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Semiannual Report

October 1, 2000 through March 31, 2001

May 2001

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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 October 1, 2000 through March 31, 2001 is given in the Reports and Abstracts section, which follows a brief description of the research in progress.

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RESEARCH IN PROGRESS

APPLIED AND NUMERICAL MATHEMATICS

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 inlet applications.

Using a compressible Navier-Stokes code developed at NASA, numerical simulations of micro-vortex generators and vortex generator jets on a flat plate and ramp have been performed. These simulations are being followed by wind tunnel experiments conducted at NASA LaRC. The wind tunnel experiments will be used to validate the numerical simulations of the vortex generators. 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. The goal is for the boundary condition to 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.

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) using the ICASE PC cluster, Coral.

Nonlinear suboptimal feedback control

Scott C. Beeler

Feedback control of nonlinear systems of ODEs is an area in which many methods have been proposed. An optimal feedback control solution is usually impossible for nonlinear systems, so various suboptimal approaches are used. These techniques can be applied to aircraft guidance and control problems including abort-type scenarios and control effector impairment situations. This work will focus on the development and study of suboptimal feedback control methods for problems of this type involving nonlinear dynamics and control inputs.

We have begun studying the methods of dynamic inversion and the state-dependent Riccati equation (SDRE) for feedback control. A preliminary version of the SDRE algorithm has been implemented for the nonlinear-dynamics-and-input systems we are interested in, and the code is being tested and modified. Early results show promise that further development of the method will produce desirable algorithm performance.

Future efforts will work on modifications to the SDRE method to improve its effectiveness and implementation of the dynamic inversion method (and possibly others) in code as well. The performance, stability, and robustness of the methods used will be studied. Application of these control techniques to aircraft guidance models is also planned for the future.

This work is done in collaboration with D. Moerder (NASA Langley).

Textbook multigrid efficiency for CFD simulations

Boris Diskin

A multigrid method is defined as having textbook multigrid efficiency (TME) if the solutions to the governing system of equations are attained in a computational work that is a small (less than 10) multiple of the operation count in one target-grid residual evaluation. The way to achieve this efficiency for the Reynolds-averaged Navier-Stokes (RANS) equations is the distributed relaxation approach separating different factors contributing to the system and treating them optimally. The design of a distributed relaxation scheme can be significantly simplified if the target discretization possesses two properties: (1) The discretization of the corresponding principally linearized system is factorizable, i.e., the determinant of the principal part of the discrete matrix operator can be represented as a product of discrete scalar factors, each of them approximating a corresponding factor of the differential matrix operator determinant. (2) The obtained scalar factor discretizations reflect the physical anisotropies and are efficiently solvable. In the last six months, the research has been focused on deriving and analyzing new factorizable schemes and extending TME to conservative discretizations of the Euler equations.

A collocated-grid scheme using second-order central differencing for the pressure gradient and the velocity divergence has been explored. The scheme being applied for compressible Euler system is factorizable in multiple dimensions. A typical difficulty associated with this type of scheme is a poor measure of h-ellipticity in the discrete approximation for the full-potential factor of the system determinant. A mechanism allowing to improve the h-ellipticity measure by obtaining *any* desired discretizations for the full-potential factor of the system determinant without compromising the scheme factorizability has been developed. The derived h-elliptic factorizable discretization has been analyzed and tested.

A direct correspondence between the primitive variable interpolations for calculating fluxes in conservative finite-volume discretizations and stencils of the discretized derivatives in the nonconservative formulation has been established. Based on this correspondence, we have arrived at a conservative discretization that is very efficiently solved with a multigrid method involving a distributed relaxation scheme based on a nonconservative formulation. TME has been demonstrated for conservative discretization of the quasi-one-dimensional Euler equations.

A review summarizing the progress and outlining a road map for achieving TME for general problem governed by RANS equations has been prepared.

Currently efforts are directed to demonstrate TME for multidimensional applications including general boundary conditions and captured shocks.

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

High-order unstructured grid methods for conservation laws

Jan Hesthaven

The increasing emphasis on the modeling of unsteady problems over very long times and in computationally very large domains requires that accurate and efficient high-order methods be developed for such problems. The geometric complexity, however, of problems of scientific and industrial interest makes such developments a very significant challenge. Unfortunately, the use of high-order/spectral methods, which seems natural due to their superior numerical properties for wave propagation and their highly efficient discretization of large computational domains, such methods have traditionally been restricted to domains that can be smoothly mapped to a unit cube, thus allowing for the construction of a well-behaved multi-dimensional approximation using tensor products. As is well known, however, automated grid generation and adaptive meshing is greatly complicated by using only hexahedrals as the fundamental element in a general curvilinear multi-element formulation.

In a long-term effort to address and, eventually, overcome these restrictions we have continued the developments of accurate high-order/spectral methods on triangles and tetrahedra. One of the novel aspects of this effort is the representation of the approximate solutions using truly multi-variate Lagrange interpolation polynomials much in the spirit of classical spectral collocation methods, resulting in highly efficient and simple implementations. The conservation law itself is satisfied in a weak sense, with the boundary conditions only weakly through a penalty term. As we have shown recently, such formulations are highly general, flexible, and robust and lend themselves well to analysis of conservation and convergence as well as highly efficient parallel implementations.

We have recently completed a thorough testing of a fully functional framework for the solution of three-dimensional conservation laws with particular emphasis being paid to Maxwell's equations and scattering and penetration applications. This successful testing period paves the way for the continuation of the effort to address techniques for handling strong shocks, efficient time-advancement, and, eventually, space-time adaptivity for geometrically complex three-dimensional problems.

This is a collaborative effort, involving David Gottlieb and members of the Electromagnetics branch at NASA Langley.

Robust optimization including model uncertainties and reliability constraints
Luc Huyse

During the preliminary design stages only crude estimates are known for many model parameters in a particular problem. Deterministic optimization using these tentative parameter values can lead to overly optimistic projections of the as-built performance. It is quite typical for the optimal design to be fairly sensitive to fluctuations in model parameters. This research develops statistical optimization methods that directly account for parameter uncertainty.

In our formulation we model the uncertainties explicitly as random variables. Based on the statistical decision theory we developed a theoretical framework for robust (or stochastic) optimization. The objective of robust optimization is to find the design with the best lifetime performance. Using analytic approximations of the stochastic integral we were able to formulate a new deterministic equivalent problem (DEP). The optimization of the DEP requires higher-order derivatives but provides additional insight in the problem. We also developed a new algorithm for the full integration of the stochastic integral. Careful analysis thereof has revealed the superiority of this method over traditional multi-point design. Statistical decision theory provides a theoretical basis for the selection of the design conditions and their respective weights in the overall objective function.

The newly developed techniques were applied to an airfoil optimization problem, using NASA Langley's 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 demonstration problem. The approximate second-order formulation leads to a considerable improvement of the robustness when compared to a deterministic single-point design. We also compared the results of the new stochastic integration algorithm to traditional multi-point design using an optimal set of weights. Our experience has been that the new algorithm is capable of drastically reducing the so-called "drag-troughs." 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). The researchers are indebted to Wu Li (Old Dominion University) for his parallelization efforts of our modifications to NASA's FUN2D code.

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 Gflop/s, with sustained performance on CFD applications of about 1.5 Gflop/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.

Extensive testing of MPI performance using LAM, MPI/Pro, MPICH, and MVICH libraries over TCP (Fast Ethernet) and VIA (Giganet cLAN) transports was completed in October 2000. The measurements reveal significantly lower MPI latency of polling implementations although interrupt driven receive can overlap computation and communication and thus, deliver higher performance in some applications.

To monitor Coral's performance, we wrote our own cluster node monitor utility whose main benefit is extremely low overhead and the ability to monitor Giganet cLAN traffic.

The Coral cluster usage has dramatically increased this year. Since October of 2000, Coral's 102 CPUs delivered 19,527 CPU*hours of computing per month on the average. 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.

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. Based on the mathematical foundations of a new active technique for control of the time-harmonic acoustic disturbances, we are developing a numerical technique that will suggest good locations for sensors and actuators.

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: only the perimeter data (the total acoustic field and its normal derivative) are required. The mathematical apparatus used for deriving the general solution is closely connected to the concepts of generalized potentials and boundary projections of Calderon's type. This exact general solution can be computed at polynomial cost, and good actuator locations determined via a procedure which progressively restricts the locations where actuators may be placed. While the actuator placement problem is still computationally challenging, this approach is much more efficient than the alternatives, which lead combinatorial computational cost. We are in the process of developing a numerical procedure that reduces the number of candidate locations based on the minimization of the control effort.

In order to develop numerically computable solutions, we intend 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.

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. Isotropic decaying turbulence has been simulated on grids of various resolutions and comparisons of the decaying turbulence spectra with experimental results has been made. These results emphasize the effect artificial dissipation can have on the turbulence spectra and are currently being used to provide guidelines for the maximum permissible levels of dissipation for properly capturing the inertial range of turbulence scales. These computations are being performed on the ICASE PC cluster, Coral.

Higher resolution simulations are currently underway as well as simulations for a stalled wing and flow over a bluff landing-gear geometry.

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

Linear and nonlinear unstructured multigrid algorithms for the solution of radiation hydrodynamic problems
Dimitri J. Mavriplis

Under the ASCI program, the simulation of radiation transport and hydrodynamic phenomena have been identified as one of the most time-consuming elements within large simulation codes. The objective of this research is to investigate the relative benefits of unstructured multigrid algorithms used as linear solvers, nonlinear solvers, or preconditioners in efficiently solving unsteady radiation hydrodynamics problems, in the radiation diffusion limit.

A linear version and a nonlinear version of an agglomeration multigrid algorithm have been developed and applied to the two-dimensional radiation diffusion system, and the two-dimensional Navier-Stokes equations, both as solvers directly, and as preconditioners for a Newton-Krylov method.

Theoretical and numerical evidence is given which shows the equivalence of the linear and nonlinear multigrid methods in the asymptotic convergence region, in terms of multigrid cycles. However, for complex nonlinear operators, the linear multigrid approach provides lower cost multigrid cycles and therefore results in a more efficient algorithm. In cases where an inexact linearization is employed, overall solution efficiency is determined by the cost of a linear versus a nonlinear multigrid cycle, and the numerical convergence effectiveness of the inexact linear system. In such cases, using the linear or nonlinear multigrid methods as preconditioners to a Newton-Krylov method can result in large gains in efficiency.

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.

Linear parameter varying control of an aircraft under adverse conditions
Jong-Yeob Shin

Recent aircraft flight control design research has concentrated on the development of control systems that stabilize an aircraft robustly and allow to recover aircraft performance under adverse conditions (actuator/sensor/engine failures and bad weather). One promising approach to designing robust flight control systems (FCS) for an aircraft under adverse conditions is use of linear parameter varying (LPV) control synthesis, since aircraft dynamics vary significantly according to angle of attack, velocity, dynamic pressure, and so on. Aircraft dynamics can be described by a quasi-LPV model with scheduling parameters, which are also states of the dynamics model.

We have currently formulated a quasi-LPV model of aircraft dynamics including longitudinal and lateral-directional axes by a function substitution method that uses linear programming optimization. In order to apply LPV control synthesis for designing a robust FCS, a quasi-LPV model of aircraft dynamics, and a model of aircraft at failure cases are required. We are currently investigating control surface failure cases and preliminary dynamic models to facilitate possible failures.

In future work, failure cases will be parameterized and integrated into LPV controller synthesis for an aircraft FCS. Due to an increasing number of scheduling parameters in LPV controller synthesis for actuator and/or sensor failure cases, blending approach of LPV controller synthesis is required to develop an LPV controller that stabilizes an aircraft robustly under adverse conditions and also minimizes aircraft performance degradation.

This research was conducted in collaboration with Christine Belcastro (NASA Langley).

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 mesh that 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 coupled with multigrid, which hopefully would dramatically increase the efficiency of time stepping for time-dependent simulations and make convergence to steady states faster, both for convection problems and for convection-diffusion problems. Jointly with Jue Yan, we have been developing a local discontinuous Galerkin method for KdV-type equations containing third derivative terms. The scheme is especially suitable for problems containing nonlinear first derivative terms and a linear or nonlinear term with small coefficients.

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

Linear programming approaches to potential function modeling for protein folding

Michael Wagner

The protein folding problem is one of the grand challenges in computational science. The recent unveiling of the human genome and the conclusion that the number of human genes is much smaller than originally thought makes the study of proteins, their function, and interactions even more important. Our effort focuses on finding good models for the energy (or potential) function that drives the folding process of proteins. There are a variety of different functional models that require the knowledge of certain parameters that appear linearly. We use linear programming to find these parameters so that the model predicts the structure of known proteins in the publicly available databases correctly. This model can then be used for structure recognition for unknown sequences or for ab-initio folding.

The resulting linear programming problems have a few hundred variables, tens (possibly hundreds) of millions of constraints and a completely dense constraint matrix and are, thus, rather challenging to solve. By exploiting LP duality theory and the structure of the problem we are able to tackle these problems by adapting the interior point solver PCx (by Czyzyk, Mehrotra, Wagner and Wright, Argonne National Lab). We use dense parallel linear algebra and a streamlined interface to Loopp (by Elber and Meller, Cornell University), the software that generates the data. We were able to solve problems with ten million constraints in 300 parameters in a few hours on 48 nodes of the Intel Pentium PC-based Velocity Cluster at the Cornell Theory Center. Details of the results were presented at the SIAM Conference on Parallel Processing in Portsmouth, VA in March of this year, a paper was submitted to the Journal of Computational Chemistry. A second, more technical writeup is in progress and will be submitted to a computational optimization journal.

Future work will include optimizing the code to allow for even larger scale problems. We believe that solving problems with 50 million constraints is well within our reach, scaling up by another order of magnitude is the next step. We are in the process of testing different functional models, the approach holds much promise to the computational chemists and biologists in the group. Finally, we are in the process of adapting the parallel LP solver to allow for the efficient solution of general LPs. Given time we will develop a version of the algorithm that is entirely independent of the underlying data structures and BLAS implementation.

This is joint work with Jarek Meller and Ron Elber (Cornell Computer Science Department).

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 particulate flow problem, 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 particle motions). 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 it 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) that 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.

This research was conducted in collaboration with Ahmed Sameh (Purdue University).

Nautilus problem solving environment (PSE)

Thomas M. Eidson

Programming efficiency has been a problem in the scientific community for many years. Attempting to extract good performance from state-of-the-art high-performance architectures can be very time consuming. The rapid changes in computing environments has inhibited the development of standards and synergetic tools. Distributed computing, especially on Grids, makes the situation worse as heterogeneous computing environments at multiple sites necessitate that an enormous amount of detail must be managed by the programmer. The situation is further complicated by the fact that larger, composite applications are becoming more common. The Nautilus Project will provide a PSE implementation both to study various PSE design issues related to programming composite applications and to provide a framework for ICASE and NASA projects to experiment with application development using a Grid/distributed programming model.

The Nautilus PSE is targeted for usage by scientific application developers who work with research-oriented applications. The programming model for Nautilus will be based on component programming concepts. Currently, the evolving specification being developed by the Common Component Architecture

(CCA) Forum is being targeted. The Nautilus design is a combination of concepts from the LAWE System (a prototype previously developed via a NASA SBIR) and concepts from the CCA Forum. A number of prototypes are under development that are being used to support the CCA specification development. Several of these prototypes are being studied for possible use as the starting point for the Nautilus development. The Nautilus design extends these basic CCA implementations to provide a richer, intuitive set of programming abstractions so that more sophisticated distributed applications can be developed. The Nautilus design also provides a more complete set of tools, in particular, to support the programming style of the research scientist. A first phase Nautilus design has been completed and a paper is being written to describe the concepts and details of that design. Two CCA prototypes, CCAFFEINE and CCAT, are being installed.

First, CCAFFEINE and CCAT will be studied and application developers will be recruited to use and to evaluate these programming frameworks. Because these prototypes are developed in a component style, the goal is to evolve one of these prototypes to the Nautilus design by gradually replacing its components. Interaction with the Grid Forum and the CCA Forum will continue so that Nautilus will include compatibility with any new standards or technology in the area of scientific PSEs for Grid computing.

Shared programming definition (SPD) project

Thomas M. Eidson

A number of Problem Solving Environments (PSE) for creating distributed applications on heterogeneous networks are under development. While many of these PSEs have similarities, such as a component-like design, they each target different application and user needs and they generally use different programming models. Since distributed applications are often composed of or developed from applications created in local environments, a degree of consistency across these different programming domains will aid code transfer. While some diversity is desired to meet the variety of different needs, application developers will benefit from some degree of homogeneity in the design and use of different PSEs.

The Advanced Programming Models Working Group (APM) of the Grid Forum is chartered with the general task of recommending standards for Grid programming. A major focus of this group has been on component-based PSEs and on understanding the similarity and differences between the various existing research prototypes. Currently, a project, led by this author, is underway to gather information in a format to support a more detailed comparison of these prototypes. As a separate effort, an ICASE/NASA Workshop on Grid Programming has been planned for April 12 and 13 to further investigate Grid programming. A small group of PSE developers with expertise in a diverse set of approaches have been invited. The format will be to discuss relevant topics with the goal of formulating a suggested approach (possibly a project to recommend to NASA) to address issues such as the need for standards to support portability and interoperability of applications across different PSEs. A proposal for Shared Programming Definitions has been developed that has/will be discussed with both of the above groups.

Work with the Grid Forum will continue with the goal of developing standards for PSEs to support programming efficiency. The results of the first workshop will be formulated into a report and a presentation. A second workshop will be organized where these results are presented to and discussed with NASA personnel.

Tidewater Research Grid Project (TRGP)

Thomas M. Eidson

A recent trend in scientific computing has been the increased use of Grid computing. Grid computing is defined as the development and execution of distributed applications across wide-area networks where administrative and security issues are non-trivial. Very high-performance computers have become increasingly expensive and researchers are looking to the use of large numbers of lower-performance machines to meet their computational needs. Unfortunately, these machines are located at various locations where the Internet (or an internet) is involved, thus the need for Grid computing. The Globus Project (Argonne National Lab and ISI Lab of Univ. of Southern California) has developed the Globus Toolkit to provide core services to run a computational Grid.

The TRGP is a project to set up a computational Grid for ICASE access. Currently, the other member organizations include labs from Old Dominion University and The College of William & Mary. A preliminary installation of the Globus Toolkit has been installed and tested at ICASE. Several meetings with representatives from member organizations have been held to agree on policies. This included the use of PGP to provide a system of trusted communication between the various organizations who are physically distributed. June 2001 has been set as a target date for initial operation.

A final installation of Globus must be completed. Communication, account management, and other procedures must be finalized. Documentation must be completed. Once these steps are done, the TRGP will be made available to the member organizations. Joint projects that use multiple sites will need to be encouraged as the success of such projects will be the measure of the success of the TRGP.

Verification of air traffic management systems

Gilles Dowek, Alfons Geser, and César Muñoz

Safety assessment of new air traffic management systems is a main issue for civil aviation authorities. Standard techniques such as testing and simulation have serious limitations in new systems that are significantly more autonomous than the older ones. The aim of this work is to develop formal techniques to verify the correctness of systems and concepts developed under the Distributed Air/Ground Traffic Management (DAG-TM) project at NASA.

Avionics systems are particularly difficult to verify because of their hybrid nature: they involve at the same time continuous behaviors, e.g., aircraft trajectories, and discrete ones, e.g., logical control. We have developed a continuous model of aircraft trajectories that is well suited for formal verification. The model consists of a mathematical model of the dynamics of an aircraft based on physical laws of kinematics and a set of theories dealing with standard calculus and continuous mathematics. Model and theories are written in the specification language of PVS. An alerting algorithm for parallel landing has been proved correct using this model. Using the same approach, we have discovered a new algorithm for tactical conflict detection and resolution (CD&R) in a three-dimensional space.

In the near future, we will formally prove the correctness of our CD&R algorithm. We will also integrate it into a more general system for strategic CD&R, which takes into account intent information such as flight plans and uncertainties such as weather conditions.

Verification of the SPIDER protocols

Alfons Geser

Systems that are used in safety-critical applications must be highly dependable. Communication between electronic equipment in such a system is particularly sensitive. For instance it is required that message exchange must not fail more than once per as much as 120,000 years. In order to arrive at such a high level of confidence, the communication hardware must operate without failure in the presence of various kinds of faults, including simultaneous faults and Byzantine faults that can exhibit a malicious, two-faced behavior. In order to avoid design errors to an extent possible by today's means, the hardware including its fault tolerance mechanism has to be formally verified.

The SPIDER architecture is designed to serve as a fault tolerant message exchange backbone between unreliable nodes of electronic equipment. For this purpose it consists of nodes that tolerate faults of each other. SPIDER has an Interactive Consistency Exchange Protocol that ensures correct transmission from good nodes to good nodes, and ensures equal views of the scenario among all good nodes. A Diagnostic Protocol must gather information about misbehavior of nodes, and exchange that information such that all good nodes arrive at an equal, correct judgment of the quality of each node.

Using a given formal verification of the Interactive Consistency Protocol, we have started and nearly finished a formal verification of the Diagnostic Protocol in PVS. We plan next to participate in the design of the Initialization Protocol, a critical phase where the nodes have to find a common timing before they can start working.

Scalable implicit solvers for PDEs and PDE-constrained optimization

David E. Keyes

The development of scalable implicit solvers for analysis and optimization of multiscale phenomena governed by PDEs are our chief objectives. Multilevel preconditioned Newton-Krylov methods, from two-level additive Schwarz to richer versions, have proven to be broadly applicable, architecturally versatile, and tunable for high performance on today's high-end commercial parallel platforms. 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 matrix-free Newton-Krylov methodology appropriate for emerging architectures.

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-Newton-Krylov.

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 performance have been met. The general approach 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 Gigaflop/s — has been extended by algorithmic performance tuning and memory system modeling to the mid-300's of Gigaflop/s, 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 will continue to develop Newton-Krylov methods in implicit parallel CFD and radiation transport, examining a variety of algorithmic, programming paradigm, and architectural issues.

One of the most exciting new areas is nonlinear additive Schwarz. This is a nonlinear preconditioning that has already proved to enlarge the domain of convergence of a Newton's method wrapped outside of it, in boundary layer and shocked duct flows. The cost is the concurrent solution of numerous smaller nonlinear problems on subsets of the unknowns, and solution of linear problems on the same subsets to apply the action of the preconditioned Jacobian. Besides robustification advantages, in the range of thousands of processors, the nonlinear preconditioning has the potential to significantly reduce the number of synchronization points, by concentrating work locally.

This research was being conducted in collaboration with Xiao-Chuan Cai (University of Colorado, Boulder), William Gropp, Barry Smith, and Paul Hovland (Argonne National Laboratory), Dinesh Kaushik and Widodo Samyono (Old Dominion University), Carol Woodward (Lawrence Livermore National Laboratory), and David P. Young (Boeing)

Heterogeneous specification formalisms for reactive systems
Gerald Lüttgen

This research is part of the NSF project CCR-9988489, which is devoted to the development of novel techniques for *heterogeneous formal specifications* of reactive systems, such as avionics systems and embedded software. The project might be seen as a response to the need that formal-methods research must start addressing multi-paradigm specifications—combining, e.g., operational and assertional styles of specification—in order to support the heterogeneous specification methodologies employed in engineering practice today.

Recent and current research within the project focuses on extending the process algebra *Calculus of Communicating Systems* (CCS), that supports an operational style of specification, by two operators that permit the inclusion of *Linear-time Temporal Logic* (LTL) formulas, thereby adding an assertional style of specification. The two operators are:

- *embed*(ϕ), where ϕ is a LTL formula; this operator facilitates the embedding of LTL formulas within process-algebraic terms.
- *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 has been given an operational semantics based on Streett automata, in terms of structural operational rules. Further, it has been investigated how exactly the notion of *Büchi/Streett testing*, which was previously developed under ICASE/NASA funding, can be adapted to the novel setting. In particular, the *Büchi/Streett must-testing preorder* would allow for an elegant theory supporting the stepwise refinement of assertional system requirements into operationally concrete system designs. Unfortunately, a straightforward adaptation of the preorder to our language leads to a subtle compositionality defect regarding parallel composition, which is currently under investigation. It should be noted that this basic research is a prerequisite for a clean semantic support of heterogeneous specification languages and methods in use today.

Regarding further work in the near future, it is planned to characterize the largest pre-congruence contained in the Büchi/Streett must-testing preorder and to investigate concurrency-theoretic issues of the resulting heterogeneous language.

The reported research was conducted in collaboration with Rance Cleaveland (SUNY at Stony Brook, New York), the principal investigator of the NSF project.

System software research plan

Merrell Patrick

The overall objective of this research is to develop software that supports the development of leading edge, large-scale distributed applications that run on networked heterogeneous computing systems. At the highest level the central focus of the research is the programming of multidisciplinary applications and application components in a way that not only supports ease of programming but also portability and interoperability across different sets of networked systems. Portability and interoperability imposes the need for development of standards for such programming languages and environments. Developing meaningful standards that will have broad impact and be of use to NASA will require collaboration with national forums and groups, researchers at universities and government labs, and commercial developers of frameworks, compilers, toolkits, shells, and portals.

Programming requirements across various application areas are very diverse and varieties of programming approaches have been or are being used. These range from (a) frameworks where software components are combined to create applications to; (b) network-aware compilers that specialize in data-parallel and task-parallel applications to; and (c) simple workflow programming systems such as shells, toolkits, and portals.

The ICASE systems software plan has been restructured to have an overarching focus on the development of a higher level programming and execution framework (PEF) with appropriate standards that supports the portability, interoperability, and scalability of integrated multi-disciplinary codes across networked computing systems. The development process will use abstractions drawn from the above mentioned approaches. These abstractions will help define standards to be used. This research will be done by ICASE at NASA Langley in collaboration with working groups of the Grid Forum and the Common Component Architecture Working Group. The ICASE team will work with NASA HPCC applications development teams and developers of commercial products so as to better address NASA needs and the shortcomings of commercial products. ICASE will develop a prototype PEF to test requirements as hypothesized by applications teams and framework developers.

The overall plan includes three projects, an overarching project focused on framework development and two important components of the framework. The tasks are:

1. Development of a component-based Programming and Execution Framework (PEF) for distributed applications.

   The programming methodology of the system will be on software component principles to support the quick development and modification of applications. Major features include:

   - a scalable, distributed computing programming and execution support system that provides state-of-the-art security and that includes the following features:
     - run-time resource discovery and resolution
     - process to resource run-time mapping
     - remote process management
     - remote task execution (in a task server process)
     - synchronizing event signals
     - data transfers for medium and high performance needs
     - remote file transfer management
     - execution steering
     - programming of host workflow and remote application servers.

- a visual, component programming system using one or more technologies such as Web-based, Java Beans.
- a set of performance monitoring and diagnostic tools to assist in the development applications codes which execute efficiently on networked systems.
- a set of executables and scripts that provide application development and execution support.
- a set of standards-based, programming abstractions to define the elements and workflow of a distributed application developed jointly with relevant standards groups.
- a set variety of communication and information discovery technologies including Globus Services and Java/Jini.

2. Development of data management component technologies for distributed scientific applications.

   The focus is an XML-based data management software component to support scientific data portability across different programs on different machines, and exploration of scientific data with tools not necessarily available locally. Both a human and program interface to the software facility is planned. Technologies to be considered will include:

   - metadata for defining data sets
   - XISL (from CACR, Caltech), an XML-based standard to represent scientific data
   - standard software components for transformation and exploring data sets
   - XSLT implementation such as Xalan-Java from Apache
   - use of extended XSL for specifying transformations.
   - systems and/or protocols for high-performance data transfers
     - stream programming
   - "add-on" techniques to filter data transfers
   - aspect-oriented programming
   - run-time data filters
   - systems and/or protocols for event management
   - publish/query programming

3. Developing language extensions for high performance and distributed computing.

   Different language approaches will be evaluated and extensions and new compilation techniques that support ease of programming while exploiting the power of parallel and distributed computers will be proposed. OpenMP will be a primary focus.

The research proposed in the above projects is targeted at meeting the programming needs of future NASA computational projects; in particular, designing complex space and aircraft systems. It is anticipated that such projects will include a large set of multidisciplinary computational codes (stand-alone executables as well as function libraries) that will interact using non-trivial communications. The research will address improved user efficiency. This will allow application developers and users to focus on quality of the physics modeled by applications rather than on the computer science details of the programming environment.

During the last six months several meetings with LaRC applications developers have been held with the goal of identifying computational framework requirements. Also a workshop involving researchers working in frameworks, compilers, toolkits, shells, and portals has been planned and will be held in April 2001. A goal is identify programming abstractions that can be used to define standards for implementing programming frameworks and to identify framework requirements as seen by the software developers.

The above projects are the joint efforts of T. Eidson (ICASE), M. Zubair (Old Dominion University and ICASE), and Barbara Chapman (University of Houston and ICASE).

Scalable parallel algorithms for incomplete factorization preconditioning

Alex Pothen

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

We create parallelism by partitioning 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 preserve the parallelism in two steps: First, we map the subgraphs to processors, form a subdomain interconnection graph, and order the subdomains by a graph coloring to reduce global dependences. Second, 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: such fill edges join only boundary vertices on one subgraph to boundary vertices on a neighboring subgraph.

We have earlier 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. We are currently implementing our algorithms on larger numbers of processors and applying them to other classes of problems. We expect to show by these experiments that our algorithm is scalable, in agreement with our analysis of the algorithm.

This is joint work with David Hysom (Old Dominion University, currently at Lawrence Livermore National Laboratory).

External memory sparse direct solvers

Alex Pothen

We consider issues in designing 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 Gigabytes of memory and 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 primary 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 model problems whose data dependence graphs (elimination trees) have simple structures. We study the influence of orderings, factorization algorithms, and blocking on the primary 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, multifrontal, and recursive, can vary by orders of magnitude for unbalanced elimination trees that occur in linear programming and related applications. We have designed 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 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).

Coloring graphs in parallel for optimization

Alex Pothen

Optimization algorithms that employ derivative information require the computation of a Jacobian or Hessian matrix. Automatic differentiation (AD) and finite differences (FD) are two techniques used to compute these matrices. It is well known that graph coloring algorithms could be used to reduce the number of function evaluations needed in estimating the Jacobian and the Hessian. We have begun to develop parallel algorithms for graph coloring applicable to optimization.

Our first contribution is a unified perspective of the various graph coloring problems, corresponding to Jacobian and Hessian estimation, and corresponding to FD or AD techniques. We show that all these problems could be formulated as a single, albeit non-traditional, graph coloring problem. We extend a recent parallel coloring algorithm for the shared memory programming model, proposed by Gebremedhin and Manne, to solve the new coloring problem.

This algorithm is being implemented, and will be applied to solve the Jacobian and Hessian estimation problems in parallel. Once this is complete, we will extend these ideas to solve the estimation problem on parallel computers with message-passing programming models.

This is joint work with Assefaw Gebremedhin (University of Bergen, Norway, who is currently visiting Old Dominion University), and Ferderik Manne (University of Bergen, Norway).

High-order compact simulation of wave propagation in non-uniform flows

Alex Povitsky

The goal of this study is to gain computational insight into physical mechanisms of angular redistribution of acoustic energy and acoustic pressure while the sound waves propagate in non-uniform compressible flow in the presence of a stagnation point. The idealized mean flows mimic real-world flows in areas of strong sound refraction such as a leading edge of a wing or a turbine blade, a protruding corner of a wall cavity, a wing-fuselage intersection, an impingement area of a jet, and an area behind a bluff body.

In terms of acoustic energy, the modified sound directivity in the presence of stagnation flow is mainly caused by redistribution of potential and kinetic components of acoustic energy (while sound propagates upstream) and by angular redistribution of acoustic energy (while directions of the mean flow and sound propagation are far from collinear). Taking into account the compressibility of the background flow, (i.e., non-uniform distribution of density and speed of sound) the maximum of acoustic pressure moderately increases (within 6%) while local Mach number $M \leq 0.6$. The pump of acoustic energy from the background flow by means of baroclinically generated vorticity is minor. The propagation of acoustic pulse upstream of the flow around the 2D circular cylinder is modeled. The time-averaged root mean square of acoustic pressure (rms) is presented as a function of angle from the centerline. To compare with the static ambient conditions, the rms of acoustic pressure at the centerline is about 40% increased for the mean velocity with $M_\infty = 0.4$. The same degree of amplification of sound remains for the 60^o sector on either side from the centerline.

In collaboration with Jan Hesthaven (Brown University), we apply his unstructured high-order code to simulate amplification of sound around more complex 2D and 3D shapes.

Trajectory-based approach to CFD optimization of HiPco reactor for production of carbon nanotubes

Alex Povitsky and Manny Salas

This study was motivated by an attempt to optimize the High Pressure carbon oxide (HiPco) process for the production of carbon nanotubes from gaseous carbon oxide. The goal is to achieve rapid and uniform heating of catalyst particles by an optimal arrangement of jets. Single- and multi-wall nanotubes are interesting nanoscale materials for aerospace applications for three reasons: A single-wall nanotube can be either metallic or semiconducting, depending on how exactly the hexagons forming the sheet line up. In addition, it is also possible to connect two nanotubes with different electrical properties. Quasi one-dimensional heterojunctions, including metal-metal and metal-semiconductor, can thus be created, resulting in nanoscale electronic components. These nanotube heterojunctions with electronic switching properties can be used for developing next-generation of computer components. Single- and multi-wall nanotubes have very good elastomechanical properties, thus they have great potential for spacecraft components requiring lightweight, highly elastic, and very strong fibrous material.

Jet mixing in a reactor for production of carbon nanotubes from gaseous carbon oxide initiated by catalyst particles is studied numerically using a mixed Eulerian and Lagrangian approach. To achieve rapid monotonic heating of catalyst particles, the behavior of particle trajectories is studied. Three types of trajectories are observed. The particle trajectories can be bent either towards the interior of the cold jet (type 1), or outward (type 2). They also can rotate in the vortical zone upstream of the intersection of cold and hot jets (type 3). Direct exposure to the action of hot jets leads to the first or to the third type of trajectory behavior that causes slow or oscillating heating, respectively. Straightforward measures such as increasing hot gas consumption, increasing the angle between hot and cold incident jets, and splitting the cold jet are not sufficient to achieve fast heating because of the behavior of particle trajectories. A modified reactor design has been proposed, Design C, which includes three parallel nozzles for cold central jets. To avoid direct exposure of trajectories to the action of hot jets, the cold jet nozzles are located between the hot peripheral jet nozzles. Type 1 trajectories are avoided and at the optimal angle between jets, $\alpha = 60^o$, the heating rate reaches $3.5^o - 4.5^o \times 10^5 K/sec$, a significant improvement compared to the rate achieved by the basic design.

This research is in the center of interdisciplinary collaboration between fluid modeling (ICASE, M. Salas and A. Povitsky), kinetic modeling (group at NASA Ames), simulation of nanotube growth (group at NASA Johnson), and physical experiments (group of Professor Smalley at Rice University). Kinetic modeling and simulation of nanotube growth require a tremendous amount of computer resources. Parallel and distributed computing, data-parallel, and task-parallel ways to exploit supercomputers will be considered in our future research.

Numerical modeling of high-incidence three-dimensional lid-driven cavity flow

Alex Povitsky

This research studies truly three-dimensional impinging flows in a spatial corner with high angle of incidence between the flow and surrounding rigid walls. To keep the simple cubic geometry, the three-dimensional rectangular cavity flow is considered where the cavity lid moves along its diagonal. The lid-driven cavity flow mimics many aeronautical, environmental, and industrial flows. The secondary flow and the strength of secondary vortices are substantially larger than those in the previous studies where the lid moves along its edge. If the lid moves along its edge (the classical CFD test case), the flow is parallel to the side walls and separation occurs due to the pressure gradient caused by its impingement into the front wall. In real life a flow is likely to be non-parallel to the cavity edges. The non-zero angle of incidence between the flow and a side wall leads to enhanced flow separation in comparison with the previous studies.

The three-dimensional lid-driven cavity flows are studied by numerical modeling using second-order upwind schemes for convective terms. This study shows that in spite of the lower level of the primary flow velocity (in the direction of moving lid), the numerous secondary vortices (in the perpendicular direction) are stronger than those in the classical case. Transition to the unsteady non-symmetric flow occurs for considerably smaller *Re* numbers.

While the steady-state solution and some transient features are predictable using second-order schemes, the detailed study of generation of unsteady Gortler vortices (i.e., lose of stability and transition to turbulence) is possible only by use of higher-order compact schemes. Our future research includes parallelization of compact schemes for incompressible elliptic solvers and use of parallel computers for simulation of transient process.

Parallel solution techniques for radiation transport equations

Linda Stals

One area of focus in the current ASCI initiative is the solution of radiation transport equations. The solution of such equations is challenging as they contain strong non-linearities and large jumps in the coefficients. We are interested in implementing efficient algorithms that will allow us to solve these problems on parallel machines containing a large number of processors.

We have investigated two different components of the solution of radiation transport equations; we have compared the parallel performance of two nonlinear solvers, and studied the use of adaptive refinement to better capture the shape of the radiation wave front as it moves through the domain. We have shown that on up to 16 processors the two nonlinear solvers are competitive with one another. These experiments need to be rerun on bigger machines to determine if this trend continues when more processors are used. The use of adaptive refinement has proved to be beneficial in aiding the solution process.

In the current work we make certain assumptions about the physical domain to help simplify the equations. Our goal now is to remove some of these assumptions.

FLUID MECHANICS

Laser-induced thermal acoustics (LITA) for flow diagnostics

Roger Hart

There is a recognized need for a seedless equivalent of laser doppler velocimetry (LDV) for use in flows where seeding is undesirable, ineffective, or impossible. The requirement for 'seedless LDV' is a severe one: what is wanted is not merely a technique that can be demonstrated in the laboratory, but a technique that can be successfully embodied in rugged, reliable hardware and applied in real-world environments by people who are not professional optics researchers. Laser-induced thermal acoustics (LITA) has been under development for several years at Langley and a few other places as a means of meeting this need. Our goal is to develop LITA to the point where it becomes widely recognized as the seedless alternative to LDV.

The major accomplishment during the current reporting period was the first test of LITA velocimetry in a real-world wind tunnel. During the previous reporting period a compact one-flow-component LITA velocimeter was constructed and tested in the laboratory. This instrument uses a novel method of quadrature-phase heterodyne detection that 1) is much more stable than previous methods, 2) recovers flow direction as well as speed, and 3) significantly improves precision and accuracy for flow velocities below 20 m/s. The LITA velocimeter was employed at the Basic Aerodynamics Research Tunnel (BART) at NASA Langley during a 40-day test period. Numerous comparisons with a pitot-static probe in the freestream showed agreement to within ± 0.5 m/s for velocities in the range 30–55 m/s, and agreement to within ± 1 m/s for velocities in the range 0–30 m/s. The flow field behind a rearward-facing step was mapped in detail and showed all the expected features, such as flow separation and reattachment, a shear layer, and recirculation and secondary separation. Comparison with LDV gave excellent agreement in the freestream, with discrepancies in turbulent regions attributable to velocity bias in the LDV measurements. Overall, our first-generation LITA apparatus proved to be already the near equal of LDV in terms of accuracy, precision, stability, and ease of use. The potential of LITA as a practical, dependable, routinely usable flow diagnostic is evident when one considers that LDV has been in use for approximately 30 years and is a thoroughly mature technology.

An improved, two-flow-component LITA velocimeter is now under design, which will incorporate the lessons learned during the BART test. It will feature improved stability and totally remote (hands-off) operation. We are currently scheduled to return to BART in April 2002 to make measurements in the slat cove region of a high-lift wing configuration; sometime after that we will make measurements on supersonic flows around a blunt body at the Probe Calibration Tunnel (PCT) at NASA Langley.

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

Mapping closure approximation to conditional dissipation rate for turbulent scalar mixing

Guowei He

This work is the first part of our research on a developing probability density function (PDF) method for turbulence modeling.

A novel mapping closure approximation (MCA) technique is developed to construct a model for the conditional dissipation rate (CDR) of a scalar in homogeneous turbulence. It is shown that the CDR model from amplitude mapping closure is incorrect in asymptotic behavior for unsymmetric binary mixing. The correct asymptotic behavior can be described by the CDR model formulated by the MCA technique. The MCA approach is outlined for constructing successive approximation to probability density function and conditional moment.

We will further develop the general principles for mapping closure approximation.

This research was conducted in collaboration with R. Rubinstein (NASA Langley).

Effects of eddy viscosity on time correlations in large eddy simulation

Guowei He

We have established a database for isotropic homogeneous turbulence. The next goal is to calibrate and develop subgrid models for turbulent flows.

Subgrid-scale (SGS) models for large eddy simulation (LES) have generally been evaluated by their ability to predict single-time statistics of turbulent flows such as kinetic energy and Reynolds stresses. Recent applications of large eddy simulation to the evaluation of sound sources in turbulent flows, a problem in which time correlations determine the frequency distribution of acoustic radiation, suggest that subgrid models should also be evaluated by their ability to predict time correlations in turbulent flows.

This work compares the two-point, two-time Eulerian velocity correlation evaluated from direct numerical simulation (DNS) with that evaluated from LES, using a spectral eddy viscosity, for isotropic homogeneous turbulence. It is found that the LES fields are too coherent, in the sense that their time correlations decay more slowly than the corresponding time correlations in the DNS fields. This observation is confirmed by theoretical estimates of time correlations using the Taylor expansion technique. The reason for the slower decay is that the eddy viscosity does not include the random backscatter, which decorrelates fluid motion at large scales. An effective eddy viscosity associated with time correlations is formulated, to which the eddy viscosity associated with energy transfer is a leading-order approximation.

This work is a collaborative effort with L.-P. Wang and R. Rubinstein (NASA Langley).

Lattice Boltzmann equation on a two-dimensional rectangular grid

Li-Shi Luo

The method of the lattice Boltzmann equation (LBE) is usually associated with uniform and symmetric meshes, such as triangular and square ones in two dimensions and a cubic one in three dimensions. This feature is due to the symmetry imposed by the discretization in the (particle) velocity space. This limits the application of the LBE method to situations in which highly asymmetric meshes are needed (such as stretched meshes with very high aspect ratio in the boundary layer). The present work proposes an LBE scheme on a rectangular grid.

We propose a generalized LBE nine-velocity model in two-dimensional space with rectangular grids. The model is based upon the previously proposed generalized LBE nine-velocity model on a square lattice that is constructed in moment space instead of velocity space, and possesses a maximum number of adjustable parameters allowed by the freedom of the LBE model. We analyzed the model and found that, in order to attain the isotropy of model, the sound speed has to be adjusted according to the grid aspect ratio. We also numerically tested the model for three cases: (a) a vortex moving with a constant velocity on a mesh with periodic boundary conditions; (b) Poiseuille flow with an arbitrary inclined angle with respect to the lattice orientation; and (c) a cylinder asymmetrically placed in a channel. The numerical results of these tests are compared with either analytic solutions or the results obtained by other methods.

A paper entitled "Lattice Boltzmann Equation on a Two-dimensional Rectangular Grid," authored by M'hamed Bouzidi, Dominique d'Humières, Pierre Lallemand, and Li-Shi Luo, has been accepted by the Journal of Computational Physics (2000). An ICASE report is under preparation.

The present work is a result of collaboration with Pierre Lallemand (Laboratoire ASCI-CNRS, Université Paris-Sud (Paris XI Orsay), France), and Dominique d'Humières (Ecole Normale Supérieure, Paris, France).

The present work has been partially funded by NASA Langley Research Center under the program of "Innovative Algorithms for Aerospace Engineering Analysis and Optimization."

We intend to extend our work to 3D LBE models or other more complicated LBE models with larger number of velocities.

Vibrationally induced instabilities in thermocapillary and binary fluid systems

J. Raymond Skarda

G-jitter is a potential source of instability in fluid systems on space based platforms. The impact of residual accelerations (g-jitter) on materials processing applications involving thermocapillary and binary fluid systems are of particular interest. This work consists of two tasks: the first is to complete analysis of and finalize reporting of a study concerning gravity modulation of a fluid layer with surface tension along its free surface. The second task is to examine bursting behavior that occurs in a binary fluid system, and the sensitivity of this behavior to g-Jitter.

Floquet theory was successfully applied to compute stability boundaries of the gravity modulated Marangoni problems. Fundamental differences in the behavior of the stability boundaries were observed with respect to the purely buoyancy (modulated Rayleigh-Bénard) problems. Simple stability criteria were obtained from reduced (one-term Galerkin) formulations of the problem. Final revisions of the paper entitled: "Instability of a Gravity Modulated Fluid Layer with Surface Tension Variation," were completed, and the paper is to appear in the Journal of Fluid Mechanics, Vol 434. Preliminary simulations of the binary fluid system have been performed using a solver written by Dr. David Jacqmin. Empirical eigenfunctions have successfully been computed using programs written by Skarda. A reduced-order model has been developed, however, preliminary results are in poor agreement with results obtained directly from the Jacqmin code.

The disagreement of the lower order model results with direct numerical simulation will be examined. Effects of vibration (in the context of gravity modulation) imposed on the binary fluid system will then be examined using both computational and reduced-order models.

STRUCTURES AND MATERIALS

Closed-shell carbon nanostructures from organo-metallic precursors

Theo Dingemans

Single-wall and multi-wall carbon nanotubes are heralded as a new generation of materials with many high-end applications in electronics, composites, and the medical field. To date, not many of these ideas have materialized and not much progress is expected until some key problems are resolved. One of the problems is the production and processability of carbon nanostructures. Practically, all carbon nanostructures production facilities rely on high temperature laser ablation techniques or high-pressure carbon monoxide techniques (HiPCO). The last method has been reasonably successful with respect to producing single-wall carbon nanotubes (SWNTs) in acceptable quantities. Nevertheless, purification with strong oxidizing agents is often necessary to remove amorphous carbon, catalyst, and other undesirable side products. Purification of nanotubes produced via HiPCO can result in a yield as low as 50% of acceptable, but not necessarily superior quality nanotubes. The solubility of nanotubes is another major point of concern. Most industries depend on solution-based processing techniques that will enable them to transport starting materials, intermediates, and products, and perform chemical transformations followed by dissolving, extracting, etc. Presently, carbon nanotubes are available in dry form ("bucky paper") or as meta-stable colloidal suspensions in toluene or other solvents. Regardless of the form in which the nanotubes are available, it remains virtually impossible to take full advantage of their unique properties because they are insoluble and very resistant towards common chemistries. Currently, we are investigating the use of organo-metallic precursors towards the synthesis of closed-shell carbon nanostructures.

As a starting point we have synthesized and characterized three isomeric phenyl-alkyne cobalt complexes. All compounds are soluble and have a high C-H ratio. The different substitution patterns (regio-isomers) will give us information about how substitution patterns affect the formation of pre-graphitic networks. Although some of the synthetic steps were challenging, we have optimized the synthetic routes and we are now able to provide multigram quantities of these organo-metallic precursors.

Future work will include processing the precursor molecules using conventional spin casting and vapor deposition techniques. We envision that this approach will allow us to fabricate ceramic, polymer, and bio-based sensors and devices from *in-situ* formed carbon nanostructures. In addition, we will explore the possibility of incorporating hetero atoms such as nitrogen (N) and Boron (B) and investigate their electronic properties in applications such as one-dimensional semiconductors and field effect transistors (FETs).

This research was conducted in collaboration with Mia Siochi (NASA Langley).

Constitutive modeling of nanostructured materials

Vasyl Michael Harik

Nanostructured materials and carbon nanotubes, in particular, appear to possess extraordinary physical properties (e.g., high stiffness-to-weight and strength-to-weight ratios and large electrical and thermal conductivities). Potential applications of these materials range from new electronic devices and electromechanical probes to multifunctional structural components and control systems for aerospace industries. The goal of this research is to develop constitutive models for advanced material systems involving various nanostructures.

To examine the validity and possible limitations of the continuum models for carbon nanotubes, the mechanical behavior of a nanotube under axial compressive loads is investigated. The underlying assumptions of continuum models are analyzed along with the governing equations and macromechanical concepts used in the models. Non-dimensional analysis of the buckling behavior and geometric and material parameters is carried out. The values of critical strains for various nanotubes are derived and compared with molecular dynamics simulations. Model applicability maps are constructed for different nanotube geometries in the parameter space.

Future research involves analysis of the nanotube-based AFM tips and other scanning probes along with further development of modeling capabilities for the constitutive behavior of nanostructured materials.

This research is conducted in collaboration with T. Gates and M. Nemeth (NASA Langley) as well as other scientists and engineers under the guidance of D. Ambur (NASA Langley).

Constitutive modeling of electromechanical effects in multifunctional materials

Vasyl Michael Harik

Design of new aerospace structures, such as flexible wings, structures with active controls, multifunctional membranes, and inflatable electromagnetic antennas require fundamental understanding of electromagnetic-thermoelastic material behavior so that they can be modeled accurately in structural analyses. The objective of this research is to develop constitutive models for multifunctional materials.

A class of nanostructured piezoelectric polymers is considered in order to identify the key physical phenomena contributing to the mechanical and electrical properties of multifunctional polymer films. The physical and materials science characterization of the key material parameters has been analyzed prior to deriving functional relations. The form of functional relations depends on the feedback from the dimensional analysis and electromechanical models that are examined for such material systems. The work performed thus far indicates that the dimensional analysis of material behavior may lead to characteristic non-dimensional parameters that would control material constitutive response.

Future work involves derivation of the general and explicit functional relations between material parameters as well as validation of such relations by experimental data.

This research is conducted in collaboration with D. Ambur (NASA Langley) and Z. Ounaies (ICASE).

Progressive failure analysis of composite materials

Vasyl Michael Harik

In-service failures of complex material systems are generally difficult to predict. In aerospace applications, the use of composite structures permits optimization of their design not only for weight and mechanical performance but also for a predictable failure pattern. In laminated structures, damage accumulation processes have progressive character which depends on the material properties, the ply-stacking configuration, and the type of loading. The goal of this research is to assess the failure criteria and damage models for advanced composite systems considered in the NASA White Paper on Progressive Failure Analysis.

The current assessment of basic concepts, mathematical and physical models of composite behavior is based on the previous reviews and some recent studies such as an International Exercise on Failure of Composites organized by DERA (UK) and the Low Cycle Fatigue Program of the U.S. Army Research Laboratory (Aberdeen, MD). The analysis of micromechanical and hierarchical modeling stems from the work carried out in cooperation with the Sandia National Laboratories (Albuquerque, NM). The first phase contribution to the NASA White Paper has been completed.

This work will be further developed by other NASA researchers.

This research is conducted under the guidance of D. Ambur (NASA Langley) and in collaboration with C. Davila (NASA Langley) and other NASA engineers.

Progressive failures studies of composite panels with and without cutout
Navin Jaunky

The use of composite materials for aircraft primary structures can result in significant benefits on aircraft structural cost and performance compared to conventional metallic structures. However, unlike conventional metallic materials, composite structures fail under different failure modes such as matrix cracking, fiber-matrix shear failure, fiber failure, and delamination. The initiation of damage in a composite laminate occurs when a single ply or part of the ply in the laminate fails in any of these failure modes over a certain area of the structure. The initiation of damage does not mean that the structure cannot carry any additional load. The residual load-bearing capability of the composite structure from the onset of material failure or initiation of damage to final failure can be quite significant. It is at the final failure load that the structure cannot carry any further load.

Accurate determination of failure modes and their progression helps either to devise structural features for damage containment or to define fail-safe criteria. Therefore, it is important to understand the damage progression in composite structures subjected to different loading conditions. Hence the objective of the present study is to develop and validate an efficient methodology that can predict the ultimate strength of composite panels by taking into account ply damage modes and geometrical nonlinear response. Geometric nonlinear response is important since aircraft structures are thin-wall structures and undergo significant deformation.

The finite element implementation of this progressive failure analysis was developed for the ABAQUS structural analysis program using the USDFLD user-written subroutine. ABAQUS calls this USDFLD subroutine at all material points of elements that have material properties defined in terms of the field variables. The field variables represent the material damage modes and in this study the damage modes considered are those defined by Hashin criteria. When a damage mode has been detected, the mechanical properties in the damaged area are degraded appropriately, according to the Chang degradation model, which is a ply discount model. Delamination failure mode is not included in the present study. The subroutine provides access points to a number of variables such as stresses, strains, material orientation, current load step, and material name, all of which can be used to compute the field variables. Stresses and strains are computed at each incremental load step and evaluated by the failure criteria to determine the occurrence and the mode of failure.

Progressive failure analyses were carried out for flat panels and curved panels with and without cutout. The flat panels were subjected to shear loading, while the curved panel was subjected to compression. A bead-stiffened panel subjected to shear loading was also considered. These test cases were considered since data from NASA-conducted experiments was available. Results from progressive failure analyses are in good agreement with experimental results when delamination is not the major damage mode. In some cases, including measured geometric imperfection in the finite element model provides better agreement with experiment results.

Future work will focus on more comparisons of progressive failure analyses with experiments that have recently been carried out.

This work was done in collaboration with Damodar R. Ambur, Carlos G. Davila, and Mark W. Hilburger (NASA Langley).

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 and to develop a methodology for cumulative life using delamination fatigue characterization data and geometric nonlinear finite element analysis.

The damage mechanisms in bonded composite skin/stringer structures under tension fatigue loading conditions was studied. Microscopic investigations of the specimen edges were used to identify typical damage patterns and to document the onset of matrix cracking and delamination as a function of fatigue cycles. Subsequently, an analytical methodology to accurately predict the onset of matrix cracking as well as delamination was demonstrated. The tension loading was simulated in a geometrically nonlinear plane-stress finite element model using the ABAQUS® FE code. A stress analysis was used to predict the location and orientation of the first transverse crack based on the principal transverse tension stress distribution in the flange tip area. Computed stresses for different load levels were compared to material characterization data from transverse tensile fatigue tests to generate a curve predicting the onset of matrix cracking. A fracture mechanics approach was used to determine delamination growth from this transverse crack. Delaminations of various lengths were discretely modeled by releasing multipoint constraints at the locations where delaminations were observed during the experiments. Mode I and II strain energy release rate contributions, GI and GII, were calculated for all load cases using the virtual crack closure technique. Computed peak G values were used with G versus N fatigue characterization data to predict the fatigue life of the skin/stringer specimens. A cumulative life prediction methodology was developed by combining the results for fatigue life for matrix crack onset and fatigue life for delamination onset.

The current studies were used to identify failure curves for the onset of the first failure in a virgin, as-designed, configuration.

Future work will focus on analyses to compare current results with (a) simulated first failure by delamination from an assumed matrix crack, (b) simulated first failure from an assumed delamination in the bond line, and (c) simulated delamination in the skin with no matrix crack present. This comparison may then also be extended to a more classical damage tolerance approach assuming delamination from a "critical size" initial flaw at the most "critical location."

This work was 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).

The influence of crosslinks on physical aging in glassy thermoplastic polyimides

Lee M. Nicholson

Durability and long-term performance are among the primary concerns for the use of advanced polymer matrix composites (PMCs) in modern aerospace structural applications. For a PMC subjected to long-term exposure at elevated temperatures, the viscoelastic nature of the polymer matrix will contribute to macroscopic changes in composite stiffness, strength, and fatigue life. Over time, changes in the polymer due to physical aging will have profound effects on the viscoelastic compliance of the material, hence affecting its long-term durability. This research aims to investigate the use of polymer viscoelasticity at the microstructural level to accurately predict how changes in chemical structure, physical structure, and state of stress in the polymer impact the mechanical properties of advanced polymers.

Experiments were performed using five variations in crosslink density to evaluate the differences in mechanical performance of an advanced polyimide. The physical aging behavior was isolated by conducting sequenced, short-term isothermal creep compliance tests in tension. These tests were performed over a range of sub-glass transition temperatures. The material constants, material master curves and physical aging-related parameters were evaluated as a function of temperature and crosslink density using time-temperature and time-aging superposition techniques. The time-temperature superposition analysis of the creep compliance showed that high crosslink density materials have increased creep compliance and increased creep rate, and are less sensitive to physical aging compared to low crosslink density materials. The temperature sensitivity of the time-temperature superposition (TTSP) shift factor was shown to increase monotonically with increasing crosslink density. This research has significant implications for the composites and resins community since it's a widely accepted practice to use crosslinks to provide thermal and mechanical stability. This research has shown that the introduction of crosslinks significantly interferes with the mechanisms of physical aging making the glassy resin behave differently than expected.

The effects of creep loading for long timescales ($>$ 1100 hours) will provide a means for evaluating a predictive model, and the long-term effects of crosslink density and temperature. The initial model predictions compare favorably with the long-term test data. This work is continuing to develop constitutive relationships to express the long-term mechanical performance of the material.

This research is done in collaboration with Thomas S. Gates, Karen S. Whitley and Jeffrey A. Hinkley (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 applications that will enable self-adaptive flight with improved performance and safety in next generation aircraft and spacecraft. One such application is the design and development of high-performance, high-temperature, flexible piezoelectric polymers. This application was the impetus for a study in which NASA LaRC has synthesized a series of polyimides containing polar functional groups. Additionally, the resultant piezoelectric response was assessed and a fundamental structure-property analysis was performed. Effects of structural changes, including variations in the type and concentration of dipolar groups, on the piezoelectric behavior is examined. The remanent polarization, the dielectric relaxation strength, and the various piezoelectric coefficients were measured. Polymers with multiple nitril groups showed out-of-plane displacement that exceeded that of state-of-the-art PVDF. Large directionality in the piezoelectric behavior was seen where the in-plane coefficients were more than one order of magnitude smaller than the out-of-plane values. The thermal stability of the piezoelectric effect was evaluated under dynamic and static thermal stimuli. These materials exhibited good thermal stability of the piezoelectric properties up to 100°C. This work was presented at the American Chemical Society Poly Millennial 2000, December 10, 2000 (Waikoloa, Hawaii). The polymers show very promising behavior for use as high-temperature sensors, and they possess distinct improvements over state-of-the-art piezoelectric film sensors including enhanced polarization, polarization stability at elevated temperatures, and improved processability.

Future work will further explore the processing and properties of the polyimide/PZT composites. This work is done in collaboration with Joycelyn S. Harrison (NASA Langley), Cheol Park (ICASE), and Dan Klein (NRC).

Piezoelectric ceramics for use as actuators

Zoubeida Ounaies

Implementing piezoelectric actuators in vibration and noise suppression applications is steered towards improving spacecraft and aircraft operation. This may lead to reduction of control electronics size and cost, and a lowering of the voltage drive by using thinner, more efficient, and better characterized actuators. THUNDER (THin UNimorph DrivER) actuators are pre-stressed piezoelectric devices developed at NASA LaRC that exhibit enhanced strain capabilities. As a result, they are of interest in a variety of aerospace and aircraft applications. Their performance as a function of electric field, temperature, and frequency is needed in order to optimize their operation. Towards that end, a number of THUNDER devices were obtained from FACE Co. with stainless steel thicknesses varying from 1 mil to 20 mils. The various devices are evaluated to determine low-field and high-field displacement as well as the polarization hysteresis loops as a function of frequency. The thermal stability of these drivers was evaluated by two different methods. First, the samples were thermally cycled under electric field by systematically increasing the maximum temperature from 25°C to 200°C while the displacement was being measured. Second, the samples were isothermally aged at an elevated temperature in air, and the isothermal decay of the displacement was measured at room temperature as a function of time. Results of this study were presented at the SPIE Smart Structures and Materials Conference, March 4–9, 2001 (Newport Beach, CA). The internal stresses present within the ceramic and metal layers, combined with restricted lateral motion, enhanced the axial displacement and caused large asymmetry in the domain switching at high fields. Asymmetry of the hysteresis is most likely due to stress domains facilitating switching and alignment with positive fields and impeding alignment with negative fields. To quantify the exact relationship between the state of stress in the ceramic and the overall performance, we are pursuing modeling of these devices, incorporating both thermoelastic relations and ferroeletric domain theory. We also plan on continuing the modeling of the nonlinear hysteresis behavior of piezoelectric ceramics as a function of frequency and temperature.

This work is done in collaboration with Ralph Smith (North Carolina State University and ICASE) and Karla Mossi (Virginia Commonwealth University and ICASE).

Molecular dynamics simulations of metallic nano-clusters

Sun Mok Paik

For the last decade the nano-sized metallic particles have attracted a lot of attention among scientists and engineers because of its potential application in a variety of fields, such as improving fracture toughness of a material, quantum devices, micro-mechanics, etc. 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 study the thermodynamic properties of the nano-sized Au clusters using the Molecular Dynamics simulation.

Using the MD technique we simulate a stable structure of Au clusters sized between five nanometers and 30 nanometers on the (001) surface at room temperature T=300K. A many-body Embedded Atomic

Method (EAM) potential is used for the interatomic interactions between the gold atoms. We then increase temperature to T=1300K and monitor structural phase transformation as a function of temperature both on in-plane and interlayer structures. We find that the large (> 10 nm) clusters are slightly off-aligned to underlying substrate ("rotated domain") with rotation angle about 1° whereas the smaller clusters (< 10 nm) are aligned to the substrate ("un-rotated domain"). The rotated domain undergoes a phase transition to an un-rotated domain at a temperature about 3/4 of the melting temperature. Unlike the bulk materials, the interlayer distance between the cluster and substrate layer decreases as the temperature increases.

In the future, we will simulate and calculate various mechanical and electric properties of other metallic nano-particles. We also plan to write a MD code for a parallel computer.

This work was done in collaboration with Min Namkung and R. A. Wincheski (NASA Langley).

A theoretical modeling of quantum transport in carbon nanotube-based magnetic tunnel junctions

Sun Mok Paik

Molecular electronics has taken a large step forward since the discovery of carbon nanotube metallic and semiconducting molecular wire. Because of the unique structure and electrical properties, the potential application of these devices are enormous, such as quantum dot, quantum wire, quantum computers, logic gates, as well as other nano-mechanical devices. The nanotube behaves as ballistic quantum conductors with long phase-coherence lengths for charge carriers and, thus, it may well be an ideal candidate for achieving molecular scale magneto-electronics in which both the charge and spin degree of freedom are utilized for the operation of a functional device. More detailed theoretical modeling and suggestions are needed.

In this project we use the tight-binding Hamiltonian model,

$$H = -V_{pp\pi} \sum_{<y>} a_i^{+} a_j,$$

to calculate the energy band of a carbon nanotube where $V_{pp\pi} = 2.75$ for a single-wall carbon nanotube, and $a^{\dagger}$ and a are the creation and destruction operators. Using this Hamiltonian, the Green's function of the carbon nanotube base magnetic tunnel junction that consists of a Single-wall Carbon NanoTubes (SWNT) connected to two ferromagnetic (FM) electrodes is calculated,

$$G^{r(a)}(E) = \frac{1}{E - H_{tube} - \sum_L^{r(a)} - \sum_R^{r(a)}},$$

where r/a stands for retarded/advanced. $\sum_L^{r(a)}$ and $\sum_R^{r(a)}$ are the retarded Green's function for the left and right electrodes, respectively. The magnetic moments of two FMs are pointing different directions so that we can investigate the spin-dependent quantum transport properties. The density of the state (DOS) and the conductivity of the system are calculated from the Green's function. We find that the resistance between two FM electrodes is minimal ($\sim 6.4k\Omega$ for armchair tube with the length obeyed by $3n+1$ rule) when the magnetic moments of two electrodes are parallel, and maximum when the magnetic moments are anti-parallel. The change in the resistance is about 20%. These results will be compared and used in an ongoing experimental project in the Nondestructive Evaluation Science Branch of NASA Langley.

In the future, we will use MD simulation techniques to find more realistic interface structure between electrode and carbon nanotube. This result will be used to more quantitative prediction for the quantum transport properties in carbon nanotube-based tunnel junctions.

This work was done in collaboration with Min Namkung and R. A. Wincheski (NASA Langley).

Corona poling of partially cured polyimide

Cheol Park

A series of amorphous piezoelectric polyimides containing polar functional groups has been developed at NASA LaRC for potential use as high-temperature sensors and actuators in aircraft and aerospace applications. They exhibited a piezoelectric response at temperatures in excess of 150°C and good thermal stability. The level of piezoelectricity in the amorphous polyimides, however, is an order of magnitude lower than what is required for practical utility in devices. In an attempt to maximize the degree of dipolar orientation and the piezoelectric response, a new poling method was introduced and evaluated.

In-situ poling and imidization of partially cured polyimides was studied to achieve the required piezoelectricity. A positive corona poling was used to minimize localized arcing during poling and allow additional variations in the poling process. The dielectric relaxation strength, remanent polarization, and piezoelectric responses were evaluated as a function of the poling profile. The partially cured, corona-poled polymers exhibited higher dielectric relaxation strength ($\Delta\varepsilon$), remanent polarization (P_r), and piezoelectric strain coefficient (d_t) than a fully cured, conventionally poled one. A response comparable to that of the piezoelectric polymer PVDF was attained from the amorphous polyimides with higher thermal stability. This study was presented at the American Chemical Society Biennial Meeting in Hawaii, December 2001.

Future research will be focused on assessing the stability of the piezoelectricity of the partially cured corona-poled polymers. Application of the in-situ poling and imidization of partially cured polyimides for amorphous polyimides containing higher dipolar concentration will be investigated.

This research was performed in collaboration with Zoubeida Ounaies (ICASE), Kris Wise (NRC), and Joycelyn Harrison (NASA Langley).

Single-wall carbon nanotube polymer composites

Cheol Park

Carbon nanotubes are of great interest because of their unique electronic and mechanical properties combined with their chemical stability. In this study, single-wall carbon nanotube (SWNT) polymer composites were prepared and characterized as part of an effort to develop polymeric materials with improved combinations of properties for potential use as thin films on future spacecraft. Next generation spacecraft will require ultra-lightweight materials that possess specific and unique combinations of properties such as radiation and atomic oxygen resistance, low solar absorptivity, high thermal emissitivity, electrical conductivity, tear resistance, ability to be folded and seamed, and good mechanical properties. The objective of this work was to incorporate sufficient electrical conductivity into space-durable polymers to mitigate static charge build-up. The challenge is to obtain this level of conductivity ($10^6 - 10^8$ S/cm) without degrading other properties.

Several different approaches were attempted to fully disperse the SWNTs into the polymer matrix. These include high shear mixing, sonication, and synthesizing the polymers in the presence of pre-dispersed SWNTs. The effect of SWNT concentration and dispersion of the nanocomposites on the conductivity, solar absorptivity, and mechanical properties were investigated. The SWNT/polyimide nanocomposite films exhibited significant increases in surface and volume conductivity at relatively low loading ($< 0.2wt\%$) levels with some loss of optical transmission and increase in color (solar absorptivity). Tensile properties and thermal stability were noticeably improved at $1wt\%$ SWNT. The dispersion of SWTNs was evaluated with optical, transmission electron, and scanning probe microscopes. This study was presented at the Nanospace 2001 conference in Galveston, TX on March 2001.

Investigation of alternative methods of dispersing SWNTs in polymer matrices are continued. Chemical modification of a SWNT surface to aid in dispersion will also be studied. Electrospinning of the SWNT/polymer solution will be studied to develop engineering nanofibers for potential use as sensors and actuators in aerospace applications.

This research was performed in collaboration with Zoubeida Ounaies (ICASE), Kent Watson (NRC), Joycelyn Harrison (NASA Langley), and John Connell (NASA Langley).

Organic-inorganic hybrid-clay nanocomposites

Cheol Park

Polymer-clay nanocomposites are of great interest for many industrial applications due to their light weight, high strength, modulus, and toughness, tear/rip resistance, radiation resistance, low coefficient of thermal expansion, low permeability of atoms, low solar absorption, and optical transparency. Layered silicates (e.g., clay) can provide efficient reinforcement as an inclusion with unique physical and chemical properties at low loading levels (1–5%) because of their high surface area and aspect ratio if the layered silicates are completely exfoliated in a host polymer matrix. However, uniform dispersion of completely exfoliated layered silicates in a polymer matrix has been a difficult task to accomplish. One of the reasons is lack of compatibility between the hydrophilic clay surfaces and organophilic polymer matrix. To overcome this thermodynamic barrier, organically modified layered silicates have often been used to intercalate and exfoliate the layered silicates in a polymer matrix. Complete dispersion of the clays as a single silicate layer in a polymer matrix, however, has rarely been achieved with the present methods due to the intrinsic strong attraction among the layers with high surface area. Successfully intercalated and swelled layered silicates often fail to exfoliate during mixing under shear or sonication, and even exfoliated clay layers tend to reform stacked layers during solvent evaporation or polymerization process. A novel approach should be designed to achieve complete dispersion of the clay inclusions in a polymer matrix to achieve the required properties. Accordingly, it is a primary objective of this research to provide a unique method to disperse layered silicates uniformly as a single layer in a host composite matrix by introducing organic-inorganic hybrid as a matrix.

These nanocomposites were prepared by dispersion of nano-sized inclusions such as layered silicates (smectite-type clay) into an organic-inorganic hybrid matrix homogeneously without flocculation. The hydrolyzed silanol groups present in the organic and inorganic precursors subsequently reacted with hydroxyl groups located on the clay layer edges to form hydrogen and/or covalent bonds. This aided in the dispersion of the clay layers more efficiently under high shear. Remaining silanol groups reacted to form a network structure through self-condensation, thus preventing the dispersed exfoliated single clay layers from collapsing back to a layered structure during polymerization and film drying and/or curing. The hybrid-clay nanocomposite exhibited an increase in tensile properties at low loadings. A transmission electron microscope was used to assess the dispersion of the nanoclays in the matrix resin, which revealed that most of the layered silicates remained exfoliated and the exfoliated clays are distributed uniformly.

Further characterization of the hybrid-clay nanocomposites is underway including the permeation and X-ray analyses. Various organic-inorganic hybrid systems will be investigated for the hybrid-clay composites.

This research was performed in collaboration with Joseph Smith (NASA Langley) and John Connell (NASA Langley).

REPORTS AND ABSTRACTS

Mehrotra, Piyush, and Hans Zima: *High performance Fortran for aerospace applications.* ICASE Report No. 2000-31, (NASA/CR-2000-210321), January 2, 2001, 27 pages. To appear in Parallel Computing.

This paper focuses on the use of High Performance Fortran (HPF) for important classes of algorithms employed in aerospace applications. HPF is a set of Fortran extensions designed to provide users with a high-level interface for programming data parallel scientific applications, while delegating to the compiler/runtime system the task of generating explicitly parallel message-passing programs. We begin by providing a short overview of the HPF language. This is followed by a detailed discussion of the efficient use of HPF for applications involving multiple structured grids such as multiblock and adaptive mesh refinement (AMR) codes as well as unstructured grid codes. We focus on the data structures and computational structures used in these codes and on the high-level strategies that can be expressed in HPF to optimally exploit the parallelism in these algorithms.

Bottasso, Carlo L., Stefano Micheletti, and Riccardo Sacco: *Discontinuous dual-primal mixed finite elements for elliptic problems.* ICASE Report No. 2000-37, (NASA/CR-2000-210543), October 18, 2000, 22 pages. To be submitted to Computer Methods in Applied Mechanics and Engineering.

We propose 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 to introduce 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.

The resulting family of discontinuous dual-primal mixed finite element methods is presented in the one and two-dimensional cases. In the one-dimensional case, we show the equivalence of the method with implicit Runge-Kutta schemes of the collocation type exhibiting optimal behavior. Numerical experiments in one and two dimensions demonstrate the order accuracy of the new method, confirming the results of the analysis.

Xu, Kun: *A gas-kinetic BGK scheme for the compressible Navier-Stokes equations.* ICASE Report No. 2000-38, (NASA/CR-2000-210544), October 30, 2000, 37 pages. To be submitted to the International Journal of Numerical Methods in Fluids.

This paper presents an improved gas-kinetic scheme based on the Bhatnagar-Gross-Krook (BGK) model for the compressible Navier-Stokes equations. The current method extends the previous gas-kinetic Navier-Stokes solver developed by Xu and Prendergast by implementing a general nonequilibrium state to represent the gas distribution function at the beginning of each time step. As a result, the requirement in the previous scheme, such as the particle collision time being less than the time step for the validity of the BGK Navier-Stokes solution, is removed. Therefore, the applicable regime of the current method is much enlarged and the Navier-Stokes solution can be obtained accurately regardless of the ratio between the collision time and the time step. The gas-kinetic Navier-Stokes solver developed by Chou and Baganoff is the limiting case of the current method, and it is valid only under such a limiting condition. Also, in this paper, the appropriate implementation of boundary condition for the kinetic scheme, different kinetic limiting cases, and the Prandtl number fix are presented. The connection among artificial dissipative central schemes, Godunov-type schemes, and the gas-kinetic BGK method is discussed. Many numerical tests are included to validate the current method.

Chen, Zhikai, Kurt Maly, Piyush Mehrotra, and Mohammad Zubair: *Arcade: A web-Java based framework for distributed computing.* ICASE Report No. 2000-39, (NASA/CR-2000-210545), October 23, 2000, 14 pages. Proceedings of WebNet 2000.

Distributed heterogeneous environments are being increasingly used to execute a variety of large size simulations and computational problems. We are developing Arcade, a web-based environment to design, execute, monitor, and control distributed applications. These targeted applications consist of independent heterogeneous modules which can be executed on a distributed heterogeneous environment. In this paper we describe the overall design of the system and discuss the prototype implementation of the core functionalities required to support such a framework.

Lockard, David P., Li-Shi Luo, and Bart A. Singer: *Evaluation of the lattice-Boltzmann equation solver PowerFLOW for aerodynamic applications.* ICASE Report No. 2000-40, (NASA/CR-2000-210550), November 1, 2000, 48 pages.

A careful comparison of the performance of a commercially available Lattice-Boltzmann Equation solver (PowerFLOW) was made with a conventional, block-structured computational fluid-dynamics code (CFL3D) for the flow over a two-dimensional NACA-0012 airfoil. The results suggest that the version of PowerFLOW used in the investigation produced solutions with large errors in the computed flow field; these errors are attributed to inadequate resolution of the boundary layer for reasons related to grid resolution and primitive turbulence modeling. The requirement of square grid cells in the PowerFLOW calculations limited the number of points that could be used to span the boundary layer on the wing and still keep the computation size small enough to fit on the available computers. Although not discussed in detail, disappointing results were also obtained with PowerFLOW for a cavity flow and for the flow around a generic helicopter configuration.

Dubrulle, B., and Guowei He: *Possible statistics of two coupled random fields: Application to passive scalar.* ICASE Report No. 2000-41, (NASA/CR-2000-210553), November 13, 2000, 21 pages. Submitted to the European Journal of Physics C.

We use the relativity postulate of scale invariance to derive the similarity transformations between two coupled scale-invariant random fields at different scales. We find the equations leading to the scaling exponents. This formulation is applied to the case of passive scalars advected i) by a random Gaussian velocity field; and ii) by a turbulent velocity field. In the Gaussian case, we show that the passive scalar increments follow a log-Levy distribution generalizing Kraichnan's solution and, in an appropriate limit, a log-normal distribution. In the turbulent case, we show that when the velocity increments follow a log-Poisson statistics, the passive scalar increments follow a statistics close to log-Poisson. This result explains the experimental observations of Ruiz et al. about the temperature increments.

Bauchau, Olivier A., Jou-Young Choi, and Carlo L. Bottasso: *On the modeling of shells in multibody dynamics.* ICASE Report No. 2000-42, (NASA/CR-2000-210556), November 13, 2000, 28 pages. Submitted to Multibody Dynamics Systems.

Energy preserving/decaying schemes are presented for the simulation of the nonlinear multibody systems involving shell components. The proposed schemes are designed to meet four specific requirements: unconditional nonlinear stability of the scheme, a rigorous treatment of both geometric and material nonlinearities, exact satisfaction of the constraints, and the presence of high frequency numerical dissipation. The kinematic nonlinearities associated with arbitrarily large displacements and rotations of shells are treated in a rigorous manner, and the material nonlinearities can be handled when the constitutive laws stem from the existence of a strain energy density function. The efficiency and robustness of the proposed approach is illustrated with specific numerical examples that also demonstrate the need for integration schemes possessing high frequency numerical dissipation.

Bottasso, Carlo L., Olivier A. Bauchau, and Jou-Young Choi: *An energy decaying scheme for nonlinear dynamics of shells.* ICASE Report No. 2000-43, (NASA/CR-2000-210557), November 13, 2000, 28 pages. Submitted to Computer Methods in Applied Mechanics and Engineering.

A novel integration scheme for nonlinear dynamics of geometrically exact shells is developed based on the inextensible director assumption. 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 nonlinear regime. Furthermore, the scheme features tunable high frequency numerical damping and it is therefore stiffly accurate. The method is tested for a finite element spatial formulation of shells based on mixed interpolations of strain tensorial components and on a two-parameter representation of director rotations. The robustness of the scheme is illustrated with the help of numerical examples.

Ditkowski, A., D. Gottlieb, and B.W. Sheldon: *Optimization of chemical vapor infiltration with simultaneous powder formation.* ICASE Report No. 2000-44, (NASA/CR-2000-210620), November 27, 2000, 21 pages. Submitted to Advanced Materials.

A key difficulty in isothermal, isobaric chemical vapor infiltration is the long processing times that are typically required. With this in mind, it is important to minimize infiltration times. This optimization problem is addressed here, using a relatively simple model for dilute gases. The results provide useful asymptotic expressions for the minimum time and corresponding conditions. These approximations are quantitatively accurate for most cases of interest, where relatively uniform infiltration is required. They also provide useful quantitative insight in cases where less uniformity is required. The effects of homogeneous nucleation were also investigated. This does not affect the governing equations for infiltration of a porous body, however, powder formation can restrict the range of permissible infiltration conditions. This was analyzed for the case of carbon infiltration from methane.

Ayala-Rincón, Mauricio, and César Muñoz: *Explicit substitutions and all that.* ICASE Report No. 2000-45, (NASA/CR-2000-210621), November 28, 2000, 27 pages. To appear in the Colombian Journal of Computation.

Explicit substitution calculi are extensions of the λ-calculus where the substitution mechanism is internalized into the theory. This feature makes them suitable for implementation and theoretical study of logic-based tools such as strongly typed programming languages and proof assistant systems. In this paper we explore new developments on two of the most successful styles of explicit substitution calculi: the $\lambda\sigma$- and λs_e-calculi.

Cockburn, Bernardo, and Chi-Wang Shu: *Runge-Kutta discontinuous Galerkin methods for convection-dominated problems.* ICASE Report No. 2000-46, (NASA/CR-2000-210624), December 5, 2000, 80 pages. Submitted to SIAM Review.

In this paper, we review the development of the Runge-Kutta discontinuous Galerkin (RKDG) methods for non-linear convection-dominated problems. These robust and accurate methods have made their way into the main stream of computational fluid dynamics and are quickly finding use in a wide variety of applications. They combine a special class of Runge-Kutta time discretizations, that allows the method to be non-linearly stable regardless of its accuracy, with a finite element space discretization by discontinuous approximations, that incorporates the ideas of numerical fluxes and slope limiters coined during the remarkable development of the high-resolution finite difference and finite volume schemes. The resulting RKDG methods are stable, high-order accurate, and highly parallelizable schemes that can easily handle complicated geometries and boundary conditions. We review the theoretical and algorithmic aspects of these methods and show several applications including nonlinear conservation laws, the compressible and incompressible Navier-Stokes equations, and Hamilton-Jacobi-like equations.

Cockburn, Bernardo, Mitchell Luskin, Chi-Wang Shu, and Endre Süli: *Enhanced accuracy by post-processing for finite element methods for hyperbolic equations.* ICASE Report No. 2000-47, (NASA/CR-2000-210625), December 14, 2000, 34 pages. Submitted to Mathematics of Computation.

We consider the enhancement of accuracy, by means of a simple post-processing technique, for finite element approximations to transient hyperbolic equations. The post-processing is a convolution with a kernel whose support has measure of order one in the case of arbitrary unstructured meshes; if the mesh is locally translation invariant, the support of the kernel is a cube whose edges are of size of the order of the mesh size only. For example, when polynomials of degree k are used in the discontinuous Galerkin (DG) method, and the exact solution is globally smooth, the DG method is of order $k + 1/2$ in the L^2 norm, whereas the post-processed approximation is of order $2k + 1$; if the exact solution is in L^2 only, in which case no order of convergence is available for the DG method, the post-processed approximation converges with order $k + 1/2$ in L^2 over a subdomain on which the exact solution is smooth. Numerical results displaying the sharpness of the estimates are presented.

He, Guowei, and R. Rubinstein: *Mapping closure approximation to conditional dissipation rate for turbulent scalar mixing.* ICASE Report No. 2000-48, (NASA/CR-2000-210631), December 14, 2000, 12 pages. To be submitted to Physics of Fluids.

A novel mapping closure approximation (MCA) technique is developed to construct a model for the conditional dissipation rate (CDR) of a scalar in homogeneous turbulence. It is shown that the CDR model from amplitude mapping closure is incorrect in asymptotic behavior for unsymmetric binary mixing. The correct asymptotic behavior can be described by the CDR model formulated by the MCA technique. The MCA approach is outlined for constructing successive approximation to probability density function (PDF) and conditional moment.

Shi, Jing, Changqing Hu, and Chi-Wang Shu: *A technique of treating negative weights in WENO schemes.* ICASE Report No. 2000-49, (NASA/CR-2000-210632), December 27, 2000, 22 pages. Submitted to the Journal of Computational Physics.

High order accurate weighted essentially non-oscillatory (WENO) schemes have recently been developed for finite difference and finite volume methods both in structured and in unstructured meshes. A key idea in WENO scheme is a linear combination of lower order fluxes or reconstructions to obtain a higher order approximation. The combination coefficients, also called linear weights, are determined by local geometry of the mesh and order of accuracy and may become negative. WENO procedures cannot be applied directly to obtain a stable scheme if negative linear weights are present. Previous strategy for handling this difficulty is by either regrouping of stencils or reducing the order of accuracy to get rid of the negative linear weights. In this paper we present a simple and effective technique for handling negative linear weights without a need to get rid of them. Test cases are shown to illustrate the stability and accuracy of this approach.

Rubinstein, Robert, and Meelan Choudhari: *Statistical prediction of laminar-turbulent transition.* ICASE Report No. 2000-50, (NASA/CR-2000-210638), January 5, 2001, 39 pages. To be submitted to Physics of Fluids.

Stochastic versions of stability equations are considered as a means to develop integrated models of transition and turbulence. Two types of stochastic models are considered: probability density function evolution equations for stability mode amplitudes, and Langevin models based on representative stability theories including the resonant triad model and the parabolized stability equations. The first type of model can describe the effect of initial phase differences among disturbance modes on transition location. The second type of model describes the growth of random disturbances as transition proceeds and provides a natural framework in which to couple transition and turbulence models. Coupling of parabolized stability equations with either subgrid stress models or with conventional turbulence models is also discussed as an alternative route to achieve the goal of integrated turbulence and transition modeling.

Huyse, Luc, and R. Michael Lewis: *Aerodynamic shape optimization of two-dimensional airfoils under uncertain operating conditions.* ICASE Report No. 2001-1, (NASA/CR-2001-210648), January 16, 2001, 13 pages. To appear in the Proceedings of the International Conference on Structural Safety and Reliability.

Practical experience with airfoil optimization techniques has revealed unexpected difficulties. Traditionally the performance of an airfoil is optimized for given, or assumed, model parameters. Experience has indicated that a deterministic optimization for discrete operating conditions may result in dramatically inferior performance when the actual conditions are different from these, somewhat arbitrarily chosen, design values. Extensions to multi-point optimization have proven unable to adequately remedy the problem of "localized optimization". This paper presents an intrinsically statistical approach and demonstrates how the shortcomings of multi-point optimization with respect to "localized optimization" can be overcome.

Lüttgen, Gerald, and Walter Vogler: *A faster-than relation for asynchronous processes.* ICASE Report No. 2001-2, (NASA/CR-2001-210651), January 16, 2001, 35 pages. To be submitted to the 12th International Conference on Concurrency Theory.

This paper introduces a novel (bi)simulation-based faster-than preorder which relates asynchronous processes with respect to their worst-case timing behavior. The studies are conducted for a conservative extension of the process algebra CCS, called TACS, which permits the specification of maximal time bounds of actions. TACS complements work in plain process algebras which compares asynchronous processes with respect to their functional reactive behavior only, and in timed process algebras which focus on analyzing synchronous processes. The most unusual contribution of this paper is in showing that the proposed faster-than preorder coincides with two other and at least equally appealing preorders, one of which considers the absolute times at which actions occur in system runs. The paper also develops the semantic theory of TACS: it characterizes the largest precongruence contained in the faster-than preorder. A small example relating two implementations of a simple storage system testifies to the practical utility of the new theory.

Mavriplis, Dimitri J.: *Multigrid approaches to non-linear diffusion problems on unstructured meshes.* ICASE Report No. 2001-3, (NASA/CR-2001-210660), February 12, 2001, 16 pages. Submitted to the Journal of Numerical Linear Algebra with Applications.

The efficiency of three multigrid methods for solving highly non-linear diffusion problems on two-dimensional unstructured meshes is examined. The three multigrid methods differ mainly in the manner in which the nonlinearities of the governing equations are handled. These comprise a non-linear full approximation storage (FAS) multigrid method which is used to solve the non-linear equations directly, a linear multigrid method which is used to solve the linear system arising from a Newton linearization of the non-linear system, and a hybrid scheme which is based on a non-linear FAS multigrid scheme, but employs a linear solver on each level as a smoother. Results indicate that all methods are equally effective at converging the non-linear residual in a given number of grid sweeps, but that the linear solver is more efficient in cpu time due to the lower cost of linear versus non-linear grid sweeps.

Povitsky, Alex, and Manuel D. Salas: *Lagrangian approach to jet mixing and optimization of the reactor for production of carbon nanotubes.* ICASE Report No. 2001-4, (NASA/CR-2001-210662), February 14, 2001, 27 pages. To be submitted to AIAA Journal.

This study was motivated by an attempt to optimize the High Pressure carbon oxide (HiPco) process for the production of carbon nanotubes from gaseous carbon oxide. The goal is to achieve rapid and uniform heating of catalyst particles by an optimal arrangement of jets. A mixed Eulerian and Lagrangian approach is implemented to track the temperature of catalyst particles along their trajectories as a function of time. The FLUENT CFD software with second-order upwind approximation of convective terms and an algebraic multigrid-based solver is used. The poor performance of the original reactor configuration is explained in terms of features of particle trajectories. The trajectories most exposed to the hot jets appear to be the most problematic for heating because they either bend towards the cold jet interior or rotate upwind of the mixing zone. To reduce undesirable slow and/or oscillatory heating of catalyst particles, a reactor configuration with three central jets is proposed and the optimal location of the central and peripheral nozzles is determined.

Ciardo, Gianfranco, Gerald Lüttgen, and Radu Siminiceanu: *Saturation: An efficient iteration strategy for symbolic state-space generation.* ICASE Report No. 2001-5, (NASA/CR-2001-210663), February 14, 2001, 21 pages. To appear in Proc. of the 7th Int'l. Conf. on Tools and Algorithms for the Construction and Analysis of Systems.

This paper presents a novel algorithm for generating state spaces of asynchronous systems using Multi-valued Decision Diagrams. In contrast to related work, the next-state function of a system is not encoded as a single Boolean function, but as cross-products of integer functions. This permits the application of various iteration strategies to build a system's state space. In particular, this paper introduces a new elegant strategy, called saturation, and implements it in the tool SMART. On top of usually performing several orders of magnitude faster than existing BDD-based state-space generators, the algorithm's required peak memory is often close to the final memory needed for storing the overall state spaces.

Hesthaven, J.S., and T. Warburton: *High-order/spectral methods on unstructured grids I. Time-domain solution of Maxwell's equations.* ICASE Report No. 2001-6, (NASA/CR-2001-210836), March 27, 2001, 45 pages. Submitted to the Journal of Computational Physics.

We present an ab initio development of a convergent high-order accurate scheme for the solution of linear conservation laws in geometrically complex domains. As our main example we present a detailed development and analysis of a scheme suitable for the time-domain solution of Maxwell's equations in a three-dimensional domain. The fully unstructured spatial discretization is made possible by the use of a high-order nodal basis, employing multivariate Lagrange polynomials defined on the triangles and tetrahedra. Careful choices of the unstructured nodal grid points ensure high-order/spectral accuracy, while the equations themselves are satisfied in a discontinuous Galerkin form with the boundary conditions being enforced weakly through a penalty term. Accuracy, stability, and convergence of the semi-discrete approximation to Maxwell's equations is established rigorously and bounds on the global divergence error are provided. Concerns related to efficient implementations are discussed in detail.

This sets the stage for the presentation of examples, verifying the theoretical results, as well as illustrating the versatility, flexibility, and robustness when solving two- and three-dimensional benchmarks in computational electromagnetics. Pure scattering as well as penetration is discussed and high parallel performance of the scheme is demonstrated.

INTERIM REPORTS

Rubinstein, R., C.L. Rumsey, M.D. Salas, and J.L. Thomas, editors, *Turbulence modeling workshop.* ICASE Interim Report No. 37, (NASA/CR-2001-210841), April 11, 2001, 193 pages.

Advances in turbulence modeling are needed in order to calculate high Reynolds number flows near the onset of separation and beyond. To this end, the participants in this workshop made the following recommendations. (1) A national/international database and standards for turbulence modeling assessment should be established. Existing experimental data sets should be reviewed and categorized. Advantage should be taken of other efforts already underway, such as that of the European Research Community on Flow, Turbulence, and Combustion (ERCOFTAC) consortium. Carefully selected "unit" experiments will be needed, as well as advances in instrumentation, to fill the gaps in existing datasets. A high priority should be given to document existing turbulence model capabilities in a standard form, including numerical implementation issues such as grid quality and resolution. (2) NASA should support long-term research on Algebraic Stress Models and Reynolds Stress Models. The emphasis should be placed on improving the length-scale equation, since it is the least understood and is a key component of two-equation and higher models. Second priority should be given to the development of improved near-wall models. Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES) would provide valuable guidance in developing and validating new Reynolds-averaged Navier-Stokes (RANS) models. Although not the focus of this workshop, DNS, LES, and hybrid methods currently represent viable approaches for analysis on a limited basis. Therefore, although computer limitations require the use of RANS methods for realistic configurations at high Reynolds number in the foreseeable future, a balanced effort in turbulence modeling development, validation, and implementation should include these approaches as well.

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Huyse, L., and R.M. Lewis, "Aerodynamic shape optimization of two-dimensional airfoils under uncertain operating conditions," International Conference on Structural Safety and Reliability, Newport Beach, CA.

Krueger, R., I.L. Paris, T.K. O'Brien, and P.J. Minguet, "Fatigue life methodology for bonded composite skin/stringer configurations," ASTM Journal of Composites Technology and Research, submitted January 2001.

Muñoz, C., R.W. Butler, V. Carreno, and G. Dowek, "On the verification of conflict detection algorithms," NASA Technical Memorandum, submitted March 2001.

Ounaies, Z., K. Mossi, R.C. Smith, and J.D. Bernd, "Low-field and high-field characterization of THUNDER actuators," SPIE: Smart Materials and Structures Spring Conference, Newport Beach, CA, March 2001.

Ounaies, Z., C. Park, D. Klein, and J.S. Harrison, "Field responsive polyimides: An analysis of their piezoelectricity," American Chemical Society Poly Millennial 2000, December 2000.

Park, C., Z. Ounaies, K. Wise, J.S. Harrison, and J.G. Smith, Jr., "Partially cured polyimides: A poling study," American Chemical Society Poly Millennial 2000, December 2000.

Povitsky, A., "Aeroacoustics of a stagnation flow near a rigid wall," Physics of Fluids, 12, No. 10 (2000), pp. 2595–2608.

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Povitsky, A., "High-order compact simulation of wave propagation in a non-uniform mean flow," AIAA Paper 2001-2628, 15th AIAA Computational Fluid Dynamics Conference, Anaheim, CA, June 2001.

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Povitsky, A., "Numerical study of wave propagation in a non-uniform compressible flow," Physics of Fluids, submitted.

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ICASE COLLOQUIA

Name/Affiliation/Title	Date
Philip Hall, Imperial College, UK "Chaotic Breakdown of Stagnation Point Flows"	October 3, 2000
Enrique Lavernia, University of California, Irvine "Processing of Nanostructured Systems: Coatings and Bulk Materials"	October 5, 2000
Julia Weertman, Northwestern University "Mechanical Behavior of Nanocrystalline Metals"	October 18, 2000
Robert Averback, University of Illinois at Urbana-Champaign "Processing and Properties of Nanostructured Bulk Metallic Alloys"	October 19, 2000
Ira Livshits, Carnegie Mellon University "Wave-ray Multigrid Methods for Highly Indefinite Helmholtz Equation"	October 20, 2000
Oren Livne, Weizmann Institute of Science, Israel "$O(N \log N)$ Multilevel Calculation of N Eigenfunctions"	October 23, 2000
Gary Shiflet, University of Virginia "Nanocrystal Formation from Aluminum-based Metallic Glass"	October 26, 2000
Michael Krane, Rutgers University "Reduced-complexity Aeroacoustic Prediction in Pipe Flows Applied to Speech Synthesis"	October 27, 2000
Bjorn Backman, University of Southern Florida ICASE Series on Risk-Based Design: "Design Innovation and Risk Management: A Structural Designer's Voyage Into Uncertainty"	November 13, 2000
Raymond Cosner, Boeing Phantom Works, St. Louis, MO ICASE Series on Risk-based Design: "Uncertainty Management in Computational Fluid Dynamics"	November 14, 2000
Jianjun Cheng, University of California, Santa Barbara "Synthesis and Studies of Optically Active Poly(beta-peptides)"	November 15, 2000
Kamen Beronov, Nagoya University, Japan "Three Topics in Two-point Closure Modeling of Anisotropic Homogeneous Turbulence"	November 16, 2000

Name/Affiliation/Title	Date
Maher Boulos, Universite de Sherbrooke, Quebec, Canada "Thermal Plasma Applications to Nano-structured Materials Synthesis"	November 17, 2000
Takashi Ishihara, Nagoya University, Japan "Lagrangian Statistics in the Inertial Subrange of Isotropic Turbulence"	November 17, 2000
David Nicholls, University of Minnesota "High Order Boundary Perturbation Methods for Free Boundary and Boundary Value Problems"	November 20, 2000
Anatole Beck, University of Wisconsin, Madison "A Fractal Example in Ordinary Differential Equations"	November 21, 2000
Zhenyuan Wang, University of Texas at El Paso "Classification by Nonlinear Integral Projection Pursuit"	December 1, 2000
Singiresu Rao, University of Miami ICASE Series on Risk-based Design: "Modeling of Uncertainty in Structural Design"	December 4, 2000
Gilbert Strang, Massachusetts Institute of Technology "Three Matrices and Their Applications"	December 15, 2000
Hanne Gottliebsen, University of St. Andrews "Transcendental Functions and Continuity Checking in PVS"	January 16, 2001
Nahum Zobin, The College of William & Mary "Math of Heart Attacks"	January 17, 2001
Scott Beeler, North Carolina State University "Nonlinear Feedback Control Methodologies and Their Application to a Thin Film Growth Process"	January 22, 2001
Timothy Hasselman, ACTA Incorporated ICASE Series on Risk-based Design: "Reliability-based Optimization for Structural Design"	January 25, 2001
Seongsin Kim, Agilent Technologies, San Jose, CA "MOCVD Growth and Characterization of Epitaxial Quantum Dots for Optoelectronic Devices"	January 29, 2001

Name/Affiliation/Title	Date
Dennis Gannon, Indiana University, Bloomington "Science Portals and Distributed Software Component Architectures"	February 2, 2001
Sarah-Jane Frankland, North Carolina State University "Evaluating Carbon Nanotube Applications with Simulation: Hydrogen Storage and Polymer Composites"	February 9, 2001
William Oberkampf, Sandia National Laboratories ICASE Series on Risk-based Design: "Error and Uncertainty in Modeling and Simulation"	February 21, 2001
Billie F. Spencer, The University of Notre Dame ICASE Series on Risk-based Design: "Control of Civil Infrastructure Systems"	February 26, 2001
Christopher Viney, Heriot-Watt University, Scotland "New Materials from the Zoo"	March 1, 2001
Matthias Heinkenschloss, Rice University "Domain Decomposition Based Optimization Methods for the Optimal Control of Partial Differential Equations"	March 9, 2001
Boris Chernyavskiy, Rutgers, The State University of New Jersey "Parallel Code Performance on Beowulf Type Clusters"	March 14, 2001
Semyon Tsynkov, North Carolina State University "Active Shielding and Control of Environmental Noise"	March 15, 2001
S. Hariharan, The University of Akron "On Phase-field Methods"	March 16, 2001
Svetlana Poroseva, Stanford University "Pressure-containing Correlations: The Main Issue in High-order Turbulence Closures"	March 19, 2001
Pin Tong, Hong Kong University of Science and Technology "Fracture of Piezoelectric Ceramics"	March 23, 2001

OTHER ACTIVITIES

On January 12–13, 2001, ICASE and NASA Langley co-sponsored a Turbulence Modeling Workshop at the Reno Hilton in Reno, Nevada. The purpose of the Workshop was to discuss current and future capabilities for predicting High Reynolds Number turbulent separated flows at flight conditions. There were 39 attendees, and an ICASE Interim Report will be published.

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