco Ciardo, Manish Malhotra, and Robin A. Sahner: *Dependability and performability analysis*. ICASE Report No. 93-85, November 17, 1993, 28 pages. *Performance Evaluation of Computer and Communication Systems, Lecture Notes in Computer Science 729*, Editors: L. Donatiello and R. Nelson, Springer-Verlag 1993, pp. 587-612.

In this tutorial, we discuss several practical issues regarding specification and solution of dependability and performability models. We compare model types with and without rewards. Continuous-time Markov chains (CTMCs) are compared with (continuous-time) Markov reward models (MRMs) and generalized stochastic Petri nets (GSPNs) are compared with stochastic reward nets (SRNs). It is shown that reward-based models could lead to more concise model specification and solution of a variety of new measures. With respect to the solution of dependability and performability models, we identify three practical issues: largeness, stiffness, and non-exponentiality, and we discuss a variety of approaches to deal with them, including some of the latest research efforts.

Buckmaster, J., and T. Jackson: *Flames in dusty mixtures - their structure and stability*. ICASE Report No. 93-86, November 17, 1993, 24 pages. Submitted to the 25th Symposium (International) on Combustion.

The structure and stability of flames in dusty mixtures is investigated. The presence of the dust leads to significant transport of energy by radiation and the fundamental goal of the analysis is to explore to what extent this displaces the classical non-hydrodynamical stability boundaries of the plane deflagration. An approximate description of the radiative transport permits analysis for arbitrary values of both the Planck length and the Boltzmann number. It is shown that the pulsating/traveling-wave instability usually associated with values of Lewis number (Le) bigger

than 1 is strongly enhanced by the presence of radiation and can be present even if $Le < 1$. On the other hand radiation tends to suppress the cellular instability normally associated with values of Le less than 1. The latter is consistent with preliminary experimental observations of Abbud-Madrid and Ronney.

Ristorcelli, J.R.: *Carrying the mass flux terms exactly in the first and second moment equations of compressible turbulence.* ICASE Report No. 93-87, November 18, 1993, 11 pages. Submitted to Physics of Fluids.

In compressible turbulence models it is assumed that the Favre-mean velocities are suitable approximations to the Reynolds-mean velocities in order to close unknown terms. This neglects, in the mean momentum and energy equations, the contribution to the stress and work terms by the mean of the fluctuating Favre velocity, a quantity proportional to the turbulent mass flux. As the stress and work terms do not introduce any new unknown correlations requiring closure in either $k - \epsilon$ or Reynolds stress closures and because the exact form of the terms can, with little additional work, be carried there is no need to make any modeling assumptions. In the Reynolds stress equations the viscous terms appear naturally in Reynolds variables while the problem is posed in Favre variables. In the process of splitting the viscous terms into the viscous transport terms, carried in Favre variables, and the dissipation terms, carried in Reynolds variables, important contributions from the mass flux appear. The accurate accounting of these terms is important for any consistent near wall modeling and the retention of the mass flux terms is important in complex compressible turbulent flows.

Ristorcelli, J.R.: *A representation for the turbulent mass flux contribution to Reynolds-stress and two-equation closures for compressible turbulence.* ICASE Report No. 93-88, November 18, 1993, 25 pages. Submitted to Physics of Fluids.

The turbulent mass flux, or equivalently the fluctuating Favre velocity mean, appears in the first and second moment equations of compressible $k - \epsilon$ and Reynolds stress closures. Mathematically it is the difference between the unweighted and density-weighted averages of the velocity field and is therefore a measure of the effects of compressibility through variations in density. It appears to be fundamental to an inhomogeneous compressible turbulence, in which it characterizes the effects of the mean density gradients, in the same way the anisotropy tensor characterizes the effects of the mean velocity gradients. An evolution equation for the turbulent mass flux is derived. A truncation of this equation produces an algebraic expression for the mass flux. The mass flux is found to be proportional to the mean density gradients with a tensor eddy-viscosity that depends on both the mean deformation and the Reynolds stresses. The model is tested in a wall bounded DNS at Mach 4.5 with notable results.

Wu, Sean F., and Lucio Maestrello: *Response of a finite plate excited by a turbulent boundary layer*. ICASE Report No. 93-89, December 1, 1993, 28 pages. Submitted to AIAA Journal.

Formulations for predicting dynamic and acoustic responses of a finite plate flush-mounted on an infinite baffle subject to turbulent and mean flow excitations are presented. In deriving these formulations, the effects of stretching due to in-plane force and coupling between structural vibration and acoustic radiation are taken into account. The resulting equation governing plate vibration contains cubic nonlinearities. To obtain an approximate solution, the plate flexural displacement is expanded into orthogonal base functions. The unknown coefficients associated with base functions are determined by solving a set of coupled nonlinear integral equations using Galerkin's method. A stability analysis is given using the basic existence-uniqueness theorem. In particular, stable conditions for a linearized system are obtained using the Routh algorithm. It is shown that structural instabilities can be induced by fluid loading and mean flow. Two unstable mechanisms are found to be attributable to added damping and stiffness due to acoustic radiation. The effect of added damping increases linearly, while that of added stiffness increases quadratically with the Mach number of mean flow. Finally, the cross-power spectral density functions of plate flexural vibration and radiated acoustic pressure are derived and expressed in terms of the cross-power spectral density function of turbulent flow.

Fischer, Paul F.: *Projection techniques for iterative solution of $Ax = b$ with successive right-hand sides*. ICASE Report No. 93-90, December 1, 1993, 13 pages. Submitted to SIAM Journal on Scientific Computing.

We present two projection techniques for computing approximate solutions to linear systems of the form $Ax^n = b^n$, for a sequence $n = 1, 2, \dots$, e.g., such as arises from time discretization of a partial differential equation. The inexpensive approximate solutions can be used as initial guesses for iterative solution of the system, resulting in significantly reduced computational expense. Examples of two- and three-dimensional incompressible Navier-Stokes calculations are presented in which \underline{x} represents the pressure, and A is a discrete Poisson operator. In flows containing significant dynamic activity, these projection techniques lead to as much as a two-fold reduction in solution time.

Nicol, David M., and Weizhen Mao: *Automated parallelization of times Petri-net simulations*. ICASE Report No. 93-91, December 1, 1993, 29 pages. Submitted to Journal of Parallel and Distributed Computing.

Timed Petri-nets are used to model numerous types of large complex systems, especially computer architectures and communication networks. While formal analysis of such models is sometimes possible, discrete-event simulation remains the most general technique available for assessing the model's behavior. However, simulation's computational requirements can be massive, especially on the large complex models that defeat analytic methods. One way of meeting these requirements is by executing the simulation on a parallel machine. This paper describes simple techniques for the

automated parallelization of timed Petri-net simulations. We address both the issue of processor synchronization, as well as the automated mapping, static and dynamic, of the Petri-net to the parallel architecture. As part of this effort we describe a new mapping algorithm, one that also applies to more general parallel computations. We establish analytic properties of the solution produced by the algorithm, including optimality on some regular topologies. The viability of our integrated approach is demonstrated empirically on the Intel iPSC/860 and Delta architectures using many processors. Excellent performance is observed on models of parallel architectures.

Chapman, Barbara, Piyush Mehrotra, Hans Moritsch, and Hans Zima: *Dynamic data distributions in Vienna fortran*. ICASE Report No. 93-92, December 1, 1993, 21 pages. To appear in the Proceedings of Supercomputing '93, November 1993, Portland, OR.

Vienna Fortran is a machine-independent language extension of Fortran, which is based upon the Single-Program-Multiple-Data (SPMD) paradigm and allows the user to write programs for distributed-memory systems using global addresses. The language features focus mainly on the issue of distributing data across virtual processor structures. In this paper, we discuss those features of Vienna Fortran that allow the data distributions of arrays to change dynamically, depending on runtime conditions. We discuss the relevant language features, outline their implementation and describe how they may be used in applications.

Debussche, A., T. Dubois, and R. Temam: *The nonlinear Galerkin method: A multi-scale method applied to the simulation of homogeneous turbulent flows*. ICASE Report No. 93-93, December 10, 1993, 87 pages. Submitted to Theoretical and Computational Fluid Dynamics (TCFD).

Using results of DNS in the case of two-dimensional homogeneous isotropic flows, we first analyze in detail the behavior of the small and large scales of Kolmogorov like flows at moderate Reynolds numbers. We derive several estimates on the time variations of the small eddies and the nonlinear interaction terms; those terms play the role of the Reynolds stress tensor in the case of LES. Since the time step of a numerical scheme is determined as a function of the energy-containing eddies of the flow, the variations of the small scales and of the nonlinear interaction terms over one iteration can become negligible by comparison with the accuracy of the computation. Based on this remark, we propose a multilevel scheme which treats differently the small and the large eddies. Using mathematical developments, we derive estimates of all the parameters involved in the algorithm, which then becomes a completely self-adaptive procedure. Finally, we perform realistic simulations of (Kolmogorov like) flows over several eddy-turnover times. The results are analyzed in detail and a parametric study of the nonlinear Galerkin method is performed.

Jameson, Leland: *On the differentiation matrix for Daubechies-based wavelets on an interval.* ICASE Report No. 93-94, December 9, 1993, 35 pages. Submitted to SIAM Journal on Scientific Computing.

The differentiation matrix for a Daubechies-based wavelet basis defined on an interval will be constructed. It will be shown that the differentiation matrix based on the currently available boundary constructions does not maintain the superconvergence encountered under periodic boundary conditions.

Jameson, Leland: *On the Daubechies-based wavelet differentiation matrix.* ICASE Report No. 93-95, December 9, 1993, 53 pages. To appear in Journal of Scientific Computing.

The differentiation matrix for a Daubechies-based wavelet basis will be constructed and 'superconvergence' will be proven. That is, it will be proven that under the assumption of periodic boundary conditions that the differentiation matrix is accurate of order $2M$, even though the approximation subspace can represent exactly only polynomials up to degree $M - 1$, where M is the number of vanishing moments of the associated wavelet. It will be illustrated that Daubechies-based wavelet methods are equivalent to finite difference methods with grid refinement in regions of the domain where small-scale structure is present.

Bryan, Kurt, Valdis Liepa, and Michael Vogelius: *Reconstruction of multiple cracks from experimental electrostatic boundary measurements.* ICASE Report No. 93-96, December 13, 1993, 28 pages. Submitted to Proceedings of the 1993 SIAM Annual Meeting, Philadelphia, PA, July 1993.

This paper describes an algorithm for recovering a collection of linear cracks in a homogeneous electrical conductor from boundary measurements of voltages induced by specified current fluxes. The technique is a variation of Newton's method and is based on taking weighted averages of the boundary data. We also describe an apparatus that was constructed specifically for generating laboratory data on which to test the algorithm. We apply the algorithm to a number of different test cases and discuss the results.

Leemis, Lawrence, and Kishor S. Trivedi: *A comparison of approximate interval estimators for the Bernoulli parameter.* ICASE Report No. 93-97, December 14, 1993, 16 pages. Submitted to the American Statistician.

The goal of this paper is to compare the accuracy of two approximate confidence interval estimators for the Bernoulli parameter p . The approximate confidence intervals are based on the normal and Poisson approximations to the binomial distribution. Charts are given to indicate which approximation is appropriate for certain sample sizes and point estimators.

Hu, Fang Q.: *The acoustic and instability waves of jets confined inside an acoustically lined rectangular duct*. ICASE Report No. 93-98, December 14, 1993, 31 pages. Submitted to the Journal of Sound and Vibration.

An analysis of linear wave modes associated with supersonic jets confined inside an acoustically lined rectangular duct is presented. Mathematical formulations are given for the vortex-sheet model and continuous mean flow model of the jet flow profiles. Detailed dispersion relations of these waves in a two-dimensional confined jet as well as an unconfined free jet are computed. Effects of the confining duct and the liners on the jet instability and acoustic waves are studied numerically. It is found that the effect of the liners is to attenuate waves that have supersonic phase velocities relative to the ambient flow. Numerical results also show that the growth rates of the instability waves could be reduced significantly by the use of liners. In addition, it is found that the upstream propagating neutral waves of an unconfined jet could become attenuated when the jet is confined.

Ponnusamy, Ravi, Joel Saltz, Alok Choudhury, Yuan-Shin Hwang, and Geoffrey Fox: *Runtime support and compilation methods for user-specified data distributions*. ICASE Report No. 93-99, December 15, 1993, 35 pages. To be submitted to IEEE Transactions on Parallel and Distributed Systems.

This paper describes two new ideas by which an HPF compiler can deal with irregular computations effectively. The first mechanism invokes a user specified mapping procedure via a set of compiler directives. The directives allow use of program arrays to describe graph connectivity, spatial location of array elements and computational load. The second mechanism is a simple conservative method that in many cases enables a compiler to recognize that it is possible to reuse previously computed information from inspectors (e.g. communication schedules, loop iteration partitions, information that associates off-processor data copies with on-processor buffer locations). We present performance results for these mechanisms from a Fortran 90D compiler implementation.

Mavriplis, C., and John Van Rosendale: *Triangular spectral elements for incompressible fluid flow*. ICASE Report No. 93-100, December 17, 1993, 18 pages. To appear in the Proceedings of the AIAA 11th CFD Conference, Orlando, FL, July 6-9, 1993.

In this paper we discuss the use of triangular elements in the spectral element method for direct simulation of incompressible flow. Triangles provide much greater geometric flexibility than quadrilateral elements and are better conditioned and more accurate when small angles arise. We employ a family of tensor product algorithms for triangles, allowing triangular elements to be handled with comparable arithmetic complexity to quadrilateral elements. The triangular discretizations are applied and validated on the Poisson equation. These discretizations are then applied to the incompressible Navier-Stokes equations and a laminar channel flow solution is given. These new triangular spectral elements can be combined with standard quadrilateral elements, yielding a general and flexible high order method for complex geometries in two dimensions. The natural generalization to tetrahedral elements in three dimensions will be described in a future work.

Bertolotti, Fabio: *Vortex generation and wave-vortex interaction over a concave plate with roughness*. ICASE Report No. 93-101, December 17, 1993, 42 pages. To be submitted to Theoretical and Computational Fluid Dynamics.

The generation and amplification of vortices by surface inhomogeneities, both in the form of surface waviness and of wall-normal velocity, is investigated using the nonlinear PSE equations. Transients and issues of algebraic growth are avoided through the use of a similarity solution as initial condition for the vortex.

In the absence of curvature, the vortex decays as $\sqrt{1/x}$ when flowing over streamwise aligned riblets of constant height, and grows as \sqrt{x} when flowing over a corresponding streamwise aligned variation of blowing/suction transpiration velocity. However, in the presence of wall inhomogeneities having both streamwise and spanwise periodicity, the growth of the vortex can be much larger. In the presence of curvature, the vortex develops into a Görtler vortex.

The “direct” and “indirect” interaction mechanisms possible in wave-vortex interaction are presented. The “direct” interaction does not lead to strong resonance with the flow conditions investigated. The “indirect” interaction leads to K-type transition.

Ristorcelli, J.R., J.L. Lumley, and R. Abid: *A rapid-pressure correlation representation consistent with the Taylor-Proudman theorem materially-frame-indifferent in the 2D limit*. ICASE Report No. 94-1, January 7, 1994, 51 pages. To be submitted to Journal of Fluid Mechanics.

A nonlinear representation for the rapid-pressure correlation appearing in the Reynolds stress equations, consistent with the Taylor-Proudman theorem, is presented. The representation insures that the modeled second-order equations are frame-invariant with respect to rotation when the flow is two-dimensional in planes perpendicular to the axis of rotation. The representation satisfies realizability in a new way: a special *ansatz* is used to obtain, analytically, the values of coefficients valid away from the realizability limit: the model coefficients are functions of the state of the turbulence that are valid for all states of the mechanical turbulence attaining their constant limiting values only when the limit state is achieved. Utilization of all the mathematical constraints are not enough to specify all the coefficients in the model. The unspecified coefficients appear as free parameters which are used to insure that the representation is asymptotically consistent with the known equilibrium states of a homogeneous sheared turbulence. This is done by insuring that the modeled evolution equations have the same fixed points as those obtained from computer and laboratory experiments for the homogeneous shear. Results of computations of the homogeneous shear, with and without rotation, and with stabilizing and destabilizing curvature, are shown. Results are consistently better, in a wide class of flows which the model not been calibrated, than those obtained with other nonlinear models.

Sun, Xian-He, and Jianping Zhu: *Shared virtual memory and generalized speedup*. ICASE Report No. 94-2, January 7, 1994, 23 pages. To appear in the Proceedings of the International Parallel Processing Symposium, 1994.

Generalized speedup is defined as parallel speed over sequential speed. In this paper the generalized speedup and its relation with other existing performance metrics, such as traditional speedup, efficiency, scalability, etc., are carefully studied. In terms of the introduced asymptotic speed, we show that the difference between the generalized speedup and the traditional speedup lies in the definition of the efficiency of uniprocessor processing, which is a very important issue in shared virtual memory machines. A scientific application has been implemented on a KSR-1 parallel computer. Experimental and theoretical results show that the generalized speedup is distinct from the traditional speedup and provides a more reasonable measurement. In the study of different speedups, various causes of superlinear speedup are also presented.

Greenberg, Albert G., Boris D. Lubachevsky, David M. Nicol, and Paul E. Wright: *Efficient massively parallel simulation of dynamic channel assignment schemes for wireless cellular communications*. ICASE Report No. 94-3, January 10, 1994, 14 pages. Submitted to the Workshop on Parallel and Distributed Simulation.

Fast, efficient parallel algorithms are presented for discrete event simulations of dynamic channel assignment schemes for wireless cellular communication networks. The driving events are call arrivals and departures, in continuous time, to cells geographically distributed across the service area. A dynamic channel assignment scheme decides which call arrivals to accept, and which channels to allocate to the accepted calls, attempting to minimize call blocking while ensuring co-channel interference is tolerably low. Specifically, the scheme ensures that the same channel is used concurrently at different cells only if the pairwise distances between those cells are sufficiently large. Much of the complexity of the system comes from ensuring this separation.

The network is modeled as a system of interacting continuous time automata, each corresponding to a cell. To simulate the model, we use conservative methods; i.e., methods in which no errors occur in the course of the simulation and so no rollback or relaxation is needed. Implemented on a 16K processor MasPar MP-1, an elegant and simple technique provides speedups of about 15x over an optimized serial simulation running on a high speed workstation. A drawback of this technique, typical of conservative methods, is that processor utilization is rather low. To overcome this, we developed new methods that exploit *slackness* in event dependencies over short intervals of time, thereby raising the utilization to above 50% and the speedup over the optimized serial code to about 120x.

Venkatkrishnan, V.: *Parallel implicit unstructured grid Euler solvers*. ICASE Report No. 94-4, January 10, 1994, 20 pages. Submitted to AIAA Journal.

A mesh-vertex finite volume scheme for solving the Euler equations on triangular unstructured meshes is implemented on an MIMD (multiple instruction/multiple data stream) parallel computer.

An explicit four-stage Runge-Kutta scheme is used to solve two-dimensional flow problems. A family of implicit schemes is also developed to solve these problems, where the linear system that arises at each time step is solved by a preconditioned GMRES algorithm. Two partitioning strategies are employed, one that partitions triangles and the other that partitions vertices. The choice of the preconditioner in a distributed memory setting is discussed. All the methods are compared both in terms of elapsed times and convergence rates. It is shown that the implicit schemes offer adequate parallelism at the expense of minimal sequential overhead. The use of a global coarse grid to further minimize this overhead is also investigated. The schemes are implemented on a distributed memory parallel computer, the iPSC/860.

Venkatakrisnan, V., and D. J. Mavriplis: *Agglomeration multigrid for the three-dimensional Euler equations*. ICASE Report No. 94-5, January 10, 1994, 28 pages. Submitted to AIAA Journal.

A multigrid procedure that makes use of coarse grids generated by the agglomeration of control volumes is advocated as a practical approach for solving the three-dimensional Euler equations on unstructured grids about complex configurations. It is shown that the agglomeration procedure can be tailored to achieve certain coarse grid properties such as the sizes of the coarse grids and aspect ratios of the coarse grid cells. The agglomeration is done as a preprocessing step and runs in linear time. The implications for multigrid of using arbitrary polyhedral coarse grids are discussed. The agglomeration multigrid technique compares very favorably with existing multigrid procedures both in terms of convergence rates and elapsed times. The main advantage of the present approach is the ease with which coarse grids of any desired degree of coarseness may be generated in three dimensions, without being constrained by considerations of geometry. Inviscid flows over a variety of complex configurations are computed using the agglomeration multigrid strategy.

Banks, David C.: *Illumination in diverse codimensions*. ICASE Report No. 94-6, January 14, 1994, 22 pages. Submitted to ACM Siggraph '94.

This paper derives a model of diffuse and specular illumination in arbitrarily large dimensions, based on a few characteristics of material and light in 3-space. It then describes how to adjust for the anomaly of excess brightness in large codimensions. If a surface is grooved or furry, it can be illuminated with a hybrid model that incorporates both the 1D geometry (the grooves or fur) and the 2D geometry (the surface).

Chen, David T., Andrei State, and David Banks: *Interactive shape metamorphosis*. ICASE Report No. 94-7, January 14, 1994, 9 pages. Submitted to July Meeting of Siggraph '94.

We describe a technique for controlled metamorphosis between surfaces in 3-space. We apply well-understood techniques to produce shape metamorphosis between models in a 2D parametric space. The user selects morphable features interactively, and the morphing process executes in real time on a high-performance graphics multicomputer.

Borggaard, Jeff, and John Burns: *A sensitivity equation approach to shape optimization in fluid flows*. ICASE Report No. 94-8, January 21, 1994, 34 pages. To appear in the IMA Workshop on Flow Control, Springer, 1993.

In this paper we apply a sensitivity equation method to shape optimization problems. An algorithm is developed and tested on a problem of designing optimal forebody simulators for a 2D, inviscid supersonic flow. The algorithm uses a BFGS/Trust Region optimization scheme with sensitivities computed by numerically approximating the linear partial differential equations that determine the flow sensitivities. Numerical examples are presented to illustrate the method.

Jameson, Leland: *On the wavelet optimized finite difference method*. ICASE Report No. 94-9, March 8, 1994, 47 pages. Submitted to Journal of Computational Physics.

When one considers the effect in the physical space, Daubechies-based wavelet methods are equivalent to finite difference methods with grid refinement in regions of the domain where small scale structure exists. Adding a wavelet basis function at a given scale and location where one has a correspondingly large wavelet coefficient is, essentially, equivalent to adding a grid point, or two, at the same location and at a grid density which corresponds to the wavelet scale. This paper introduces a wavelet-optimized finite difference method which is equivalent to a wavelet method in its multiresolution approach but which does not suffer from difficulties with nonlinear terms and boundary conditions, since all calculations are done in the physical space. With this method one can obtain an arbitrarily good approximation to a conservative difference method for solving nonlinear conservation laws.

Speziale, Charles G., and Thomas B. Gatski: *An alternative assessment of second-order closure models in turbulent shear flows*. ICASE Report No. 94-10, March 9, 1994, 20 pages. Submitted to AIAA Journal.

The performance of three recently proposed second-order closure models is tested in benchmark turbulent shear flows. Both homogeneous shear flow and the log-layer of an equilibrium turbulent boundary layer are considered for this purpose. An objective analysis of the results leads to an assessment of these models that stands in contrast to that recently published by other authors. A variety of pitfalls in the formulation and testing of second-order closure models are uncovered by this analysis.

Singer, Bart A., and David C. Banks: *A predictor-corrector scheme for vortex identification*. ICASE Report No. 94-11, March 9, 1994, 20 pages. Submitted to Physics of Fluids.

A new algorithm for identifying and characterizing vortices in complex flows is presented. The scheme uses both the vorticity and pressure fields. A skeleton line along the center of a vortex is produced by a two-step predictor-corrector scheme. The technique uses the vector field to move

in the direction of the skeleton line and the scalar field to correct the location in the plane perpendicular to the skeleton line. A general vortex cross section can be concisely defined with five parameters at each point along the skeleton line. The details of the method and examples of its use are discussed

Ciardo, Gianfranco, Lawrence M. Leemis, and David Nicol: *On the minimum of independent geometrically distributed random variables*. ICASE Report No. 94-12, March 10, 1994, 17 pages. To appear in *Statistics and Probability Letters*.

The expectations $E[X_{(1)}]$, $E[Z_{(1)}]$, and $E[Y_{(1)}]$ of the minimum of n independent geometric, modified geometric, or exponential random variables with matching expectations differ. We show how this is accounted for by stochastic variability and how $E[X_{(1)}]/E[Y_{(1)}]$ equals the expected number of ties at the minimum for the geometric random variables. We then introduce the “shifted geometric distribution”, and show that there is a unique value of the shift for which the individual shifted geometric and exponential random variables match expectations both individually and in their minimums.

Harari, Isaac, and Eli Turkel: *Accurate finite difference methods for time-harmonic wave propagation*. ICASE Report No. 94-13, March 18, 1994, 40 pages. Submitted to *Journal of Computational Physics*.

Finite difference methods for solving problems of time-harmonic acoustics are developed and analyzed. Multi-dimensional inhomogeneous problems with variable, possibly discontinuous, coefficients are considered, accounting for the effects of employing non-uniform grids. A weighted-average representation is less sensitive to transition in wave resolution (due to variable wave numbers or non-uniform grids) than the standard pointwise representation. Further enhancement in method performance is obtained by basing the stencils on generalizations of Padé approximation, or generalized definitions of the derivative, reducing spurious dispersion, anisotropy and reflection, and by improving the representation of source terms. The resulting schemes have fourth-order accurate local truncation error on uniform grids and third order in the non-uniform case. Guidelines for discretization pertaining to grid orientation and resolution are presented.

Ta'asan, Shlomo: *Canonical-variables multigrid method for steady-state Euler equations*. ICASE Report No. 94-14, March 18, 1994, 13 pages. Submitted to *Proceedings of the 14th International Conference on Multigrid Methods in Fluid Dynamics*, Bangalore, India, July 1994.

In this paper we describe a novel approach for the solution of inviscid flow problems for subsonic compressible flows. The approach is based on canonical forms of the equations, in which subsystems governed by hyperbolic operators are separated from those governed by elliptic ones. The discretizations used as well as the iterative techniques for the different subsystems, are inherently different. Hyperbolic parts, which describe, in general, propagation phenomena, are discretized

using upwind schemes and are solved by marching techniques. Elliptic parts, which are directionally unbiased, are discretized using *h-elliptic* central discretizations, and are solved by pointwise relaxations together with coarse grid acceleration. The resulting discretization schemes introduce artificial viscosity only for the hyperbolic parts of the system; thus a smaller total artificial viscosity is used, while the multigrid solvers used are much more efficient. Solutions of the subsonic compressible Euler equations are achieved at the same efficiency as the full potential equation.

Hu, Fang Q.: *A spectral boundary integral equation method for the 2-D Helmholtz equation*. ICASE Report No. 94-15, March 21, 1994, 25 pages. To be submitted to Journal of Computational Physics.

In this paper, we present a new numerical formulation of solving the Boundary Integral Equations reformulated from the Helmholtz equation. The boundaries of the problems are assumed to be smooth closed contours. The solution on the boundary is treated as a periodic function, which is in turn approximated by a truncated Fourier series. A Fourier collocation method is followed in which the boundary integral equation is transformed into a system of algebraic equations. It is shown that in order to achieve spectral accuracy for the numerical formulation, the non-smoothness of the integral kernels, associated with the Helmholtz equation, must be carefully removed. The emphasis of the paper is on investigating the essential elements of removing the nonsmoothness of the integral kernels in the spectral implementation. The present method is robust for a general boundary contour. Aspects of efficient implementation of the method using FFT are also discussed. A numerical example of wave scattering is given in which the exponential accuracy of the present numerical method is demonstrated.

Gunzburger, Max D. and L. Steven Hou: *Finite dimensional approximation of a class of constrained nonlinear optimal control*. ICASE Report No. 94-16, March 28, 1994, 48 pages. Submitted to SIAM Review.

An abstract framework for the analysis and approximation of a class of nonlinear optimal control and optimization problems is constructed. Nonlinearities occur in both the objective functional and in the constraints. The framework includes an abstract nonlinear optimization problem posed on infinite dimensional spaces, an approximate problem posed on finite dimensional spaces, together with a number of hypotheses concerning the two problems. The framework is used to show that optimal solutions exist, to show that Lagrange multipliers may be used to enforce the constraints, to derive an optimality system from which optimal states and controls may be deduced, and to derive existence results and error estimates for solutions of the approximate problem. The abstract framework and the results derived from that framework are then applied to three concrete control or optimization problems and their approximation by finite element methods. The first involves the von Kármán plate equations of nonlinear elasticity, the second the Ginzburg-Landau equations of superconductivity, and the third the Navier-Stokes equations for incompressible, viscous flows.

Speziale, C.G., R. Abid, and N.N. Mansour: *Evaluation of Reynolds stress turbulence closures in compressible homogeneous shear flow*. ICASE Report No. 94-17, March 31, 1994, 30 pages. To appear in ZAMP.

Direct numerical simulation data bases for compressible homogeneous shear flow are used to evaluate the performance of recently proposed Reynolds stress closures for compressible turbulence. Three independent pressure-strain models are considered along with a variety of explicit compressible corrections that account for dilatational dissipation and pressure-dilatation effects. The ability of the models to predict both time evolving fields and equilibrium states is systematically tested. Consistent with earlier studies, it is found that the addition of simple dilatational models allows for the prediction of the reduced growth rate of turbulent kinetic energy in compressible homogeneous shear flow. However, a closer examination of the equilibrium structural parameters uncovers a major problem. None of the models are able to predict the dramatic increase in the normal Reynolds stress anisotropies or the significant decrease in the Reynolds shear stress anisotropy that arise from compressible effects. The physical origin of this deficiency is attributed to the neglect of compressible terms in the modeling of the deviatoric part of the pressure-strain correlation.

Chapman, Barbara, Piyush Mehrotra, John Van Rosendale, and Hans Zima: *A software architecture for multidisciplinary applications: integrating task and data parallelism*. ICASE Report No. 94-18, March 30, 1994, 25 pages. Submitted to CONPAR '94 - International Conference on Parallel Processing '94.

Data parallel languages such as Vienna Fortran and HPF can be successfully applied to a wide range of numerical applications. However, many advanced scientific and engineering applications are of a multidisciplinary and heterogeneous nature and thus do not fit well into the data parallel paradigm. In this paper we present new Fortran 90 language extensions to fill this gap. Tasks can be spawned as asynchronous activities in a homogeneous or heterogeneous computing environment; they interact by sharing access to Shared Data Abstractions (SDAs). SDAs are an extension of Fortran 90 modules, representing a pool of common data, together with a set of methods for controlled access to these data and a mechanism for providing persistent storage. Our language supports the integration of data and task parallelism as well as nested task parallelism and thus can be used to express multidisciplinary applications in a natural and efficient way.

Otto, S.R., and James P. Denier: *The effect of crossflow on Görtler vortices*. ICASE Report No. 94-19, March 29, 1994, 30 pages. Submitted to the Journal of Fluid Mechanics.

It is well known that the boundary layer flow over a surface with a region of concave curvature is susceptible to centrifugal instabilities in the form of Görtler vortices. In the limit of large Görtler number (a parameter which is a measure of the curvature of the surface) the effect of a crossflow component in the underlying basic flow has been shown to stabilise these modes and thus render the Görtler vortex mechanism inoperable in these situations. Here we consider the effect of crossflow when the Görtler number (and the scaled spanwise wavenumber of the vortex) are both order one

quantities. The parabolic partial differential equations governing the linear evolution of a Görtler vortex in a three-dimensional boundary layer are solved numerically. Our results suggest that, at least for small magnitude crossflows, the Görtler vortex instability mechanism is still operable. In addition we consider the effect of an applied pressure gradient within the boundary layer on the instability mechanism and demonstrate that a favourable pressure gradient renders the boundary layer more susceptible to the Görtler vortex instability; this is in stark contrast to the case of Tollmien-Schlichting waves where a favourable pressure gradient stabilises the flow.

Burns, John A. and Belinda B. King: *A note on the regularity of solutions of infinite dimensional Riccati equations*. ICASE Report No. 94-20, March 30, 1994, 18 pages. Submitted to Applied Math Letters.

This note is concerned with the regularity of solutions of algebraic Riccati equations arising from infinite dimensional LQR and LQG control problems. We show that distributed parameter systems described by certain parabolic partial differential equations often have a special structure that smoothes solutions of the corresponding Riccati equation. This analysis is motivated by the need to find specific representations for Riccati operators that can be used in the development of computational schemes for problems where the input and output operators are not Hilbert-Schmidt. This situation occurs in many boundary control problems and in certain distributed control problems associated with optimal sensor/actuator placement.

ICASE COLLOQUIA

October 1, 1993 - March 31, 1994

Name/Affiliation/Title	Date
K. R. Rajagopal, University of Pittsburgh "Boundary Layers in Non-Linear Materials"	October 5
Max D. Gunzburger, Virginia Polytechnic Institute and State University "Computations and Analyses of Flow Control and Optimization Problems"	October 7 & 8
Natalia Alexandrov, Rice University "Multilevel Algorithms for Nonlinear Equations and Equality Constrained Optimization"	October 19
Don Delisi, Northwest Research Associates "Some New Experimental Results on Vortex Decay"	October 27
Michael S. Howe, Boston University "Interaction of Flexural Waves with Open and Closed Cracks, Joints and Ribs, and with Bias Flow Perforations"	October 28
James Martin, Christopher Newport University "Three-Dimensional Flow Structures in Swirling and Nonswirling Jets"	November 2
Geoffrey Lilley, University of Southampton, United Kingdom, "Fundamentals of Aerodynamic Noise"	November 2, 9, & 15
Christian H. Bischof, Argonne National Laboratory "Opportunities for Parallelism in Derivative Computations"	November 4
Ian Foster, Argonne National Laboratory "Fortran M: A Language for Modular Parallel Programming"	November 4
Stephen R. Wheat, Sandia National Laboratories "SUNMOS - Sandia University of New Mexico Operating System"	November 5
David Womble, Sandia National Laboratories "Implementing LU Factorization on Massively Parallel Machines"	November 5

Name/Affiliation/Title	Date
Douglas A. Feikema, Propulsion Research Center “Degenerate Four Wave Mixing Combustion Diagnostics for Turbulent Reactive Flow”	November 5
Andrew Grimshaw, University of Virginia “From Mentat to Legion: The Evolution of a High-Performance Parallel Processing System”	November 8
Roy Nicolaides, Carnegie-Mellon University “Computational Challenges in Non-Convex Optimization for Smart Materials”	November 9
Russell Taylor, University of North Carolina “Visualization via Virtual Reality”	November 12
Julian D. Cole, Rensselaer Polytechnic Institute “Hodograph Design of Lifting Airfoils with High Critical Mach Numbers”	November 15
Robert V. Wilson, Old Dominion University “Numerical Simulation of Two-Dimension Spatially Developing Mixing Layers”	November 18
Abdou Youssef, The George Washington University “Randomized Routing on Benes-Clos Networks”	December 2
Michael A. Palis, New Jersey Institute of Technology “Grain-Size Optimization and Scheduling for Message-Passing Architectures”	December 17
Wei Cai, University of North Carolina at Charlotte “Wavelet Collocation Methods for Initial Value Boundary Problems”	January 4
Jamal A. Masad, High Technology Corporation “A Method for Direct Computation of Boundary-Layer Stability Characteristics”	January 12
Ulrich Neumann, University of North Carolina, Chapel Hill “Parallel Volume Renderer Design”	February 4

Name/Affiliation/Title	Date
Pearl Y. Wang, George Mason University “PEC: A Scalable Network for Massively Parallel Systems”	February 14
Oleg S. Ryzhov, Rensselaer Polytechnic Institute “Stability of Transonic Boundary Layers”	February 17
Yihong Cai, The Florida State University “Iterative Domain Decomposition Algorithms: Theory and Applications”	February 18
Eyal Arian, The Weizmann Institute of Science “The Multigrid One Shot Method for Optimal Shape Problems”	February 23
David P. Young, “Boeing Commercial Airplane Company & Boeing Computer Services “Issues in Design Optimization Methodology”	February 24
Victor Milenkovic, Harvard University “Placement and Compaction of Nonconvex Polygons for Clothing Manufacture”	February 25
Nathaniel Whitaker, University of Massachusetts “Computations of Statistical Equilibrium Solutions of the Euler Equations”	February 28
Kelly Black, North Carolina State University “A Petrov-Galerkin Spectral Element Technique for Heterogeneous Porous Media”	March 4
Vijay Shukla, Columbia University “A Study of Asymmetry and Variability in Convectively Driven Flows”	March 21
Muhammad R. Hajj, Virginia Polytechnic Institute and State University “Nonlinear and Parametric Mode Interactions in Transitioning Shear Flows”	March 22
Jiro Nakamichi, National Aerospace Laboratory, Japan “Aeroelastic Characteristics of a Tailored Forward Swept Wing”	March 24

Name/Affiliation/Title	Date
Michael Navon, The Florida State University "Variational Data Assimilation Experiments with Variable Resolution Finite-Element Shallow-Water Equations Model"	March 25
George S. Dulikravich, The Pennsylvania State University "Inverse Problems in Engineering"	March 28
Philip Hall, University of Manchester, United Kingdom "Phase Equations: A New Approach to Strongly Nonlinear Shear Flow Instabilities"	March 29

OTHER ACTIVITIES

On March 14-18, 1994, ICASE and NASA LaRC co-sponsored a Short Course on Turbulent Flow Modeling and Prediction at the OMNI Hotel in Newport News, VA. The objective of this course was to provide the scientists and engineers with the necessary understanding of turbulence physics, modeling and predictive methodologies including direct numerical simulation (DNS) and large eddy simulation (LES). There were 81 attendees and a formal proceedings will be published.

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