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April 1, 2000 through September 30, 2000

ICASE
NASA Langley Research Center
Hampton, Virginia

Operated by Universities Space Research Association

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INTRODUCTION

ICASE* is operated at the Langley Research Center (LaRC) of NASA by the Universities Space Research Association (USRA) under a contract with the Center. USRA is a nonprofit consortium of major U.S. colleges and universities.

The Institute conducts unclassified basic research in applied mathematics, numerical analysis and algorithm development, computer science, fluid mechanics, and structures and materials 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 its permanent staff and 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 multidisciplinary design optimization;
- Applied computer science: system software, systems engineering, and parallel algorithms;
- Theoretical, computational, and experimental research in fluid mechanics in selected areas of interest to LaRC, such as transition, turbulence, flow control, and acoustics; and
- Theoretical, computational, and experimental research in structures and material sciences with emphasis on smart materials and nanotechnologies.

ICASE reports are primarily considered to be preprints of manuscripts that have been submitted to appropriate research journals or that are to appear in conference proceedings. A list of these reports for the period April 1, 2000 through September 30, 2000 is given in the Reports and Abstracts section, which follows a brief description of the research in progress.

RESEARCH IN PROGRESS

APPLIED AND NUMERICAL MATHEMATICS

Active flow control research tool development
Brian G. Allan

The use of secondary flow control devices on inlets, such as vortex generators and small synthetic jets, has recently attracted interest. Significant improvements in engine flow distortion and pressure loss have been demonstrated using these small flow control devices. This technology has shown a great potential for improving existing inlet configurations and enabling more advanced inlet designs, allowing for reduced inlet lengths and sharper turning angles. In order to take advantage of these devices, computational tools need to be developed in order to evaluate potential engine inlet designs. The goal of this research is to develop computational boundary conditions and techniques for a CFD code, in order to model vortex generators and synthetic jets for an inlet application.

Using a compressible Navier-Stokes code, developed at NASA, numerical simulations of micro-vortex generators and synthetic jets on a flat plate and inlet duct flows, will be performed. These simulations are to be performed in conjunction with wind tunnel experiments conducted at NASA Langley Research Center. From these simulations and experiments, a better understanding of the flow physics of the flow control devices will be gained. Using these insights into the flow physics of the control devices, a computational boundary condition can then be developed. This boundary condition will capture the general behavior of the flow control devices without having to simulate them directly. This will result in a reduced computational cost by eliminating the need to include fine grids for the vortex generators and synthetic jets. By reducing the computational cost, the inlet design cycle time can also be significantly reduced. High resolution calculations of the flow about micro-vortex generator fins and jets on a flat plate, have been performed using a Reynolds averaged Navier-Stokes code.

Future work will include a comparison of the numerical results to experimental data for a better understanding of the flow physics of these devices. Once an understanding of the flow physics is known, the development of computational boundary conditions, which model the flow control devices, can be performed.

This work was done in collaboration with Pieter Buning (NASA Langley).

Anisotropic mesh adaption
Carlo L. Bottasso

Many problems in fluid and solid mechanics present solution features that are inherently directional. For example shock waves are characterized by gradients that are very high in one local direction, while substantially smaller in the other two. Similarly, a vortex shed by the tip of a wing presents gradients in the radial direction that are much higher than in the direction of its core. In all these cases, anisotropic meshes are highly desirable for their evident economic advantages.

We are developing a methodology for introducing regions of high anisotropy in existing isotropic unstructured grids in complex, curved, three-dimensional domains. The new procedures can be used for refining solution features internal to the computational domain (e.g., shock waves) or in the proximity of its boundaries (e.g., boundary layers). In both cases, suitable voids are created in the existing grid in the regions of localization using a mesh motion algorithm that solves a fictitious elasticity problem. The voids are then filled with stacks of prisms that are subsequently tetrahedronized to yield a simplicial mesh. The mesh

motion algorithm allows dealing in a simple and effective manner with the problem of self-intersection of elements in concave regions of the model boundaries and in the case of closely spaced model faces, avoiding the need for cross-over checks and complex grid correction procedures.

The capabilities and performance of the new methodology are being tested with the help of practical examples involving the growth of boundary layers and the refinement of shock waves.

Discontinuous dual-primal mixed finite elements
Carlo L. Bottasso

Discontinuous Galerkin methods are the subject of active research for the solution of partial differential equations in a number of problems in mathematical physics. Great insight on the characteristics of such methods can be gained from the study of model problems, for example the Laplacian.

We have developed a novel discontinuous mixed finite-element formulation for the solution of second-order elliptic problems. Fully discontinuous piecewise polynomial finite-element spaces are used for the trial and test functions. The discontinuous nature of the test functions at the element interfaces allows the introduction of new boundary unknowns that, on the one hand enforce the weak continuity of the trial functions, and on the other avoid the need to define a priori algorithmic fluxes as in standard discontinuous Galerkin methods. Static condensation is performed at the element level, leading to a solution procedure based on the sole interface unknowns. In the one-dimensional case, we can show the equivalence of the method with implicit Runge-Kutta schemes of the collocation type exhibiting optimal behavior. This clearly provides a strong incentive towards the generalization to multiple space dimensions. Numerical experiments in one and two dimensions demonstrate the order accuracy of the new method, confirming the results of the analysis.

Future efforts will concentrate on the extension of these ideas to other model problems, and on comparisons of this class of methods with alternative, well established solution procedures.

This work is done in collaboration with S. Micheletti and R. Sacco (Politecnico di Milano).

Geometric integration theory for multibody dynamics
Carlo L. Bottasso

The partial differential equations governing the dynamics of nonlinear multibody systems composed of beams, shells and rigid bodies are known to present a rich mathematical structure. In particular, the resulting models are Hamiltonian systems characterized by a symplectic nature and associated with conservation laws that stem from symmetries of the Hamiltonian. The linear and angular momentum as well as the total mechanical energy are conserved for free motions of such systems. Classical integration methods rarely preserve the underlying structure of the problem being solved, and hence, such structure is lost in the numerical solution.

We have developed a novel integration scheme for the nonlinear dynamics of geometrically exact shells based on the inextensible director assumption. This method extends previous work done on the dynamics of rigid bodies, geometrically exact beams and flexible multibody systems. The new algorithm is designed so as to imply the strict decay of the system total mechanical energy at each time step, and consequently unconditional stability is achieved in the fully nonlinear regime. Furthermore, the scheme features tunable high frequency numerical damping and it is, therefore, stiffly accurate. The method was implemented in a general-purpose multibody code. Numerical test examples have been solved for verifying the characteristics of the new method.

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Future efforts will concentrate on the use of the code for solving more complex problems, in particular for the modeling of helicopters and tiltrotors.

This work is done in collaboration with O.A. Bauchau (Georgia Institute of Technology).

Textbook multigrid efficiency for CFD applications
Boris Diskin

State-of-the-art multigrid methodologies for large-scale compressible flow applications use a block-matrix relaxation and/or a pseudo-time-dependent approach to solve the equations; significant improvements have been demonstrated using multigrid approaches, but the methods are not optimally convergent. The Reynolds-averaged Navier-Stokes (RANS) equation sets are systems of coupled nonlinear equations which are not, even for subsonic Mach numbers, fully elliptic, but contain hyperbolic partitions. There is a potential gain of several orders of magnitude in operation count reduction if the textbook multigrid efficiency (TME) could be attained for the RANS equations. The objective of the research is to develop TME methods for large-scale CFD applications.

The method proposed for achieving TME is the distributed relaxation approach of Brandt which decomposes the system of equations into separable, usually scalar, factors that can be treated with optimal methods. The distributed relaxation is applied in regular (smoothly varying) flow regions. Near boundaries and discontinuities, the general approach is to relax the governing equations directly in terms of primitive variables. Several sweeps of robust (but possibly slowly converging) relaxation, such as Newton-Kacmarcz relaxation, can be made in these regions. The additional sweeps will not affect the overall complexity because the number of boundary and/or discontinuity points is usually negligible in comparison with the number of interior points. Recently, TME has been demonstrated for viscous compressible flow applications and for high-Reynolds-number incompressible viscous flow. The main accomplishment of this half-year period is the formulation of the general framework expected to be required for achieving TME for large-scale compressible flow applications. This framework was tested by solving the quasi-one-dimensional Euler equations.

Currently efforts are directed to extension of the proposed TME methodology to different (subsonic, transonic, and supersonic; compressible and incompressible; free, wake, boundary-layer, stagnation, lifting, etc.) flow regimes on different structured (staggered and non-staggered; Cartesian and body-fitted) grids for different (conservative and non-conservative; low and high order) discretizations of Navier-Stokes equations.

The research in these directions is conducted in collaboration with with J.L. Thomas (NASA Langley) and A. Brandt (The Weizmann Institute of Science).

Materials science: Optimization of chemical vapor infiltration with simultaneous powder formation
Adi Ditkowski

A variety of materials are produced by infiltration processes. In these techniques a fluid phase (i.e., a gas or a liquid) is transported into a porous structure, where it then reacts to form a solid product. These methods are particularly important for producing composite materials, where the initial porous perform is composed of the reinforcement phase (i.e., fibers, whiskers, or particles) and infiltration produces the matrix. A detailed assessment of the relevant reaction and mass transport rates during infiltration requires mathematical modeling, using a minimum of two coupled partial differential equations which describe changes in the reactant concentration and the solid structure as a function of both position and time. A key difficulty in chemical vapor infiltration (CVI) is the long processing times that are typically required. With this in

mind, it is important to minimize infiltration times. The goal of the research is to find the optimal conditions (i.e., pressure and temperature) to run this process.

This study specifically considers optimization for a set of two equations which describe isothermal, isobaric CVI. This work was divided into the following stages. (1) A set of PDEs which model the process was derived. (2) An analytic analysis was made on this model to determine its proper ties. (3) Asymptotic solutions were found and an optimization procedure was established on these asymptotic solutions. These results are an estimate of the optimal conditions. (4) Two numerical methods were used to verify the asymptotic results and to study their limits. (5) The numerical optimization procedure was developed and used for this problem. Our work presents a framework for treating the problem of determining the optimal pressure and temperature which corresponds to the minimum infiltration time.

In the future the methodology developed here will be used to find the optimal operation condition for other CVI processes as well as other problems in materials science, such as silicone oxidation and trench-filling.

This work was done in collaboration with David Gottlieb and Brian W. Sheldon.

On error bounds of finite difference approximations to partial differential equations — temporal behavior and rate of convergence
Adi Ditkowski

The question of the role of numerically imposed boundary conditions in the solution of parabolic and hyperbolic PDE's has been with us for many years. Many investigators have studied the effect of boundary conditions on the stability of the overall scheme, (i.e., the 'inner algorithm' + boundary conditions). In this context stability implies convergence of the scheme, at a fixed time t, as the mesh is refined. The question of the temporal behavior of the error was usually not considered. When constructing higher order schemes, third-order accuracy and above, it turns out that it is difficult to state boundary conditions such that the overall scheme remains stable. The question then arises: What happens to the overall accuracy of the numerical solution if the order of accuracy of the inner stencil, (m), is higher than the order of the boundary conditions, $(m - s)$. This problem has been tackled by Gustafsson in his papers from 1975 and 1981. His main result, for both parabolic and hyperbolic PDE's, is that if the accuracy of the extra boundary conditions, required for 'numerical closure' of the problem, are one less than that of the inner scheme, then the overall accuracy is not affected. The physical boundary conditions, however, must be approximated to the same order as the inner scheme. The goal of this work was to derive error bounds which are *functions of grid space and time.*

In this work we had considered a form of differentiation matrices, both hyperbolic and parabolic, which represent a fairly wide family of boundary condition formulations plus central inner schemes. We investigate the dependence of the error on time as well as on mesh size. The main results are as follows:

- In the parabolic case, the overall convergence rate is of order m if $s = 0, 1$, and $m - s + 3/2$ if $s \geq 2$. The error is uniformly bounded independent of t for all t, $t \geq 0$.
- In the hyperbolic case, the overall convergence rate is of order of $\min(m, m - s + 1)$ for all s, in agreement with the results given by Gustafsson. For $s = 0, 1$, the temporal bound of the error behaves as $\sqrt{t}$ for $t \ll 1$, and bends over smoothly to a linear bound as t increases. For $s \geq 2$, the temporal behavior is $\sim \sqrt{t}$ for all t, $t \geq 0$.

The parabolic and hyperbolic results for the case $s \geq 2$ were found by using standard energy methods. In order to derive the hyperbolic results for the case $s = 1$, however, a new method had to be developed. The

approach we took here is to define a new problem, which is somewhat similar to the original one and to show that the solution of this auxiliary problem bounds the error of the original problem.

In the near future we would like to refine the bounds, derive error bound for different numerical schemes and to use the new approach to other applications such as stability analysis of flows.

This work was done in collaboration with Saul Abarbanel and Bertil Gustafsson.

High order finite element methods for electromagnetics
D. Gottlieb, J.S. Hesthaven, and T. Warburton

It is becoming increasingly apparent that there is a need in the electromagnetics community for improved numerical methods for simulation of electromagnetic wave propagation in complex media. With this in mind, we are proposing the use of high order methods that can be used on unstructured grids. This enables the use of standard finite element meshes for complex geometries with the additional feature that field profiles can be accurately and efficiently propagated through the domain without the phase errors typically seen with lower order methods.

We have created a two-dimensional code that uses triangular elements which are up to 13th order in space and fourth order in time accurate. We have tested this against standard test cases and have shown exponential accuracy. For a specific case we see that increasing the order of the element decreases the error in the calculated radar cross section (RCS) by a factor of ten. Additionally, we have shown theoretically that this kind of convergence will be expected whenever the solution we are trying to represent is smooth enough. We are currently collaborating with Sherwin (Imperial College) and Morgan (University of Swansea) to compare the efficiency of this code against an optimized finite volume code.

We have also created a three-dimensional code that uses tetrahedral elements which are up to tenth order in space and fourth order accurate in time. We have spent the summer interfacing this code with an industrial mesh generator (Gambit from Fluent). We have also verified this code against results from Hypercomp Inc. and have shown reasonable agreement with bistatic RCS data for scattering from a zero-thickness business card geometry. Additionally, we have been computing results for geometries (from the EMCC test case database) suggested by the Electromagnetics Research Branch at NASA Langley, under the supervision of Truong Nguyen and Fred Beck (now retired). We have compared results from the 3D code with results from an axisymmetric multi-domain code of Hesthaven for scattering from a geometry constructed as the union of a cone and a hemisphere. They have shown good agreement for incident fields at certain angles, however this test case has indicated that further work is required to understand and account for the singularities in fields caused by the sharp point of the cone.

We intend to continue optimizing the three-dimensional code as well as calculating results for the cone-sphere scattering problem and for the cavity penetration problems suggested by Truong Nguyen, Fred Beck and M.C. Bailey from the Electromagnetics Research Branch. These geometries have proved to be extremely interesting in the way that they stretch certain features of these time-domain methods. These difficulties are certainly not unique to our method but pose problems for almost all numerical methods used to solve the time-domain Maxwell's equations. We also intend to investigate mixed implicit/explicit time integration to treat the thinly coated cone-sphere problem that was proposed by the Electromagnetics Research Branch.

Robust optimization including model uncertainties and reliability constraints
Luc Huyse

Current formal aerodynamic optimization procedures assume that airfoil performance is perfectly predicted by CFD analysis and that all operating conditions (e.g., cruise Mach number) are fixed. During the

early stages of the design process many parameters are merely estimates of desired operating conditions. Single point designs using these uncertain parameters can lead to overly optimistic projections of as-built performance. Such assumptions can lead to designs with poor performance at off-design conditions. This research will develop new optimization methods that anticipate parameter uncertainty.

A theoretical framework for robust (or stochastic) optimization has been developed and its superiority over existing multi-point optimization techniques has been demonstrated through analytic examples. Based on a second-order expansion of a mean-value analysis, substantial computational savings can also be achieved when only moderate levels of uncertainty exist for some of the variables or parameters in the mathematical model.

The newly developed techniques were applied to an airfoil optimization problem, using the FUN2D code. The minimization of the drag in cruise regime while maintaining a constant lift is chosen as the objective function. Only the Mach number is assumed to be uncertain in this preliminary analysis. The performance of the resulting robust design is considerably better than the expected value of the performance of an optimal design, obtained at selected deterministic or fixed operating conditions. Currently, we are combining the FUN2D code with the iSight optimization framework so that constrained optimization with a more realistic set of design variables can be studied. The ultimate goal is to develop general-purpose robust optimization methods for use in multidisciplinary design.

This work was conducted in collaboration with Sharon Padula (NASA Langley).

Active shielding and control of environmental noise
Josip Lončarić, Victor S. Ryaben'kii, and Semyon V. Tsynkov

Rejection of exterior noise caused by periodic sources such as propellers or turbines would significantly enhance passenger comfort and reduce noise fatigue on long flights. Passive sound absorbing materials help at high frequencies, but to be effective below about 1 kHz their weight penalty becomes significant. Active noise control can reduce low frequency noise with less weight penalty. We present the mathematical foundations of a new active technique for control of the time-harmonic acoustic disturbances.

Unlike many existing methodologies, the new approach provides for the exact volumetric cancellation of the unwanted noise in a given predetermined region of space while leaving those components of the total sound field deemed as friendly unaltered in the same region. Besides, the analysis allows us to conclude that to eliminate the unwanted component of the acoustic field in a given area, one needs to know relatively little; in particular, neither the locations nor the structure of the external noise sources need to be known. We constructed the general solution for the aforementioned noise control problem. The apparatus used for deriving the general solution is closely connected to the concepts of generalized potentials and boundary projections of Calderon's type. To prove that the new technique is appropriate, we thoroughly worked out a simple two-dimensional model example that allows full analytical consideration, including optimalization of the control effort.

In order to develop numerically computable solutions, we plan to describe the discrete framework for the noise control problem parallel to the continuous one. This discrete framework is obtained using difference potentials method; in the future it is going to be used for analyzing complex configurations that originate from practical designs. Once we have computed the solution for a particular configuration, we intend to investigate the possibilities of optimizing it according to the different criteria that would fit different practical requirements. We expect to discuss the applicability of the technique to quasi-stationary problems, future extensions to the cases of the broad-band spectra of disturbances, as well as other possible applications

which may include different physics, such as electrodynamics, and different formulations of the boundary-value problems, such as scattering.

Performance of different communication patterns on the Coral system
Ignacio M. Llorente

The evaluation of the message passing performance of a parallel system should not only consider the performance of the interconnection system, but also the impact of the memory hierarchy exploitation. The communication cost in a parallel application depends not only on the amount of data exchanged between the processes, but also on how they are structured in the local memories. In fact, the bandwidth reduction due to local memory access with poor data locality may be more important than the reduction due to contention in the network. This situation might influence, for example, the optimal data partitioning of domain decomposition applications. Although 3-D decompositions exhibit lower inherent communication-to-computation ratios, lower dimensional decompositions, where boundaries with poor spatial locality are not needed, may be more efficient. This behavior has been previously reported for some current parallel architectures as the Cray T3E and the SGI Origin 2000. The aim of this research is to evaluate the performance of the Coral system for different communication patterns using LAM/MPI 6.3. Since the study is focused on the Coral subsystem based on dual-CPU nodes (500MHz Pentium III), we have also studied the influence of the processor mapping. In this case, an optimal mapping does not only reduce network contention, but also allows the exploitation of shared memory communications.

We have performed the following communication tests:

- Unidirectional Communications: First, we have used the classical Ping-Pong test to establish the achievable bandwidths. Then, this base experiment has been modified by increasing the network load and by decreasing the spatial locality properties of the messages. For contiguous messages, preliminary results show an asymptotic bandwidth of 80 Mbytes/s between processors in the same node (shared memory communication) and 11 Mbytes/s for processors in different nodes. For strided data, the bandwidth drops down to 20 (25% the asymptotic bandwidth) and 8 Mbytes/s (73%) respectively. With network saturation, the bandwidth between different nodes for contiguous and strided data is 6 (55%) and 5 Mbytes/s (45%) respectively. Summing up these results, for inter-node communications, the bandwidth reduction due to network saturation is more important than the reduction due to non-contiguous messages, while for intra-node communications, message performance strongly depends on data locality and is not affected by the network contention.

- Processor Mapping: It is clear that an optimal processor mapping should exploit the faster communication of contiguous messages inside the nodes which also helps to reduce the network contention. For example, the processor mapping of a 1-D topology should be made to assign neighboring processes to the same node. The communication bandwidth has been measured to be 30% higher in such a situation.

- Domain Decomposition Technique: The relation between computation and communication times is much higher on the Coral system than in current parallel architectures, so the 3-D decomposition achieves the best performance, requiring 30% less time than the 1-D decomposition and 8% less than the 2-D one.

- Set of Tridiagonal Systems of Equations: A set of tridiagonal systems of equations has been solved using different approaches: pipelined sequential algorithms (Pipelined Gaussian Elimination method), matrix transpose algorithms (Mapping Transposition algorithm) and different parallel im-

plicit solvers (Cyclic Reduction method, Mattor's algorithm, and Wang's partition method). Each one of those methods exhibits a different communication pattern: pipelined communication, collective communications, binary tree communications, etc. The Mattor's algorithm combined with Cyclic Reduction shows the best results in terms of execution time and so parallel efficiency.

The work performed will provide guidance for efficient programming on the Coral system.

The results will be compared with those obtained on some current parallel architectures (Cray T3E and SGI Origin 2000) considering not only performance issues, but also the performance-cost ratio.

This research was conducted in collaboration with M. Prieto-Matias and E. Huedo-Cuesta (Universidad Complutense, Spain).

A robust and parallel multigrid method for the simulation of a yawed flat plate
Ignacio M. Llorente

The combination of implicit plane relaxation with partial and full coarsening has been found to be fully robust for solving the incompressible Navier-Stokes equations on highly stretched grids in the simulation of the driven cavity and a boundary layer over a flat plate. In particular, the combination of plane smoothing and semi-coarsening achieves a convergence rate independent of grid size, stretching and Reynolds number for the boundary layer simulation. Moreover, a tri-plane ordering in the smoothing sweep exhibits similar convergence to the lexicographic ordering and allows the efficient parallel implementation of the algorithm. The objective of this research is to study whether those convergence properties are maintained in the simulation of a boundary layer at high Reynolds numbers over a yawed flat plate, where the leading edge is not perpendicular to the stream. This simulation exhibits some basic problems that may prevent optimal multigrid efficiencies from being achieved, namely, a highly stretched grid near the yawed plate in order to capture small scale physical phenomena and an entering flow not aligned with the discretization grid.

A FAS multigrid code has been used to solve the incompressible Navier-Stokes equations on a single-block grid with stretching. The discrete equations are obtained using a finite volume approach in a staggered grid. For the convective terms a first order upwind discretization is used. Second-order accuracy is achieved with a defect-correction procedure based on a QUICK scheme inside the multigrid cycle. The smoothing operator is a cell-implicit Symmetric Coupled Gauss Seidel method, where the momentum and continuity equations are relaxed in a coupled manner. The combination of plane smoothing (where each plane consists of a slab of cells) and semi-coarsening has been found to be robust in the simulation of the yawed flat plate for angles up to 45 degrees. The smoothing process is not computationally expensive because each slab of cells is approximately solved with a 2-D robust multigrid algorithm consisting of one FAS F(1,1) cycle that combines a cell-implicit smoother and semi-coarsening. *Textbook multigrid convergence* is attained for the model problem, i.e., preliminary results show that the convergence rate is independent of the grid size, grid stretching, Reynolds number, and angle of yaw. In fact, the full multigrid algorithm converges the solution to below the truncation error with one F(2,1) cycle per level. The parallel version of the code is being implemented on the Coral system by using the MPI communication library in order to obtain results in finer grids up to 256 cells per side.

We intend to continue working on parallel and robust multigrid methods for block-structured applications. In particular, we will compare the numerical and architectural properties of coupled and distributive relaxation for the incompressible Navier-Stokes equations.

This research was conducted in collaboration with R.S. Montero and M. Prieto-Matias (Universidad Complutense, Spain), and M.D. Salas (ICASE).

Large eddy simulation using a parallel multigrid solver

Dimitri J. Mavriplis

The failure to develop a universally valid turbulence model coupled with recent advances in computational technology have generated a greater interest in the large-eddy simulation approach for computing flows with large amounts of separation. This approach involves resolving the large-scale unsteady turbulent eddies down to a universally valid range in the hope of yielding a more generally valid simulation tool. The purpose of this work is to develop a large-eddy simulation capability based on an existing unstructured grid Navier-Stokes solver. The use of unstructured grids, which facilitates the discretization of complex geometries and adaptive meshing techniques, is expected to enhance the flexibility of the resulting simulation capability.

An unsteady Reynolds-averaged Navier-Stokes (RANS) flow solver based on unstructured meshes has been developed and validated on the case of a circular cylinder. A Detached Eddy Simulation (DES) model based on modifications to the one-equation Spalart-Allmaras RANS turbulence model has been implemented and validated for the case of flow over a sphere. Flow over a wing at post-stall incidences has also been computed using the unsteady RANS and the DES methods. These computations are being performed on the ICASE PC cluster, Coral.

The simulation of decaying isotropic turbulence in a periodic domain is underway in order to enable the calibration of the model constant and to study the effect of artificial dissipation on the simulation of eddies in the inertial range. Higher resolution simulations for the stalled wing and flow over a bluff landing gear geometry are to be performed in the near future.

This work is being carried out in collaboration with Juan Pelaez (Old Dominion University).

Unstructured multigrid algorithms for the solution of radiation diffusion problems

Dimitri J. Mavriplis

Under the ASCI program, the simulation of radiation transport phenomena has been identified as one of the most time consuming elements within large simulation codes. The objective of this research is to investigate the effectiveness of unstructured multigrid algorithms in efficiently solving unsteady radiation transport problems, in the radiation diffusion limit.

A two-dimensional unstructured grid radiation diffusion solver has been developed which employs agglomeration multigrid to converge the nonlinear problem at each physical time step. In a first approach, a nonlinear FAS multigrid scheme is used to directly converge the nonlinear problem at each time step, whereas in the second approach, a Newton iteration scheme is applied to the nonlinear problem and a linear multigrid algorithm is employed to solve the linear system at each Newton iteration. A hybrid scheme based on a nonlinear FAS multigrid scheme but using a linear solver on each grid level has also been implemented. Results indicate that while all three schemes converge at the same rate based on the number of (linear or nonlinear) grid sweeps, the linear multigrid solver is more efficient due to the smaller number of expensive nonlinear function evaluations.

These results are to be extended into the three-dimensional setting and effects of scalability on large numbers of processors will be studied in addition to algorithmic efficiency. A complete validation of the solver in terms of accuracy will also be completed in the near future.

On the extension of compressible flow solvers to incompressible flows

C.-C. Rossow

The extension of methods designed to solve compressible flows near the incompressible flow regime still remains a challenge. The usual way to make compressible codes applicable for the solution of low Mach number flows is to precondition the system of compressible equations. This is done in such a way that the disparity in the eigenvalues is reduced and the condition number of the resulting system becomes of the order of unity. However, in regions of very low Mach number, e.g., near stagnation points and in recirculation regions, the preconditioning matrix may become singular and the robustness of the computation may be impaired. Therefore, to make compressible codes applicable to incompressible flow problems with the same reliability as for compressible flows, further effort seems to be required to understand the basic mechanisms of computing incompressible flows.

Due to the robustness problems encountered when using preconditioning techniques, the question may be asked whether some elements are missing in this approach. It is well known that in the incompressible limit, the velocity field of the flow must be divergence free. This is an essential requirement, and it may be argued whether this condition has to be satisfied on a discrete level, too. Analysis of unsuccessful computations with preconditioning revealed that this constraint was violated in these cases. Based on this observation, a possibility was sought to respect this constraint for the discrete equations. Based on the Mach number expansion of the classical Flux Difference Splitting scheme, the discrete mass flux was investigated. In the incompressible limit, the discrete mass flux is mainly governed by pressure differences arising in the artificial dissipation due to the solution of a Riemann problem. Using these pressure differences, an equation for a correction of the pressure, such that a divergence free velocity field will be enforced, could be derived. In the incompressible limit, this equation is of purely elliptic nature. Solving this equation in the framework of an unstructured, compressible code allowed the computation of completely incompressible (M=0) flows.

It could be shown that this formulation of a pressure correction equation is equivalent to classical methods for solving incompressible flows. However, in the present formulation, no heuristic arguments are required, but the derivation is based on the solution of the corresponding Riemann problem in combination with the divergence free velocity field constraint. As a result, the discrete incompressible method arises consistently from the compressible formulation.

During the research, the observation was made that the pressure equation is not well suited for the computation of compressible flows with shocks. This may be consistently understood with the vanishing pressure differences in the mass flux when the Mach number approaches unity. An attempt was made to turn the basic elliptic equation into a hyberbolic equation for supersonic flows, as is practice for other pressure-based methods used for the computation of compressible flows. However, the experience was made that very small timesteps were required to obtain a stable integration towards steady state, and this approach was recognized as not efficient for compressible flows. Therefore, a blending technique was derived which allows a transition from the pressure-based incompressible formulation to the density-based compressible formulation.

With this formulation, completely incompressible and compressible, transonic flows around airfoils were computed. The method was used to simulate inviscid as well as viscous flowfields, and the implementation into the multigrid framework of the basic unstructured code was straightforward. A comparison with the standard preconditioning technique used in the same code showed an increased robustness of the pressure correction method for high lift flows close to separation. This may be attributed to the fact that the pressure correction equation enforces the divergence free velocity field on a discrete level during each timestep. It was

found that for highly stretched meshes, the elliptic equation became stiff due to the high aspect ratios, and the number of Jacobi-iterations had to be increased.

The results obtained during this work indicate that it is crucial for convergence to respect the divergence free constraint. Furthermore, care has to be taken when regarding incompressible or nearly incompressible unsteady flow: this constraint applies here also, and the violation of it may lead to wrong interpretations. This holds especially for the computation of flows at maximum lift conditions, where unsteadiness is likely to occur, and recirculation zones with very low speeds are present.

Future work will be directed towards an enhanced method for the solution of the pressure correction equation to ensure convergence for more severe conditions. Furthermore, it will be investigated whether the additional evaluation of the continuity equation could be avoided to reduce computational cost.

High-order discontinuous Galerkin method and WENO schemes
Chi-Wang Shu

Our motivation is to have high order non-oscillatory methods for structured and unstructured meshes which are easy to implement for parallel machines. The objective is to develop and apply high order discontinuous Galerkin finite element methods and weighted ENO schemes for convection dominated problems. The applications will be problems in aeroacoustics and other time dependent problems with complicated solution structure.

Jointly with Harold Atkins at NASA Langley, we are continuing in the investigation of developing the discontinuous Galerkin method to solve the convection dominated convection-diffusion equations. We have been continuing in our investigation of local preconditioners which hopefully would dramatically increase the time step restriction on the time dependent simulations and make convergence to steady states much faster, both for convection problems and for convection-diffusion problems. Jointly with Cockburn, Luskin and Suli, we have been developing a local post processing technique for the discontinuous Galerkin method applied to linear PDEs which will effectively double the order of accuracy of the scheme with minimal additional computational cost.

Research will be continued for high order discontinuous Galerkin methods and weighted ENO methods and their applications.

High-order two-way artificial boundary conditions for nonlinear wave propagation with backscattering
Semyon Tsynkov

When solving linear scattering problems, one typically first solves for the impinging wave in the absence of obstacles. Then, by linear superposition, the original problem is reduced to one that involves only the scattered waves driven by the values of the impinging field at the surface of the obstacles. In addition, when the original domain is unbounded, special artificial boundary conditions (ABCs) that would guarantee the reflectionless propagation of waves have to be set at the outer boundary of the finite computational domain. The situation becomes conceptually different when the propagation equation is nonlinear. In this case the impinging and scattered waves can no longer be separated, and the problem has to be solved in its entirety. In particular, the boundary on which the incoming field values are prescribed, should transmit the given incoming waves in one direction and simultaneously be transparent to all the outgoing waves that travel in the opposite direction. We call this type of boundary conditions two-way ABCs.

In the paper, we construct the two-way ABCs for the nonlinear Helmholtz equation that models the laser beam propagation in a medium with nonlinear index of refraction. In this case, the forward propagation is

accompanied by backscattering, i.e., generation of waves in the direction opposite to that of the incoming signal. Our two-way ABCs generate no reflection of the backscattered waves and at the same time impose the correct values of the incoming wave. The ABCs are obtained for a fourth-order accurate discretization to the Helmholtz operator; the fourth-order grid convergence is corroborated experimentally by solving linear model problems. We also present solutions in the nonlinear case using the two-way ABC which, unlike the traditional Dirichlet boundary condition, allows for direct calculation of the magnitude of backscattering.

Future work will include building a more efficient iteration procedure than the one currently employed, numerical studies of both subcritical and supercritical regimes, comparing the results obtained in the framework of the nonlinear Helmholtz equation with those obtained for the nonlinear Schroedinger equation, and finally casting the ABCs that we have constructed into the general framework of Calderon's pseudo-differential boundary equations.

This research was conducted in collaboration with Gadi Fibich (Tel Aviv University).

COMPUTER SCIENCE

Preconditioning techniques for solving the particulate flow problem in parallel
Abdelkader Baggag

To extract the implicit information that is in the equations of the motion of the flow of particulates, it is necessary to numerically solve the coupled system of PDEs consisting of the equations of the fluid motion, and the equations of the rigid-body motion governing the particles. These equations are coupled through the no-slip boundary condition on the particle surfaces, and through the hydrodynamic forces and torques exerted by the fluid on the particles. To solve numerically, the particulate flow problem is discretized by a standard Galerkin finite element scheme, in which both the fluid and particle equations of motion are incorporated into a single variational equation where the fluid and particle velocities appear as primitive unknowns. The computation is then performed on an unstructured grid, and an arbitrary Lagrangian-Eulerian moving mesh technique is adopted to deal with the motion of the particles.

The numerical simulation of the particulate flow problem is extremely computationally intensive, since it is nonstationary, i.e., it evolves over many time steps, and within each time step a nonlinear system of equations must be solved, and within each nonlinear iteration several linear systems are solved. The time stepping is handled by a backward Euler scheme, and a Newton method is used to deal with the nonlinearity. The various algebraic systems (Jacobians) which arise thereafter are large, sparse, nonsymmetric, and often indefinite, and their solution can consume up to 90% of the total CPU time of the entire simulation. The main focus of this research is to address the efficient solution of the linear systems and to implement them on parallel computers, and to optimize them in particular on the Origin 2000.

Although the methods based on the Krylov subspaces have excellent parallelization properties, they lack robustness without good preconditioning. In this research some novel techniques are investigated and devised. These techniques include the balance scheme, the multilevel method, and the augmentation method. These algorithms are implemented in a Particle Mover object-oriented code, called PM++, and extensively validated for the particulate flow problem of the Grand-Challenge project.

Parallel implicit solvers for PDEs and PDE-constrained optimization
David E. Keyes

The development and application of parallel implicit solvers for multiscale phenomena governed by PDEs are our chief objectives. Newton-Krylov-Schwarz (NKS) methods have proven to be broadly applicable, architecturally versatile, and tunable for high performance on today's high-end commercial parallel platforms (e.g., Cray T3E, SGI Origin, IBM SP, Compaq AlphaServer). The challenge of obtaining high performance is likely to be increased on coming generations of high-end machines, as represented, for instance, by the ASCI "white" machine at Lawrence Livermore National Laboratory, and also on Beowulf clusters, such as ICASE's "Coral." Our primary efforts are concentrated on algorithmic adaptations of NKS methodology appropriate for emerging architectures and on evaluation of new software tools and methodology.

Since we employ Newton's method as the solver, we can also apply our techniques to nonlinear systems that augment the original PDE discrete equations by additional equations that represent the first-order necessary conditions (the Karush-Kuhn-Tucker equations) for optimality. Working through the Lagrange formulation for PDE-constrained optimization, we designate this approach Lagrange-NKS, or simply LNKS.

Both structured-grid and unstructured-grid CFD legacy codes have been ported to advanced platforms and reasonable objectives for algorithmic convergence rate, parallel efficiency, and raw floating point perfor-

mance have been met. The general approach embodied in the NKS family of algorithms is documented in previous ICASE technical reports, among other places. Newton's method, robustified by pseudo-transient continuation, generates global linear systems that are solved in a matrix-free manner by Krylov iteration, and preconditioned locally. In the absence of timestepping, a non-local two-level preconditioner based on a coarsening of the problem is also required to maintain algorithmic scalability at a modest cost to asymptotic parallel efficiency, but most nonlinear problems require some form of timestepping, even for the computations of steady states.

During the past year, our 1999 Bell Prize-winning work — an implementation of the NASA code FUN3D running on up to 3,072 dual-processor nodes of the ASCI Red machine at 227 Gigaflops/s — has been extended by algorithmic performance tuning and memory system modeling, while we await access to the next larger machine.

Domain-decomposition algorithms for PDEs and Lagrange-based algorithms for PDE-constrained optimization are special cases of partitioned solvers, where the partitions are geometrically or functionally based, respectively. We are examining a variety of partitioned solvers, where the variety arises from the type of partitioning and also the order of nestedness of the partitioning with respect to the linearization required in any nonlinear problem. A key decision in the trade-off between globalized convergence properties and parallel computational cost per iteration is whether a global Newton linearization is employed, or multiple independent Newton linearizations within partitions. We have recently begun to explore nonlinear preconditioning which is expected to be well suited for machines with 10,000 processors or more. In this range conventional NKS methods begin to lose efficiency to the cost of global synchronization.

We will continue to develop NKS methods in implicit parallel CFD and radiation transport, examining a variety of algorithmic, programming paradigm, and architectural issues.

The Coral Project
Josip Lončarić, Thomas W. Crockett, Piyush Mehrotra, Peter Kearney, and Manuel D. Salas

The cost of developing complex computer components such as CPUs has become so high that scientific applications alone cannot carry the full burden. In the future, scientific computing will have to use mass market leverage to overcome the cost barrier. A cost-effective alternative to high-end supercomputing was pioneered by Beowulf, a cluster of commodity PCs. By now, high performance Beowulf clusters can be built using fast commodity PCs and switched Fast Ethernet. We are exploring the benefits and the limitations of this approach, based on applications of interest to ICASE.

The initial phase of the Coral project, consisting of 32 Pentium II 400 MHz nodes and a dual-CPU server, demonstrated aggregate peak performance in excess of 10 Gflops/s, with sustained performance on CFD applications of about 1.5 Gflops/s. In order to provide a richer environment for further experimentation, a dual-CPU configuration was chosen for the second phase of the Coral project. We have added 16 dual Pentium III 500 MHz machines and two dual-CPU file servers. The third stage of this project added 16 dual Pentium III 800 MHz machines and a 32-node low latency 1.25 Gbps Giganet cLAN network fabric. The resulting system contains 96 compute CPUs with an aggregate of 36 GB of RAM and 981 GB of local disk space. Coral's three dual-CPU servers provide an additional 1.5 GB of RAM and 246 GB of disk space.

Coral has an excellent price/performance ratio, almost an order of magnitude better than an equivalent proprietary supercomputer design. This conclusion is based on our experience with a variety of applications, ranging from coarse-grained domain decomposition codes to communication-intensive parallel renderers.

For a computer system with this much memory and disk capacity, the ability to move data around

within the cluster, as well as to and from other systems, becomes an important consideration. In conjunction with the second phase of the Coral project, we have built a small Gigabit Ethernet testbed which connects the Coral servers, one of the dual-CPU compute nodes, and one of ICASE's graphics workstations. Based on our measurements, the Gigabit Ethernet based on Alteon's chipset is best suited for bulk data movement. Latency sensitive parallel codes would be better served by another network technology. This was confirmed by our test of Giganet cLAN in May, which also demonstrated a strong influence of the MPI library implementation on dual CPU nodes.

The Coral cluster usage has dramatically increased this year. In August of 2000, Coral's existing 64 compute CPUs delivered 15,890 CPU*hours of computing. We will continue to use this cluster to develop and run research codes of interest to ICASE and NASA Langley, and to evaluate price/performance tradeoffs among various hardware, software, and networking configurations.

Integrating process algebra and linear-time temporal logic
Gerald Lüttgen

This research is devoted to the development of novel techniques for *heterogeneous formal specifications* of reactive systems such as avionics systems and embedded software. Traditional formal-methods research in this area has focused on homogeneous specification methodologies in which all specifications are given in the same notation. In practice, however, heterogeneous methodologies supporting multi-paradigm specifications are desired for the following reasons. First, different system components have different characteristics. Second, components of real-world systems are often developed within different teams. Third, system requirements, which are often stated using assertions (e.g., via *temporal logics*), should be refinable into system designs that are operationally concrete (e.g., represented in *process algebra*).

The taken approach extends the process algebra *Calculus of Communicating Systems* (CCS) by two operators that permit the inclusion of *Linear-time Temporal Logic* (LTL) formulas: (i) *embed*(ϕ), where ϕ is a LTL formula; this operator facilitates the embedding of LTL formulas within process-algebraic terms; and (ii) *constraint*(P,ϕ), where P is a process term and ϕ is a LTL formula; this operator allows one to restrict the behavior of P as specified by ϕ. The resulting mixed language was intended to be given a semantics in terms of *Büchi testing*, a semantic framework which was previously developed under ICASE/NASA funding. In the context of compositionality, however, it turned out that *Streett automata* provide a notationally more convenient, albeit equally expressive, semantic domain than Büchi automata. Consequently, our Büchi-testing theory has been re-developed for Streett automata, and the resulting framework has been interfaced to our mixed language via structural-operational rules.

Regarding future work, we plan to investigate concurrency-theoretic issues of our heterogeneous language. Also, an efficient algorithm for determining whether one specification refines another within our semantic theory should be developed.

This work is done in collaboration with Rance Cleaveland (SUNY at Stony Brook, New York) and is supported by NSF Grant CCR-9988489.

Relating asynchronous systems with respect to speed
Gerald Lüttgen

Classical *process algebras* model concurrent systems whose components are assumed to have arbitrary relative speeds. To consider the temporal behavior of systems, several timed process algebras have been proposed. Remarkably, most of these assume a synchronous system model where all system components have

fixed speeds. The objective of our research is to develop a timed process algebra for evaluating the temporal worst-case efficiency of *asynchronous* concurrent systems, in which every system component potentially performs at a different speed, but guarantees an *upper time bound* on all of its actions.

Our approach extends Milner's *Calculus of Communicating Systems* (CCS) by a clock-prefix operator. This operator allows for specifying a discrete amount of time a process is being permitted to delay before it must engage in an enabled communication with its environment. Since the semantic theory of CCS is based on the behavioral equivalence *bisimulation*, we aimed at refining this relation to a preorder that compares functionally equivalent processes with respect to their speed. To this end, we studied several possible definitions for such a preorder, all of which are intuitively justifiable, and formally proved them to coincide. For the resulting preorder, we characterized the fully abstract pre-congruence contained in it and axiomatized this pre-congruence for finite sequential processes. Finally, we also investigated a corresponding 'weak' pre-congruence which abstracts from internal computation. Our work concludes long overdue research in process algebra. The obtained results testify to the elegance of bisimulation-based behavioral relations when compared to related preorders built on top of DeNicola and Hennessy's testing theory.

Regarding future work, we plan to complete the concurrency-theoretic study of our faster-than preorder and to publish our findings in a technical report.

This work is done in collaboration with Walter Vogler (University of Augsburg, Germany).

Saturation: An efficient iteration strategy for implicit state-space generators
Gerald Lüttgen

Many state-of-the-art verification techniques rely on the automated construction of the reachable state space of the system under consideration. In previous work we developed an algorithm for the *MDD-based* construction of state spaces of *asynchronous* system models, such as Petri nets. By avoiding to encode a given global next-state function implicitly as MDD, but splitting it in several explicitly represented local next-state functions instead, we gained the freedom to choose the sequencing of firing events, which controls the fixed-point iteration calculating the desired global state spaces. The objective of this research is to develop a suitable strategy for firing events which increases the time and space efficiency of state-space generation.

Our approach is based on the observation that an MDD node is not modified any more, when all events affecting the considered node have been fired exhaustively, i.e., when the node is *saturated*. Having the specific representation of state-spaces using MDDs in mind, this results in a depth-first strategy for saturating MDD nodes. The intuitive benefits of this strategy are threefold. First, it brings MDD-nodes early into their final shapes. This eliminates much of the overhead necessary in our previous algorithm. For example, it makes many checks determining whether some event is enabled at a given snap-shot during the algorithm's execution unnecessary. Second, it permits an easy cache management in which cache entries do not need to be invalidated, as they either concern MDD nodes which are not updated any further or are guaranteed never to be accessed again. Third, it allows for considering event locality naturally, thereby eliminating the need for accessing nodes rather randomly and, thus, making the corresponding infrastructure obsolete. Our novel iteration strategy leads to a new state-space generation algorithm which has been implemented in the Petri net tool SMART. The algorithm's utility has been proved by experimental studies which show that it often performs several orders of magnitude faster than existing algorithms. Equally important, it keeps the peak sizes of MDDs usually quite close to their final sizes. Our results will soon enable the verification of larger systems in less time and, thus, will help to employ automated formal verification techniques into

engineering practice.

Regarding future work, we plan to employ our idea of saturation for implementing an MDD-based CTL model checker within SMART. Moreover, we intend to investigate whether our new algorithm is suitable for parallelization.

This work is done in collaboration with Gianfranco Ciardo and Radu Siminiceanu (The College of William & Mary).

Arcade: A distributed computing environment for ICASE
Piyush Mehrotra

Distributed heterogeneous computing is being increasingly applied to a variety of large size computational problems. Such computations, for example, the multidisciplinary design optimization of an aircraft, generally consists of multiple heterogeneous modules interacting with each other to solve the problem at hand. These applications are generally developed by a team in which each discipline is the responsibility of experts in the field. The objective of this project is to develop a GUI-based environment which supports the multi-user design of such applications and their execution and monitoring in a heterogeneous environment consisting of a network of workstations, specialized machines and parallel architectures.

We have been implementing a Java-based three-tier prototype system which supports a thin client interface for the design and execution of multi-module codes. The middle tier consists of logic to process the user input and also to manage the resource controllers which comprise the third tier. We have continued implementation of our Jini-based resource monitoring and management system. The system is being designed to be modular with well-defined interfaces so that it can be used with other frameworks also. For the specification of the resources, we are closely following the standards being set by the Grid Forum Information services group and are implementing the specification using XML. Similarly we have also designed an XML-based project specification language such that both the work-flow and the inter-module data flow can be easily specified. We have implemented the translators for converting back and forth between the XML specification and our internal Java-based project specification. We have also started a new subproject focused on using XML for managing scientific data used in multi-module applications. This approach will allow meta-data describing the data to be specified using XML thus allowing the descriptions to be manipulated directly by machines. Thus, translations between different forms of the same data, e.g., cell-centered vs. vertex-centered unstructured grid data, can be automatically translated.

In the future we will continue to work on the enhancements outlined above. In addition we will enhance the current Arcade monitoring system by adding more visualization tools. We will also add support for dynamic steering of executing simulation codes.

This work is being performed in collaboration with A. Al-Theneyan and M. Zubair (Old Dominion University).

Languages for high performance and distributed computing
Piyush Mehrotra

There are many approaches to exploiting the power of parallel and distributed computers. Under this project, our focus is to evaluate these different approaches, proposing extensions and new compilation techniques where appropriate.

OpenMP is a set of directives extending C, C++ and Fortran which provide a shared-memory parallel programming model. Current parallel architectures are built by interconnecting nodes which internally

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provide true-shared memory across a small number of processors. Both hardware- and software-based approaches are used to provide a shared address space across the physically distributed memories of the nodes in larger systems. OpenMP provides an easy and incremental approach for small scale shared memory systems. However, controlling and exploiting data locality becomes an issue as the latency for data transfers across the nodes increases for larger systems. We have designed a set of directives extending OpenMP which allow users to directly express the data-locality of their programs. Such directives can then be translated by a compiler to take advantage of the underlying target architecture. In order to test our ideas, we hand-translated directives for two different programs targeting two different architectures: a) a simple Jacobi program on an IBM SP2 using the Treadmarks software based DSM system from Rice University, and b) a program implementing lattice Boltzmann equations for solving flows (provided by L.-S. Luo and group) on the SGI Origin 2000. For both the programs we wrote at least two versions, a pure OpenMP version and one in which most of the data is declared private with only buffers being shared between the threads. In both cases we found that the second version gave much better performance reinforcing the fact that data-locality is important even on shared memory systems.

We plan to continue our investigations on providing data-locality in OpenMP programs, including designing and implementing compiler transformations required to translate the distribution directives so as to exploit the underlying architectures.

This work is being done in collaboration with B. Chapman, A. Patil and A. Prabhakar (University of Houston).

On the initial condition for LBGK scheme for unsteady flow simulations
Renwei Mei

In the computational simulation for unsteady flow problems using the method of lattice Boltzmann equation, it is critically important to have a good initial condition for the particle distribution functions. Otherwise, the error in the initial condition could contaminate the whole solution. A typical approach is to set the initial particle distribution function fi's equal to the equilibrium particle distribution function based on the known velocity and pressure field. This method is, however, shown to have larger initial error.

We propose an initialization scheme to obtain improved initial condition for fi's. Let the equilibrium function based on the initial velocity and density field be $f^{(eq,0)}$. This initialization scheme let the initial field for fi's to stream and collide based on the $f^{(eq,0)}$. During this initialization procedure, macroscopic flow variables remain unchanged. One of the advantages of this initialization scheme is that one can use the existing code to obtain easily an improved initial condition for fi's. The improvement is measured for velocity and stress field in two cases: decaying Taylor vortex flow, and decaying shear flow. Significant improvement is obtained for low viscosity (or high Reynolds number).

The results of this work will be written for an archival journal.

This work is an collaborative effort with Dr. Li-Shi Luo, Profs. Domonique d'Humieres and Lian-Ping Wang.

Formal analysis of the AILS alerting algorithm
César Muñoz

The Airborne Information for Lateral Spacing (AILS) is a project being conducted at NASA Langley Research Center. Its global objective is to increase airport efficiency by enabling approaches to closely spaced parallel runways in Instrument Meteorological Conditions. One of the most critical components of the AILS

concept is the alerting algorithm. It provides situational awareness to pilots involved in a parallel approach. The aim of this work is to conduct a formal analysis of the AILS alerting algorithm in order to discover possible misbehaviors that have not been detected during simulation and testing.

An abstraction of the AILS alerting algorithm has been formalized in the specification language of the PVS verification tool. Several models of collision trajectories, which vary from a pure discrete model to a completely continuous one, have been considered. Discrete models allow the use of efficient state exploration techniques to validate formal properties. However, they have proven to be too inaccurate. An accurate continuous model of trajectories has been refined by gradually removing discrete parameters of the discrete models. As result of the formal analysis, maximum and minimum times when an alarm will first sound prior to a collision have been found.

Techniques and models developed in the formal analysis of the AILS concept will be used to study a more general concept called Distributed Air-Ground Traffic Management (DAG/TM). DAG/TM is a gate-to-gate concept being designed as part of the NASA Aviation System Capacity Program to improve the overall performance of the National Airspace System.

This work is done in collaboration with Víctor Carreño (NASA Langley).

Verification of Java byte-code
César Muñoz

A key aspect of the Java language is the definition of a standard execution model, called the Java Virtual Machine (JVM), which executes machine-independent byte-code. In this work we apply Formal Methods techniques to formally analyze multi-thread executions of Java programs.

A formal model of concurrent Java byte-code based on transition systems has been developed. Given a particular Java program, a specification of its execution is written as an infinite state transition system. This model, that we write in the SAL specification language, can then be simplified into a finite system by using predicate abstraction techniques. Properties such as mutual-exclusion have been verified for classical examples of Java programs.

Aspects not considered in the first approach, such as exceptions and a richer set of instructions of the Java byte-code, will be considered in future research.

This work is done in collaboration with Peter Habermehl (University of Paris 7).

External memory sparse direct solvers
Alex Pothen

We are developing external memory algorithms and software for solving large, sparse systems of equations by means of direct solvers. Such methods will enable sparse direct solvers to make effective use of the Terabytes of storage available on serial computers; parallel algorithms running on PC clusters like Coral and Teraflop parallel computers with multiple levels of memory hierarchy will also benefit.

We formalize two problems for external memory sparse matrix factorizations: minimizing the core memory required in a read-once/write-once model, and minimizing the data movement needed in a read-many/write-many model. We compute bounds on these quantities for sparse problems whose computational graphs have good separators. We show that a data structure called the elimination tree determines the core memory requirements and the data movement costs of a sparse factorization algorithm. The relative performance of the three commonly used variants of the factorization algorithm, viz. left-looking, right-looking, and multifrontal, can vary a great deal for unbalanced elimination trees that occur in mathematical

programming and related applications. We are designing fast simulators that compute the data movement costs of these algorithms in time proportional to the size of the factors rather than the flops required to compute them.

We also propose to extend OBLIO, our object-oriented sparse direct solver library, with serial and parallel implementations of external memory solvers.

This is joint work with Florin Dobrian (Old Dominion University).

Scalable parallel algorithms for incomplete factorization preconditioning
Alex Pothen

The parallel computation of robust preconditioners is necessary for solving large systems of equations iteratively in scientific computing. We are developing scalable parallel algorithms and software that can compute incomplete factorization preconditioners for high levels of fill.

We partition the adjacency graph of the coefficient matrix into subgraphs of roughly equal sizes such that each subgraph has few boundary nodes relative to the number of interior nodes. We map the subgraphs to processors, form a subdomain interconnection graph, and order the subdomains by a graph coloring to reduce global dependences. On each subdomain, we locally reorder the interior vertices before the boundary vertices. This reordering limits the fill that joins a subgraph on one processor to a subgraph on another, and enhances the concurrency in the computation. The preconditioner computation takes place in two phases: in the first phase, each processor computes the rows of the preconditioner corresponding to the interior vertices of their subdomains. In the second phase, the rows corresponding to the boundary nodes are computed.

We have reported results on problem sizes of up to 20 million rows and columns on up to 216 processors of the SGI Origin, the Cray T3E, the Sun HPC 10000, and Coral, the ICASE Beowulf cluster. Our results show that the algorithm is scalable, in agreement with our analysis of the algorithm. We are currently implementing our parallel algorithm on parallel computers with Teraflop performances. We are also developing multi-threaded implementations on computers with shared address-space programming models.

This is joint work with David Hysom (Lawrence Livermore National Laboratory).

Enhancing the performance of unstructured mesh codes
Alex Pothen

Irregular computations such as unstructured mesh algorithms or sparse matrix algorithms achieve only a small fraction of the available peak performance on modern microprocessors. Understanding the reasons for this low performance is difficult on modern microprocessors since they issue multiple instructions in each clock cycle, and permit them to execute out of issue-order by exploiting multiple functional units and multiple levels of caches. We have initiated a study measuring the performance of these codes using hardware performance counters and simulation tools to first understand and then improve the performance.

We have studied the performance of the kernel of an unstructured mesh code for solving Euler's equations. By measuring various performance metrics, we find that on an SGI architecture the performance is limited primarily by the number of loads and stores that can be issued in a clock cycle, and that the level 1 and level 2 caches play a less important role in determining performance on the SGI. We have also studied the role of scheduling data accesses and computations by reordering the irregular data structures. We have experimented with ordering algorithms such as nested dissection, Cuthill-McKee, and space-filling curve based orderings. These improve performance for different reasons: some of them improve spatial locality, while others improve temporal locality.

We are continuing our work to find general principles for improving the performance of irregular computations. This is joint work with Jinghua Fu (Old Dominion University), and Dimitri Mavriplis (ICASE).

Numerical modeling of sound radiation and propagation in a non-uniform flow
Alex Povitsky

The propagation of disturbances in a non-uniform mean flow in the presence of a reflecting wall is investigated by high-order numerical scheme using compact approximation of spatial derivatives. Simulations were performed on serial and parallel computers for three-dimensional flows. Stagnation flows and flow around a cylinder are taken as prototypes of real world flows with strong pressure gradients. Monopole and dipole acoustic, vortical and entropy pulses are embedded in an incompressible inviscid background flow. The intensity and directivity of near-field wave patterns appear to be quite different from the benchmark solutions obtained in a uniform flow or in a static environment.

Near-wall stretching of a vortical monopole pulse by the stagnation flow leads to formation of a wave with two maximums apart from the centerline whereas a vortical dipole evolves into a three-spot wave with maximum acoustic pressure at the centerline. For an entropy pulse, the baroclinically induced vortex pair produces a sound wave similar to that originated from a vorticity dipole. Initial superposition of vorticity and entropy pulses forms non-symmetrical wave patterns. For an acoustic wave in the flow around a cylinder, the observed mean acoustic pressure is approximately doubled (upstream pulse position) and halved (downstream pulse position) in comparison with the benchmark. Angular redistribution of acoustic energy and its components and energy transfer between the mean flow and the wave are discussed in ICASE Report No. 2000-35.

Our future plans include the study of sound generation and propagation in non-uniform compressible flows and flows with vortex shedding (cavity noise). To get realistic distribution of acoustic sources in a turbulent flow, we plan to use the LES approach.

Optimization of jet mixing reactor for production of carbon nanotubes
Alex Povitsky

The high-pressure jet mixing reactor has been proposed for the industrial production of fullerene carbon nanotubes by the Nanotechnology Lab at Rice University. The C_{60} molecules combined in nanotubes have unusual and very useful electronic and mechanical properties. However, the mass production of nanotubes still presents a challenge. The single-walled carbon nanotubes may be produced from CO with the help of a catalyst whose rapid and uniform heating is critical for feasibility of this technology. Catalyst particles get into the reaction chamber via the central CO jet. The particles must be heated from $200°C$ (central jet temperature) to temperatures close to $1000°C$ as rapidly as possible, since slowly heated catalytic particles quickly loose their catalytic ability. To increase mixing, hot turbulent jets issuing from several nozzles surrounding the central nozzle are used. The goal of our numerical modeling and optimization of the reactor is to obtain a uniformly high temperature of the catalyst.

The maximum strength of each peripheral jet and the constraint on a total mass flux of peripheral jets suggests a configuration of two peripheral jets with high intersection angle between the central and peripheral jets. The optimal distance between peripheral nozzles and the central jet results from the tradeoff between the strength of a peripheral jet while it hits the central jet and the co-flowing effect delaying mixing of the central jet. Then, the FLUENT CFD software and GAMBIT grid generator were used in a detailed simulation of two-phase flow in the reactor. In addition to solving transport equations for the continuous

phase, FLUENT has an option to simulate a discrete second phase in a Lagrangian frame of reference. The analysis of velocity field and particle trajectories shows that strong recirculation zone at the centerline may lead to undesirable clustering of catalyst particles. Thus, the Eulerian optimization of reactor should be refined by the Lagrangian simulation of the discrete phase.

In our future research, the refined models of turbulence (as the RNG $k - \epsilon$) and a precise thermal radiation model should be evaluated to predict a correct rate of chemical reactions leading to formation of nano-tubes in presence of the catalyst. Dr. Carl Scott (NASA Johnson Space Center) applied his chemical model of the catalyst behavior and CHEMKIN software to the particle trajectories obtained by our CFD computations and his results are indicative of the time it takes to produce iron clusters as large as 20 or 40 atoms. To verify our results by physical experiments, we collaborate with the Nanotechnology Laboratory at Rice University (Prof. Richard Smalley).

Solving radiation transport equations with the multigrid method
Linda Stals

Radiation transport equations arise in the study of many different fields such as combustion, astrophysics and hypersonic flow. The solution of these equations presents interesting challenges due to large jumps in the coefficients and strong nonlinearities. In this project we compare the efficiency of several different solution techniques. Specifically, we focus on the performance of an inexact Newton multigrid scheme and compare it to the Full Approximation Scheme (FAS).

We have currently investigated the case where all temperatures are in equilibrium and the model reduces to a single equation. This equation contains many of the features inherent in the full model such as the strong nonlinearities and large jumps in the coefficients. We found that the Newton-Multigrid method worked better because it did not need to calculate the diffusion coefficient as often. Such an observation is of interest because including more physics in the model will increase the complexity of the diffusion coefficient even further and thus the Newton-Multigrid method is the method of choice. A flux limiter can also be included in the equation which changes its behavior from being locally parabolic to locally hyperbolic. We found that in such a case the use of adaptive refinement helped the solvers to better handle the steep wave front.

In future work we want to include more physics in the equations. The PI's for the ASCI II project are David Keyes and Alex Pothen (Old Dominion University and ICASE) and Dimitri Mavriplis (ICASE).

FLUID MECHANICS

Receptivity and transition in laminar boundary layers
W.O. Criminale and D.G. Lasseigne

This work has been the principal area of research and a comprehensive and thorough treatise based on first principles has been made. This report is entitled "A new paradigm for investigating receptivity and bypass dynamics in laminar boundary layers," by W.O. Criminale, R.D. Joslin, and T.L. Jackson and will be submitted to the Journal of Fluid Mechanics for publication.

Flow control and drag reduction
W.O. Criminale and D.G. Lasseigne

This problem is a natural extension of the work done on boundary layer receptivity. More specifically, by using the framework of initial-value problems for vorticity in the boundary layer, it is possible to determine the full range of the temporal dynamics. As a result it is then possible to design feedback in such a way as to suppress any damaging response in this system. The question remaining now is how to transpose such results into physically realizeable mechanisms for the boundary layer. Not only is the analysis able to investigate such behavior, but it has led to a more rational method for analytically solving the stability equations in this field. A second report is in progress that deals with the general technique (W.O. Criminale and D.G. Lasseigne).

Laser-induced thermal acoustics for flow diagnostics
Roger C. Hart

Off-body nonintrusive measurement of flow velocities is currently routinely done with laser doppler velocimetry (LDV) and particle interval velocimetry (PIV). Both techniques require seeding the flow with silica particles or droplets of liquid which serve as scatterers for the incident laser light. Seeding is undesirable in some circumstances (e.g., highly polished high-Reynolds number facilities or supersonic facilities, where the seed may literally sandblast models and tunnel surfaces), and impossible in others (there may be locations on models, behind rearward facing steps for instance, where you simply cannot get the seed to go). Laser-induced thermal acoustics (LITA) is a relatively new technique being developed at Langley and a few other places which allows truly seedless point velocimetry, and additionally measures temperature and pressure. Our goal is to explore and demonstrate the potential of this method by a combination of laboratory research and tunnel measurements.

In LITA a powerful pulsed laser creates a pair of counterpropagating acoustic wave packets at the measurement point. A second CW or long-pulse probe laser illuminates the wave packets at the Bragg diffraction angle. Doppler-shifted light diffracted from each packet is mixed on a detector with a small fraction of the unshifted probe beam. Analysis of the three resulting beat frequencies allows determination of both a component of flow velocity and the speed of sound (and thus temperature). Additionally, pressure can be found by analysis of the temporal decay of the signal. A measurement is made in a few microseconds over a volume of 100's of microns (transverse) by $\sim$ a centimeter (longitudinally). A first-generation prototype LITA apparatus has been constructed using compact, fieldable, "user-friendly" lasers and employing a novel technique for performing the heterodyne signal detection that is vastly more stable than our earlier efforts. The apparatus consists of transmitter and receiver units, each with a volume of about three cubic feet and

weighing less than 100 pounds each, plus one or two racks of electronics, power supplies, computers, and other ancillary equipment. Development of this instrument is continuing, but currently we observe one-sigma single-shot uncertainties of 0.7 to 1.0 m/s over the range of 8 m/s to 35 m/s. Performance is limited largely by signal/noise level.

We currently expect to begin a 40 day test/demonstration of LITA at BART during the second week of October 2000. We will compare LITA velocity measurements with pitot tube measurements of free stream velocity, and then attempt to map the separation, reattachment, and recirculation behind a rearward-facing step.

This research was conducted in collaboration with R.J. Balla and G.C. Herring (NASA Langley).

The probability density function (PDF) approach to turbulence modeling
Guowei He

The primary motivation of this research is to develop a PDF method for turbulence modeling. In comparison with the moment method, the PDF method takes advantage to exactly model nonlinear terms, but needs to model molecular diffusion and pressure. We will develop a mapping closure approximation (MCA) for scalar diffusion in turbulent shear flows. The second motivation of this research is to investigate the effect of shear on small-scale statistics in turbulence. The current turbulence models are mainly based on the assumption of isotropy. We will develop a model to incorporate small scale anisotropy.

We have developed a two-dimensional MCA approach to calculate the PDFs of scalar gradients in turbulent shear flows, where velocity is designed to be a superposition of isotropic Gaussian random filed and a directed shear flow. We derived and analyzed the governing equation of mapping function by exactly modeling "rapid-change" shear flows. The result obtained shows that shear does enhance more intense intermittency of scalar gradient in the direction of shear than the one transversal to the direction of shear and induces difference of their PDFs. Therefore, scalar field in shear flow is anisotropic at the level of dissipation.

We plan to numerically verify the above theoretical results.

This work is accomplished in collaboration with Dr. R. Rubinstein.

Direct numerical simulation (DNS) of isotropic homogeneous turbulence
Guowei He

In a collaborative effort with L.P. Wang (University of Delaware), we have developed a spectrum code specially for the cluster computer at ICASE for DNS of isotropic homogeneous turbulence. Several test cases have been successfully run at the grid size 64^3, 128^3 and 256^3. The largest case at the grid size 512^3 allowed by current capacity of the cluster computer is running for the largest database which can resolve small scale fluctuations in turbulence.

The database from DNS can be used to investigate the mechanism and modeling of turbulence. In collaboration with R. Rubinstein, we have calculated the time correlations of velocity fields from the DNS database and will compare them with the results obtained from LES subgrid models. The comparison allows us to estimate the predictability of the current LES subgrid models, which has not been investigated so far.

We plan to apply the comparison methodology to investigate a variety of turbulence models.

Eigen-solution analysis of the discontinuous Galerkin method

Fang Hu

It is well known that for a discontinuous Galerkin scheme employing basis polynomials of order p, the rate of convergence has been shown to be $h^{p+1/2}$ in general and h^{p+1} in some special cases. In contrast to the many studies on the convergence rates there have been relatively few works on the wave propagation properties of DGM, especially with non-uniform grids. Our work is motivated by the need to understand DGM with non-uniform grids.

A detailed study on spatially propagating waves in a discontinuous Galerkin scheme has been carried out. We are especially interested in wave propagation properties when there is an abrupt change of element sizes, as well as the influences the flux formula has on these properties. By analyzing the semi-discrete system, it is found that, for any given order of the basis functions, there are only, at most, two spatially propagating numerical wave modes for each physical wave of the PDE. One of the modes can accurately represent the physical wave and the other is spurious. The directions of propagation of these two numerical modes are opposite. In most cases, the spurious mode has a large damping rate. When full (exact) upwind flux formula is used, however, the spurious mode is non-existent. It is also shown analytically that, for the physically accurate mode, the numerical dispersion relation is accurate to order $2p + 2$ where p is the highest order of the basis polynomials. The results of the eigen-solutions are then used to study the propagation of waves through an interface of abrupt change of element sizes. Closed form numerical reflection and transmission coefficients are derived and analyzed.

Works on 2-D and 3-D equations will be carried out in the future.

This work is in collaboration with H.L. Atkins (NASA Langley).

Dispersion, dissipation, isotropy, Galilean invariance, and stability of the lattice Boltzmann equation

Li-Shi Luo

Like any numerical schemes to solve partial differential equations, the lattice Boltzmann equation (LBE) has a number of numerical artifacts due to the discretization. These artifacts are yet to be fully understood. Our objective is to analyze the artifacts of the lattice Boltzmann equation, such as its dissipation for non-zero wavenumber (hyper-viscosities), its isotropy (wave-number dependence of the transport coefficients), and non-Galilean invariant effects due to discretization.

We construct a 2D generalized lattice Bhatnagar-Gross-Krook (LBGK) Boltzmann model with multiple relaxation parameters in moment space. We analyze the linearized dispersion equation of the generalized LBGK model to obtain its generalized hydrodynamics.

We have obtained the wave-number dependence of transport coefficients theoretically, and verified the results by various numerical simulations. By introducing multiple relaxation parameters in the collision process of the LBE model, we can drastically improve the numerical stability of the LBE method. We have also quantitatively analyzed the impact of interpolations to the LBE method. This work has been published in Physical Review E.

We will extend the model to 3D and for complex fluids.

This work is accomplished in collaboration with Prof. P. Lallemand (Laboratoire C.N.R.S.-A.S.C.I., France), and it is partially supported by the program of Innovative Algorithms for Aerospace Engineering Analysis and Optimization at NASA LaRC.

Stochastic description of transitional flows

Robert Rubinstein

There is still no well-established procedure for incorporating transition in turbulence calculations. While aerodynamic flows can be computed successfully using any of several different turbulence models if the transition location is prescribed in advance, no single turbulence model can reliably predict transition. If transition is computed incorrectly, the entire flow calculation is generally unsatisfactory.

The analysis of the growth of subharmonics due to three-wave interactions was applied to an experiment performed by Kachanov and collaborators. Analysis of this experiment had suggested an important effect of initial phase correlations; the present work quantifies this effect by evaluating the joint probability density of modal amplitudes and phases. The probability that the subharmonic amplitude exceeds the primary has also been evaluated as a function of local Reynolds number; it is possible that this condition can serve as a simple transition criterion.

Work on the stochastic formulation of the parabolized stability equations is continuing.

This work was performed in collaboration with Meelan Choudhari (NASA Langley).

STRUCTURES AND MATERIALS

Decohesion elements for the simulation of progressive delamination in composites
Pedro P. Camanho

The fracture process of high performance composite laminates is quite complex, involving both intralaminar damage mechanisms (e.g., matrix cracking, fibre fracture) and interlaminar damage (delamination). Although progress has been made lately in the development of accurate tools for the prediction of intralaminar damage growth, similar tools for delamination are still difficult to implement, and thus delamination is generally not considered. Without delamination, the predictive capabilities of progressive failure analyses will remain limited. The analysis of delamination is commonly divided into the study of the initiation and the analysis of the propagation of an already initiated area. Delamination initiation analysis are usually based on stresses and use criteria such as the quadratic interaction of the interlaminar stresses in conjunction with a characteristic distance. This distance is a function of geometry and material properties, so its determination always requires extensive testing.

One approach to simulate both delamination onset and growth in composite materials is the use of interfacial decohesion elements placed between the composite layers. This approach is based on a Dudgale-Barenblatt type cohesive zone. Cohesive zone models are particularly attractive when interfacial strengths are relatively weak when compared with the adjoining material, as in the case of composite laminates. The proposed constitutive equations for the interface are phenomenological mechanical relations between the tractions and interfacial separations. The work of normal and tangential separation can be related to the critical values of energy release rates. In fact, it can be shown that the cohesive zone formulation is identical to Griffith's theory of fracture.

In order to predict delamination onset and growth, an eight-node decohesion element with interpolating shape functions for the top and bottom faces compatible with those of the elements being connected will be developed. The material response built into the element represents damage using Barenblatt's model in which a cohesive zone ahead of crack tip is used to predict delamination growth. A bilinear strain softening constitutive equation will be implemented such that the element does not carry any tensile or shear loads after the interfacial fracture energy has been consumed. Such an element will be used to model the interface between sublaminates or between bonded components.

Update of Dr. Jer-Nan Juang's system observer/controller identification toolbox
Joshua Grohs

Due to the increasing use of Dr. Juang's System Observer/Controller Identification Toolbox (SOCIT) the necessity of expanding its compatibility and support became imperative. With the current reliance on the internet, Dr. Juang felt it necessary to provide online support for his toolbox. In addition to text-based support, he also believed that it needed to support a couple of different platforms, therefore translation of the toolbox began. These projects were the focus of my summer research.

In order to satisfy the need for online support I designed a webpage dedicated to the toolbox. This website offers support for his Graphical User Interface (GUI) version of SOCIT as well as a comprehensive user guide. This user guide describes each function in depth and was modeled after MATLAB's help pages. In addition to these online aids, Dr. Juang's toolbox was translated from MATLAB to SCILAB in order to increase its platform support. SCILAB is a matrix-based scientific software package resembling MATLAB

with one very big difference. SCILAB is freeware and can be downloaded from the French National Institute for Research in Computer Science and Control SCILAB Homepage. By increasing the support of Dr. Juang's toolbox it will become more user-friendly and this will result in more people using it.

Future applications of my work will include connecting this support webpage to the NASA Research site, instead of its current link from Dr. Juang's personal webpage. Perhaps, in the future even more translations of SOCIT will be created, thus furthering its software support.

Debonding in stringer reinforced composite components
Ronald Krueger

Many composite components in aerospace structures are made of flat or curved panels with co-cured or adhesively bonded frames and stiffeners. Testing of stiffened panels designed for pressurized aircraft fuselage has shown that bond failure at the tip of the frame flange is an important and very likely failure mode. Comparatively simple specimens consisting of a stringer flange bonded onto a skin were developed in previous investigations. The failure that initiates at the tip of the flange in these specimens is identical to the failure observed in the full-scale panels and the frame pull-off specimens. The objective of this work is to investigate the damage mechanisms in composite bonded skin/stringer constructions under uniaxial and biaxial (in-plane/out-of-plane) loading conditions using experimental and numerical approaches.

Based upon experimental findings, a two-dimensional nonlinear plane-strain finite element (FE) analysis was performed using the ABAQUS(r) FE code. A stress analysis was used to investigate the onset of failure. This approach showed that the location and orientation of the initial transverse ply crack in the flange are dependent on the stress distribution in the critical area near the flange tip. For all three loading conditions, computed maximum principal tensile stresses were almost identical and exceeded the transverse tension strength of the material. A fracture mechanics approach was used to determine the potential for delamination growth from the initial transverse crack. In this approach, delaminations of various lengths originating from the transverse crack as observed in the experiments were simulated. Mode I and mode II strain energy release rate contributions were calculated for all load cases using the virtual crack closure technique. Computed total strain energy release rates were compared to critical values obtained from an existing mixed-mode failure criterion. The results suggest that once a matrix ply crack has initiated in the flange, a delamination will form and grow in an unstable manner between the adhesive film and the top 0° skin ply as observed in the micrographs.

Future work will focus on the development of a methodology for determining the fatigue life of bonded composite skin/stringer structures using delamination fatigue characterization data and a geometric nonlinear finite element analysis. Results will be compared to fatigue tests on stringer flange/skin specimens to verify the methodology.

This work is done in collaboration with Isabelle L. Paris (National Research Council), T. Kevin O'Brien (Army Research Laboratory, Vehicle Technology Directorate located at NASA Langley) and Pierre J. Minguet (The Boeing Company, Philadelphia).

Molecular weight effects on the mechanical response of a glassy thermoplastic polyimide
Lee M. Nicholson

The objective of this work is to detail and summarize the physical and mechanical testing of an advanced polymer (LaRC$^{\text{TM}}$-SI). Using five known variations in molecular weight, the results of mechanical tests were compared over a range of temperatures below the glass transition. Results from these tests will be presented

along with descriptions of the material, test methods and an interpretation of the polymer's mechanical response.

The molecular weights, molecular weight distributions, glass transition temperatures and the mechanical response of an advanced thermoplastic, glassy polyimide have been determined. The notched tensile strength is a strong function of both temperature and molecular weight. A critical molecular weight (M_c) is observed to occur at a $\overline{M}_w \sim 22000$ g/mol below which, the notched tensile strength decreases rapidly. This critical molecular weight transition is not temperature dependent. The observed microstructures and nonlinear (inelastic) behavior have helped to characterize further, the brittle to ductile transition as a function of molecular weight and temperature. Independent of temperature, high molecular weight materials ($\overline{M}_w > M_c$) will tend to fail in a ductile manner and low molecular weight materials ($\overline{M}_w < M_c$) will tend to exhibit brittle failure. The Young's Modulus and Shear Modulus are strong functions of temperature only. Using time-temperature superposition analysis of the creep compliance, low molecular weight materials have increased creep compliance and increased creep rate, over that seen in the high molecular weight materials. This fundamental understanding of how the molecular structure affects the macroscopic mechanical performance of a polymer matrix composite is extremely important for the efficiency of design of new materials and resulting engineered components. It not only reduces material developmental costs, but also reduces time to market for components.

Future research areas are, to establish the connectivity between nano-meso-micro scale of materials through experimentation and analysis, validation of computational tools, and establishment of key parameters that link synthesis and assembly to macro-level engineering performance.

This research was conducted in collaboration with Karen S. Whitley and Thomas S. Gates (NASA Langley).

High temperature piezoelectric films
Zoubeida Ounaies

Developing high performance, high temperature flexible piezoelectric materials for active flow control sensors and airframe health monitoring sensors is a critical component of NASA's Morphing Program, which is focused on investigating smart and biomimetic material technologies that will enable self-adaptive flight with improved performance and safety air and space travel.

Early molecular modeling by NASA scientists indicated the potential of forcing piezoelectricity in amorphous polyimides by adding dipoles to the polymer structure. This was the impetus for the current study in which we have synthesized a series of polyimides to investigate the potential piezoelectric response resulting from incorporating various dipoles into the structure.

Structure-property Studies: Structure-property relationship in piezoelectric polyimides shed some light into the effects of dipole nature, concentration, location, chain flexibility and glass transition temperature on piezoelectricity in polyimides.

Thermal Stability: We have shown that the piezoelectricity of this polymer was stable under both dynamic and static thermal stimuli and statistically no loss was observed up to 100°C. Since this amorphous piezoelectric polyimide can generate a piezoelectric response at elevated temperatures, its thermal stability should be beneficial for high temperature aerospace applications.

Piezocomposite Processing: We propose to combine the polyimides with piezoelectric powder, namely lead zirconate titanate (PZT) to make a 0–3 piezocomposite. Such a composite would exhibit the piezoelectric coefficients of the ceramic and the flexibility, strength and lightweight of the polymer. The relative ease of

processing and potential high temperature use make this material an attractive candidate for various sensing applications.

The feasibility of developing new monomers and polymers with larger dipole concentrations while maintaining chain flexibility and favorable geometries is still pursued in an attempt to increase the piezoelectric behavior and the use temperature. Future work will further explore the processing and properties of the polyimide/PZT composite.

This work is done in collaboration with Joycelyn S. Harrison (NASA Langley) and Cheol Park (ICASE).

Piezoelectric ceramics for use as actuators
Zoubeida Ounaies

The goal is to implement piezoelectric actuators in vibration and noise suppression applications steered towards improving aircraft operation. This will lead to reduction of control electronics size and cost, and a lowering of the voltage drive by using thinner, more efficient, better characterized actuators.

We have completed the determination of capacitive behavior and power consumption of piezoelectric actuators. This is an important step in order to optimize the system configuration and to provide efficient driving electronics when using the piezoelectric wafers as actuators. Empirical relations were developed from experimental data to predict the capacitance and loss tangent of a piezoelectric ceramic as nonlinear functions of both applied peak voltage and driving frequency. It was demonstrated that by incorporating the variation of capacitance and power loss with voltage and frequency, satisfactory estimates of power requirements can be obtained. These relations allow general guidelines in selection and application of piezoelectric actuators and driving electronics for active control applications.

To gain a fundamental understanding of how processing variables affect actuator performance, we have recently completed displacement measurements as a function of temperature (25 to 200°C), voltage and frequency on pre-stressed piezoelectric ceramic transducers. Results show that the pre-stressed ceramics can have large displacements stable up to these high temperatures.

Future work includes understanding the effect of pre-stressing inherent to the material on nonlinear behavior as a function of applied field and frequency. Towards that end, we will determine the power efficiency, the electro-mechanical conversion coefficient as well as the resonance behavior as a function of geometry.

We also plan on continuing the modeling of the hysteresis behavior of piezoelectric ceramics as a function of frequency and temperature. Modeling the doming behavior and the displacement characteristics of THUNDER actuators is done in collaboration with Dr. R.C. Smith and Mr. R.E. Wieman.

This research was conducted in collaboration with Ralph Smith (North Carolina State University) and Thomas Jordan (NASA Langley).

Molecular dynamics simulations for mechanical and electrical properties of metallic and polymer systems
Sun Mok Paik

For a quantitative understanding of the underlying mechanisms for mechanical and electrical failures, it is necessary to investigate and quantify the effects of atomistic structures and defects on the materials properties. The Molecular Dynamics (MD) simulation technique is an exact (within numerical accuracy of the computer) deterministic numerical simulation method, and one of the best-suited methods to study local structures of a system. In this investigation, we will study the mechanical properties of metallic systems, and

the dielectric properties of polymers using the Molecular Dynamics simulation technique providing failure sensing and preventing mechanisms.

The materials simulations fall into three different categories: (1) deterministic simulations such as the MD simulation, (2) stochastic such as a Monte Carlo (MC) simulation, and (3) ab initio calculation. These methods have both pros and cons but the MD method is best suited for our purpose. Using the MD technique, we will simulate a stable structure of metallic alloy systems, and the effects of the structure factors, like alloy composition ratio, segregation, grain boundaries, impurities, defects, etc., on the crack formation and propagation. A many-body Embedded Atomic Method (EAM) potential is used for the interatomic interactions between the metal atoms. We have completed coding the MD program in C for a single metallic (Au) system, and are extending it to the alloy systems. For polymer systems, we are in the stage of developing a suitable empirical molecular interaction potential.

In the future, we will simulate and calculate various mechanical and dielectric properties of more complicated metallic alloys and polymer systems. We also plan to write an MD code for a parallel computer.

This work is done in collaboration with Dr. Min Namkung (NASA Langley).

Theoretical study of pulsed eddy current decay
Sun Mok Paik

The pulsed eddy current testing method has been widely used in Non-destructive Evaluation (NDE) and depth measurement of the conducting plates. The method measures the change of the field near the metal surface, and can predict the depth and flaw of the plate quite accurately. However, there are two serious problems in real applications: (1) the fact that the result is very sensitive to experimental conditions such as the sensor position and direction has made the experiments difficult, and (2) the thickness of the plates that can be measured are limited to less than about 6 mm. In this investigation, we study the eddy current decay mechanism theoretically and find a way to circumvent the above mentioned problems.

The second-order differential equation for vector potential A, is derived from Maxwell's equations,

$$\Delta^2 A = -\mu i_0 + \mu\sigma\frac{\partial A}{\partial t} + \mu\varepsilon\frac{\partial^2 A}{\partial t^2} + \mu\Delta\left(\frac{1}{\mu}\right) \times (\Delta \times A),$$

and solved for a system of two-conducting plates as a function of sensor position, r, sensor height, z, and the lift-off, l of the drive-coil and sensor. We find that the field, A, decays as time increases after applying a voltage pulse with a decay constant τ that depends on the thickness of the first conducting plate. For the different lift-off l, the signal, A, changes but the decay behavior does not change. Thus, with a suitable scaling, the tilting and lift-off problems can be avoided in an eddy current measurement.

In the future we will investigate a method to increase the maximum thickness of the plate that can be measured using the eddy current decay method.

This work is done in collaboration with Dr. Min Namkung (NASA Langley).

Sensor-actuator dual functional electroactive polymeric hybrid systems
Ji Su

Sensor and actuation functions are two important concerns in smart structures and biomimetic technologies. Piezoelectric and electrostrictive materials are two promising candidates for being employed in these areas. Piezoelectric and electrostrictive polymeric materials have been drawing more and more attention due to their lightweight, excellent processability, and electrical/mechanical toughness as well as very promising properties exhibited in some polymer materials. Among them, poly (vinylidene fluoride) (PVDF)

and its copolymers are widely used as sensor materials. Recently, several electrostrictive polymers have been developed for actuation applications due to their large electric-field-induced strain and high mechanical energy density, superior to PVDF and its copolymers. For actuation applications, both the piezoelectric mechanism and electrostrictive mechanism are utilizable. However, the piezoelectric mechanism needs a remanent polarization and the electrostrictive mechanism does not need a remanent polarization, these two mechanisms usually do not appear in the same material. The recently developed NASA-LaRC electrostrictive graft elastomer offers not only promising electromechanical properties, but also excellent processability. This allows the development of a piezoelectric-electrostrictive polymeric molecular hybrid composite system using conventional processing methods.

A piezoelectric PVDF-based copolymer-electrostrictive graft elastomer molecular composite system was developed using the solution casting method. The measurements of mechanical modulus, dielectric constant, and piezoelectric strain coefficient were conducted as a function of temperature and frequency. The electric field induced strain response of the molecular composite films was also tested. Both piezoelectric and electrostrictive contributions were observed in the strain measurement. The research results offer a material which can be utilized for unified sensor/actuator devices and structure.

More characterization work on the newly developed materials is needed for understanding the mechanisms further and developing prototype devices using their materials. The characterization work will be conducted in the near future.

This research was conducted in collaboration with Joycelyn S. Harrison (NASA Langley) and Zoubeida Ounaies (ICASE).

REPORTS AND ABSTRACTS

Gottlieb, Sigal, Chi-Wang Shu, and Eitan Tadmor: *Strong stability preserving high-order time discretization methods.* ICASE Report No. 2000-15, (NASA/CR-2000-210093), April 7, 2000, 28 pages. Submitted to SIAM Review.

In this paper we review and further develop a class of strong-stability preserving (SSP) high-order time discretizations for semi-discrete method-of-lines approximations of partial differential equations. Termed TVD (total variation diminishing) time discretizations before, this class of high-order time discretization methods preserves the strong-stability properties of first-order Euler time stepping and has proved very useful especially in solving hyperbolic partial differential equations. The new contributions in this paper include the development of optimal explicit SSP linear Runge-Kutta methods, their application to the strong stability of coercive approximations, a systematic study of explicit SSP multi-step methods, and a study of the strong-stability preserving property of implicit Runge-Kutta and multi-step methods.

Muñoz, César, and Victor Carreño: *Aircraft trajectory modeling and alerting algorithm verification.* ICASE Report No. 2000-16, (NASA/CR-2000-210097), April 12, 2000, 25 pages. Submitted to the International Conference on Theorem Proving in Higher Order Logics (TPHOL2000).

The Airborne Information for Lateral Spacing (AILS) program at NASA Langley Research Center aims at giving pilots the information necessary to make independent approaches to parallel runways with spacing down to 2500 feet in Instrument Meteorological Conditions. The AILS concept consists of accurate traffic information visible at the navigation display and an alerting algorithm which warns the crew when one of the aircraft involved in a parallel landing is diverting from the intended flight path. In this paper we present a model of aircraft approaches to parallel runways. Based on this model, we analyze the alerting algorithm with the objective of verifying its correctness. The formalization is conducted in the general verification system PVS.

Lallemand, Pierre, and Li-Shi Luo: *Theory of the lattice Boltzmann method: Dispersion, dissipation, isotropy, Galilean invariance, and stability.* ICASE Report No. 2000-17, (NASA/CR-2000-210103), April 19, 2000, 33 pages. To appear in Physical Review E.

The generalized hydrodynamics (the wave vector dependence of the transport coefficients) of a generalized lattice Boltzmann equation (LBE) is studied in detail. The generalized lattice Boltzmann equation is constructed in moment space rather than in discrete velocity space. The generalized hydrodynamics of the model is obtained by solving the dispersion equation of the linearized LBE either analytically by using perturbation technique or numerically. The proposed LBE model has a maximum number of adjustable parameters for the given set of discrete velocities. Generalized hydrodynamics characterizes dispersion, dissipation (hyper-viscosities), anisotropy, and lack of Galilean invariance of the model, and can be applied to select the values of the adjustable parameters which optimize the properties of the model. The proposed generalized hydrodynamic analysis also provides some insights into stability and proper initial conditions for LBE simulations. The stability properties of some 2D LBE models are analyzed and compared with each other in the parameter space of the mean streaming velocity and the viscous relaxation time. The procedure described in this work can be applied to analyze other LBE models. As examples, LBE models with various

interpolation schemes are analyzed. Numerical results on shear flow with an initially discontinuous velocity profile (shock) with or without a constant streaming velocity are shown to demonstrate the dispersion effects in the LBE model; the results compare favorably with our theoretical analysis. We also show that whereas linear analysis of the LBE evolution operator is equivalent to Chapman-Enskog analysis in the long wave-length limit (wave vector $k = 0$), it can also provide results for large values of k. Such results are important for the stability and other hydrodynamic properties of the LBE method and cannot be obtained through Chapman-Enskog analysis.

Povitsky, Alex: *Improving jet reactor configuration for production of carbon nanotubes*. ICASE Report No. 2000-18, (NASA/CR-2000-210108), April 20, 2000, 25 pages. To be submitted to Computers and Fluids.

The jet mixing reactor has been proposed for the industrial production of fullerene carbon nanotubes. Here we study the flowfield of this reactor using the SIMPLER algorithm. Hot peripheral jets are used to enhance heating of the central jet by mixing with the ambiance of reactor. Numerous configurations of peripheral jets with various number of jets, distance between nozzles, angles between the central jet and a peripheral jet, and twisted configuration of nozzles are considered. Unlike the previous studies of jet mixing, the optimal configuration of peripheral jets produces strong non-uniformity of the central jet in a cross-section. The geometrical shape of reactor is designed to obtain a uniform temperature of a catalyst.

Allan, Brian G.: *A reduced order model of the linearized incompressible Navier-Stokes equations for the sensor/actuator placement problem*. ICASE Report No. 2000-19, (NASA/CR-2000-210110), April 20, 2000, 30 pages. Presented at the 3rd ASME/JSME Joint Fluids Engineering Conference, FEDSM99-6927, San Francisco, CA, July 1999.

A reduced order modeling approach of the Navier-Stokes equations is presented for the design of a distributed optimal feedback kernel. This approach is based on a Krylov subspace method where significant modes of the flow are captured in the model. This model is then used in an optimal feedback control design where sensing and actuation is performed on the entire flow field. This control design approach yields an optimal feedback kernel which provides insight into the placement of sensors and actuators in the flow field. As an evaluation of this approach, a two-dimensional shear layer and driven cavity flow are investigated.

Hart, Roger C., R. Jeffrey Balla, and G.C. Herring: *Optical measurement of the speed of sound in air over the temperature range 300-650 K*. ICASE Report No. 2000-20, (NASA/CR-2000-210114), April 25, 2000, 9 pages. Submitted to the Journal of the Acoustical Society of America.

Using laser-induced thermal acoustics (LITA), the speed of sound in room air (1 atm) is measured over the temperature range 300-650 K. Since the LITA apparatus maintains a fixed sound wavelength as temperature is varied, this temperature range simultaneously corresponds to a sound frequency range 10-15 MHz. The data are compared to a published model and typically agree within 0.1-0.4% at each of 21 temperatures.

Roberts, T.W., D. Sidilkover, and S.V. Tsynkov: *On the combined performance of non-local artificial boundary conditions with the new generation of advanced multigrid flow solvers.* ICASE Report No. 2000-21, (NASA/CR-2000-210115), April 28, 2000, 43 pages. To be submitted to Computers and Fluids.

We develop theoretically and implement numerically a unified flow solution methodology that combines the advantages relevant to two independent groups of methods in CFD that have recently proven successful: The new factorizable schemes for the equations of hydrodynamics that facilitate the construction of optimally convergent multigrid algorithms, and highly accurate global far-field artificial boundary conditions (ABCs). The primary result that we have obtained is the following. Global ABCs do not hamper the optimal (i.e., unimprovable) multigrid convergence rate pertinent to the solver. At the same time, contrary to the standard local ABCs, the solution accuracy provided by the global ABCs deteriorates very slightly or does not deteriorate at all when the computational domain shrinks, which clearly translates into substantial savings of computer resources.

Hart, Roger C., R. Jeffrey Balla, and G.C. Herring: *Simultaneous velocimetry and thermometry of air using nonresonant heterodyned laser-induced thermal acoustics.* ICASE Report No. 2000-22, (NASA/CR-2000-210118), May 5, 2000, 12 pages. Submitted to Applied Optics.

Non-resonant laser-induced thermal acoustics (LITA) is employed with heterodyne detection to measure temperature (285-295K) and a single component of velocity (20-150 m/s) in an atmospheric pressure, subsonic, unseeded air jet. Good agreement is found with pitot-tube measurements of velocity (0.2% at 150 m/s and 2% at 20 m/s) and the isentropic expansion model for temperature (0.3%).

Hysom, David, and Alex Pothen: *Efficient parallel computation of ILU(k) preconditioners.* ICASE Report No. 2000-23, (NASA/CR-2000-210120), May 5, 2000, 21 pages. Proceedings of SC'99, ACM, November 1999.

We report the development of a parallel algorithm for computing ILU preconditioners. The algorithm attains a high degree of parallelism through employment of a two-level ordering strategy, coupled with a subdomain graph constraint that regulates the location of nonzeros in the Schur complement. Experimental results include timings on four parallel platforms, for problems with up to 20 million unknowns running on up to 216 processors. The results support our theoretic analysis that the algorithm is highly scalable, for both preconditioner computation (factorization) and application (triangular solve) stages.

Hysom, David, and Alex Pothen: *Parallel ILU ordering and convergence relationships: Numerical experiments.* ICASE Report No. 2000-24, (NASA/CR-2000-210119), May 5, 2000, 23 pages. To be submitted to SIAM.

We recently developed a parallel algorithm for computing ILU preconditioners, which was presented at Super Computing 1999. The algorithm has been shown to be highly scalable, in terms of execution time required for preconditioner factorization and application, for problems with up to 20 million unknowns running on up to 216 processors. However, since the algorithm reorders the matrix, and it is widely known that ordering can significantly affect convergence, questions were raised concerning the quality of the computed preconditioners. In this report we present experimental results demonstrating that the orderings imposed by the algorithm do not significantly degrade convergence, as long as the number of unknowns per subdomain

is not too small. We report on two model problems, Poisson's equation, and a special case of the convection-diffusion equation, which other researchers have used for ordering and convergence studies. We show that convergence behavior is fairly flat as long as subdomains contain at least 512 nodes.

Arian, E., M. Fahl, and E.W. Sachs: *Trust-region proper orthogonal decomposition for flow control*. <u>ICASE Report No. 2000-25</u>, (NASA/CR-2000-210124), May 11, 2000, 23 pages. To be submitted to the Journal of Computational Physics.

The proper orthogonal decomposition (POD) is a model reduction technique for the simulation of physical processes governed by partial differential equations, e.g. fluid flows. It can also be used to develop reduced order control models. Fundamental is the computation of POD basis functions that represent the influence of the control action on the system in order to get a suitable control model. We present an approach where suitable reduced order models are derived successively and give global convergence results.

Lewis, Robert Michael, Virginia Torczon, and Michael W. Trosset: *Direct search methods: Then and now*. <u>ICASE Report No. 2000-26</u>, (NASA/CR-2000-210125), May 11, 2000, 21 pages. To appear in a special issue of the Journal of Computational and Applied Mathematics.

We discuss direct search methods for unconstrained optimization. We give a modern perspective on this classical family of derivative-free algorithms, focusing on the development of direct search methods during their golden age from 1960 to 1971. We discuss how direct search methods are characterized by the absence of the construction of a model of the objective. We then consider a number of the classical direct search methods and discuss what research in the intervening years has uncovered about these algorithms. In particular, while the original direct search methods were consciously based on straightforward heuristics, more recent analysis has shown that in most - but not all - cases these heuristics actually suffice to ensure global convergence of at least one subsequence of the sequence of iterates to a first-order stationary point of the objective function.

Montero, Ruben S., and Ignacio M. Llorente: *Robust multigrid algorithms for the incompressible Navier-Stokes equations*. <u>ICASE Report No. 2000-27</u>, (NASA/CR-2000-210126), May 12, 2000, 24 pages. To be submitted to the Journal of Computational Physics.

Anisotropies occur naturally in CFD where the simulation of small scale physical phenomena, such as boundary layers at high Reynolds numbers, causes the grid to be highly stretched leading to a slow down in convergence of multigrid methods. Several approaches aimed at making multigrid a robust solver have been proposed and analyzed in literature using the scalar diffusion equation. However, they have been rarely applied to solving more complicated models, like the incompressible Navier-Stokes equations. This paper contains the first published numerical results of the behavior of two popular robust multigrid approaches (alternating-plane smoothers combined with standard coarsening and plane implicit smoothers combined with semi-coarsening) for solving the 3-D incompressible Navier-Stokes equations in the simulation of the driven cavity and a boundary layer over a flat plate on a stretched grid. The discrete operator is obtained using a staggered-grid arrangement of variables with a finite volume technique and second-order accuracy is achieved using defect correction within the multigrid cycle. Grid size, grid stretching and Reynolds number are the factors considered in evaluating the robustness of the multigrid methods. Both approaches yield large increases in convergence rates over cell-implicit smoothers on stretched grids. The combination of

plane implicit smoothers and semi-coarsening was found to be fully robust in the flat plate simulation up to Reynolds numbers 10^6 and the best alternative in the driven cavity simulation for Reynolds numbers above 10^3. The alternating-plane approach exhibits a better behavior for lower Reynolds numbers (below to 10^3) in the driven cavity simulation. A parallel variant of the smoother, tri-plane ordering, presents a good trade-off between convergence and parallel properties.

Lüttgen, Gerald, and Michael Mendler: *The intuitionism behind Statecharts steps.* ICASE Report No. 2000-28, (NASA/CR-2000-210302), July 31, 2000, 45 pages. To appear in the 27th International Colloquium on Automata, Languages, and Programming (ICALP 2000).

The semantics of Statecharts macro steps, as introduced by Pnueli and Shalev, lacks compositionality. This report first analyzes the compositionality problem and traces it back to the invalidity of the Law of the Excluded Middle. It then characterizes the semantics via a particular class of linear, intuitionistic Kripke models, namely stabilization sequences. This yields, for the first time in the literature, a simple fully-abstract semantics which interprets Pnueli and Shalev's concept of failure naturally. The results not only give insight into the semantic subtleties of Statecharts, but also provide a basis for an implementation, for developing algebraic theories for macro steps, and for comparing different Statecharts variants.

Llorente, Ignacio M., Manuel Prieto-Matias, and Boris Diskin: *An efficient parallel multigrid solver for 3-d convection-dominated problems.* ICASE Report No. 2000-29, (NASA/CR-2000-210319), August 24, 2000, 33 pages. To be submitted to the Parallel Computing Journal.

Multigrid algorithms are known to be highly efficient in solving systems of elliptic equations. However, standard multigrid algorithms fail to achieve optimal grid-independent convergence rates in solving non-elliptic problems. In many practical cases, the non-elliptic part of a problem is represented by the convection operator. Downstream marching, when it is viable, is the simplest and most efficient way to solve this operator. However, in a parallel setting, the sequential nature of marching degrades the efficiency of the algorithm. The aim of this report is to present, evaluate and analyze an alternative highly parallel multigrid method for 3-D convection-dominated problems. This method employs semicoarsening, a four-color plane-implicit smoother, and discretization rules allowing the same cross-characteristic interactions on all the grids involved to be maintained. The resulting multigrid solver exhibits a fast grid-independent convergence rate for solving the convection-diffusion operator on cell-centered grids with stretching. The load imbalance below the critical level is the main source of inefficiency in its parallel implementation. A hybrid smoother that degrades the convergence properties of the method but improves its granularity has been found to be the best choice in a parallel setting. The numerical and parallel properties of the multigrid algorithm with the four-color and hybrid smoothers are studied on SGI Origin 2000 and Cray T3E systems.

Thomas, James L., Boris Diskin, Achi Brandt, and Jerry C. South, Jr.: *General framework for achieving textbook multigrid efficiency: One-dimensional Euler example.* ICASE Report No. 2000-30, (NASA/CR-2000-210320), August 24, 2000, 21 pages. Submitted to Frontiers of Computational Fluid Dynamics - 2000.

A general multigrid framework is discussed for obtaining textbook efficiency to solutions of the compressible Euler and Navier-Stokes equations in conservation law form. The general methodology relies on a distributed relaxation procedure to reduce errors in regular (smoothly varying) flow regions; separate and

distinct treatments for each of the factors (elliptic and/or hyperbolic) are used to attain optimal reductions of errors. Near boundaries and discontinuities (shocks), additional local relaxations of the conservative equations are necessary. Example calculations are made for the quasi-one-dimensional Euler equations; the calculations illustrate the general procedure.

Allan, Brian G., Jer-Nan Juang, David L. Raney, Avi Seifert, Latunia G. Pack, and Donald E. Brown: *Closed-loop separation control using oscillatory flow excitation.* ICASE Report No. 2000-32, (NASA/CR-2000-210324), August 30, 2000, 27 pages.

Design and implementation of a digital feedback controller for a flow control experiment was performed. The experiment was conducted in a cryogenic pressurized wind tunnel on a generic separated configuration at a chord Reynolds number of 16 million and a Mach number of 0.25. The model simulates the upper surface of a 20airfoil at zero angle-of-attack. A moderate favorable pressure gradient, up to 55pressure gradient which is relaxed towards the trailing edge. The turbulent separation bubble, behind the adverse pressure gradient, is then reduced by introducing oscillatory flow excitation just upstream of the point of flow separation. The degree of reduction in the separation region can be controlled by the amplitude of the oscillatory excitation. A feedback controller was designed to track a given trajectory for the desired degree of flow reattachment and to improve the transient behavior of the flow system. Closed-loop experiments demonstrated that the feedback controller was able to track step input commands and improve the transient behavior of the open-loop response.

Fibich, Gadi, and Semyon Tsynkov: *High-order two-way artificial boundary conditions for nonlinear wave propagation with backscattering.* ICASE Report No. 2000-33, (NASA/CR-2000-210326), September 6, 2000, 44 pages. To be submitted to the Journal of Computational Physics.

When solving linear scattering problems, one typically first solves for the impinging wave in the absence of obstacles. Then, using the linear superposition principle, the original problem is reduced to one which involves only the scattered wave (which is driven by the values of the impinging field at the surface of the obstacles). When the original domain is unbounded, special artificial boundary conditions (ABCs) have to be set at the outer (artificial) boundary of the finite computational domain, in order to guarantee the reflectionless propagation of waves through this external artificial boundary. The situation becomes conceptually different when the propagation equation is nonlinear. In this case the impinging and scattered waves can no longer be separated, and the problem has to be solved in its entirety. In particular, the boundary on which the incoming field values are prescribed, should transmit the given incoming waves in one direction and simultaneously be transparent to all the outgoing waves that travel in the opposite direction. We call this type of boundary condition two-way ABCs. In the paper, we construct the two-way ABCs for the nonlinear Helmholtz equation, which models a continuous-wave (CW) laser beam propagation in a medium with nonlinear index of refraction. In this case, the forward propagation of the beam is accompanied by backscattering, i.e., generation of waves in the opposite direction to that of the incoming signal. Our two-way ABCs generate no reflection of the backscattered waves and at the same time impose the correct values of the incoming wave. The ABCs are obtained in the framework of a fourth-order accurate discretization to the Helmholtz operator inside the computational domain. The fourth-order convergence of our methodology is corroborated experimentally by solving linear model problems. We also present solutions in the nonlinear case using the two-way ABC which, unlike the traditional Dirichlet boundary condition approach, allows for direct calculation of the magnitude of backscattering.

Al-Theneyan, Ahmed, Piyush Mehrotra, and Mohammad Zubair: *Enhancing Jini for use across non-multicastable networks.* ICASE Report No. 2000-34, (NASA/CR-2000-210329), September 20, 2000, 13 pages. To appear in Operating Systems Review.

Distributed heterogeneous systems are being increasingly used to execute a variety of large size simulation and computational problems. Resource management is one of the most important issues in building such systems. Recently, Sun introduced the Jini connection technology for building plug-and-play networks of resources. Jini relies on multicasting across the network for its internal protocols. However, in a distributed environment, such as the one under consideration here, multicasting may not be supported across the subnets for various reasons. In this paper we describe enhancements to Jini required to use it for building a middleware resource management system in a distributed environment that does not support multicasting. In particular, we introduce a lightweight service, called the Tunneling Service, which tunnels multicast messages across the subnets. We have implemented our mechanism and used it to successfully tunnel messages between subnets in a single domain and also between different domains. In this paper we describe our design choices and our implementation of the system.

Povitsky, Alex: *Numerical study of wave propagation in a non-uniform flow.* ICASE Report No. 2000-35, (NASA/CR-2000-210533), September 26, 2000, 31 pages. To be submitted to the Journal of Computational Physics.

The propagation of acoustic waves originating from cylindrical and spherical pulses, in a non-uniform mean flow, and in the presence of a reflecting wall is investigated by Hardin and Pope approach using compact approximation of spatial derivatives. The 2-D and 3-D stagnation flows and a flow around a cylinder are taken as prototypes of real world flows with strong gradients of mean pressure and velocity. The intensity and directivity of acoustic wave patterns appear to be quite different from the benchmark solutions obtained in a static environment for the same geometry. The physical reasons for amplification and weakening of sound are discussed in terms of dynamics of wave profile and redistribution of acoustic energy and its potential and kinetic components. For an acoustic wave in the flow around a cylinder, the observed mean acoustic pressure is approximately doubled (upstream pulse position) and halved (downstream pulse position) in comparison with the sound propagation in static ambient conditions.

Dolan, Elizabeth D., Robert Michael Lewis, and Virginia Torczon: *On the local convergence of pattern search.* ICASE Report No. 2000-36, (NASA/CR-2000-210535), September 26, 2000, 20 pages. Submitted to the SIAM Journal on Optimization.

We examine the local convergence properties of pattern search methods, complementing the previously established global convergence properties for this class of algorithms. We show that the step-length control parameter which appears in the definition of pattern search algorithms provides a reliable asymptotic measure of first-order stationarity. This gives an analytical justification for a traditional stopping criterion for pattern search methods. Using this measure of first-order stationarity, we analyze the behavior of pattern search in the neighborhood of an isolated local minimizer. We show that a recognizable subsequence converges r-linearly to the minimizer.

ICASE COLLOQUIA

Name/Affiliation/Title	Date
Walter Vogler, Universitaet Augsburg, Germany "Efficiency of Asynchronous Systems"	April 13
Bruce Hendrickson, Sandia National Labs "Devising Effective Parallel Algorithms"	April 18

Bruce M. Boghosian, Center for Computational Science, Boston University
  ICASE Series on Computational Nanotechnology: "A Macroscopic, Mesoscopic and
  Microscopic Look at Amphiphilic Fluids"
	April 19

Deepak Srivastava, CSC/NAS, NASA Ames Research Center
  ICASE Series on Computational Nanotechnology: "Nanotechnology of Molecular
  Electronics and Machines: Carbon Nanotubes"
	May 3

Reto Luginbuehl, University of Washington, Seattle "Bioengineering the Way to Smart Nanomaterials: Phase Transitions at the Nanoscale"	May 5
Mario Rodriguez, Massachusetts Institute of Technology "Identifying Mode Confusion Potential in Software Design"	May 8
Michael Mendler, Sheffield University, United Kingdom "What is in a Statecharts Step, Exactly?"	May 18
Suvranu De, Massachusetts Institute of Technology "The Method of Finite Spheres"	May 26
Michael Barton, Analytical Methods, Inc., Redmond, WA "The Role of Instability in Modeling Wall-bounded Turbulent Flows"	June 8
Peter Habermehl, University Paris 7, Paris, France "On the Verification of Infinite-state Systems"	June 9

Sivaram Arepalli, G.B. Tech/Lockheed Martin
  "Progress in Production, Purification and Applications of Single Wall Carbon
  Nanotubes at NASA/JSC"
	June 13

Alfons Geser, University of Tubingen, Germany "More Correct Hardware"	June 19

Name/Affiliation/Title	Date
Bassam Bamieh, University of California, Santa Barbara "Modeling and Control of Transition to Turbulence in Wall Bounded Shear Flows"	June 20
Andrew Adams, University of St. Andrews, Scotland "Real Number Theorem Proving in PVS, with Transcendental Function Support"	June 26
Ana Cavalli, Institut National des Telecomunications, France "Application of Formal Methods to Conformance Test Generation"	June 30

Raymond Ristorcelli, Los Alamos National Laboratory
    "Turbulent Dispersion and Turbulent Diffusivities in the Presence of Stationary Mean
    Deformations"
	July 5

Gilles Dowek, INRIA - Rocquencourt, France "What are Explicit Proof-terms Needed For?"	July 6
Steven Cox, University of Florida, Gainesville "Global Optimization of the High Speed Civil Transport"	July 14

Myron Ginsberg, HPC Research & Education and University of Michigan
    "Opportunity to Utilize NASA-supported Computer Technology to Improve the
    Performance for Large Industrial Applications"
	July 26

Alex Povitsky, ICASE "Aeroacoustics of a Non-uniform Mean Flow"	July 27
Peter Bernard, University of Maryland, College Park "The Structure of Turbulent Boundary Layers"	August 2
David Montgomery, Dartmouth College "Turbulence Computations with Viscous Boundary Conditions"	August 2
Murali Rangarajan, University of Cincinnati "Analysis of Requirements Through Automated Application of Proof Obligations"	August 7
Sharath Girimaji, Texas A&M University "Turbulence Modeling of Complex Flows: An Integrated Approach"	August 8
Yukio Kaneda, Nagoya University, Japan "Some Results of High-resolution DNS of Homogeneous and 'Isotropic' Turbulence"	August 9

Name/Affiliation/Title	Date

Semyon Tsynkov, Tel Aviv University, Israel
  "Non-deteriorating Numerical Methods for the Propagation of Waves Over
  Unbounded Domains"
	August 10

Tom Girardeau, Georgia Institute of Technology "Synthesis and Dynamics of Poly(ethylene glycol)/Cyclodextrin Rotaxanes"	August 14
Ching Loh, Taitech Inc. and NASA Glenn Research Center "Computational Aeroacoustics by the Space-time CE/SE Method"	August 15
Eli Turkel, Tel Aviv University, Israel "Robust Preconditioning Methods"	August 23
Saul Abarbanel, Tel Aviv University, Israel "On the Analysis and Construction of Absorbing Layers in CEM and CFD"	August 24

Jason Rouse, Lehigh University
  "Understanding and Controlling the Swellability of Polyelectrolyte/Clay Multilayer
  Films"
	August 25

Carlo Bottasso, Politecnico di Milano, Italy "Aerodynamic and Structural Modeling of Rotorcraft Systems"	August 28

Pedro Camanho, University of Porto, Portugal
  "A Progressive Damage Model for Mechanically Fastened Joints in Composite
  Laminates"
	August 29

Jean-Pierre Bertoglio, Ecole Centrale de Lyon, France "Towards Applications of Spectral Turbulence Models to CFD"	September 5
Peter Bakker, Delft University of Technology, The Netherlands "Topology of Three-dimensional Separations"	September 7
Robert Yates, Lawrence Livermore National Laboratory "Denotational Semantics of Dataflow Networks with Nonmonotonic Processes"	September 8
Cord Rossow, German Aerospace Center "On the Extension of Compressible Flow Solvers to Incompressible Flows"	September 13

Tim Clark, Los Alamos National Laboratory
  "A Lattice Boltzmann Method Applied to the Turbulent Rayleigh-Taylor Mixing
  Layer"
	September 18

Name/Affiliation/Title	Date

Gerhard Goldbeck-Wood, Polymer Consortium Molecular Simulations, Inc., UK
  "Mesoscale Simulations of Polymers and Soft Materials: Software Tools and
  Applications"
	September 21

Kiyosi Horiuti, Tokyo Institute of Technology
  "Analysis of the Structures Responsible for Subgrid-scale Energy Transfer in Large
  Eddy Simulation"
	September 26

Paul Hovland, Argonne National Laboratory
  "Matrix-free Newton-Krylov Methods Using a Hybrid Automatic Differentiation-
  finite Difference Strategy"
	September 28

ICASE SUMMER ACTIVITIES

The summer program for 2000 included the following visitors:

VISITOR and AREA OF RESEARCH	AFFILIATION	DATE OF VISIT
Abarbanel, Saul *Applied & Numerical Math*	Tel Aviv University, Israel	7/03 – 9/01
Attar, Peter J. *Structures and Materials*	Duke University	6/01 – 7/28
Avihar, Edan A. *Fluid Mechanics*	Tel Aviv University, Israel	7/31 – 9/01
Baggag, Abdelkader *Computer Science*	Purdue University	6/05 – 9/08
Banks, H. Thomas *Applied & Numerical Math*	North Carolina State University	6/05 – 6/09
Barton, J. Michael *Fluid Mechanics*	Analytical Methods, Inc.	6/05 – 6/09
Bernard, Peter S. *Fluid Mechanics*	University of Maryland	8/01 – 8/04
Bertoglio, Jean-Pierre E. *Fluid Mechanics*	Universite Claude Bernard - Lyon 1, France	8/28 – 9/08
Bottasso, Carlo L. *Applied & Numerical Math*	Politecnico di Milano, Italy	8/21 – 9/29
Brandt, Achi *Applied & Numerical Math*	The Weizmann Institute of Science, Israel	7/10 – 7/28
Camanho, Pedro M. *Structures*	University of Portugal	7/31 – 9/29

VISITOR and AREA OF RESEARCH	AFFILIATION	DATE OF VISIT
Chapman, Barbara M. *Computer Science*	University of Houston	5/15 – 6/09 7/24 – 8/04
Chepfer, Helene *Atmospheric Sciences*	University of Paris 6, France	7/03 – 9/30
Ciardo, Gianfranco *Computer Science*	The College of William & Mary	5/31 – 6/09 8/14 – 8/18
Clark, Timothy *Fluid Mechanics*	Los Alamos National Laboratory	9/06 – 9/20
Cox, Steven E. *Applied & Numerical Math*	University of Florida, Gainesville	5/15 – 7/28
Criminale, William *Fluid Mechanics*	University of Washington, Seattle	6/19 – 6/30
d'Humieres, Dominique G. *Computer Science*	Laboratoire de Physique Statistique, France	7/31 – 9/01
Ditkowski, Adi *Applied & Numerical Math*	Brown University	8/07 – 8/18
Dowek, Gilles A. *Computer Science*	INRIA, France	6/28 – 7/07
Dowell, Earl *Structures and Materials*	Duke University	7/10 – 7/12
Girimaji, Sharath S. *Fluid Mechanics*	Texas A&M University	7/03 – 8/18 9/19 – 9/21
Goozee, Richard *Fluid Mechanics*	The University of Queensland, Australia	9/25 – 10/06
Gotoh, Toshiyuki *Fluid Mechanics*	Nagoya Institute of Technology, Japan	7/31 – 8/04

VISITOR and AREA OF RESEARCH	AFFILIATION	DATE OF VISIT
Gottlieb, David *Applied & Numerical Math*	Brown University	7/10 – 7/21
Griffith, D. Todd *Structures and Materials*	University of Kentucky	5/30 – 8/04
Grohs, Joshua W. *Structures and Materials*	Virginia Polytechnic Institute and State University	5/15 – 8/16
Habermehl, Peter Franz-Joseph *Computer Science*	University of Paris 7, France	5/30 – 6/ 09
Hafez, Mohammed *Applied & Numerical Math*	University of California, Davis	7/31 – 8/04
Hattori, Yuji *Applied & Numerical Math*	Kyushu Institute of Technology, Japan	8/21 – 8/25
Hesthaven, Jan *Applied & Numerical Math*	Brown University	7/24 – 7/28 8/07 – 8/18
Horiuchi, Kiyoshi *Fluid Mechanics*	Tokyo Institute of Technology, Japan	9/18 – 9/29
Hu, Fang *Applied & Numerical Math*	Old Dominion University	5/08 – 6/16
Huedo-Cuesta, Eduardo *Applied & Numerical Math*	Universidad Complutense, Spain	7/03 – 7/28
Jakatdar, Amol S. *Computer Science*	Old Dominion University	5/22 – 8/25
Kandil, Osama *Applied & Numerical Math*	Old Dominion University	5/23 – 6/29 Intermittently
Kaneda, Yukio *Fluid Mechanics*	Nagoya University, Japan	7/31 – 8/11

VISITOR and AREA OF RESEARCH	AFFILIATION	DATE OF VISIT
Keyes, David *Computer Science*	Old Dominion University	6/01 – 8/31 Intermittently
Kholodar, Denis B. *Structures and Materials*	Duke University	6/26 – 8/18
Kulkarni, Prashanth P. *Computer Science*	Old Dominion University	5/22 – 8/25
Lallemand, Pierre *Computer Science*	Universita Paris Sud, France	9/25 – 11/03
Lee, Min Hee *Materials*	Inha University, Korea	7/03 – 8/30
Li, Yawei *Computer Science*	University of Florida, Gainesville	5/22 – 8/10
Llorente, Ignacio M. *Applied & Numerical Math*	Universidad Complutense, Spain	7/03 – 7/28
Loh, Ken *Fluid Mechanics*	Taitech, Inc.	8/14 – 8/18
Longman, Richard *Structures and Materials*	Columbia University	5/01 – 5/05 5/15 – 6/16 7/03 – 9/01
Mattsson, Ken R. *Applied & Numerical Math*	The Aeronautical Research Institute of Sweden	8/21 – 9/15
Mei, Renwei *Computer Science*	University of Florida, Gainesville	7/21 – 8/18
Mendler, Michael V. *Computer Science*	Sheffield University, United Kingdom	5/15 – 5/26
Milder, Seth *Computer Science*	George Mason University	5/23 – 8/04

VISITOR and AREA OF RESEARCH	AFFILIATION	DATE OF VISIT
Montero, Ruben S. *Applied & Numerical Math*	Universidad Complutense, Spain	7/03 – 7/28
Naguib, Ahmed *Structures and Materials*	Michigan State University	6/05 – 6/16
Nordstrom, Jan M. *Applied & Numerical Math*	The Aeronautical Research Institute of Sweden	6/10 – 7/15
Patil, Amit J. *Computer Science*	University of Houston	5/15 – 9/01
Pothen, Alex *Computer Science*	Old Dominion University	6/01 – 8/31 Intermittently
Prabhakar, Achal *Computer Science*	University of Houston	5/15 – 9/01
Prieto-Matias, Manuel *Applied & Numerical Math*	Universidad Complutense, Spain	7/03 – 7/28
Qi, Dewei *Fluid Mechanics*	Western Michigan University	7/10 – 8/25
Ristorcelli, J. Raymond *Fluid Mechanics*	Los Alamos National Laboratory	7/03 – 7/07
Rossow, Cord C. *Applied & Numerical Math*	German Aerospace Center	8/18 – 9/15
Ryaben'kii, Viktor S. *Applied & Numerical Math*	Russian Academy of Sciences	6/26 – 7/10
Seifert, Avraham *Fluid Mechanics*	Tel Aviv University, Israel	6/15 – 9/01
Shu, Chi-Wang *Applied & Numerical Math*	Brown University	7/17 – 8/04

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Tsynkov, Semyon *Applied & Numerical Math*	Tel Aviv University, Israel	6/26 – 8/15
Turkel, Eli *Applied & Numerical Math*	Tel Aviv University, Israel	6/19 – 8/25
Wang, Lian-Ping *Fluid Mechanics*	University of Delaware	6/05 – 6/23 7/31 – 8/11
Warburton, Timothy C. *Applied & Numerical Math*	Brown University	5/08 – 5/12 6/12 – 8/11
Woodruff, Stephen L. *Fluid Mechanics*	Florida State University	6/19 – 6/30
Xu, Kun *Fluid Mechanics*	The Hong Kong University of Science and Technology	6/05 – 6/30
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Zhou, Ye *Fluid Mechanics*	Lawrence Livermore National Laboratory	9/11 – 9/15

OTHER ACTIVITIES

On August 3–4, 2000, ICASE sponsored a Workshop on Kinetic Methods for CFD and Parallel Computing at ICASE. The purposes of the Workshop were (1) to review the LBE method, (2) to evaluate the range of its potential applications to CFD, (3) to discuss the important issues which remain to be solved in the future and (4) to assess the future of the method. A number of experts on the LBE method and CFD gave presentations.

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13. ABSTRACT *(Maximum 200 words)*

This report summarizes research conducted at ICASE in applied mathematics, fluid mechanics, computer science, and structures and material sciences during the period April 1, 2000 through September 30, 2000.

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