NASA/CR-2002-211436

Semiannual Report

April 1, 2001 through September 30, 2001

20020325 143

February 2002

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NASA/CR-2002-211436

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ICASE
NASA Langley Research Center
Hampton, Virginia

Operated by Universities Space Research Association

CONTENTS

INTRODUCTION

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

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

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

The major categories of the current ICASE research program are:

- Applied and numerical mathematics, including multidisciplinary design optimization;
- Applied computer science: system software, systems engineering, and parallel algorithms;
- Theoretical, computational, and experimental research in fluid mechanics in selected areas of interest to LaRC, such as transition, turbulence, flow control, and acoustics; and
- Theoretical, computational, and experimental research in structures and material sciences with emphasis on smart materials and nanotechnologies.

ICASE reports are primarily considered to be preprints of manuscripts that have been submitted to appropriate research journals or that are to appear in conference proceedings. A list of these reports for the period April 1, 2001 through September 30, 2001 is given in the Reports and Abstracts section, which follows a brief description of the research in progress.

RESEARCH IN PROGRESS

APPLIED AND NUMERICAL MATHEMATICS

Active flow control research tool development
Brian G. Allan

The design of future aircraft engine inlets are evolving into more compact and exotic shapes. These future inlet designs are driven by the need for propulsion systems to be much lighter and compact. However, inlet designs are restricted by pressure loss and flow non-uniformity at the engine face. In order to accommodate the need for lighter and more compact propulsion systems, the use of secondary flow control devices are needed to overcome inlet design restrictions. Secondary flow control devices being used now include vortex generator vanes and jets. It has been shown that these devices can allow for reduced inlet lengths and sharper turning angles while maintaining a desired flow distortion at the engine face. In order to take advantage of these devices, computational tools need to be developed in order to evaluate future inlet designs. The goal of this research is to develop computational boundary conditions and techniques for a computational fluid dynamics code, in order to model vortex generator vanes and synthetic jets for inlet applications.

Using a compressible Reynolds averaged Navier-Stokes code, developed at NASA, numerical simulations of micro-vortex generator vanes and jets on a flat plate and ramp have been performed. Experiments for a single micro-vortex generator vane on a flat plate have been performed at NASA Langley Research Center. Comparisons of the numerical results and the experimental data for the single vane have shown that the turbulence modeling has a large effect on the computed flow field. A comparison between a numerical simulation using the Spalart-Allmaras (SA) and Mentor SST models showed the vortex produced by the vane to be over damped for both cases. However, the simulations using the SST model were able to predict the trajectory of the vortex and the peak vorticity, much better than the simulation using the SA model. The vortex generator vanes used in this study have a height which is 20% of boundary layer thickness. This generates a much weaker vortex than a standard vane which has a height equal to the boundary layer thickness, and a vortex which is much closer to the wall, increasing wall damping effects. Experiments using various height vanes will be conducted at NASA Langley providing further comparisons with numerical simulations. From these comparisons a better understanding of the numerical modeling of vortex generators in a boundary layer will be realized.

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, Chung-Sheng Yao, and John Lin (NASA Langley). Numerical results were computed using the ICASE PC cluster, Coral.

Feedback control of nonlinear systems
Scott C. Beeler

We are studying the feedback control problem for nonlinear systems of ODEs, concentrating on an optimality-based feedback control approach. The state-dependent Riccati equation (SDRE) algorithm is one such method, derived from the optimal control conditions. It seeks to include the nonlinear elements of the problem in the control formulation in an attempt to achieve greater optimality than linear-based methods, while still maintaining desired robustness properties. Our work in this area looks to develop SDRE-based

techniques for problems involving nonlinear dynamics and control inputs. These techniques can be applied to aircraft guidance and control problems including abort-type scenarios and control actuator impairment situations. Another possible application is to small remote-controlled gliders in significant ambient winds. This lightweight unpowered flight has a smaller velocity and so the winds have a greater effect on the craft's flight dynamics and maneuvering capabilities.

We have implemented in MATLAB code several versions of the SDRE algorithm for feedback control, and have tested them on example problems with nonlinearities in both the state and control dynamics (for which the performance has been encouraging). One possible application for this, a glider in ambient winds, has been formulated in MATLAB and Fortran code, and is ready to be studied and controlled. In addition, research into fuzzy logic control is underway, for application to the glider problem. For higher-level control problems, such as the glider surveying certain areas at certain times while maintaining altitude, fuzzy logic control may be very useful due to somewhat vague and possibly conflicting goals. With this groundwork laid for problems to be studied and techniques to be used, we can proceed with applying the newly-developed control methods to the more complex examples of interest.

Future efforts include fine-tuning of the SDRE methods to improve its performance and robustness, and study of the methods in application to a more realistic nonlinear control problem than the rather artificial examples used so far. Various control problems using the glider example will be constructed and control methods will be applied to them. Once these mid-level scenarios have been studied, things such as larger-scale glider surveying problems can be constructed, with fuzzy logic control probably used in some capacity in the control design. Other control techniques may be implemented as well to study and compare their performance, and other aircraft guidance and control models may be subjected to the controls as well.

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

Scaling and performance of DSMC simulations
Przemyslaw Bogacki and David E. Keyes

The objective of this effort is to develop highly performant and scalable implementations of the Direct Simulation Monte Carlo (DSMC) method. DSMC is a discrete approximation to the Boltzmann formulation of gas dynamics that is well established for simulating rarefied flows. It is also of interest to NASA in the context of nonrarefied flows, where it is expected to provide insight into transitional and turbulent flows. As such, it is the focus of a multinational initiative, of which this research is a part.

A domain-decomposed implementation of a DSMC code, using MPI-based message passing, has been created from an original sequential implementation by Graeme Bird. This implementation facilitates a possible overlap of communication and computation, to the extent that the architecture supports the latter (i.e., there is separate communication hardware). Flexibility has been preserved in the distributed data structures handling assignment of cells to processors and communication between processors to allow for the possibility of adaptive load balancing. The code has been debugged against the original sequential code by Bird. The ICASE Coral cluster and Old Dominion University Sun LIONS systems have been the implementation platforms.

Future plans include establishing benchmark per-node and scalability performance, undertaking detailed profiling from the level of the sequential inner loops through the interprocessor message passing to isolate performance bottlenecks. Then heuristics will be employed based on memory locality and communication/computation trade-offs to implement performance enhancements. The effectiveness of these enhancements will be evaluated across a variety of architectures. Ultimately, based on these experiments, and in

2

cooperation with other collaborators closer to the modeling and the motivating engineering applications, possible modifications of the DSMC method will be suggested to allow further enhancements and evaluate their trade-offs.

Textbook multigrid efficiency for CFD simulations
Boris Diskin

The major goal of my research is to demonstrate textbook multigrid efficiency (TME) in solving basic computational fluid dynamics models associated with the Reynolds-averaged Navier-Stokes (RANS) equations. A multigrid method demonstrates TME if the solution to the governing system of equations is attained in a computational work that is a small (less than 10) multiple of the operation count in one target-grid residual evaluation. One can think about TME as efficiency typical for multigrid solutions of the Laplace equation. The methodology proposed for achieving such efficiency for the RANS equations is the distributed relaxation method separating different factors contributing to the system and treating them optimally. Recently, a new approach to discretizing the RANS equation has been developed. Following this approach one can design a family of factorizable discretization schemes that are very suitable for distributed relaxation. Computational tests with representatives of these new discrete schemes have corroborated accuracy of the schemes; TME in solutions of these schemes has been demonstrated. However, it was observed that, in spite of demonstrating TME, the multigrid solvers employed did not quite match the efficiency typical for the Laplace equation. The most notable difference was the fact that, for achieving TME for RANS simulations, it was required to employ F or W cycles, while simple V cycles, very efficient for Laplacian, were either slow or unstable, even for constant-coefficient models. In the past six months, we thoroughly investigated the sources for such a deterioration and worked out the recipes to avoid it.

We have identified two main reasons for possible V-cycle efficiency deterioration:

1. *Treatment of boundary conditions:* The distributed relaxation approach decouples equations in the interior, while, at the boundary, equations remain strongly coupled. In the general framework for achieving TME, several sweeps of local relaxation near the boundaries are recommended. It has been realized, however, that an arbitrary choice for internal boundary conditions accompanying the local relaxation procedure can undermine the stability of the global iterative algorithm. Using a constant-coefficient analysis for stability of boundary conditions, we have developed an analytical criterion to identify suitable sets of the boundary conditions for the local relaxation procedure.

2. *Coarse-grid correction prolongation:* The multigrid methodology for TME solutions of the RANS equations envisions that the coarse-grid corrections are interpolated (prolonged) in terms of primitive variables. On the other hand, decoupling of the discrete equations occurs in terms of auxiliary variables related to primitive ones through some transformation. Prolongation in terms of primitive variables implies some large (often non-local) interpolation stencils for auxiliary variables. Thus, efficiency of the RANS equations solver corresponds to (deteriorated) efficiency of a scalar-equation solver employing those large interpolation stencils. Two ways to cure the difficulty have been proposed. (1) The first way is an implementation of a general recipe to include some "inner multigrid cycle" already at the relaxation stage. In other words, a multigrid cycle (rather than a simple relaxation pass) is applied to a scalar factor before transferring residuals to the coarse grid in framework of an outer multigrid cycle. This approach is a part of a general multigrid methodology for achieving TME and is considered necessary for multidimensional compressible RANS problems. If an "inner multigrid cycle" is applied, the precise form of prolongation in the outer multigrid cycle is

less important for overall efficiency. (2) The second approach is to modify the prolongation stencil in the outer multigrid cycle such that the corrections obtained by auxiliary variables approximate the corrections they would obtain in an "inner multigrid cycle." Sometimes such a modification can be done by local changes, sometimes it requires a global (but inexpensive) solution of a scalar equation.

Numerical tests have been performed with modified algorithms solving the RANS equations, and the convergence typical for Laplace equation has been restored.

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

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

Incorporating a Mars atmospheric model into a least squares environment for 2001 Mars Odyssey aerobraking operations
Alicia M. Dwyer

The method of aerobraking has proved successful in missions to both Mars and Venus. Aerobraking uses the atmosphere of the planet, rather than chemical propulsion, to reduce the size of the orbit of a spacecraft. In October 2001, aerobraking will again be used by the 2001 Mars Odyssey orbiter to obtain a desired science mapping orbit. The success of the aerobraking mission depends on how accurately the behavior of the atmosphere is known. Knowledge of the Mars atmosphere is obtained from previous passes through the atmosphere by landers such as Viking and Pathfinder, and aerobraking passes recorded by orbiters like the Mars Global Surveyor. The previous mission data, combined with an understanding of the physics of the atmosphere, become the basis of atmospheric models. The models, used in the design and operation of spacecraft, are critical to mission success.

One engineering-oriented model of the atmosphere being used for the 2001 Odyssey mission is the Mars Global Reference Atmospheric Model (Mars-GRAM). Mars-GRAM, developed at the Marshall Space Flight Center, calculates the mean density for any location (altitude, latitude, and longitude) and time (seasonal and diurnal) on the planet. However, in the polar regions where the majority of the Odyssey mission will take place, the error between modeled and observed values increases. The author's work involves analyzing the use of Mars-GRAM in a least squares environment. By including small variations to input parameters, which effect peak density and the atmospheric drag duration of a trajectory, analysis will determine if Mars-GRAM densities calculated using the least squares approach will more accurately represent aerobraking observations.

Currently, Mars-GRAM is being incorporated into the least squares software and will be validated using past aerobraking mission data from the Mars Global Surveyor. In the future, the software will also tested using a simulated nominal 2001 Odyssey mission. Upon successful completion of the tests and validation, the software will be implemented as part of the Odyssey operational software and used to determine a wave model of the atmosphere.

This work is done in collaboration with Robert Tolson (George Washington University, Joint Institute for Advancement of Flight Sciences).

Analysis of accelerometer measurements and six degree-of-freedom simulations for aerobraking operations of Mars 2001 Odyssey
Jill Hanna

Atmospheric aerobraking has been used in two different planetary missions, Magellan at Venus and Mars Global Surveyor, to change an elliptical orbit to a nearly circular orbit. This process will be used again for the Mars 2001 Odyssey. The Odyssey spacecraft will enter the atmosphere of Mars on October 24th and the operations teams at the Jet Propulsion Laboratory, Lockheed Martin Astronautics, and NASA Langley Research Center will begin a three-month process of guiding the spacecraft safely through the atmosphere, reducing the orbital energy, and bringing the spacecraft into a circular science orbit.

As part of the Langley operations team, the author is serving as part of the Flight Mechanics team and the Accelerometer team. As a Flight Mechanics team member, she is simulating the flight path of the spacecraft through the atmosphere with a six degree-of-freedom simulation. She compares the simulated data to the rotational characteristics of the flight data, while at the same time determining the uncertainties in the spacecraft aerodynamics. All of the operations software will be automated so that little human interaction is required to process the data. The software for the simulation comparison for the Flight Mechanics team has been completed and the process has begun for validation of all software. Accelerometers are an essential part of the aerobraking operations. From accelerometer data, important properties of the atmosphere, such as density and density scale height, are obtained. As part of the Accelerometer team, the author is responsible for obtaining these properties after each orbit and relaying this information to other facilities as well as to all other teams here at Langley. The Accelerometer team software is operational with only minor changes yet to be completed. There have been four Operations Readiness Tests in which the Langley operations team has been an active participant. In these tests, spacecraft telemetry was simulated and used to reproduce several expected flight passes through the atmosphere. All tests were successful and demonstrated that NASA Langley is well prepared for the upcoming aerobraking phase of Mars Odyssey.

From October 2001 to February 2002, the Langley operations team will analyze the functions of the spacecraft during aerobraking. Much of this analysis will be based on results from the Accelerometer team. The author also will recommend updates to the aerodynamics database of the spacecraft due to results from six degree-of-freedom simulations of the Flight Mechanics team.

Robust optimization including model uncertainties
Luc Huyse

During the preliminary stages of a design process only crude estimates are known for many model parameters. In addition, operational uncertainty associated with certain parameters (Mach number, flight path) cannot be avoided. Deterministic optimization using pre-determined 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. In previous work, we have developed a statistical framework to reduce this sensitivity.

Our objective of robust optimization is to find the design with the best overall, i.e., expected, 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. We applied the newly developed techniques 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.

Current formal aerodynamic optimization procedures assume that airfoil performance is perfectly predicted by CFD analysis. The next development step in this project is to account for the effects of the model uncertainty itself in the optimization procedure. Turbulence models are subject to considerable uncertainty. Special attention will also be paid to the effects of boundary condition uncertainty. This uncertainty is introduced during the numerical solution phase when the infinite or semi-infinite integration domain is cut-off at some "far-field" boundary.

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

Stochastic methods for CFD applications
Luc Huyse and Robert W. Walters

Non-deterministic analysis methods for CFD have gained considerable attention in recent years. In the first phase of this project, we have provided an overview of existing non-deterministic approaches to computational fluid dynamics problems. The computation of stochastic solutions to the governing equations of fluid dynamics faces some specific challenges. In this research we will perform a thorough uncertainty assessment, considering the impact of inherent uncertainty as well as uncertainty due to an incomplete understanding of the physics and uncertainty introduced when the integration domain is cut off at some "far field" boundary.

Methods that are covered include interval analysis, Monte Carlo simulation, moment methods, and polynomial chaos. Both random variable and random field models are considered. Applications include nonlinear convection-diffusion; supersonic flow over wedges, expansions and an airfoil; and a two-dimensional boundary layer flow. Particular attention is paid to an accurate modeling of the uncertainty associated with the mathematical model description of the actual physics and the boundary conditions.

Current research focuses on algorithmic aspects of the polynomial chaos expansions as well as on a probabilistically accurate modeling of the boundary condition uncertainty.

Study of the efficiency and accuracy of physical time integration schemes for the unsteady Navier-Stokes equations
Giridhar Jothiprasad

Many physical phenomena of interest are inherently unsteady and with the continuous reduction of computer costs more attention is devoted to the simulation of these flows. However, there is a need for further reduction of computer time for unsteady flows. The purpose of this work is to investigate possible reductions in computer time due to choice of an efficient time integration scheme from a series of schemes differing in the order of accuracy. In any comparison of efficiency a precise error tolerance is a requirement. It is well known that high-order schemes (fourth-, fifth-) outperform low-order schemes at small error tolerances. We investigate whether these schemes are optimal at large (engineering) tolerances ($10^{-1} - 10^{-2}$) as well.

For the purpose of comparison, an existing unstructured multigrid Navier-Stokes solver developed by Dimitri Mavriplis was modified to incorporate various physical time-stepping schemes. The modified program allows time to be discretized in a fully implicit sense using both multistep BDF and multistage RK schemes. The resulting nonlinear algebraic equations are solved iteratively with multigrid acceleration to speed up the convergence. Also, we focused on the ESDIRK (Explicit first stage, Single diagonal coefficient, Diagonally Implicit Runge-Kutta) class of RK schemes. We have completed coding the various modifications in FORTRAN 77 and are currently analyzing whether the expected asymptotic order of accuracy was achieved for the various schemes.

We need to establish the asymptotic order of accuracy of various BDF and RK schemes. A major contributor to the inefficiency of implicit methods is solving the nonlinear systems at each stage to inappropriate sub-iteration tolerance levels. Hence, the level to which the implicit equations should be converged given the desired order of accuracy should also be studied. We also hope to incorporate a turbulence model into the equations and study how this affects the convergence and efficiency results. Also, the use of RK schemes also enables us to incorporate an error estimator into the solver which could further be used to automate the process of choosing a timestep given the desired accuracy.

This work was carried out with the guidance of Dimitri Mavriplis.

Unstructured nonconforming multigrid algorithms for the solution of radiation transport problems
Kab Seok Kang

The simulation of radiation transport in the optically thick flux-limited diffusion regime has been identified as one of the most time-consuming tasks within large simulation codes. Due to multimaterial complex geometry, the radiation transport system must often be solved on unstructured grids. A variety of finite volume and conforming finite element schemes have been employed in research at ICASE and at numerous national laboratories on this so-called "radiation diffusion" system. Meanwhile, multilevel, nonconforming finite element or covolume method have proven flexible and effective on incompressible fluid flow problems. The objective of this research is to investigate the behavior and the benefits of unstructured nonconforming multigrid algorithms used as linear solvers (inside of Newton approaches), directly as nonlinear solvers, or simply as preconditioners in solving steady and unsteady implicit radiation diffusion problems.

We have completed coding linear and nonlinear versions of a two-dimensional unstructured nonconforming multigrid algorithm and have begun comparisons with earlier methods and parallelization. We use the P_1 nonconforming finite element space on triangular mesh and nested-mesh subdivision to automatically generate a sequence of unstructured meshes on the domain.

We plan to document the relative advantages of this method and measure its scalability on large numbers of processors of the ICASE Coral cluster and other machines, and extend into three-dimensional settings.

An approximation management framework for nonlinear programming
R. Michael Lewis

We have previously developed a trust region approximation management framework, AMMO, for the use of general non-quadratic approximations in optimization that insures robust global behavior. This work is one of the few systematic approaches to the use of non-quadratic approximations and surrogates in nonlinear programming and provides an analytical justification for such strategies.

We have continued numerical tests of AMMO on aerodynamic optimization problems. Most recently we have experimented with variable physics models, with both the Euler and Navier-Stokes equations for

modeling the flow around a two-element airfoil. The Euler equations provided the low-fidelity model and the Navier-Stokes equations the high-fidelity model. In our tests, the low-fidelity model is adjusted using a multiplicative correction due to Chang, Haftka, et al. so that it agrees to first order with the high-fidelity model. Use of the corrected low-fidelity model to guide the optimization led to a five-fold improvement in computational cost over relying purely on the high-fidelity model.

We are currently investigating how we might improve these results by relaxing the degree of optimization performed in the AMMO subproblem, which involves the minimization based on the lower-fidelity approximation. We are currently solving this problem to a high degree of precision; however, we need only solve it to a point that yields a suitable improvement in the merit function for the high-fidelity problem.

This research was done in collaboration with Natalia Alexandrov, Eric Nielsen, and Kyle Anderson (NASA Langley).

Analysis of bilevel approaches to MDO
R. Michael Lewis

Bilevel problem formulations have received considerable attention as an approach to multidisciplinary optimization (MDO) in engineering. However, careful consideration of the analytical and computational consequences of using bilevel methods has been largely lacking. We have continued our study of the analytical and computational properties of bilevel approaches to MDO, including optimization by linear decomposition (OLD) and collaborative optimization (CO).

Our analysis of OLD and CO reveals that the resulting system-level optimization problem suffers from some inherent computational difficulties due to the stability properties of the resulting system-level optimization problem. Most notably, the standard Karush-Kuhn-Tucker (KKT) conditions that usually characterize solutions of nonlinear programs necessarily fail to apply to solutions of the system-level problems that result in OLD and CO. This breakdown of the KKT conditions derives from the bilevel nature of the method, and the characterization of interdisciplinary consistency at the system level in terms of the optimal value functions of certain disciplinary optimization problems.

The analytical features of the system-level problem have serious consequences for the application of conventional nonlinear programming algorithms to finding its solution, and, we believe, explain numerical difficulties with collaborative optimization that have been reported in the MDO literature.

We are currently exploring alternative approaches to MDO problems that avoid these analytical and computational difficulties. We conjecture that one can show in a more or less rigorous way that there is no approach that manifests a high degree of disciplinary autonomy that is also both robust and efficient.

This research was done in collaboration with Natalia Alexandrov (NASA Langley).

Robust airfoil optimization over a range of free-stream Mach numbers
Wu Li and Luc Huyse

The ultimate goal is to develop next-generation design tools that are insensitive to fuzziness or uncertainty in design specifications. One important example is aerodynamic shape optimization for achieving drag reduction over a specified range of free-stream Mach numbers. This new method avoids the over-optimization at a single design point that is characteristic of traditional methods while conserving computer resources.

A theoretical study of the multipoint optimization method suggests that the number of design points must be greater than the number of free-design variables for the multipoint optimization method to avoid undesirable trade-off of marginal improvements at the design points for significant performance degradation

at off-design points. A new optimization method called the profile optimization method uses a common descent direction for all design points to achieve a consistent drag reduction over the given range of free-stream Mach numbers in each iteration. The profile optimization method is tested on a lift-constrained drag minimization problem for a two-dimensional airfoil in Euler flow, which is formulated with 20 free-design variables. An unstructured grid computational fluid dynamics code, FUN2D, is used to compute the lift/drag coefficients and their gradients with respect to airfoil shapes and angles-of-attack. A parallel implementation of FUN2D on the ICASE Coral computer system returns the lift/drag and their gradients for multiple free-stream Mach numbers simultaneously.

The numerical simulation results indicate that the profile optimization method is not sensitive to the number of design points used, it avoids unnecessary shape distortions during optimization iterations, and consistently reduces the drag over the given Mach range in each iteration. With only four design points, the profile optimization method generates smooth optimal airfoils with smooth drag profiles over the given Mach range. It is important to note that at each iteration the profile optimization method produces a smooth airfoil and that each airfoil has improved performance over the previous one. The final airfoil shape is significantly better than the initial NACA-0012 airfoil.

Optimization techniques can automate many design tasks, providing better designs in a shorter time. However, traditional optimization methods require precise specification of the objectives and constraints. By contrast, the profile optimization method allows uncertainty in design specifications. It prevents severe degradation in the off-design performance. It produces a smooth airfoil shape with improved drag characteristics at each optimization iteration. Thus, it allows the designer to make an educated trade-off between the amount of computer resources used and the amount of expected improvement.

This robust optimization method will be extended to study optimization of three-dimensional wings under realistic operating conditions. The mathematical properties of the method will be analyzed in order to generalize the method for use in future MDO applications.

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

Parallel and robust multigrid method for the simulation of a turbulent boundary layer
Ignacio M. Llorente

Multigrid algorithms based on a plane implicit solver in combination with semicoarsening have been found to be fully robust for the simulation of laminar boundary layers. In particular, we have considered the flow over a flat plate with a non-trivial angle of yaw, where the leading edge is not perpendicular to the stream. This simulation presents two basic problems, namely highly stretched grids and non-aligned flows with open characteristics, which both prevent optimal multigrid efficiencies from being achieved. In this situation the multigrid solver considered solves the governing system of equations in a fixed amount of work units, independently of the grid size, grid stretching factor and the non-alignment parameter. Moreover, a four-color ordering in the smoothing sweep exhibits similar convergence to the lexicographic ordering and allows the efficient parallel implementation of the algorithm. The objective of this research is to study whether those convergence properties are maintained in the simulation of a steady turbulent boundary layer at high Reynolds numbers over a yawed flat plate.

We are introducing in our code a Reynolds-averaged approach to turbulence based on the one-equation model of Spalart and Allmaras, since this approach is reasonably robust, inexpensive, and has been previously reported to achieve favorable results. The turbulence equation is discretized using the same finite volume techniques as the flow equations. Second-order accuracy in the convective terms is achieved with a defect-

correction procedure based on a QUICK scheme inside the multigrid cycle and the diffusion terms are treated using a second-order formulation. The turbulence and flow equations are only coupled in the finer grid where the eddy viscosity from the turbulence model is added to the flow solutions. The turbulence equation is solved decoupled from the flow equations by using a robust multigrid approach that combines implicit smoothing and semicoarsening. We have almost completed coding the turbulent solver and we will begin the debugging phase shortly.

The parallel implementation of the multigrid solver outlined above can be done on the basis of two different approaches: domain decomposition (DD) or a global multigrid partitioning (GMP). The scalability and efficiencies obtained in Coral with the GMP technique have been quite satisfactory. The combination of semicoarsening and plane implicit solvers results in an efficient exploitation of the underlying hardware due to the inherent locality of the smoothing process. Nevertheless, the GMP approach is not well suited to dealing with complex geometries in general situations. DD methods are easier to implement, imply fewer communications since there are only required on the finer grid, and can be applied to complex geometries. However, they lead to algorithms which have negative impact on the convergence rate. A hybrid approach that applies the multigrid cycle on the entire domain while the smoothers are performed in a domain decomposition way has been previously proposed for the elliptic operator. This multiblock smoothing strategy opens the possibility of using an adaptive smoother, that is, different smoothers for different portions of the domain, where choice of the smoother is based on a minimization of operation count while retaining optimum smoothing performance. An example of this should be using a plane-implicit smoother in the portions of the domain that have strong anisotropies while using a point smoother in the regions that are isotropic. These alternatives are being studied in order to implement the parallel version of the turbulent solver on the Coral system.

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

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

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 have developed a numerical technique which can 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. The answer depends on the chosen optimality criterion.

While L_2 optimality of control inputs is typically sought, this criterion is not physically meaningful. Minimizing the L_1 norm of the control effort has a clear physical interpretation, but it is very difficult to solve numerically. Fortunately, our numerical results for the two-dimensional case and our analytic proof for the one-dimensional case show that perimeter controls are L_1 optimal. This is a strong basis for our conjecture that perimeter controls are L_1 optimal in general. Finally, we've shown that noise control can absorb power. The power optimal controls load the noise sources to increase their power output, then absorb half of the power increase as the other half radiates to infinity.

These results on L_2 optimality, L_1 optimality, and power optimality provide useful guidance for the exact volumetric cancellation of noise. Once our paper is written, we hope to seek funding for further work on approximate noise cancellation, 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.

The Coral Project
Josip Lončarić, Ryan Cresawn, 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. Scientific computing needs 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, very 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. This year the project is in its fourth stage, and 24 of the original 400 MHz machines were replaced with much faster 1.7 GHz machines. The resulting system contains 96 compute CPUs and six server CPUs with an aggregate of 54.5 GB of RAM and 1.2 TB 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 continued. The measurements reveal $75-300\%$ performance gains thanks to VIA transport for CG, FT, IS, and SP benchmarks, while BT, LU, and MG show modest $27-33\%$ performance gains. Comparing TCP performance shows that interrupt driven receive in MPI/Pro is particularly helpful for the FT case.

The Coral cluster usage has dramatically increased this year. 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.

Human/robotic exploration of the Solar System

Robert Cassanova, Josip Lončarić, Lewis Peach, and Manuel Salas

Exploration of the solar system will be most effective if both humans and robots are synergistically combined. Done correctly, this approach can reduce risks, improve efficiency and accomplish goals faster. The challenge is to understand the ways in which this could be accomplished and how this mix might evolve over the next 10–40 years with the incorporation of revolutionary aerospace systems concepts. We are organizing a workshop which will bring together experts from academia, government, and industry to address these challenges.

This workshop, to be held on Nov. 6–7, 2001, aims to support the development of a preliminary plan which would maximize the scientific return and enable the human exploration and development of space.

The scope of this effort includes both planetary science and "in space" platform science applications beyond low Earth orbit. Specific objectives are: (1) identification of advanced revolutionary systems concepts, (2) identification of required technologies to enable these capabilities, (3) an evaluation of the evolution of the relative roles of humans and machines to implement these concepts, and (4) an identification of the science that would be enabled by these capabilities.

Support for this project was provided by the Revolutionary Aerospace Systems Concepts (RASC) activity at NASA Langley Research Center.

We have invited over 125 experts and received over 70 confirmations.

After the workshop, session leaders will gather at ICASE on Nov. 8th, 2001 to draft the final report. Additional visual illustrations of the exploration concepts presented at the workshop will also be prepared. The final NASA Conference Proceedings should be published in early 2002.

Aerodynamic transonic drag prediction using an unstructured multigrid Navier-Stokes solver

Dimitri J. Mavriplis

A drag-prediction workshop was organized by the AIAA Applied Aerodynamics Committee and held in Anaheim, CA, June 2001. This work constitutes the computations performed as part of our participation in the workshop. The objective of the workshop was to assess the capability of a variety of current day Navier-Stokes solvers at predicting drag in the transonic cruise regime of a transport aircraft.

The flow over a wing-body transport aircraft configuration was computed on a grid of 1.6 million points and a grid of 13 million points at various Mach numbers and lift coefficient values. The results were compiled as a series of drag polars and drag rise (drag versus Mach number at fixed lift coefficient) curves. A total of 72 individual cases were computed on the 1.6 million point grid, which was performed in about one week on the ICASE PC cluster using 16 to 32 processors. A total of six cases were computed on the 13 million point grid which was performed on the SGI NAS Origin 2000 machine using 64 to 128 processors. The drag results were found to be in relatively close agreement with results from other validated structured, unstructured and overset grid method codes in the workshop, although a consistent bias in the lift at a given angle of attack existed between these numerical results and the experimental wind tunnel values. The ability to compute large numbers of cases with good accuracy on unstructured grids using inexpensive PC clusters was demonstrated through this exercise.

More computations on additional grids are to be performed and the ability of adaptively generated meshes to reduce solution time and increase accuracy are also to be studied.

Comparison of linear and nonlinear unstructured multigrid algorithms

Dimitri J. Mavriplis

In previous work, linear multigrid methods were shown to be substantially more efficient for solving the transient radiation diffusion equations on unstructured grids as compared to nonlinear full-approximation-storage (FAS) multigrid methods. This work is concerned with developing a better understanding of the underlying mechanisms involved in linear and nonlinear multigrid methods, and investigating the relative performance of these multigrid methods for the solution of Reynolds-averaged Navier-Stokes problems.

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 additional gains in efficiency. For the Navier-Stokes equations, the linear multigrid algorithm was shown to be up to three times faster than the nonlinear multigrid method on simple problems such as flow over a single airfoil. However, on more complex problems such as the high-lift flow over a multi-element airfoil, both schemes provide substantially slower convergence and are roughly equivalent in terms of asymptotic convergence efficiency, while the nonlinear multigrid method exhibits more robust and faster initial convergence from a poor initial guess. The slower convergence of both schemes in this case is shown to be due to the use of an inexact (first-order accurate) linearization. This work was presented at the 15th AIAA Computational Fluid Dynamics Conference, Anaheim, CA, June 11–14, 2001.

These results are to be extended into the three-dimensional setting and for transient Navier-Stokes problems. Effects of scalability on large numbers of processors will also be studied in addition to algorithmic efficiency.

Large eddy simulation using a parallel multigrid solver

Dimitri J. Mavriplis and Juan Pelaez

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. This model has been validated in the large-eddy simulation (LES) regime (in the absence of boundary layers) by simulating the decay of isotropic turbulence in a periodic box. The effect of grid resolution and artificial

dissipation on the ability to capture the small scale turbulence characteristics has been determined through numerical experiments. Using these guidelines, the DES simulation of flow over a sphere and flow over a wing at near stall conditions is being computed. These computations are being performed on the ICASE PC cluster, Coral. Results of this work were presented at the Third AFOSR International Conference on Direct Numerical Simulation and Large Eddy Simulation, in Arlington, TX, August 5–9, 2001.

Higher resolution simulations are currently underway as well as simulations for flow over a bluff landing-gear geometry. Techniques for improving accuracy and reducing solution time are also under consideration.

Investigation of multigrid-implicit higher-order accurate time-stepping procedures for unstructured mesh Navier-Stokes simulations

Dimitri J. Mavriplis and Giridhar Jothiprasad

The accurate solution of transient fluid flow problems as required in large-eddy simulations, can become very CPU-time intensive due to the long simulation times required and large number of time steps employed. This work explores the feasibility of reducing the overall simulation time for a given level of accuracy by resorting to a smaller number of higher-order accurate time steps.

Based on the work of H. Bijl, M. Carpenter, and V. Vatsa, an implicit Runge-Kutta time-stepping scheme has been implemented in an existing two-dimensional unstructured Navier-Stokes solver. A four-stage and a six-stage Runge-Kutta scheme are employed, which are third-order and fourth-order accurate in time, respectively. Each stage of the Runge-Kutta schemes represents an implicit nonlinear problem that is solved using the agglomeration multigrid scheme previously developed for steady-state problems. This multigrid solver has also been used as a solver for a second-order backwards difference time-stepping scheme. Design accuracy for both Runge-Kutta schemes has been demonstrated for laminar flow over a circular cylinder.

The relative efficiencies for a given accuracy level of the various Runge-Kutta schemes and the second-order backwards differencing scheme are to be compared, and additional calculations of turbulent flow cases are to be performed.

High-order upwind finite difference methods

Jan Nordstrom

Although progress has been made using high-order central finite difference methods, increased dissipation to stabilize these methods for nonlinear calculations are necessary.

We have worked on upwind methods of summation-by-parts type implemented in the Fax-Friedrich formulation. Stability and boundary procedures have been studied for a hyperbolic system (Euler).

Including of second derivatives to enable Navier-Stokes calculations is planned.

The work was done together with Mark H. Carpenter (NASA Langley).

Post-parameterization of aircraft geometry using free-form deformation in combination with structured grid generation

Arno Ronzheimer

Numerical methods in computational fluid dynamics (CFD) have been continuously improved and have become a reliable tool in industry during the complete process of aircraft development. Particularly unstructured CFD methods have gained a degree of automation and reliability to perform analysis on geometries routinely, having nearly any detail of a final aircraft. However, to improve an aircraft design in a late phase, especially when aerodynamic interference effects occur, which may degrade the promised performance of

the aircraft, the turnaround time for further design studies is mainly governed by the ability of the present CAD System and CAD designer to provide alternate geometries to be used in CFD. To eliminate this lag of automation in redesign, a post-parameterization method, based on free-form deformation techniques and structured grid generation methods, has been proposed to perform modifications fast and systematically.

In the first step, the classical method of free-form deformation was coded. As this method was not sufficient and flexible enough to achieve the target objective, eventually the so-called extended method was coded as well. Both methods are based on a mapping and re-mapping procedure of object points into Bezier- or B-spline-hyperpatches. Finally the result of the deformation is determined by two control-point lattices, defining a first hyperpatch into which the object points are mapped in, and a second hyperpatch used for re-mapping, to obtain new object points. To provide deformation lattices for a specific application of free-form deformation, the present functionality of the structured grid generation system MegaCads from DLR was used. In addition to standard grid generation techniques, such as bilinear and trilinear interpolation methods, also a basic CAD functionality is included in MegaCads. But at last, due to the underlying parametric concept, which allows to replay the complete grid generation sequence with new parameter settings, it is extremely well suited to control free-form deformation. Several examples, dealing with possible applications in aircraft design, showed a significant potential of this approach. Preferably the present approach of free-form deformation in combination with grid-generation, will be applied to modify the geometry which is already prepared to be used in the grid generation step of a CFD-cycle. As for this task, a closed volume topology is indispensable, further functionalities have been coded to import geometry and topology and to split the volume topology. To rebuild a closed volume topology after parts of the geometry have been deformed, a merging procedure similar to morphing techniques is considered.

Before the present approach will be used in practice, primarily the merging of parts of the geometry has to be completed. To grant a stable and versatile use in practice, further applicative case studies have to be performed.

Accuracy enhancement of the discontinuous Galerkin method through negative norm estimates and post-processing
Jennifer Ryan

Using negative norm error estimates, a highly efficient and local post-processor has already been shown to improve the accuracy of the discontinuous Galerkin method for linear hyperbolic equations (by Cockburn, Luskin, Shu, and Süli). This approach has great potential in making the discontinuous Galerkin method more effective for aeroacoustic simulations, where usually linear Euler equations are solved for long-time intervals.

Part of our research efforts for the post-processor are directed toward finding the effects of applying the post-processor to multi-domains with different mesh sizes and separately, the effects of limiting for nonlinear equations. Our hope is to be able to extend the use of the post-processor to more complex domains. Initial evidence suggests that the post-processor does improve the accuracy of the approximation. Additionally, we have extended the application of the TVB-Limiter previously proposed by Shu to higher order discontinuous Galerkin methods, i.e., $k > 2$, by first projecting the approximation to lower-order polynomial spaces and limiting the projection of the approximation and then limiting again in the original approximation space.

Future work will be to extend these results to two dimensions and establish the theoretical framework for applying the post-processor to nonlinear equations such as the Euler equations.

This research is done in collaboration with Harold Atkins (NASA Langley) and Chi-Wang Shu (Brown

University).

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 which 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.

The infinite number of quasi-LPV models can be generated for a certain class of a nonlinear system in which control inputs enter linearly. We have currently formulated an analysis method to choose which quasi-LPV model leads to a less conservative result to present the reachable set of the nonlinear system. In the conventional LPV synthesis methodology an LPV controller is designed solving linear matrix inequality (LMI) optimization over the entire parameter spaces. To generate an LPV controller under adverse conditions, the conventional LPV synthesis methodology may not be appropriate, since solving the LMI optimization over the entire parameter spaces leads to a conservative result that the performance would be degraded too much. One of the approaches to reduce conservatism in an LPV controller is the "blending approach" in which the LMI optimization problem is solved over parameter subspaces, respectively. An LPV controller is synthesized based on the blended solution matrices over the parameter intersection subspace. We have completed coding the LMI optimization problem of blending LPV controllers in MATLAB to determine optimal blending functions to minimize performance index γ over the parameter intersection subspaces.

In future work, the analysis method on quasi-LPV models will be integrated into the current function substitution method to generate a quasi-LPV model of aircraft dynamics. Also, parameterized failure cases of an aircraft will be integrated into a quasi-LPV model to facilitate synthesis of an LPV controller of an aircraft under adverse conditions. Since the failure parameter cannot be measured exactly, an LPV synthesis methodology based on the estimated parameter will be investigated. In the design process based on the estimated failure parameter, parameter uncertainties are introduced into the LPV controller synthesis and may lead to conservative results. A method to reduce the conservatism will be investigated using dynamic D scaling.

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

Jointly with Harold Atkins (NASA Langley), we are continuing in the investigation of developing the discontinuous Galerkin method to solve the convection-dominated, convection-diffusion equations. Local preconditioners and post-processing techniques for enhancing accuracy are two main areas of investigation.

Jointly with Jue Yan, we have been generalizing the local discontinuous Galerkin method to PDEs with higher derivatives, including the bi-harmonic equations with four derivatives. These schemes are especially suitable for problems containing nonlinear first derivative terms and a linear or nonlinear higher derivative term with small coefficients.

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

System risk assessment and allocation in conceptual design
Natasha Smith

This research addresses the problem of system risk assessment during the conceptual design of multi-disciplinary engineering systems. Currently, most reliability assessment is based on full-scale testing, after detailed design, manufacture and assembly of the system when design adjustments are often prohibitively expensive. Inclusion of reliability information earlier in the design process has the potential to provide considerable savings in time and cost. Specifically, this research is aimed at employing probabilistic analysis and optimization techniques for the conceptual design of a NASA reusable launch vehicle.

The first phase of this project involved employing probabilistic optimization on a response surface based design. The Vehicle Analysis Branch at NASA Langley provided a deterministic optimization model based on response surfaces generated from their analysis codes for weights and sizing, geometry, and aerodynamics. We added a First Order Reliability Method (FORM) analysis to this program and performed probabilistic optimization. We have also completed wrapping a response surface based FORM analysis in Model Center, a software program for process integration. Now that we have the basic reliability analysis algorithm and an understanding of how to use Model Center, we can proceed with applying reliability analysis to a multi-disciplinary system using actual analysis tools.

Our plans include using the Model Center environment to apply probabilistic analysis to an existing conceptual design analysis algorithm for a reusable launch vehicle. This algorithm incorporates codes for geometry, weights and sizing, aerodynamics, and trajectory. This will involve generalizing the FORM algorithm, coding loops of the analysis codes for partial derivatives and FORM convergence, and developing a Model Center driver to optimize the system.

Convergence acceleration and acoustics
Eli Turkel

Solving the compressible steady-state Navier-Stokes equations in three-dimensional complex geometries requires thousands of sweeps through the mesh in order to reduce the residual by several orders of magnitude. In contrast, when solving the inviscid equations around an isolated three-dimensional wing, one can frequently get solutions to within engineering in only one to two hundred sweeps through the mesh (i.e., minimal work units). The main difference between the two cases is the high stretching needed to resolve the boundary layer at flight number Reynolds numbers. Because of this stretching the aspect ratio between the directions normal and tangential to the boundary layer can be of the order of thousands or even ten thousands. This high-aspect ratio severely deteriorates the convergence rates of any explicit schemes. Implicit schemes such as the ADI approach do not overcome this deficiency. This is a bigger problem than low Mach numbers where the ratio of the acoustic to convective speeds becomes very large.

To partially overcome the grid problems, we have introduced a GMRES algorithm as an additional smoother into the three-dimensional Navier-Stokes solver. Testing of this acceleration technique is still continuing.

For low speeds it is well known that the standard algorithms do not converge very well. To overcome this difficulty preconditioning techniques have been devised to alter the wave speeds. These new systems have all the speeds approximately equal as the Mach number approaches zero.

However, these preconditioned systems continue to have robustness problems whenever a range of Mach numbers occur in the flow rather than just low-speed flow. We have added a Mach-number dependence to the basic parameter, beta, of the preconditioning. This is done in such a manner that the preconditioning is turned off at intermediate Mach numbers. Hence, the preconditioning is active only when the Mach number is sufficiently small. The standard preconditioning uses (p,u,v,w,T) variables. While this is appropriate for very low speeds it implies that even when the preconditioning matrix is the identity matrix that the algorithm does not revert to the standard nonpreconditioning scheme. Hence, the preconditioning has been reformulated to use conservation variables in an efficient manner. This allows the preconditioning to be completely removed at some specified, subsonic Mach number.

We plan on combining this with both the complex and real versions of TLNS#D to be able to better solve both time-dependent and time-harmonic problems.

This was joint work with Veer Vatsa (NASA Langley).

Terminal descent engine controller for three-DoF planetary entry simulation
David W. Way

The Mars Smart Lander will be the first mission to employ a second-generation capability for precision landing and hazard avoidance. The new generation of Mars landers with lifting body designs, aerodynamic steering, active terrain sensing, and powered divert capabilities requires a new generation of simulation technology to support their development. A high-fidelity engineering computer simulation capable of supporting end-to-end mission studies, trades and algorithm development for Mars entries is desired. The Program to Optimize Simulated Trajectories (POST) software has been modified to include many system models to provide such analysis capability. One of the various spacecraft subsystem models needed for this simulation is a terminal descent controller. While higher fidelity six degrees-of-freedom (DoF) simulations are being developed, it is desired to maintain a lower fidelity three-DoF simulation that executes faster while providing similar results. We want to simulate the behavior of a six-DoF terminal descent controller in a three-DoF simulation of the Entry, Descent, and Landing (EDL) phase of a planetary entry vehicle.

Three independent modules are necessary to implement the terminal descent model. The first is a controller, which takes the guidance commanded thrust and attitude and solves for the necessary throttle settings. This module extracts the required propulsive moment from the attitude quaternions and solves a constrained optimization problem using the method of LaGrange multipliers. The second module is a simulator, which takes the current throttle settings and solves for the new vehicle attitude. This module solves Euler's equations of motion and performs a simple integration. The third module is a navigator, which integrates the sensed body rates and calculates the current navigated attitude. This module performs a task similar to the simulator, except that dispersions are added to the rates to model navigational uncertainty. We have completed coding all three modules of the algorithm in C++ and testing the controller response in a stand-alone setting against various command functions. Now that the controller is complete, it can be included in the POST simulation.

We are currently adding the controller to the three-DoF EDL simulation. Next, the code will be compared and validated with existing results, which allow the guidance system to obtain the desired attitude instantaneously. Finally, we will assess the impact of the controller on the landing accuracy by performing

Monte Carlo analyses. These results will be compared to 6-DoF simulations.

This research was conducted in collaboration with Scott Striepe (NASA Langley).

Kinetic scheme for rarefied gas flow
Kun Xu

The rarefied gas flow is defined as the flow with Knudsen number $Kn = l/L \geq 0.1$, where l the particle mean free path and L is the length scale of the device. For such a flow, the traditional DSMC method with intrinsic fluctuation due to individual particle movement is very expensive in order to reduce its noise to the level lower than the flow speed, such as $0.1 m/s$, in the MEMS devices which are operated in the room temperature. The objective of this research is to develop a gas-kinetic scheme by solving the gas-kinetic BGK model for the rarefied gas flow.

The gas-kinetic BGK scheme for the Navier-Stokes equations has been successfully developed in recent years. The gas-kinetic Navier-Stokes solver basically captures the time evolution of the gas distribution function to the first-order Chapman-Enskog expansion $f = f_0(1 + Kn\psi_1)$. In order to extend the scheme to the transition regime with large Knudsen number, we need to go further to solve the Burnett equations, which correspond to the second-order Chapman-Enskog expansion $f = f_0(1 + Kn\psi_1 + Kn^2\psi_2)$. To the current stage, we have completed all theoretical work about the determination of ψ_2 and its spatial and temporal derivatives.

In the near future, we are going to code the gas-kinetic Burnett solver, test, and validate it in many cases, such as Couette and Poiseuille flows.

COMPUTER SCIENCE

Development of a simulation model for suspensions in a fluctuating fluid

Yu Chen and Yasuhiro Inoue

A series of discrete mesoscopic fluid models, which include lattice gas automata (LGA), lattice Boltzmann method (LBM), and dissipative particle dynamics (DPD), have been introduced during the past decade for the analysis of fluid flows. Characteristics of these models in common can be summarized as follows: The detailed microscopic description of fluids has been greatly simplified from the viewpoint of molecular dynamics (MD), though the essential properties to ensure the conservation of mass, momentum, and energy (only in some extended models) are preserved without a compromise. On the other hand, the collective or coarse-grained dynamics of the underlying particles approaches the continuum mechanics of real fluids. The reason why these fluid models are appealing lies in several aspects. First, comparing with those conventional numerical methods for fluid simulation, such as the finite-difference or the finite-element solution of Navier-Stokes equations, particle-based methods (LGA and DPD) are free from numerical instability. Next, comparing with the more robust microscopic models, such as MD and DSMC (for direct Simulation Monte Carlo) these methods are more practical in terms of their computational cost. Note that a very wide spectral of time and length scales would, in general, characterize the behavior of complex fluids, a fact which requires a higher resolution as well as a longer time progression for the numerical simulation. Third, pattern formation and dynamic flow of complex fluids are often much easier to be modeled in a universal way by intuitively introducing particle interactions or particle structures, rather than trying to establish constitutive relationships from a huge experimental database, in a framework of partial differential equations for the macroscopic quantities.

Recently, a new mesoscopic model was suggested by Malevanets and Kapral. This model resembles LGA in synchronous discrete time evolution and in discretizing space with regular lattices. On the other hand, positions and velocities of particles are treated as continuous variables. Hence, we name the model real-coded lattice-gas (RLG). Other differences between RLG and LGA are the abandonment of exclusion law on particle residence and the use of a stochastic rotational rule for particle interactions. Particle dynamics consists of two processes, namely, streaming and collision. The position of every particle is renewed in the streaming process, and the update of velocity is done in the collision process. Since there is no longer an exclusion law, an arbitrary number of particles can enter into a single cell and multi-particle collisions (in a DSMC style) are carried out there by rotating the relative velocity (to the averaged velocity over the cell) of every particle with a random angle. Kinetic theory of such particle dynamics tells that the equilibrium velocity distribution function is Maxwell-Boltzmann and that the existence of an H-theorem can be proved. Furthermore, a set of Galilean-invariant hydrodynamic equations including the transport equation for internal energy can be derived using the Chapman-Enskog expansion. Also, the extension to a three-dimensional model can be done in a straightforward way. All these conclusions from previous studies seem very encouraging, as most of the peculiarities of LGA are cured in this model. There are also numerical evidences showing that RLG is computationally much efficient than LGA or DPD. Regarding RLG's advantage over LBM, one may mention the absolute numerical stability and the natural reproduction of fluctuating hydrodynamics, the latter of which would be very useful, for example, in studying problems with flow instability or the Brownian motions.

Although research on RLG is still in its infancy and fundamental questions of the model, such as the expression of transport coefficients, the validity of molecular chaos and the proof for Galilean invariance, are to be clarified, various applications have already been challenged in simulations of complex fluids: the

solvent dynamics, the dynamics of short polymer chains, the extension to immiscible two-phase models, the amphiphilic surfactant models, and the simulation of a single rising bubble, etc. In this study, we shall develop a new scheme for the application of RLG to suspended solid objects in a fluctuating fluid environment. A large number of documents on direct numerical simulation of solid-liquid flow using the conventional Navier-Stokes solver can be found from previous literatures. On the other hand, the same kind of work has been done with the use of mesoscopic fluid models (mainly with LBM models), all of which showed impressive agreement with experiments and the mainstream studies. The goal for this study lies in, however, two folds. First, by employing the RLG as the model for the background fluid, where hydrodynamic flows are strongly coupled with thermal fluctuations, we want to develop a more efficient simulation model for suspensions. Second, we are going to use such a simulation model to further investigate the complex dynamics of suspending solid objects in the fluctuating fluids. The latter is also concerned with another research theme in authors' research group, namely on the development of a "bottom-up" LBM model of liquid crystal, where the stable or meta-stable states of orientation need to be investigated under fluctuations and flows.

So far, the basic version of a two-dimensional simulation model was developed. First, we found a simple method to detect the reflections of RLG particles on the solid boundaries. Next, particle-solid interactions were calculated by replacing particle velocities in tangential and normal directions, according to different probability density distributions (PDFs). The derivation of these PDFs are based on diffused boundary condition, namely, the solid is a heat bath and the impinging particles relaxed to Maxwellian quickly. The solid-solid interactions, on the other hand, are disposed as two-body collisions through a colliding impulse, which can be decided once the relative velocities, the moment of inertia, and two masses of solids are known. We also carried out two numerical simulations to show the effectiveness of the model. The first simulation is for a single object in a fluctuating fluid. In this case, we show that displacements of the object follow a Gaussian distribution, a piece of evidence for the Brownian motions. The second simulation is a N-body simulation, where we show that the solid-solid collision model works correctly in a qualitative sense. During the stay in ICASE, we further checked the possibility for the use of a new particle-solid interaction rule, namely, the rule of bounce-back with rescaling. It was demonstrated that the new rule is faster and worked quite well if the averages are smooth enough. This has enabled us to bring out a strategy for the future simulations: if the density of suspension is high, bounce-back with scaling can be used to calculate the particle-solid interactions more efficiently; if the density of suspension is not so high, diffused boundary condition should be used instead.

This study will be continued in the following aspects: 1) Investigations of boundary conditions (further), lattice resolution and noise effects will be carried out; 2) Investigation of both the static and the dynamic structure factors will be done in order to show that the RLG fluctuation is similar to that of real fluids; and 3) Polygon description of suspending objects will be used so that three-dimensional simulation of suspensions in complex shapes can be performed.

Object-oriented software correctness issues in safety critical applications
Maria Consiglio

A new approach to air traffic operations that addresses limitations and shortcomings of the current system is being developed. In this initial phase of the project different elements of the system are being in-

vestigated and possible solutions evaluated. Within this framework, it is important to estimate the reliability of automated tools, in particular of software systems recommended for use in air traffic control.

The utilization of object-oriented technology (OOT) for the implementation of automated air traffic management tools is being considered. The goal of this study is to assess the technical implications of OOT as a software design paradigm.

In addressing the adequacy of OOT for air traffic management (ATM) software applications it is important to distinguish between object-oriented program decomposition as it was conceived more than three decades ago as an approach to manage program complexity, and popular object-oriented programming languages/practices and their many idiosyncrasies. Equally important is to understand the magnitude and complexity of the ATM system involving multiple organizations and components, intricate procedures, distributed control and highly dynamic real time problems. An in-depth, systematic study of object-based program decomposition and programming practices will help identify advantages and disadvantages of the approach as well as sources of problems and venues for solutions.

This work is in its initial phase. Research is currently underway on issues pertaining to air traffic operations as well as software engineering questions.

Flow control
William O. Criminale and D. Glenn Lasseigne

The possibility that specific flows can be controlled has long been a desired goal in fluid mechanics. On the one hand this can mean enhancement so that mixing is more efficient, for example; the contrary means that of maintaining a well-defined laminar state so that drag is reduced. It is the latter problem — as applied to boundary layers that has been the focus of this work.

Linearized stability analysis for parallel or almost parallel flows is re-examined so that (a) a more tractable means for analytical solutions can be established; (b) a method that is capable of treating the full range of the dynamics; and (c) ability to use feedback to control the flow. Traditionally, when viscous effects are included (boundary layers in particular), this problem has been one necessitating singular perturbations and has been devoted almost exclusively to the determination of discrete eigen modes. It is now clear that using this approach in order to affect flow control is of questionable application since the results that are achieved represent only a part of the bases required for the examination of the full dynamics. Indeed, the results of normal modes are essentially tantamount to predicting only the asymptotic fate of any perturbation. Instead, a means for explicitly examining a general arbitrary initial-value problem for all time is the fundamental first step in understanding real-time flow control. This work offers an alternative means to achieve this purpose by using a moving coordinate transformation that then allows for the introduction of multiple spatial and temporal scales. As a result, the full three-dimensional problem can be comprehensively and analytically investigated. Moreover, the basis for this approach permits the problem to be changed to one of regular rather than singular perturbations. The early transient period as well as the asymptotic fate can be analytically ascertained. The method can be applied to all shear flows but this work has concentrated on the flat plate boundary layer. Not only is the analysis less complex and explicit, but also exhibits the essential and salient physical processes that transpire in the flow. All analytical results are supported by numerical evaluation of the full set of governing equations.

There remains the final goal of the feedback design for the control. Likewise, there is the question of the actual physical design that will be required for this operation. Among other considerations will be the task of minimizing the drag.

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. A number of Problem Solving Environments (PSE) or frameworks 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. The Nautilus Project will be based on standards for components and application element metadata to support portability and interoperability between different PSEs/frameworks.

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. ICASE is participating in the CCA Forum to help develop the concepts. The CCA component encapsulates primarily the user code that will be used to build a composite application. The CCA service-component concepts will provide support for other application elements such as events, file transfers, data transfers, information discovery, remote process management, machine resource management, site management, and file system management. However, the CCA specification does not address several programming issues. These issues relate to the description of an application in a complete and consistent manner. This means in a manner that the application (at a minimum the high-level details) can be described to others in an efficient manner. This is a complicated objective for large, applications composed of many elements. The Application Metadata Working Group of the Grid Forum is attempting to define standards for describing the various application elements. Previous ICASE work on Shared Programming Definitions is being presented to this group as a starting point. Any proposed standards developed by this working group will be used in the Nautilus project as the basis for a programming model. This programming model will be used to design and implement any programming support tools for Nautilus.

A proposal is being written, jointly with Jack Dongarra from the University of Tennessee, to continue the development of the Nautilus Project. Dr. Dongarra brings ideas on the use of smart components to the proposal. As applications get larger, the developers will not have sufficient knowledge about every application elements. Smart components will allow the framework to assist the developer in choosing the best application components as well as in fine tuning those components to fit into the overall application environment. Work will continue with the CCA and Grid Forums to foster the development of standards and best practices for use in the development of programming environments such as the one in the Nautilus Project.

Systems software research for grid environments
Thomas M. Eidson and Merrell Patrick

Next Generation Software (NGS) for scientific and engineering computing is critical to the long-term success of NASA LaRC programs and activities. To help identify some of NASA's software systems needs, a workshop titled "Programming Computational Grids" was held at ICASE on April 12–13, 2001. A workshop report with two major parts has been written. One part focuses on technical requirements of a component-based programming model for computational frameworks. The second part contains a set of recommendations addressing a strategy for NASA to consider in using the potential offered by software component technologies and their use in programming composite applications. Details can be found in ICASE Report No. 38, NASA/CR-2001-211224.

As reported in the last Semiannual Report, ICASE developed a five-year systems software research and development plan. This plan depended on ICASE continuing to receive NASA HPCC funds via the LaRC HPCCP Office. During the spring of 2001 NASA discontinued funding of the HPCC program commencing in FY 2002. Attempts by the LaRC HPCCP Office and by ICASE to obtain funding under the new CICT program commencing in FY 2002 that was defined and will be managed by NASA ARC failed. This called for a scaling back and refocusing of projects previously planned and a new strategy in developing funding to support these efforts. These projects, namely, the Tidewater Research Grid Partnership and the Nautilus Component-based Framework project will be discussed below. Proposals to develop funding for systems software research from other sources are being written.

Tidewater Research Grid Partnership (TRGP)
Thomas M. Eidson and Josip Lončarić

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. A number of projects around the world are focusing on the technology and security of remote-job execution, few are looking at the security issues involved with managing a distributed user base located at multiple sites. TRGP was formed to assist ICASE and other related organizations in learning Grid software basic technology and to provide a base platform for the development of Grid programming environments. Additionally, the user-management security/trust issues are being studied.

The TRGP is a project to set up a computational Grid for use by government organizations and universities located in the Tidewater Region or otherwise related to ICASE. Currently, the Computational Science Group at the College of William and Mary has become a TRGP site. Old Dominion University, Jefferson Labs, other William and Mary Labs, and NASA Langley are some of the organizations currently involved in discussions about joining TRGP. The Globus Toolkit has been installed as the core software to provide communication and other remote Grid functionality. PGP-based software, the TRGP Trust System, has also been developed to provide distributed-user management functionality. This allows a user at one site to interact with Grid administrators at other sites in a secure manner. Initial testing of the TRGP Grid between ICASE and William and Mary has exercised the account management and trust procedures, verified the underlying Globus functionality, and demonstrated the ability to submit jobs to remote sites. The

documentation has been designed and draft versions developed.

An immediate goal is to finish the development of documentation and a web site so that new members can join TRGP in an efficient manner. Grid usage tests will be developed so that new users will have examples to guide them. Several reasonably sophisticated applications are being sought and TRGP will assist the owners of these applications in porting to a Grid environment. These applications will provide further examples for new users. New organizations and users will be actively recruited. After the core Grid functionality has been made available to a modest group of users and sites, more advanced functionality will be studied for implementation by TRGP. There are a large number of research projects around the world, including several TRGP current or potential members, where Grid software is being developed. This includes information discovery, problem solving environments, and visual programming and execution interfaces.

This work was conducted in collaboration with Tom Crockett (The College of William & Mary).

Conflict resolution and recovery in three-dimensional airspace
Alfons Geser and César Muñoz

The flight path of an airplane is supposed to be composed of straight line segments. If one of these line segments of one airplane, the ownship, violates required separation to another airplane, then the ownship has to pursue another flight path to avoid the conflict. In previous work we presented an algorithm, KB3D, that proposes a straight half-line that avoids the conflict. This algorithm did not address the problem of getting back to the original flight path. In the current work we modify and extend our algorithm. The new algorithm proposes two line segments. The first line segment lets the ownship avoid the conflict and the second line segment brings the ownship back to the next trajectory change point of the original flight path. Thus the conflict is avoided with only a little modification to the flight path.

Our analysis of the problem shows a remarkable variety of solutions. One may choose from four constraints that the ownship has to satisfy. Moreover in the first line segment, the ownship may dodge the protected zone vertically or horizontally; likewise and independently so for the second line segment. Like in the KB3D approach we avoid the use of trigonometric functions. The new algorithm, called RR3D, is implemented in Java. The analysis and the design and implementation of RR3D are finished. Formal verification in PVS has begun.

We plan to continue the formal verification effort and to do extensive simulation in a realistic environment.

This work was done in collaboration with Florent Kirchner (ENAC) and Andreas Kaiser (University of Tuebingen).

Optimal unconstrained conflict resolution in three-dimensional airspace
Alfons Geser and César Muñoz

Two airplanes are said to be in predicted conflict if their trajectories come too close. Conflict resolution has to provide an alternative trajectory for one of the airplanes such that there is no longer a predicted conflict. An optimal solution to a conflict is defined as the minimum magnitude change of velocity vector that allows conflict avoidance. Previous work, such as Karl Bilimoria's (NASA Ames) Geometric Optimization algorithm or our KB3D algorithm (see above), seeks solutions that moreover satisfy given constraints. The present work addresses optimal solutions in the absence of constraints.

Thus far we have designed the algorithm and sketched proofs of its correctness and optimality.

We are going to do formal proofs of these properties in PVS. We will also integrate it in a more general system for conflict detection and resolution, allowing a graphical representation of the solutions.

This work was done in collaboration with Florent Kirchner (ENAC).

Formal verification of the SPIDER diagnosis protocol
Alfons Geser

SPIDER is an architecture for broadcast communication in a safety-critical environment. For this reason it provides a high degree of fault tolerance. Even in the presence of multiple, simultaneous faults and malicious faults, it is required to operate without failure. For this purpose the hardware is split into nodes that fail independently. Every hardware node must be aware that any other node is faulty. The Interactive Consistency Protocol takes care that all good nodes receive the same information (Agreement), and that every message from a good node arrives unchanged at all good nodes (Validity). The Diagnosis Protocol distributes the local information about misbehavior of other nodes in such a way that all good nodes arrive at the same judgment of which is good and which is bad.

The formal verification of the Diagnostic Protocol in PVS is finished. A good deal of the proof effort is spent for exploitation of symmetry properties and parameterization of the PVS theories. Still the proof is heavy and hard to communicate. As the SPIDER project is intended to provide training material for the Federal Aviation Agency, the proofs must be conceivable and clear. One of the short-term goals is, therefore, to simplify the proof.

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.

This work is done in collaboration with Paul Miner (NASA Langley).

An alternative verification method applied to the SPIDER interactive consistency protocol
Alfons Geser

For ultra-dependable systems, i.e., systems that have a failure rate of less than 10^{-10} during a 10-hour mission, correctness checks by inspection and simulation are no longer reliable enough. They must be accompanied by a rigorous mathematical proof of correctness, called *formal verification*, that is checked by a computer. For the various levels of design, different formal verification methods are appropriate. For the hardware level, Model Checking has been applied successfully. At a high level of abstraction, Theorem Proving has shown its merits. A severe shortcoming of Model Checking is its inability to handle infinite value domains, such as the integer numbers. Theorem Proving, on the other hand, requires a sophisticated user interaction. The SPIDER protocols have been proved by Theorem Proving techniques whereas other approaches to fault tolerance use Model Checking. To be able to assess advantages and disadvantages of either approach, we have begun a case study with Propositional Satisfiability Checking, a restricted form of Model Checking, at the SPIDER Interactive Consistency Protocol. If not an alternative, this is a useful supplement to the given proof by Theorem Proving.

This project has just started. Preliminary results show that a simple case of the protocol can be checked.

Future work includes an analysis of the range of applicability of the technique, and application to other SPIDER protocols.

This work was done in collaboration with Carsten Sinz (University of Tuebingen).

Formal proof of the optimality of KB3D
Hanne Gottliebsen, Alfons Geser, and César Muñoz

Distributed Air Ground Traffic Management (DAG-TM) is a NASA project aiming the redefinition of the National Aerospace System. KB3D is a new algorithm for Conflict Detection and Resolution (CD&R) in

three-dimensional airspace. The objective of this work is to verify that the flight path corrections suggested by KB3D are optimal.

KB3D gives a set of solutions, each of which modifies only one stated parameter of the ownship: ground speed, vertical speed, or ground track. By making some basic assumptions on the KB3D solutions one can attempt to formally verify that any of the solutions are optimal in the sense that they are as close to the original flight path as possible while still resolving the conflict. The basic assumptions on KB3D were verified as part of the verification of KB3D. Using the general verification system PVS, the cases where the ground speed or the vertical speed is changed have been formally verified to be optimal.

Future work includes verifying the solutions modifying the ground track and the KB3D algorithm outputs every optimal solution.

This work was done in collaboration with Jacques Fleuriot (University of Edinburgh).

Spacing, sequencing, and safety in airport terminal areas
Saraswati Kalvala

This work is part of ongoing work on managing airspace traffic, with particular emphasis on autonomy of pilots from ground-based operators. In particular, we have studied the issues arising from aircraft within what is called the Terminal Area and the final approach to landing. This space has several unique characteristics, such as the high concentration of aircraft, restricted number of runways for which the aircraft compete, the need for maintaining paths which preserve spatial separation while packing aircraft as close as possible, and the determination of a fixed sequence of arrival at runways.

We have developed an abstract model of Terminal Areas for studying feasibility of autonomous operations, efficiency, separation, etc., in the context of predetermined paths and operational restrictions in the Terminal Area. This graph-theoretic model serves as a platform for formal reasoning about conflicts in the Terminal Area and the safety of algorithms which may supply directives to the aircraft, on issues such as sequencing, choice of flight-path, speed, etc., whether these decisions are made centrally by ground operators or by more distributed strategies.

The model is currently being refined to cope with the maneuverability allowed for pilots to make local changes to speed and path, and to capture more information about the state of aircraft and complexities of Terminal Areas. Further plans include generating suggestions of flight-plans and sequences to aircraft which can improve throughput. Collaboration with John Knight (University of Virginia) will allow us to integrate the formal model with a simulation model of Terminal Areas.

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

Formal development of conflict detection and resolution algorithms
César Muñoz and Alfons Geser

Distributed Air Ground Traffic Management (DAG-TM) is a NASA project aiming the redefinition of the National Aerospace System. A critical component of this concept is a Conflict Detection and Resolution (CD&R) system which warns pilots of potential conflicts with other aircraft and outputs resolution maneuvers to avoid conflicts. The objective of this work is to provide a formal framework for the development and verification of CD&R algorithms.

By using a rigorous mathematical model of the problem, a new algorithm for CD&R in a three-dimensional airspace, namely KB3D, has been designed and implemented in Java. KB3D is a three-dimensional extension of the two-dimensional geometric optimization algorithm developed by Karl Bilimoria

(NASA Ames). In contrast to Bilimoria's approach, KB3D only uses basic arithmetic operations over real numbers and the square root function. In particular, trigonometric functions, which may be computationally expensive, are avoided. The algorithm outputs a set of solutions. Each solution modifies only one state parameter of the ownship: ground track, ground speed, or vertical speed. Special attention was given to singularities and exceptional cases. The algorithm and its implementation in Java have been formally verified using the general verification system PVS.

Several extensions to KB3D are planned. Future work will concentrate on resolution and recovery trajectories, optimal trajectories, and the integration with simulation tools developed within the DAG-TM project.

This work was done in collaboration with Gilles Dowek (INRIA).

Proof automation of nonlinear arithmetic in PVS
César Muñoz and Alfons Geser

Verification and analysis of air traffic management systems require a considerable amount of work on nonlinear algebra and continuous mathematics. PVS, and theorem provers in general, provide only limited support for nonlinear arithmetic. This work aims at the development of libraries and tools that improve the capabilities of the PVS theorem prover in this domain.

First, a set of libraries for continuous mathematics were developed in PVS. They include a trigonometric library containing logical and numerical properties of the trigonometric functions and their inverses, and a library of numerical approximations (upper and lower bound) for sine, cosine, tangent, and square root. Finally, strategies dealing with equalities and inequalities on real numbers were developed. In particular, a new decision procedure for the field of real numbers (named FIELD) was developed. FIELD is originally based on a similar tactic implemented in Coq V7, but it has been extensively adapted to cope with PVS idiosyncrasies.

In the future, a new mechanism for higher order rewriting in PVS will be developed.

Part of this work was done in collaboration with Rick Butler (NASA Langley), Víctor Carreño (NASA Langley), Gilles Dowek (INRIA), Micaela Mayero (INRIA), Jacques Fleuriot (University of Edinburgh), and Delia Kesner (University of Paris 11).

Verification of Java programs
César Muñoz

Verification of imperative programs is a very active research area with rather few success stories in real-life applications. Given the nature of Java, that is, a simple language with a well-understood semantics, verification of programs that use an imperative subset of the Java language is well suited for formal verification. The objective of this work is to sustain the above claim by formally verifying avionics systems written · in Java.

The approach is based on a structural shallow embedding of Java in PVS. An automatic translator from Java to PVS was implemented. The translator takes a compliant Java program and produces a logical embedding of the program in the PVS specification language. The correctness property of the program can be expressed using the embedding. Furthermore, several strategies that implement Hoare's Logic rules have been developed. The translator and the strategies were used in the formal verification of KB3D (Conflict Detection and Resolution in 3-D).

Future work will extend the capabilities of the translator and make use of the Integrated Canonizer and Solver tool developed at SRI International.

Part of this work was done in collaboration with Jean Christophe Filliatre (University of Paris 11).

Simulation of automation technologies in terminal area
Stavan Parikh, Alfons Geser, and César Muñoz

NASA Langley is involved in the development of a Free Flight implementation under the Distributed Air/Ground Traffic Management plan. Terminal area is one of the areas identified within this plan that can benefit from automation. Research in the development and then analysis of self-spacing and self-merging algorithms is an ongoing effort. The analysis of these algorithms needs to focus not only on the feasibility and functionality of the technology itself, but also on its effect on the overall system in terms of performance and dependability. Due to the high cost and risk associated with actual testing it is not possible to test every new algorithm in an actual test environment. A practical alternative to an actual testing environment is provided by simulation. A successful technology at the simulation level can then be further verified via formal analysis and then in real-life conditions.

A viable self-spacing algorithm for terminal area, developed by T. Abbott, has been identified. A simple self-merging algorithm built around the self-spacing algorithm was developed. For the testing of these algorithms a simulator modeling terminal area flight was developed. The simulator is developed in modules such that different self-spacing, self-merging, and other terminal area algorithms can be tested within the same framework. The simulator was built around a network modeling system called RAPTOR developed at the University of Virginia (UVA). Currently Dallas Fort Worth International Airport has been modeled and analysis has been done on the self-spacing and self-merging algorithms for up to 250 airplanes in the airspace.

The simulator developed here provides a powerful tool for rapid prototyping of new automation technologies. It provides a means for testing for fault-tolerance of the terminal area system. The analysis of the algorithms provides valuable data to be used for further research. Future plans include collaboration with the DAG-TM group at Langley for testing new algorithms with this simulator. Also identification and the study of critical fault areas in the system are planned.

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

Scalable parallel algorithms for incomplete factor preconditioners
Alex Pothen

The parallel computation of robust preconditioners is needed to solve large systems of equations by Krylov space solvers. We are developing scalable parallel algorithms and software that can compute incomplete factorization preconditioners.

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: by suitably ordering the subdomains by means of a coloring, and by ordering the interior nodes within each subdomain before the boundary nodes. We have shown by analysis on model problems, and by computations on convection-diffusion problems that this algorithmic approach is scalable when the problem size per processor is fixed, and the number of processors are increased. Our results on up to 400 processors of various parallel computers (the SGI Origin, the Cray T3E, the Sun HPC 10000, and Coral, the ICASE Beowulf cluster) confirm our analyses. Our software for computing incomplete factors in parallel, EUCLID, is available with interfaces for Hypre and PETSc, and is included in Hypre release 1.6.0.

We are continuing to improve our parallel implementation; apply the preconditioners to application problems in electromagnetics and radiation transport; and relate our work to a novel combinatorial class of preconditioners, support-based preconditioners.

This is joint work with David Hysom (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 connectivity, branching in the elimination tree, and balance of the tree in determining the minimum memory required. We also study the influence of algorithms and blocking on the data movement costs. We have designed fast simulators that compute the data movement costs of these algorithms, and experimentally measured the number of data reorganizations needed as a function of the core memory available. We show that the relative performance of three commonly used variants of the factorization algorithm, viz. left-looking, right-looking, and multifrontal algorithms can vary by orders of magnitude for unbalanced elimination trees that occur in linear programming and related applications.

This study will help us make design choices in extending 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.

We have been able to provide 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 then 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 developed and implemented, and will be applied to solve the Jacobian and Hessian estimation problems in parallel on shared-memory computers. 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 and Ferderik Manne (University of Bergen).

Three-dimensional flow in cavity at yaw

Alex Povitsky

This study is motivated by three-dimensional flows about protrusions and cavities with an arbitrary angle between the external flow and rigid elements. The motivation comes from the problem of airframe noise. The deployment of the trailing-edge flaps, the leading-edge slats, and the undercarriage become one of the important sources of aircraft noise at landing phase of flight. Enclosures of quite different scales are formed by wheel wells, brace boxes, and pin cavities in various joints linking different gear components. Wheels and axles comprise a series of short cylinders of different aspect ratios and inclinations relative to the flow direction. The novel type of a "building block" cavity flow is proposed where the cavity lid moves along its diagonal (Case A). The proposed case is taken as a typical representative of essentially three-dimensional highly separated vortical flows having simple single-block rectangular geometry of computational domain.

The considered flow (Case A) is substantially different from that in the benchmark case where the cavity lid moves parallel to the side walls of the cavity (Case B). Enhanced transverse fluid motion in the direction perpendicular to the direction of moving lid is observed in Case A. The integral of momentum in this direction is about one order of magnitude higher than that in Case B. The flow in the three-dimensional elongated cavity driven by the cavity lid has the curvilinear separation line and non-symmetric vortices in the mid-plane. Again, the integral of transverse momentum is approximately one order of magnitude higher than those in benchmark cases B, where the lid moves parallel to either long or short side walls. For diagonal-driven fully developed turbulent cavity flow in a cube, modeled by the Reynolds Stress model of turbulence, the vortical pattern is qualitatively similar to that for the laminar flow at $Re = 2000$. For Case B, significantly more secondary vortices are observed in planes perpendicular to the lid direction than for laminar flow case. Nevertheless, the transverse momentum for Case A remains more than one order of magnitude higher than that for Case B, i.e., the strong yaw-related amplification of transversed flow holds for turbulent Re numbers.

Our future research includes modeling of transition to turbulence in cavity flows, generation, propagation and suppression of noise in opened cavities. The latter part of research will be conducted in collaboration with S. Tsynkov (North Carolina State University) and J. Loncaric.

Solving radiation transport equations with the multigrid method

Linda Stals

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

Our recent research has mainly focused on the use of adaptive refinement techniques to aid in the solution process. We have implemented a parallel adaptive grid refinement routine that changes the shape of the grid to match the wave front as it moves through the domain. This gives a far more accurate solution.

In our future work we want to look at adaptive time-stepping routines.

FLUID MECHANICS

Seedless laser velocimetry with laser-induced thermal acoustics
Roger Hart

Non-intrusive measurement of flow velocity by various laser-based methods provides information of great significance to the experimental fluid dynamics community. However, the only methods to have achieved widespread use to date are laser Doppler velocimetry and particle interval velocimetry, both of which require the flow to be seeded with small (~ 1 micron) particles to serve as light scatterers. Seeding is not feasible in some wind tunnels due to concerns over removal of spent seed, clogging of flow straightening screens, or abrasion of finely polished surfaces. Additionally, there are regions in airflows of interest, such as vortex cores over delta wings or in recirculation regions behind rearward facing steps or leading-edge slats, where useful seed concentrations may be difficult or impossible to achieve. There is thus considerable (although not universal) interest in the experimental fluid dynamics community in a laser velocimetry technique that can provide the dependability, ease of use, and quality of data of existing methods without seeding. Laser-induced thermal acoustics (LITA) is a relatively new technique which has great promise as a robust, reliable seedless laser velocimetry method. Our objective is to further develop the theoretical and technical basis for LITA velocimetry in the laboratory, and to demonstrate the utility of LITA velocimetry through a variety of 'real-world' wind tunnel measurements at NASA Langley.

Considerable theoretical and laboratory evaluation of LITA velocimetry has already been accomplished, although work continues in support of the improvement of our designs for fieldable measurement systems. Our overall design philosophy springs from the realization that a system must be relatively easy to install and use and must reliably produce dependable data; a system that does not meet these requirements will be of no interest to our user community. To that end our designs stress modularity, easy transport and installation, and the use of compact, turn-key laser systems. Of great significance in regard to stability and accuracy is our use of a novel grating demodulation technique (invented by us). The current reporting period has been devoted to: the preparation of reports documenting our very successful demonstration of a one-component LITA velocimeter at BART late last year; theoretical and laboratory exploration of various possible improvements to the method; and design, parts procurement, and initial phases of construction of a much more sophisticated two-component velocimeter. The new instrument will feature remote operation and greater stability and ease of use than the original prototype. All experience to date indicates that an instrument of considerable practical utility is within reach.

We are currently scheduled to return to BART with the new two-component instrument in April 2002 to make measurements behind the deployed leading-edge slat of a high-lift wing configuration. Comparison with PIV in the flow above the wing will also be made. Somewhat later, we will take the new instrument to PCT to attempt a variety of measurements in a supersonic flow. Possible use of LITA velocimetry at other facilities such as LTPT is being discussed.

This work is being pursued in collaboration with R.J. Balla and G.C. Herring (NASA Langley).

Predicting time correlations by large-eddy simulation
Guowei He

Sound generated by turbulence is an important source of noise and raises many questions of fundamental and engineering interest. In sound radiation, the Lighthill acoustic analogy shows that the sound source de-

pends on time correlation. The objective of the current research is to study the properties of time correlation in turbulence and develop subgrid scale (SGS) models for Large Eddy Simulation (LES) in sound radiation.

This work starts with evaluating the eddy viscosity SGS model using the database for isotropic turbulence on a Beowulf 96 CPU cluster computer at ICASE. It is shown that the eddy viscosity SGS model over-predicts time correlations. The necessary conditions for SGS models to correctly predict time correlation are derived analytically. These conditions can be used to evaluate the performance of SGS models. We have developed a two-parameter expression for the time correlation. The two-parameter expression can fit the measurements from the database by fixing its "sweeping" and "oscillation" parameters.

Our future work will include evaluating the currently existing SGS models and developing the effective SGS models for LES in predicting time correlation.

This work is performed in collaboration with R. Rubinstein.

Mapping closure approximation to a joint probability density function
Guowei He

There is no well-established procedure for calculating a joint probability density function (PDF) in turbulence modeling, especially in turbulent mixing. While the transport equation of the joint PDF has been formulated, some models associated with the transport equation, such as conditional dissipations on two given components, still need to be improved. The goal of this research is to develop the mapping closure approximation approach (MCA) for a joint PDF.

The previous work on MCA for a single scalar has been extended to multiple scalars. The conditional diffusion and dissipation have been derived for differential diffusions. The shape of the joint PDF has been formulated. Moreover, MCA also provides the models for other conditional statistics, such as ensemble average of one component conditioned on another given component. Those results are compared with direct numerical simulation. The primary comparison shows good agreement.

Future work will include a comparison of the numerical results to the MCA's predictions in more complex situations, in order to develop the models of conditional moments in PDF as well as conditional-moment equations.

Bypass dynamics in laminar boundary layer
D. Glenn Lasseigne and William O. Criminale

In previous work we have investigated the two-dimensional response of the laminar boundary layer to exterior disturbances using a new paradigm for the linearized stability analysis for parallel and almost parallel flows. The approach taken is to capture the entire range of dynamics, which includes the significant contribution of the continuum modes. This is done by formulating the problem as an inhomogeneous initial value problem. It can be shown that disturbances that reside in the continuum modes can directly feed into the discrete modes as the boundary layer expands downstream.

This same modeling approach is taken to study the three-dimensional response of the laminar boundary layer in order to determine possible bypass mechanisms. The chosen method is particularly suitable to this endeavor since it is known that in the limit of completely spanwise disturbances, only the continuum modes exist. In particular, it is investigated as to the nature of the forcing terms that will produce significant growth of disturbances within the boundary layer. Both parallel and non-parallel calculations help to highlight the details of the boundary-layer response.

This work will lead directly to a weak, nonlinear theory in which the same modeling approach can be used to determine the effects of mode interaction has on the total response.

Moving boundaries in lattice Boltzmann method
Li-Shi Luo

So far the method of the lattice Boltzmann equation (LBE) has been mostly applied to CFD problems with non-moving boundaries, except in case of particular suspensions in fluids where the Reynolds number is relatively small and the accuracy of boundary geometry is not the most crucial part in the calculation. However, in many CFD problems the accurate simulation of moving boundaries is very important. The present work extends the LBE method to the problems with moving boundaries.

We propose a lattice Boltzmann method to treat moving boundary problems for solid objects moving in a fluid. The method is based on the simple bounce-back boundary condition and interpolations at boundaries. The proposed method is tested in two flows past an impulsively started cylinder moving in a channel in two dimensions: (a) the flow past an impulsively started cylinder moving in a transient Couette flow; and (b) the flow past an impulsively started cylinder moving in a channel flow at rest. We obtain satisfactory results and also verify the Galilean invariance of the lattice Boltzmann method.

A paper entitled "Lattice Boltzmann Method for Moving Boundaries," authored by Pierre Lallemand and Li-Shi Luo, has been submitted to the Journal of Computational Physics (2001). An ICASE report is in preparation.

The present work is a result of collaboration with Pierre Lallemand (Laboratoire ASCI-CNRS, Université Paris-Sud (Paris XI Orsay), France). The present work has been partly funded by NASA Langley under the program of "Innovative Algorithms for Aerospace Engineering Analysis and Optimization."

We intend to extend our work to three-dimensional LBE models or other more complicated LBE models with larger number of velocities.

Numerical investigation of non-Boussinesq lock exchange flows
James E. Martin

Gravity currents are horizontal flows that occur when a density difference exists across a lateral contact boundary. One particularly simple arrangement which allows for the study of gravity currents is the lock exchange configuration. To study lock exchange flow, we initially divide a channel into a right and a left reservoir, with each half of the channel initially filled with a fluid of different density. Upon release of the separating membrane, gravity currents ensue as each fluid mutually intrudes upon the other. As a first step in examining the potential problem in industry of accidental release of a dense (and potentially dangerous) gas, one may consider lock exchange flow as a simple model.

Our approach is to perform high-resolution, two-dimensional simulations of lock exchange flow. We take care to avoid application of the common Boussinesq assumption, thus making our results valid for two fluids with any density ratio. With the governing equations, we take a streamfunction vorticity approach. In addition, we study the mixing of the two fluids by simultaneously solving a diffusion equation. Spectral Galerkin methods are used to represent the streamwise dependence of both the streamfunction and the vorticity fields. For the density field, differencing is accomplished exclusively through compact finite difference techniques. For large density ratio, we find that the Kelvin-Helmholtz instability (familiar from the previous Boussinesq studies of this problem by Hartel, Meiburg, and Necker) occurs only near the dense front. Analysis of the flow within the protruding gravity current head reveals a new topology in the form of a strong recirculation zone which entrains light fluid toward the channel bottom. The thickness of the lighter fluid layer situated beneath the dense front is seen to increase with larger density ratio. Over the complete range of density

ratios, we have computed Froude numbers for both the light and dense fronts and found agreement with the experimental measurements of Grobelbauer, Fannelop, and Britter (1993), thus verifying our code.

To date, we have limited our attention to gravity currents over horizontal no-slip walls. In the future, we will consider what differences occur for slip boundaries and we will consider the effect of a sloping channel.

This research was done in collaboration with Eckart Meiburg (University of California at Santa Barbara).

Biological application of laser-induced thermal acoustics
Toshiharu Mizukaki

We have been trying to develop a new measurement technique of water temperature for medical applications, which is based on laser-induced thermal acoustics (LITA). This measurement technique has several advantages over ordinary techniques, for it proposes such as measurement using thermocouples. One of the advantages is its quick response time, which is less than 100 nanoseconds. The fastest response time that ordinary thermocouples have is about three milliseconds, which is 30,000 times longer than LITA at this moment. Ordinary thermocouples cannot measure the temperature changes behind shock waves since shock waves in water create sudden temperature rises and drops, which duration will be less than several microseconds. Then the fast response time of LITA can make temperature measurement behind shock waves in water possible. Water temperature measurement behind shock waves in water has been strongly desired to develop medical applications of shock waves such as a cancer-removing technique, which could only kill cancer by the heat generated by shock waves. Then, the objective of this research is to show by means of evidence that LITA can be applied as a water temperature measurement technique.

The most important point for our objective is to obtain clear LITA signals in water, which is a low signal-to-noise ratio that is enough to bring precise water temperature within less than one percent error. We had two problems for this purpose. One was high-frequency LITA signals that were higher than 75 MHz must be observed in pure water, and the other was noise reduction to distinguish pure LITA signals from other unwanted light which were generated by the exciting and probing laser beams. A LITA signal is an oscillated one which frequency depends upon the speed of sound of its medium. The medium that has faster speed of sound will bring us high frequent LITA signals. In air, the speed of sound is 345 meters per second at room temperature, while the speed of sound is about 1500 meters per second in pure water. The LITA signal has more than 70 MHz frequency in water. To obtain such high-frequency LITA signals precisely, we assembled a fast-speed data acquisition system, which consisted of a four-gig sampling rate digital oscilloscope, a multi-channel programmable trigger generator, and a photomultiplier tube. This system helped us obtain LITA signals that were enough quality to analyze their frequency. To overcome the second problem, we applied spectroscopic techniques such as a Perrein-Broca prism, a monochrometer, and a spatial filter for our LITA signal-detection system. Those devices helped us distinguish pure LITA signals from any kind of unwanted light. By means of efforts that were described above, we have successfully demonstrated new measurement techniques for water temperature with short measurement time, and high special resolution. The analyzed results showed that this technique had 10 percent error. The fact that the obtained data has a relatively large error, however, can be improved by using a short-duration laser such as a Pico second laser. To obtain more precise measurement results, much more oscillation must be needed within measurement duration. This research, however, shows applicability of LITA for water temperature measurement. Now that fundamental technique has been established, we can increase the precision of measurement.

Future plans of this research are as follows: a) Utilize Pico second laser for pump laser to obtain much more ringing, b) Utilize fast digital oscilloscope that has more than 1 GHz sampling rate to interoperate

LITA signal, c) Apply this technique for temperature measurement behind shock waves, and d) Continue research on application for shock wave measurement at Shock Wave Research Center in Japan, which the author is working in.

This research was conducted in collaboration with Paul M. Danehy, Greg C. Herring, David Aldrafer, and Steve Jones (NASA Langley).

STRUCTURES AND MATERIALS

Mixed-mode decohesion finite elements for the simulation of delamination in composite materials

P.P. Camanho

Delamination is one of the predominant forms of failure in laminated composites due to the lack of reinforcement in the thickness direction. Delamination as a result of impact or a manufacturing defect can cause a significant reduction in the compressive load-carrying capacity of a structure. The stress gradients that occur near geometric discontinuities such as ply drop-offs, stiffener terminations and flanges, bonded and bolted joints, and access holes promote delamination initiation, trigger intraply damage mechanisms, and may cause a significant loss of structural integrity.

The objective of the research is to develop zero-thickness decohesion finite elements capable of simulating delamination onset and growth under mixed-mode loading conditions. Interactive criteria to predict delamination onset and growth are proposed and implemented in a softening constitutive equation, which represents the way by which the interface loses its load-carrying capability.

Future activities will include the application of decohesion elements to the analysis of aircraft structural components.

The current work has been performed with the collaboration of Carlos Dávila (NASA Langley).

Closed-shell carbon nanostructures from organo-metallic precursors

Theo Dingemans

To circumvent some of the processing problems associated with single-wall and multi-wall carbon nanotubes, we have designed and synthesized several organo-metallic compounds with high C-H ratios. These precursors are highly soluble and can be processed using a variety of processing techniques. Once in place, as a thin film or dispersed in organic and inorganic hosts, the temperature is increased and a variety of closed-shell carbon nanostructures are formed. Although extensive literature is available on different catalyst systems that can be used in mixed graphite feedstocks, little information is available on organo-metallic compounds and their usefulness as precursors towards closed-shell carbon nanostructures.

To date we have synthesized and characterized three isomeric phenyl-alkyne cobalt complexes. The different substitution patterns, or regio-isomers, will give us information about how the substitution patterns affect the formation of graphitic networks. Thermo gravimetric analysis (TGA) shows two distinct weight-loss regions. The low-temperature event is associated with the loss of carbon monoxide (CO), caused by catalyst decomposition, and the high-temperature event is due to the formation of the graphitic network. Differential scanning calorimetry (DSC) experiments show that the high-temperature event is highly exothermic in nature. We used scanning electron microscopy coupled with an energy dispersive x-ray analyzer (SEM/EDX) to obtain information about the morphology and composition of the crude products. Preliminary results show the presence of two different morphologies, i.e., both amorphous and crystalline regions can easily be distinguished. The most abundant are the crystalline structures, which are approximately 1 μm in diameter and appear to be covered with — or comprised of — cobalt. Although the amorphous regions are more difficult to characterize, they appear to be covered with cobalt as well.

Future work will include temperature-dependent NMR and Raman experiments, which will allow us to follow the carbonization process *(in-situ)*. We will use transition electron microscopy (TEM) and atomic force

microscopy (AFM) to determine what type of carbon structures were formed using this method. In addition, we will explore different chemistries that will allow us to incorporate 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 and Peter Lillehei (NASA Langley).

Molecular dynamics simulations of polymer-nanotube composites
Sarah-Jane V. Frankland

Composite materials of polymers and carbon nanotubes are being developed as lightweight materials with potentially good mechanical and electrical properties. In this work, the interface between the nanotube and the polymer is proposed as the chemical key to understanding the mechanical behavior of the composite with regard to such features as the load transfer mechanism, the elastic moduli, the strength of the composite, and its failure mechanism. Molecular modeling of this interface, and properties generated from the molecular models via molecular dynamics (MD) simulation are being used to construct a detailed chemical representation of the polymer-nanotube interactions. However, there is an inherent length-scale issue as the aspect ratio of the carbon nanotube, which is possibly a major contributor, is large enough to make a fully atomic description intractable. Therefore, a concerted effort will be made with other researchers to utilize the nanoscale data in higher-level micromechanical or continuum-level models. These systems present an ideal challenge for beginning to bridge the length-scale gap between the nanoscale and the continuum.

To date, three prospective models are being developed that rely on input from molecular dynamics simulation. The first one takes elastic constants as input for finite element analysis, the second one also uses the elastic constants this time as the basis for a micromechanical model of a functionally graded material, and the third one is a rheological model of the polymer-nanotube interfacial failure. A parallel MD code is now available, and has been optimized sufficiently to run on Coral. As a test case, MD simulation of a carbon nanotube in a crystalline polyethylene matrix was performed, and the stress at which the nanotube yields from the matrix compared satisfactorily with earlier work. We are now ready to begin supplying information for each of the proposed models.

Simulation data will be generated for non-bonded and chemically functionalized polymer-nanotube composites. The interface will be modeled with varying degrees of chemical detail.

This work was done in collaboration with J.A. Hinkley (NASA Langley), T.S. Gates (NASA Langley), E. Saether (NASA Langley), V.M. Harik (ICASE), C. Park (ICASE), G.M. Odegard (National Research Council), and K.E. Wise (National Research Council).

Mechanics of carbon nanotubes
Vasyl Michael Harik

Carbon nanotubes possess extraordinary physical properties (e.g., high stiffness-to-weight and strength-to-weight ratios and enormous electrical and thermal conductivities). Potential applications range from new electronic devices and nanotube-based scanning probes to multifunctional polymer films and sensors for new aerospace structures. The goal of this research is to develop constitutive models for carbon nanotubes and a methodology for the implementation of continuum models at nano-scale.

Ranges of validity and length-scale limitations of the continuum models for carbon nanotubes under compressive loads are examined. Hierarchical dimensional analysis of the nanomechanical buckling problem and the geometric and material parameters involved is carried out. As a result, three classes of carbon

nanotubes are identified. One of the classes consists of the newly predicted carbon nanobeams. The scaling laws and the key non-dimensional parameters controlling the deformation process of nanotubes have been derived. Expressions for critical strains are tailored for various nanotubes and their values are compared with the 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 the effects of nanotube geometry on the constitutive properties of nano-structured materials. Applicability of advanced shell theories will be examined as well.

This research is conducted in collaboration with T.S. Gates, M.P. Nemeth and D.R. Ambur (NASA Langley).

Modeling-for-design of multifunctional composite materials
Vasyl Michael Harik

Design of new aerospace structures, such as flexible wings, structures with active controls, multifunctional membranes, and inflatable antennas require fundamental understanding of electromechanical coupling and 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 composite materials.

A class of nano-structured piezoelectric polymers is considered in order to identify the key physical phenomena contributing to electromechanical coupling and mechanical and electrical properties of multifunctional polymer films and polymer matrices. The physical and materials science characterization of the key material parameters has been analyzed before a number of functional relations between them are derived. The work performed thus far indicates that the dimensional analysis of material behavior may lead to the key non-dimensional group of parameters that would control material constitutive response. A thermal analogy for electromechanical effects is examined for microcomposites with the fiber-matrix interphase.

Future work involves derivation of functional relations for material parameters in terms of non-dimensional groups and the development of new constitutive models.

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

Constitutive modeling of nanocomposites
Vasyl Michael Harik

Numerous aerospace applications involve the use of composite materials which permit optimization of structural designs for weight, mechanical, and electromechanical performance. Nano-structured materials offer additional benefits that stem from their superior physical properties. The goal of this research is to develop hierarchical constitutive models that link the nano-scale molecular structures with continuum micromechanics. Such models are critical for the development, design, and optimization of novel nanocomposites.

A novel modeling technique, which was originally developed for planar lattice structures and carbon sheets, has been generalized for three-dimensional arbitrary molecular networks that interact through structural bonding and van der Waals forces. Under certain conditions, the multi-scale connectivity and thermodynamically consistent material averaging is achieved for nanotube-reinforced polymer composite systems via an energy-equivalence principle. This modeling approach has been smoothly linked with molecular dynamics simulations for nanotube-polyethylene material systems.

The future work is directed toward a better understanding of applicability and limitations of this novel methodology and alternative techniques for multi-scale modeling.

Intralaminar and interlaminar progressive failure analysis of composite panels with cutout
Navin Jaunky

The phenomenon of interlaminar failure (or delamination) in composite structures usually originates from discontinuities such as intraply failure, free edge, and at the skin-flange location of stiffened panel. Delamination may lead to failure of the structure or reduce its strength. Progressive intraply failure (or PFA) may not be accurate in predicting failure load of composite panels depending on the interaction between intraply damage and delamination. Intraply failure such as matrix cracking may initiate delamination long before final failure of the panel. In such a case delamination may contribute significantly to the panel failure. Therefore, including progressive interlaminar failure or delamination in a progressive intraply failure analysis is essential. However, very few researchers have considered both progressive failure and delamination, and studies on the interaction between failure, delamination, and buckling is non-existent in the literature.

A unified treatment involving the interaction of buckling and postbuckling with progressive failure and delamination is investigated. A recently postulated irreversible constitutive law for the formulation of interface element to predict delamination is used in conjunction with failure criteria and a material degradation model is used. The failure criteria and the material degradation model were discussed in the previous Semiannual Report. Interlaminar damage is simulated using interface elements placed between composite sublaminate. A softening constitutive law is generally used to formulate the interface elements that are of zero thickness. The interlaminar traction T is related to the relative displacement Δ via a constitutive law such that with increasing separation, the interlaminar traction across the surface attains a peak value, which is the maximum interfacial strength T^{max}, and then decreases to zero. Fracture mechanics is incorporated by equating the area under the $T - \Delta$ to the critical energy release rate G_c. Hence delamination is initiated when the interlaminar strength equates the maximum interfacial strength and the delamination front is advanced when the local surface energy is consumed. The mathematical form of the constitutive law is chosen to be exponential because the tangent stiffness is smooth, and help to suppress numerical oscillations associated with nonlinear solution. The form of irreversible constitutive law is such that:

- The energy consumed in the process of delamination is not recoverable.
- The constitutive law satisfies a multi-axial stress criterion for the onset of delamination.
- The delamination progresses according to a mixed-mode fracture criterion.

An eight-node interface element formulation with the irreversible constitutive law was implemented in the commercial finite element code ABAQUS as a user-defined element through a user-defined subroutine (UEL).

Interface elements as described above can be used in a variety of problems. In the past when using fracture mechanics, self-similar delamination growth and an initial delamination zone are assumed. These limitations can be overcome by positioning interface elements between sublaminates of a composite panel where the prediction of initiation and progression of delamination becomes natural without imposing constraint on the progressive failure analysis.

The interface elements were first assessed using double cantilever problems with available analytical solutions. Finite element solutions were found to be in close agreement with analytical solutions. Computational efficiency was found to be much better than when using interface elements with bilinear constitutive law.

Progressive failure with delamination was carried out for a flat panel with a centrally located circular cutout subjected to shear loading. Analysis results suggest that delamination initiates shortly after matrix cracking is initiated. Both delamination and intraply damage progress in the postbuckling regime. Better agreement was obtained with experimental data as compared with a progressive failure analysis without delamination.

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

This work is done in collaboration with Vinay Goyal and Eric Johnson (Virginia Polytechnic Institute and State University). Damodar R. Ambur and Mark W. Hilburger (NASA Langley) were also involved.

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 was to compare previous results with analytical models where the matrix crack initiation was neglected and to illustrate the difference in delamination onset predictions based on the type and location of the assumed initial damage. The goal is to extend these comparisons to a more classical damage tolerance approach assuming delamination from a "critical size" initial flaw at the most "critical location."

Finite Element analyses were performed for simple skin/flange specimens subjected to tension and bending loads. Delaminations of various lengths were discretely modeled by releasing multipoint constraints starting from different assumed flaws locations. A fracture mechanics approach was used to determine delamination growth from these flaws. Mode I and II strain energy release rate contributions were calculated for all load cases using the virtual crack closure technique. Computed total strain energy release rates were compared to critical values obtained from an existing mixed-mode failure criterion to determine the critical load. Previous experimental work showed that damage starts as a matrix crack in the top skin layer followed by a delamination between the top and second skin layer. Therefore, the first model represented the actual failure pattern as observed in the experiment. Although this case is the most realistic, it would be difficult to manufacture a specimen with an embedded flaw that simulates both the delamination and the matrix crack. Hence, in a second model a flaw was assumed to exist in the bondline, creating a delamination. This case would be the easiest to simulate experimentally and would simplify modeling, but the approach is different from the actual situation. In the third case, a delamination was assumed at the actual location observed in the experiment, however without the matrix crack. Although the delamination is located at the correct interface, the approach is simplified by the absence of the matrix crack. The goal of this study was to verify if the simplifications made in two cases were conservative.

For the skin/flange specimen configuration studied, it was found that there is a considerable reduction in critical load if the matrix crack initiation is ignored, both under tension and bending loads. For both load cases, the delamination onset load for an assumed initial flaw in the bondline is slightly higher than the critical load for delamination onset from an assumed skin matrix crack. In the case of an assumed flaw in the actual location without a skin matrix crack, the delamination onset load is even higher. As a result, assuming an initial flaw in the bondline is simpler while providing a critical load relatively close to the real

case. For the tension load and the configuration studied, the ratio of computed total strain energy release rates versus the critical values decreases with crack length. Therefore, assuming an initial flaw of 12.7 mm (0.5") as suggested by industry would be unconservative, as the critical load for delamination onset is higher. For the bending case however, assuming an initial flaw of 12.7 mm (0.5") is conservative. These results are valid for the configuration studied, and might not hold for a different configuration.

For the studies to date two-dimensional models of a longitudinal cut through the specimen were used to allow for a detailed modeling of the individual plies and the adhesive in thickness direction. Due to the complex nature of the failure a three-dimensional analysis appears appropriate. Since many layers of brick elements through the thickness would be required to model the individual plies, the size of three-dimensional finite element models, however, may become prohibitively large. A generalized plane-strain model, which requires about the same modeling effort as a simple two-dimensional model, may be viewed as an alternative to a full three-dimensional simulation. Future work will therefore focus on the comparison of results from two-dimensional plane stress, plane strain, and generalized plane strain models to data obtained from full three-dimensional simulations. This will allow study of the feasibility of using simple two-dimensional models and determine the limitations of the approach.

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

Recommendations for power amplifier development for the morphing program
Douglas K. Lindner

The objective of this project was to assess the state of power electronics development in the Langley Morphing Program and to suggest new research directions for power amplifiers for smart materials.

Currently the Morphing Program has relied primarily on the benchtop amplifiers and linear amplifiers. These amplifiers will have limited application in future smart structure applications. Assessment of the Morphing programs lead to the following recommendations for future research: 1) Classification of various power electronic circuit topologies for smart structure applications, 2) Determine the minimum size and weight for each targeted circuit topology, 3) Investigation of high-voltage amplifiers, 4) Investigate the power bus design issues for systems with multiple actuators, 5) Characterize linear and nonlinear load impedances due to the actuators, and 6) Investigation of potential energy savings for microfliers. It is recommended that these research topics be incorporated into a demonstration project that showcases the development issues of power electronic amplifiers. In addition, the preparation of a report outlining power electronic design issues is recommended.

No future work is planned.

These recommendations were developed based on discussions with the following people: Lucas Horta, Anna McGowen, Rob Bryant, Dave Cox, Garnett Horner, Tom Jordan, Zoubeida Ounaies, Gary Gibb, Rich Silcox, Travis Turner, Paul Robinson, Bob Fox, Qamar Shams, Frank Chen, and Norm Shaeffler.

Intelligent optics
Mark Little

Intelligent optics, materials or devices whose optical properties may be controlled by external means, have a significant role in many areas of today's society. Some include the communications industry, scientific research, and space applications. Examples of intelligent optics can be found everywhere, the most common

being self-darkening lenses and automobile rearview mirrors. One problem with current intelligent optical materials is a characteristically slow response time. For use in communications and space it is imperative to have fast optical devices. One possible solution is to exploit the Stark and Zeeman effects in materials. These quantum mechanical liftings of electronic degeneracy by electric or magnetic fields may induce a change in the materials optical properties that can be exploited. Since these transitions are quantum in nature their response times will be very fast. The goal of this research is to fabricate new optical thin film (OTF) materials that use either the Stark or Zeeman effect as its active optical 'switch.'

To date, work has been concentrated on acquiring the capability to produce and characterize these materials. Optical thin films require very controlled growth conditions. Several growth systems are currently being worked on to provide a wide range of growth methods. A multi-target sputtering chamber was purchased from Ohio University and will serve as the primary growth tool due to its flexibility and rapid cycle time. A Direct Metal Ion Beam deposition chamber was just delivered. These systems are in place in the lab and awaiting the contractor's installation of the necessary electrical connections, which should be complete by mid-October. A physical vapor deposition system is being worked on and should be operational by December. Film optical properties will be measured with a newly purchased variable angle spectroscopic ellipsometer. This machine is in place, operational, and producing excellent data. The preliminary laboratory setup phase is nearly complete. This is significant because once finished new films will be able to be produced and characterized in an assembly line fashion, necessary when 'hunting' for new materials.

Future plans are to begin the exploration growth for new OTF materials. The Stark and Zeeman effect will require an atomically isolated dopant level residing in a host material. Likely dopant candidates will be transition metals and rare earths with f-shell electrons. Rare earths are known to produce atomic-like levels in host matrices. Host materials will initially include standard optical glasses, oxides, wide band gap semiconductors (both crystalline and amorphous), and ferroelectric materials. There are plans to establish basic electronic testing capabilities on these materials shortly after production begins in the advent a new electronic material is developed serendipitously.

I would like to thank Glen King and Sang Choi for their help and guidance with this research.

A modular approach to multifunctional materials
Edward Locke

Future advances in aerospace and space technologies will require the fabrication of materials with tailored properties and multifunctional capabilities. Materials that are lightweight, thermally and structurally robust, and which possess the characteristics to withstand the damaging elements of multiple orbital environments will be essential in the design of safer, more economical, and highly technologically evolved aircraft and spacecraft. The multifunctional nature of future materials will enable properties such as photoreactivity, optical transparency, dielectric strength, and electrical conductivity to be engineered to desired specifications in a single material. We are currently developing synthetic methods for the construction and integration of functional modules into high-performance polymers in a geometrically defined manner for the design of novel multifunctional nanostructured materials.

Subsequent to initial design efforts toward photoreactive materials, we synthesized suitably functionalized azo monomers that were incorporated into space-durable polymer systems. The degree of intramolecular and intermolecular (cross-linked) incorporation of the optically active modules was controlled through reaction conditions and stoichiometry. Characterization of these materials upon laser irradiation with respect to the degree of dimensional control versus azo monomer content and orientation is currently underway. These

materials may provide space-durable "smart" films that facilitate laser-induced remote active shape control for applications in precision optical space membranes to be used in the Next Generation Space Telescope and Larger Gossamer space structures.

Future efforts will be directed toward the development of synthetic strategies for the integration of additional functional modules into space-durable thin films to expand the multifunctional nature of these materials.

This research was conducted in collaboration with Catharine Fay, Diane Stoakley (NASA Langley), and Oak Ridge National Laboratories.

High-temperature piezoelectric films
Zoubeida Ounaies

Polymers offer the advantage of processing flexibility because they are lightweight, durable, readily manufactured into large areas, and conformable to complex shapes. Other notable features of polymers are low dielectric constant, low elastic stiffness, and low density, which result in a high-voltage sensitivity (excellent sensor characteristics) and low acoustic and mechanical impedance (crucial for medical and underwater applications). Polymers also typically possess a high dielectric breakdown and high operating field strength, which means that they can withstand much higher driving fields than ceramics. Based on these features, piezoelectric polymers possess their own established niche areas for technical applications and useful device configurations where single crystals and ceramics are incapable of performing as effectively.

Developing high-performance, high-temperature flexible piezoelectric polymers 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 development of active flow control sensors and airframe health monitoring sensors. To achieve the goal of improved piezoelectric polymer design, amorphous polyimides containing polar functional groups have been synthesized and investigated for potential use as high-temperature piezoelectric sensors. Effect 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 are reported. The thermal stability of the piezoelectric effect was evaluated under dynamic and static thermal stimuli. To characterize the measured physical responses exhibited by the polyimides, a hierarchy of models will be considered. The goals in model development will focus on both microscopic properties inherent to the materials and macroscopic averages which facilitate structural design and future control implementation.

This fundamental structure-piezoelectric property analysis will enable molecular design of polymers that possess distinct improvements over state-of-the-art piezoelectric polymers including enhanced polarization, polarization stability at elevated temperatures, and improved process design.

Future work will further explore the processing and properties of the polyimide/PZT composite.

This work is done in collaboration with Joycelyn S. Harrison (NASA Langley), Cheol Park (ICASE), and Dan Klein (National Research Council).

Piezoelectric ceramics for use as actuators
Zoubeida Ounaies

The piezoelectric ceramic effort focuses on understanding basic mechanisms and widening their scope of application. Two main areas of concentration are 1) investigating pre-stressed piezoelectric actuators, and

2) studying energy harvesting using piezoelectric materials. Bender-type THUNDER actuators are used in both of these studies.

Two mechanisms are responsible for the high electromechanical performance of THUNDER actuators, namely the presence of stress-bias (may enhance domain reorientation) and the restricted lateral motion (domed geometry results in a d31 effect). The internal stresses present within the ceramic and metal layers, combined with restricted lateral motion, enhance the axial displacement and cause 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 ferroelectric domain theory.

In the second study, the effects of length, width, thickness of the metal substrates and the PZT are investigated in an attempt to identify the parameters responsible for optimizing the energy harvesting characteristics of the actuators. Recently, it has been demonstrated that THUNDER could be improved significantly for energy production without detrimentally affecting its electromechanical response. Current results show a correlation between the geometry of the actuators and energy production. The dome height of the device, and, thus, the volume under the device are undoubtedly dependent upon the type of metal used. The results show that the actuator can be adjusted in such a way that the same energy output could be obtained with different materials by adjusting the thickness ratios, width and length. In the future, mathematical models will be employed to predict the energy output for given geometric constraints and results will be validated through comparison with experimental data.

This work is done in collaboration with R.C. Smith (North Carolina State University) and Karla Mossi (Virginia Commonwealth University). It resulted in the publication of three ICASE reports.

Corona poling of partially cured polyimide
Cheol Park

In-situ poling and imidization of the partially cured (β-CN)APB/ODPA was studied in an attempt to maximize the degree of dipolar orientation and the resultant piezoelectric response. The dielectric relaxation strength, remnant polarization, and piezoelectric responses were evaluated as a function of the poling profile. The partially cured, corona poled polymers exhibited higher dielectric relaxation strength ($\delta\varepsilon$), remnant polarization (P_r) and piezoelectric strain coefficient (d_{33}) than the fully cured, conventionally poled ones.

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, Kristopher E. Wise (NRC), and Joycelyn S. 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. Single wall carbon nanotubes (SWNTs), however, have been rarely used as an electrical or mechanical inclusion in a polymer matrix mainly because of the difficulty in efficient dispersion. A novel process to effectively disperse SWNTs in an aromatic polymer was developed. This process involves an in-situ polymerization of monomers of interest in the presence of sonication during the polymerization process. The goal of this study is to develop a method to disperse SWNTs into polymer matrices on a nanoscale level. The resultant SWNT-polymer nanocomposite exhibited significant conductivity

enhancement (10^{10} order of magnitude) at a very low loading (0.1 wt%) without sacrificing significant optical transmission. Mechanical properties as well as thermal stability mechanical properties were also improved with the increase of the SWNT incorporation. The SWNT-polymer nanocomposites are useful in aerospace and terrestrial applications. This study was presented at Rice University in Houston, TX on July 2001. High-resolution imaging and image processing of SWNT and SWNT-polyimide composites were studied at Oak Ridge National Lab (ORNL).

SWNT/polymer nanocomposites will be further characterized microscopically (SPM, HRTEM, and HRSEM). A combined experimental and theoretical study will be performed to understand the nature of the interaction and identifying new complexes with improved properties.

This research was performed in collaboration with Zoubeida Ounaies, Sarah J. Frankland, Kristopher E. Wise (NRC), Kent Watson (NRC), Peter Lillehei (NASA Langley), John Connell (NASA Langley), Mia Siochi (NASA Langley), Joycelyn S. Harrison (NASA Langley), Roy Crooks (Lockheed-Martin), Neal D. Evans (ORNL), Edward A. Kenik (ORNL), and Jim Bentley (ORNL).

Organic-inorganic hybrid-clay nanocomposites
Cheol Park

Polymer-clay nanocomposites are of great interest for many industrial applications due to their lightweight, radiation resistance, low coefficient of thermal expansion, low permeability of atoms, low solar absorption, and optical transparency. Layered silicates (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. However, uniform dispersion of completely exfoliated layered silicates in a polymer matrix has been a difficult task to accomplish. The objective of this research is 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. This nanocomposites were prepared by dispersion layered silicates into an organic-inorganic hybrid matrix homogeneously. The hydrolyzed silanol groups present in the organic and inorganic precursors subsequently reacted with hydroxyl groups located on the clay layer edges and themselves to form hydrogen and/or covalent bonds. The hybrid-clay nanocomposite exhibited increase in tensile properties. Transmission electron microscopy and x-ray diffraction revealed that most of the layered silicates remained exfoliated and the exfoliated clays are distributed uniformly.

Various organic-inorganic hybrid systems will be studied to develop new hybrid-clay nanocomposites. A journal paper is in preparation.

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

Electrospinning
Cheol Park

Electrospinning is a process that produces continuous polymer fibers with diameters in the sub-micron range through the action of an external electric field imposed on a polymer solution or melt. Electrostatic atomization occurs when the surface tension of a polymer solution is overcome by an applied electric field, thereby ejecting elongated jets from the surface. Various polymer solutions with nano inclusions (CNR, clay, and piezoceramics) were studied to develop nanocomposite fibers for potential use in biomedical and space applications. Sub-micrometer fiber non-woven mats were produced with polyimide/CNT solutions. The goal of this study is to understand how to control the electrospinning process as a function of electric field and solution variables.

New spinneret systems will be developed for controlling the electrospinning process and patterning spun mats. Various polymer and polymer composite systems will be studied to develop electroactive fiber systems.

This research was performed in collaboration with Mia Siochi (NASA Langley), Harry Belvin (NASA Langley), and Kristin Pawlowski (NASA Langley).

Formation of novel organic-inorganic electroactive composites
Jason Rouse

A program to synthesize novel organic-inorganic composites containing electroactive functionalities has been undertaken. We envision that by minimizing the amount of organic material contained within an electroactive composite, we can increase the stability of the system to the oxidative processes that occur in space. While system stability is paramount, the inorganic matrix must also possess the flexibility afforded by organic-based polymers. With these goals in mind, we have chosen to explore the possibility of incorporating electroactive functionality within the very flexible poly(dimethylsiloxane) system to produce organic-inorganic electroactive composites.

The first route explored for the formation of such materials utilized acid-catalyzed hydrolysis and condensation of functional-group containing orthosilicate precursors in the presence of hydroxy-terminated poly(dimethylsiloxanes) (PDMS). While such chemistry did allow the formation of organic-inorganic composites, the material produced was brittle and did not allow for crack-free films. Currently, we are exploring the use of tin-catalyzed condensation of the orthosilicate precursors with the hydroxy-terminated PDMS. This chemistry has allowed the formation of high-quality films with a range of stiffness.

Future work with these materials involves exploring the variety and reproducibility of the materials prepared using the tin catalyst system. Secondly, the electroactivity of these materials needs to be determined. The incompatibility of metals to adhere to PDMS systems is a challenge that needs to be overcome first.

This research is conducted in collaboration with Zoubeida Ounaies (ICASE), Mia Siochi (NASA Langley), and Joycelyn S. Harrison (NASA Langley).

Space durable carbon nanotube polymer composites
Kent Watson

Large, deployable, ultra-light weight Gossamer spacecraft will require film-based polymeric materials that possess a unique combination of physical, mechanical, and optical properties. The requirements are dependent on the intended mission and orbital environment of the spacecraft. Recently the preparation and characterization of [2,4-bis(3-aminophenoxy)phenyl]-diphenylphosphine oxide (3-APPO) and space environmentally durable polyimides therefrom was reported. These polyimides contain a unique combination of properties including atomic oxygen (AO) and ultraviolet (UV) radiation resistance, low solar absorptivity, high thermal emissivity, solubility in common organic solvents, good mechanical properties, and formed colorless to near colorless thin films ($\sim 25\mu m$ thick). The next phase of this research has focused on modification of these polymers to incorporate conductivity sufficient for static charge mitigation without imparting color to the films or significantly reducing other desired properties.

Carbon nanotubes, both single and multi-wall, prepared by different methods (laser ablation, chemical vapor deposition, and catalytically grown carbon fibers) with various lengths and diameters were used for this study. The polymer nanocomposites were prepared by reacting 3-APPO and oxydiphthalic anhydride (ODPA) in a polar aprotic solvent in the presence of the carbon nanotubes with loadings of 0.1 and 0.2% nanomaterial. Thin films were subsequently cast and dried to form the polyimide/carbon nanocomposites.

The effects of the different types of nanotubes on the polymers' solar absorptivity, thermal emissivity, and thin-film tensile properties were studied. Low loadings of carbon nanotubes caused a decrease in the glass transition temperature (Tg) as well as a lowering of the optical transmission at 500 nm. The lowered optical transmission values may be improved with better dispersion of the carbon nanotubes. The addition of low-weight percents of carbon nanotubes appears to have caused a slight decrease in tensile strength and a slight increase in modulus. Solar absorptivities were increased slightly, with the laser ablated single-wall carbon nanotubes having the least effect out of the various nano materials. Thermal emissivity values were improved presumably due to the high thermal conductive properties of the nano materials.

Future work includes additional characterization including conductivity measurements. In addition, other types of single-wall carbon nanotubes will be used such as those prepared via the HiPCO (High Pressure Carbon Monoxide) method.

This research was performed in collaboration with John Connell (NASA Langley), Joe Smith, Jr. (NASA Langley), and Zoubeida Ounaies (ICASE).

Smart material actuators driven by microwave
Won Yi

An experimental study of smart materials actuator driven by a microwave is presented in this paper. A proof of concept experiment using THUNDER (Thin Layer Composite Unimorph Ferroelectric Driver and Sensor) Materials has been setup and demonstrated by using a microwave. The feasibility of smart material actuator systems driven by a microwave may be applied for the applications, such as the Next Generation Space Telescope's (NGST) fragmented optics control.

As a result, the Narda horn antenna's 20 W microwave power was converted into a measured 192 V DC by a digital multimeter. The estimated current being produced from the 6×6 rectenna array was 0.38mA. This was computed by using various measured resistor values and the measured voltage across each resistor. The DC voltage output of the 6×6 rectenna array was connected to the resistors in separate operations, and the current through each of the resistors was calculated. The positive terminal of the rectenna was connected to the normally open connection of the recycle timer, and the negative terminal was connected to the common/ground connection. A R-C circuit was constructed using a THUNDER and a 27K ohm resistor. One of the two terminal connections of the R-C circuit was connected to the 9 V DC recycle timer's normally open connection, and the other was connected to the common/ground. The 9 V DC recycle timer setting was set at .5 seconds, which was the recycle timer's fastest setting possible. The Amperite recycle timer had a range setting from .5 seconds to 24 hours. This time setting was verified by the Hameg Instruments Oscilloscope. The measured capacitance of THUNDER was 260nF. When the recycle timer switch was closed, the path of least resistance on the R-C circuit was via THUNDER, thus charging the circuit. When the recycle timer switch changed to the open position, the connection between the rectenna and the THUNDER was broken. The voltage polarity at this point was reversed. The THUNDER and the resistor circuit performed in the same manner as a capacitor and a resistor in a R-C circuit when a voltage was applied or removed. This on/off switching of the 9 V DC recycle timer created a pulse to show that the THUNDER could be actuated by a microwave power. This pulse was captured in a pictorial. The pulse recycle and decay times were measured as 0.5 and 0.3 sec, respectively.

THUNDER is a ferroelectric device made of multiple layers of materials, typically stainless steel, aluminum, and PZT (Lead Zirconate Titanate) piezoceramic. These layers of materials are sandwiched together with an adhesive bond. A piezoceramic material is composed of randomly oriented crystals or grains. By

applying electrodes to the ceramic and a strong DC electric field, the dipoles will tend to align themselves to the direction of the electric field. By aligning in this manner, the smart material will have a permanent residual polarization. The result of this polarization is a change in the geometric dimension. THUNDER has the capability to expand or contract, based on the polarity of the voltage applied. When the applied voltage is positive, THUNDER will flatten, and if the applied voltage were negative, the THUNDER would arch.

REPORTS AND ABSTRACTS

Dowek, Gilles, César Muñoz, and Alfons Geser: *Tactical conflict detection and resolution in a 3-d airspace.* ICASE Report No. 2001-7, (NASA/CR-2001-210853), April 30, 2001, 20 pages. Submitted to the Fourth International Air Traffic Management R&D Seminar ATM-2001.

This paper presents an algorithm for detection and resolution of air traffic conflicts in a 3-dimensional (3-D) airspace for two aircraft, namely ownship and intruder. A conflict is a projected incursion of the intruder aircraft within the protected zone of the ownship. A solution is a single maneuver, to be performed by the ownship, that effectively keeps the required minimum separation without cooperation of the intruder aircraft. The input to the algorithm is the state information, i.e., horizontal position, altitude, ground track, and vertical and ground speed, of both aircraft. The algorithm outputs a set of solutions. Each solution modifies only one state parameter of the ownship: ground track, ground speed, or vertical speed. The proposed algorithm is suitable for formal verification.

Luo, Li-Shi: *Theory of the lattice Boltzmann method: Lattice Boltzmann models for non-ideal gases.* ICASE Report No. 2001-8, (NASA/CR-2001-210858), April 30, 2001, 31 pages. Physical Review E, 62 (2000), pp. 4982–4996.

In this paper a procedure for systematic *a priori* derivation of the lattice Boltzmann models for non-ideal gases from the Enskog equation (the modified Boltzmann equation for dense gases) is presented. This treatment provides a unified theory of lattice Boltzmann models for non-ideal gases. The lattice Boltzmann equation is systematically obtained by discretizing the Enskog equation in phase space and time. The lattice Boltzmann model derived in this paper is thermodynamically consistent up to the order of discretization error. Existing lattice Boltzmann models for non-ideal gases are analyzed and compared in detail. Evaluation of these models are made in light of the general procedure to construct the lattice Boltzmann model for non-ideal gases presented in this work.

Ounaies, Z., K. Mossi, R. Smith, and J. Bernd: *Low-field and high-field characterization of THUNDER actuators.* ICASE Report No. 2001-9, (NASA/CR-2001-210859), May 9, 2001, 15 pages. To be submitted to SPIE Proceedings.

THUNDER (THin UNimorph DrivER) actuators are pre-stressed piezoelectric devices developed at NASA Langley Research Center (LaRC) that exhibit enhanced strain capabilities. As a result, they are of interest in a variety of aerospace applications. Characterization of 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 International Co. with a stainless steel substrate varying in thickness from 1 mil to 20 mils. The various devices were evaluated to determine low-field and high-field displacement as well as the polarization hysteresis loops. 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 25C to 200C while the displacement was being measured. Second, the samples were isothermally aged at 0C, 50C, 100C, and 150C in air, and the isothermal decay of the displacement was measured at room temperature as a function of time.

He, Guowei, R. Rubinstein, and Lian-Ping Wang: *Effects of eddy viscosity on time correlations in large eddy simulation.* ICASE Report No. 2001-10, (NASA/CR-2001-210860), May 3, 2001, 13 pages. To be submitted to Physics of Fluids.

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 paper 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.

Shu, Chi-Wang: *High order finite difference and finite volume WENO schemes and discontinuous Galerkin methods for CFD.* ICASE Report No. 2001-11, (NASA/CR-2001-210865), May 16, 2001, 21 pages. Submitted to the International Journal of Computational Fluid Dynamics.

In recent years high order numerical methods have been widely used in computational fluid dynamics (CFD), to effectively resolve complex flow features using meshes which are reasonable for today's computers. In this paper we review and compare three types of high order methods being used in CFD, namely the weighted essentially non-oscillatory (WENO) finite difference methods, the WENO finite volume methods, and the discontinuous Galerkin (DG) finite element methods. We summarize the main features of these methods, from a practical user's point of view, indicate their applicability and relative strength, and show a few selected numerical examples to demonstrate their performance on illustrative model CFD problems.

Mavriplis, Dimitri J.: *An assessment of linear versus non-linear multigrid methods for unstructured mesh solvers.* ICASE Report No. 2001-12, (NASA/CR-2001-210870), May 16, 2001, 26 pages. Submitted to the Journal of Computational Physics.

The relative performance of a non-linear FAS multigrid algorithm and an equivalent linear multigrid algorithm for solving two different non-linear problems is investigated. The first case consists of a transient radiation-diffusion problem for which an exact linearization is available, while the second problem involves the solution of the steady-state Navier-Stokes equations, where a first-order discrete Jacobian is employed as an approximation to the Jacobian of a second-order accurate discretization. When an exact linearization is employed, the linear and non-linear multigrid methods converge at identical rates, asymptotically, and the linear method is found to be more efficient due to its lower cost per cycle. When an approximate linearization is employed, as in the Navier-Stokes cases, the relative efficiency of the linear approach versus the non-linear approach depends both on the degree to which the linear system approximates the full Jacobian as well as the relative cost of linear versus non-linear multigrid cycles. For cases where convergence is limited by

a poor Jacobian approximation, substantial speedup can be obtained using either multigrid method as a preconditioner to a Newton-Krylov method.

Montero, Ruben S., Ignacio M. Llorente, and Manuel D. Salas: *Semicoarsening and implicit smoothers for the simulation of a flat plate at yaw.* ICASE Report No. 2001-13, (NASA/CR-2001-210871), May 16, 2001, 22 pages. To be submitted to the Journal of Computers and Fluids.

This paper presents a full multigrid solver for the simulation of flow over a yawed flat plate. The two problems associated with this simulation; boundary layers and entering flows with non-aligned characteristics, have been successfully overcome through the combination of a plane-implicit solver and semicoarsening. In fact, this multigrid algorithm exhibits a textbook multigrid convergence rate, i.e., the solution of the discrete system of equations is obtained in a fixed amount of computational work, independently of the grid size, grid stretching factor and non-alignment parameter. Also, a parallel variant of the smoother based on a four-color ordering of planes is investigated.

Ryaben'kii, V.S., S.V. Tsynkov, and V.I. Turchaninov: *Global discrete artificial boundary conditions for time-dependent wave propagation.* ICASE Report No. 2001-14, (NASA/CR-2001-210872), May 31, 2001, 40 pages. To be submitted to the Journal of Computational Physics.

We construct global artificial boundary conditions (ABCs) for the numerical simulation of wave processes on unbounded domains using a special non-deteriorating algorithm that has been developed previously for the long-term computation of wave-radiation solutions. The ABCs are obtained directly for the discrete formulation of the problem; in so doing, neither a rational approximation of "non-reflecting kernels," nor discretization of the continuous boundary conditions is required. The extent of temporal nonlocality of the new ABCs appears fixed and limited; in addition, the ABCs can handle artificial boundaries of irregular shape on regular grids with no fitting/adaptation needed and no accuracy loss induced.

The non-deteriorating algorithm, which is the core of the new ABCs, is inherently three-dimensional, it guarantees temporally uniform grid convergence of the solution driven by a continuously operating source on arbitrarily long time intervals, and provides unimprovable linear computational complexity with respect to the grid dimension. The algorithm is based on the presence of lacunae, i.e., aft fronts of the waves, in wave-type solutions in odd-dimension spaces. It can, in fact, be built as a modification on top of any consistent and stable finite-difference scheme, making its grid convergence uniform in time and at the same time keeping the rate of convergence the same as that of the non-modified scheme.

In the paper, we delineate the construction of the global lacunae-based ABCs in the framework of a discretized wave equation. The ABCs are obtained for the most general formulation of the problem that involves radiation of waves by moving sources (e.g., radiation of acoustic waves by a maneuvering aircraft). We also present systematic numerical results that corroborate the theoretical design properties of the ABCs' algorithm.

Eidson, Thomas M.: *A component-based programming model for composite, distributed applications.* ICASE Report No. 2001-15, (NASA/CR-2001-210873), May 31, 2001, 18 pages. Submitted to the Second International Workshop on Grid Computing.

The nature of scientific programming is evolving to larger, composite applications that are composed of smaller element applications. These composite applications are more frequently being targeted for distributed, heterogeneous networks of computers. They are most likely programmed by a group of developers.

Software component technology and computational frameworks are being proposed and developed to meet the programming requirements of these new applications. Historically, programming systems have had a hard time being accepted by the scientific programming community. In this paper, a programming model is outlined that attempts to organize the software component concepts and fundamental programming entities into programming abstractions that will be better understood by the application developers. The programming model is designed to support computational frameworks that manage many of the tedious programming details, but also that allow sufficient programmer control to design an accurate, high-performance application.

Harik, Vasyl Michael: *Ranges of applicability for the continuum-beam model in the constitutive analysis of carbon nanotubes: Nanotubes or nano-beams?* ICASE Report No. 2001-16, (NASA/CR-2001-211013), June 20, 2001, 25 pages. To appear in Computational Materials Science.

Ranges of validity for the continuum-beam model, the length-scale effects and continuum assumptions are analyzed in the framework of scaling analysis of NT structure. Two coupled criteria for the applicability of the continuum model are presented. Scaling analysis of NT buckling and geometric parameters (e.g., diameter and length) is carried out to determine the key non-dimensional parameters that control the buckling strains and modes of NT buckling. A model applicability map, which represents two classes of NTs, is constructed in the space of non-dimensional parameters. In an analogy with continuum mechanics, a mechanical law of geometric similitude is presented for two classes of beam-like NTs having different geometries. Expressions for the critical buckling loads and strains are tailored for the distinct groups of NTs and compared with the data provided by the molecular dynamics simulations. Implications for molecular dynamics simulations and the NT-based scanning probes are discussed.

Paik, Sun M., Sung M. Yoo, Min Namkung, and Russell A. Wincheski: *Thermodynamic behavior of nano-sized gold clusters on the (001) surface.* ICASE Report No. 2001-17, (NASA/CR-2001-211014), June 20, 2001, 10 pages. Presented at the ICCN 2001 Conference.

We have studied thermal expansion of the surface layers of the hexagonally reconstructed Au (001) surface using a classical Molecular Dynamics (MD) simulation technique with an Embedded Atomic Method (EAM) type many-body potential. We find that the top-most hexagonal layer contracts as temperature increases, whereas the second layer expands or contracts depending on the system size. The magnitude of expansion coefficient of the top layer is much larger than that of the other layers. The calculated thermal expansion coefficients of the top-most layer are about $-4.93 \times 10^{-5} \mathring{A}/K$ for the $(262 \times 227)\mathring{A}$ cluster and $-3.05 \times 10^{-5}\mathring{A}/K$ for $(101 \times 87)\mathring{A}$ cluster. The Fast Fourier Transform (FFT) image of the atomic density shows that there exists a rotated domain of the top-most hexagonal cluster with rotation angle close to 1 degree at temperature $T < 1000K$. As the temperature increases this domain undergoes a surface orientational phase transition. These predictions are in good agreement with previous phenomenological theories and experimental studies.

Huyse, Luc: *Free-form airfoil shape optimization under uncertainty using maximum expected value and second-order second-moment strategies.* ICASE Report No. 2001-18, (NASA/CR-2001-211020), June 20, 2001, 29 pages. To be submitted to the AIAA Journal.

Free-form shape optimization of airfoils poses unexpected difficulties. Practical experience has indicated that a deterministic optimization for discrete operating conditions can result in dramatically inferior performance when the actual operating conditions are different from the - somewhat arbitrary - design values used for the optimization. Extensions to multi-point optimization have proven unable to adequately remedy this problem of "localized optimization" near the sampled operating conditions. This paper presents an intrinsically statistical approach and demonstrates how the shortcomings of multi-point optimization with respect to "localized optimization" can be overcome. The practical examples also reveal how the relative likelihood of each of the operating conditions is automatically taken into consideration during the optimization process. This is a key advantage over the use of multipoint methods.

Hart, Roger C., R. Jeffrey Balla, G.C. Herring, and Luther N. Jenkins: *Seedless laser velocimetry using heterodyne laser-induced thermal acoustics.* ICASE Report No. 2001-19, (NASA/CR-2001-211021), August 28, 2001, 18 pages. To be submitted to the 19th International Conference on Instrumentation in Aerospace Simulation Facilities.

A need exists for a seedless equivalent of laser Doppler velocimetry (LDV) for use in low-turbulence or supersonic flows or elsewhere where seeding is undesirable or impractical. A compact laser velocimeter using heterodyne non-resonant laser-induced thermal acoustics (LITA) to measure a single component of velocity is described. Neither molecular (e.g. NO2) nor particulate seed is added to the flow. In non-resonant LITA two beams split from a short-pulse pump laser are crossed; interference produces two counterpropagating sound waves by electrostriction. A CW probe laser incident on the sound waves at the proper angle is diffracted towards a detector. Measurement of the beating between the Doppler-shifted light and a highly attenuated portion of the probe beam allows determination of one component of flow velocity, speed of sound, and temperature. The sound waves essentially take the place of the particulate seed used in LDV. The velocimeter was used to study the flow behind a rearward-facing step in NASA Langley Research Center's Basic Aerodynamics Research Tunnel. Comparison is made with pitot-static probe data in the freestream over the range 0 m/s-55 m/s. Comparison with LDV is made in the recirculation region behind the step and in a well-developed boundary layer in front of the step. Good agreement is found in all cases.

Yan, Jue, and Chi-Wang Shu: *A local discontinuous Galerkin method for KdV-type equations.* ICASE Report No. 2001-20, (NASA/CR-2001-211026), June 29, 2001, 28 pages. Submitted to the SIAM Journal on Numerical Analysis.

In this paper we develop a local discontinuous Galerkin method for solving KdV type equations containing third derivative terms in one and two space dimensions. The method is based on the framework of the discontinuous Galerkin method for conservation laws and the local discontinuous Galerkin method for viscous equations containing second derivatives, however the guiding principle for inter-cell fluxes and nonlinear stability is new. We prove L^2 stability and a cell entropy inequality for the square entropy for a class of nonlinear PDEs of this type both in one and multiple spatial dimensions, and give an error estimate for the linear cases in the one dimensional case. The stability result holds in the limit case when the coefficients to the third derivative terms vanish, hence the method is especially suitable for problems which are "convection

dominate", i.e. those with small second and third derivative terms. Numerical examples are shown to illustrate the capability of this method. The method has the usual advantage of local discontinuous Galerkin methods, namely it is extremely local and hence efficient for parallel implementations and easy for *h-p* adaptivity.

Fibich, G., B. Ilan, and S. Tsynkov: *Computation of nonlinear backscattering using a high-order numerical method.* ICASE Report No. 2001-21, (NASA/CR-2001-211036), August 8, 2001, 15 pages. To be submitted to the Journal of Scientific Computing.

The nonlinear Schrödinger equation (NLS) is the standard model for propagation of intense laser beams in Kerr media. The NLS is derived from the nonlinear Helmholtz equation (NLH) by employing the paraxial approximation and neglecting the backscattered waves. In this study we use a fourth-order finite-difference method supplemented by special two-way artificial boundary conditions (ABCs) to solve the NLH as a boundary value problem. Our numerical methodology allows for a direct comparison of the NLH and NLS models and for an accurate quantitative assessment of the backscattered signal.

Li, Wu, Luc Huyse, and Sharon Padula: *Robust airfoil optimization to achieve consistent drag reduction over a Mach number.* ICASE Report No. 2001-22, (NASA/CR-2001-211042), August 20, 2001, 25 pages. To be submitted to Structural Optimization.

We prove mathematically that in order to avoid point-optimization at the sampled design points for multipoint airfoil optimization, the number of design points must be greater than the number of free-design variables. To overcome point-optimization at the sampled design points, a robust airfoil optimization method (called the profile optimization method) is developed and analyzed. This optimization method aims at a consistent drag reduction over a given Mach range and has three advantages: (a) it prevents severe degradation in the off-design performance by using a smart descent direction in each optimization iteration, (b) there is no random airfoil shape distortion for any iterate it generates, and (c) it allows a designer to make a trade-off between a truly optimized airfoil and the amount of computing time consumed. For illustration purposes, we use the profile optimization method to solve a lift-constrained drag minimization problem for 2-D airfoil in Euler flow with 20 free-design variables. A comparison with other airfoil optimization methods is also included.

Tsynkov, S.V.: *On the definition of surface potentials for finite-difference operators.* ICASE Report No. 2001-23, (NASA/CR-2001-211059), September 17, 2001, 29 pages. To be submitted to the Journal of Scientific Computing.

For a class of linear constant-coefficient finite-difference operators of the second order, we introduce the concepts similar to those of conventional single- and double-layer potentials for differential operators. The discrete potentials are defined completely independently of any notion related to the approximation of the continuous potentials on the grid. We rather use an approach based on differentiating, and then inverting the differentiation of, a function with surface discontinuity of a particular kind, which is the most general way of introducing surface potentials in the theory of distributions. The resulting finite-difference "surface" potentials appear to be solutions of the corresponding system of linear algebraic equations driven by special source terms. The properties of the discrete potentials in many respects resemble those of the corresponding continuous potentials. Primarily, this pertains to the possibility of representing a given solution to the

homogeneous equation on the domain as a variety of surface potentials with the density defined on the domain's boundary. At the same time, the discrete surface potentials can be interpreted as one specific realization of the generalized potentials of Calderon's type, and consequently, their approximation properties can be studied independently in the framework of the difference potentials method by Ryaben'kii. The motivation for introducing and analyzing the discrete surface potentials was provided by the problems of active shielding and control of sound, in which the aforementioned source terms that drive the potentials are interpreted as the acoustic control sources that cancel out the unwanted noise on a predetermined region of interest.

Rubinstein, Robert, and Ye Zhou: *Schiestel's derivation of the epsilon equation and two equation modeling of rotating turbulence.* ICASE Report No. 2001-24, (NASA/CR-2001-211060), September 17, 2001, 11 pages. To appear in Computers and Mathematics with Applications.

As part of a more general program of developing multiple-scale models of turbulence, Schiestel suggested a derivation of the homogeneous part of the dissipation rate transport equation. Schiestel's approach is generalized to rotating turbulence. The resulting model reproduces the main features observed in decaying rotating turbulence.

Wieman, Robert, Ralph C. Smith, Tyson Kackley, Zoubeida Ounaies, and Jeff Bernd: *Displacement models for THUNDER actuators having general loads and boundary conditions.* ICASE Report No. 2001-25, (NASA/CR-2001-211061), September 17, 2001, 17 pages. To appear in the Proceedings of the SPIE, Smart Structures and Materials, Newport Beach, CA, 2001.

This paper summarizes techniques for quantifying the displacements generated in THUNDER actuators in response to applied voltages for a variety of boundary conditions and exogenous loads. The PDE models for the actuators are constructed in two steps. In the first, previously developed theory quantifying thermal and electrostatic strains is employed to model the actuator shapes which result from the manufacturing process and subsequent repoling. Newtonian principles are then employed to develop PDE models which quantify displacements in the actuator due to voltage inputs to the piezoceramic patch. For this analysis, drive levels are assumed to be moderate so that linear piezoelectric relations can be employed. Finite element methods for discretizing the models are developed and the performance of the discretized models are illustrated through comparison with experimental data.

Smith, Ralph C., Zoubeida Ounaies, and Robert Wieman: *A model for rate-dependent hysteresis in piezoceramic materials operating at low frequencies.* ICASE Report No. 2001-26, (NASA/CR-2001-211062), September 17, 2001, 15 pages. Proceedings of the SPIE, Smart Structures and Materials 2000, Newport Beach, CA, Vol. 3992, pp. 128-136, 2000.

This paper addresses the modeling of certain rate-dependent mechanisms which contribute to hysteresis inherent to piezoelectric materials operating at low frequencies. While quasistatic models are suitable for initial material characterization in some applications, the reduction in coercive field and polarization values which occur as frequencies increase must be accommodated to achieve the full capabilities of the materials. The model employed here quantifies the hysteresis in two steps. In the first, anhysteretic polarization switching is modeled through the application of Boltzmann principles to balance the electrostatic and thermal energy. Hysteresis is then incorporated through the quantification of energy required to translate and bend

domain walls pinned at inclusions inherent to the materials. The performance of the model is illustrated through a fit to low frequency data (0.1 Hz - 1 Hz) from a PZT5A wafer.

Jaunky, Navin, Damodar R. Ambur, Carlos G. Davila, and Mark Hilburger: *Progressive failure studies of composite panels with and without cutouts.* ICASE Report No. 2001-27, (NASA/CR-2001-211223), September 26, 2001, 27 pages. To be submitted to Composite Structures.

Progressive failure analyses results are presented for composite panels with and without a cutout and subjected to in-plane shear loading and compression loading well into their postbuckling regime. Ply damage modes such as matrix cracking, fiber-matrix shear, and fiber failure are modeled by degrading the material properties. Results from finite element analyses are compared with experimental data. Good agreement between experimental data and numerical results are observed for most structural configurations when initial geometric imperfections are appropriately modeled.

Jordan, T.L., and Z. Ounaies: *Piezoelectric ceramics characterization.* ICASE Report No. 2001-28, (NASA/CR-2001-211225), September 26, 2001, 27 pages. To appear in the Encyclopedia of Smart Materials, John Wiley.

This review explores piezoelectric ceramics analysis and characterization. The focus is on polycrystalline ceramics; therefore, single crystals, polymeric materials and organic/inorganic composites are outside the scope of this review. To thoroughly grasp the behavior of a piezoelectric polycrystalline ceramic, a basic understanding of the ceramic itself should not be overlooked. To this end, we have presented a brief introduction of the history of piezoelectricity and a discussion on processing of the ceramic and development of the constitutive relations that define the behavior of a piezoelectric material. We have attempted to cover the most common measurement methods as well as introduce parameters of interest. Excellent sources for more in-depth coverage of specific topics can be found in the bibliography. In most cases, we refer to lead zirconate titanate (PZT) to illustrate some of the concepts since it is the most widely used and studied piezoelectric ceramic to date.

INTERIM REPORTS

Eidson, Thomas M., and Merrell L. Patrick: *ICASE Workshop on Programming Computational Grids.* ICASE Interim Report No. 38, (NASA/CR-2001211224), October 15, 2001, 21 pages.

A workshop on Programming Computational Grids for distributed applications was held on April 12-13, 2001 at ICASE, NASA Langley Research Center. The stated objective of the workshop was to define, discuss, and clarify issues critical to the advancement of Problem Solving Environments/Computational Frameworks for solving large multi-scale, multi-component scientific applications using distributed, heterogeneous computing systems. This report documents a set of recommendations for NASA that suggest an approach for developing an application development environment that will meet future application needs.

OTHER REPORTS

Bodeveix, J.-P., M. Filali, and C. Muñoz, "Formalisation de la me'thode B en Coq et PVS," Technique et Science Informatique, 20, No. 7 (2001), pp. 901–926.

Brandt, A., B. Diskin, and J.L. Thomas, "Textbook multigrid efficiency for computational fluid dynamics simulations," AIAA Paper 2001-2570, invited paper for the 15th AIAA CFD Conference, Anaheim, CA, June 2001.

Diskin, B., and J.L. Thomas, "Distributed relaxation for conservative discretizations," AIAA Paper 2001-2571, Proceedings of the 15th AIAA CFD Conference, Anaheim, CA, June 2001.

Harik, V.M., "Optimization of structural designs for a safe failure pattern: Layered material systems," Materials and Design, 22, No. 4 (June 2001), pp. 317–324.

Harik, V.M., "Ranges of applicability for the continuum beam model in the mechanics of carbon nanotubes and nanorods," to appear in Solid State Communications (International Journal).

Harik, V.M., T.S. Gates, and M.P. Nemeth, "Limitations of the thin shell and beam models for carbon nanotubes," 2001 Mechanics and Materials Summer Conference, June 27–29, San Diego, CA, p. 131, 2001.

Harik, V.M., and J. Lambros, "The net-shape forming of composite micro-rods: Effects of the fiber-matrix interphase," Proceedings of the 16th Technical Conference on American Society for Composites, ASC CD, September 9–12, Blacksburg, VA, pp. 1–12, 2001.

Krueger, R., I.L. Paris, T.K. O'Brien, and P.J. Minguet, "Fatigue life methodology for bonded composite skin-stringer configurations," NASA/TM-2001-210842, ARL-TR-2432, April 2001.

Muñoz, C., R.W. Butler, V. Carreno, and G. Dowek, "On the verification of conflict detection algorithms," NASA/TM-2001-210864, May 2001.

O'Brien, T.K., A.D. Chawan, R. Krueger, and I.L. Paris, "Transverse tension fatigue life characterization through flexure testing of composite materials," NASA/TM-2001-211035, ARL-TR-2544, July 2001.

Odegard, G.M., V.M. Harik, K.E. Wise, and T.S. Gates, "Constitutive modeling of nanotube-reinforced polymer composite systems," NASA/TM-2001-211044, August 2001.

Shin, J.Y., "Blending approach of linear parameter varying control synthesis for F-16 aircraft," AIAA Guidance, Navigation, and Control Conference, August 6, 2001.

PATENTS

Kim, Jachwan, "Electro-active paper actuator," Disclosure of Invention and New Technology filed August 24, 2001.

ICASE COLLOQUIA

Name/Affiliation/Title	Date

Chenghai Sun, Indiana University-Purdue University
  "Adaptive Lattice Boltzmann Model for Compressible Flows and Parallel
  Computation"
	April 6

David Miller, Massachusetts Institute of Technology
  ICASE Series on Risk-based Design:"Uncertainty Analysis and Reliability
  Optimization for Space Systems"
	April 11

Steve Parker, University of Utah
  ICASE Series on Modern Programming Practices:"Achieving Scalability and
  Integration with the Uintah Problem Solving Environment"
	April 11

Dana Knoll, Los Alamos National Laboratory "Recent Progress in Preconditioning Jacobian-free Newton-Krylov Methods"	April 18
Laurie Williams, North Carolina State University ICASE Series on Modern Programming Practices:"Pair Programming"	May 1

Roger Hart, ICASE
  "Practical Seedless Laser Velocimetry using Heterodyne Laser-induced Thermal
  Acoustics (LITA)"
	May 3

Dimitri Mavris, Georgia Institute of Technology
  ICASE Series on Risk-based Design:"Probabilistic Approaches to Designing
  Affordable Aerospace Systems with New Technologies"
	May 3

Robert Dudley, University of Texas at Austin
  ICASE Series on Morphing:"Mechanisms of Animal Flight Maneuverability:
  Hummingbirds as Case Example"
	May 7

Wei Chen, University of Illinois at Chicago
  ICASE Series on Risk-based Design:"Efficient Methods for Robustness and
  Reliability Assessments in Engineering Design"
	May 9

Stephen Morris, MLB Company, Palo Alto, CA
  ICASE Series on Morphing:"Micro Air Vehicle Design Optimization and Flight
  Test Results"
	May 23

Name/Affiliation/Title	Date
Sutanu Sarkar, University of California, San Diego "Turbulent Jets and Shear Layers: Large Eddy Simulation and Direct Numerical Simulation"	May 24
Hamid Garmestani, FAMU-FSU College of Engineering "Advanced Processing and Micro-chbaracterization Techniques for the Production of Highly Textured Nano-powdered Magnetic Materials"	May 31
Rina Tannenbaum, Georgia Institute of Technology "Segregation of Metal Nanoclusters by Self-assembly in Block Copolymers"	May 31
James Quirk, Los Alamos National Laboratory ICASE Series on Modern Programming Practices:"Literate Programming for Scientific Computing"	June 1
Zhenan Bao, Bell Laboratories, Lucent Technologies "Self-assembled Materials and Low Cost Patterning Methods for Device Applications"	June 5
Narasimhan Sundararajan, Nanyang Technological University, Singapore "Minimal Resource Allocation Network (MRAN) — A New Minimal Radial Basis Function Network and Its Applications"	June 7
Narasimhan Sundararajan, Nanyang Technological University, Singapore "ATM Traffic Congestion Control Using MRAN Neural Networks"	June 8
Narasimhan Sundararajan, Nanyang Technological University, Singapore "Adaptive Flight Controller Design Using RBF Neural Networks"	June 8
Alyson Wilson, Los Alamos National Laboratory ICASE Series on Risk-based Design:"Information Integration Technology"	June 15
Siva Parameswaran, Texas Tech University "Turbulence Models that Work for Unsteady Buoyant Flows"	June 18
Kab-Seok Kang, Korea Advanced Institute of Science and Technology "Multigrid and the Covolume Method"	June 20
Ken Auer, RoleModel Software, Inc. ICASE Series on Modern Programming Practices:"Keeping Software Soft"	June 25

Name/Affiliation/Title	Date
Antony Jameson, Stanford University "How Many Steps are Required to Solve the Euler Equations of Steady Flow: A Query"	June 25
George Karniadakis, Brown University "Modeling Uncertainty in CFD via Polynomial Chaos"	June 25
Robert Martin, Object Mentor, Inc. ICASE Series on Modern Programming Practices:"Extreme Programming: Test First Design"	June 26
Kenneth Dial, The University of Montana ICASE Series on Morphing:"Birds Morphing: Escaping the U-shaped Power Curve and Performing Extraordinary Maneuverability"	June 29
Peyman Givi, University at Buffalo, SUNY "Velocity Filtered Density Function for Subgrid Scale Modeling of Turbulent Flows"	July 10
Ignacio Llorente, Universidad Complutense, Spain "Parallel and Robust Multigrid Techniques on Structured Grids"	July 13
David Keyes, Old Dominion University and ICASE "Terascale Optimal PDE Simulations — A Project Briefing"	July 23
Keith Bolte, Mallett Technology, Inc. "ANSYS: Modeling for Multiphysics Applications"	August 3
Roger Simpson, Virginia Polytechnic Institute and State University ICASE Series on Risk-based Design:"Some Flows for Which We Need Complete Experimental Data Sets"	August 6
Roy Kornbluh, SRI International ICASE Series on Morphing:"Dielectric Elastomer Actuators: Muscles that Morph"	August 7
Roger Simpson, Virginia Polytechnic Institute and State University ICASE Series on Risk-based Design:"Measurements that are Needed for Improved Turbulence Modeling"	August 7
Darrell Reneker, The University of Akron "Polymer Nanofibers"	August 8

Name/Affiliation/Title	Date
Michael Heath, University of Illinois at Urbana-Champaign "Integrated Simulation of Multicomponent Systems"	August 10

Bob Jacobsen, Lawrence Berkeley National Laboratory
  ICASE Series on Modern Programming Practices:"Programming in the
  Large: Experiences in Computing for High Energy Physics"
	August 13

Ching Loh, Taitech Inc./NASA Glenn Research Center "Applied Computational Aeroacoustics by the CE/SE Method"	August 14

Kun Xu, The Hong Kong University of Science and Technology
  "Gas-kinetic Schemes for Compressible Navier-Stokes Equations and
  Physical Analysis of the Godunov Method"
	August 15

Joachim Hochwarth, University of Minnesota "Comprehensive Dynamic Air Traffic System Simulation"	August 17
Frederica Darema, National Science Foundation "Symbiotic Measurement & Simulation Application Systems"	August 20
Frank Harris, The University of Akron "Nylon 6/Polyimide Nanocomposites"	August 21
Ali Beskok, Texas A&M University "Physical Challenges and Numerical Simulation of Microfluidic Transport"	August 22
Diann Brei, University of Michigan, Ann Arbor ICASE Series on Morphing:"Smart Material Actuation Systems"	August 27

Arno Ronzheimer, German Aerospace Center
  "Post-parameterization of Aircraft Geometry Using Free Form
  Deformation in Combination with Structured Grid Generation Methods"
	August 30

Cynthia DeBisschop, Old Dominion University "Mathematical Modeling of Frontal Polymerization"	September 5
Robert Walters, Virginia Polytechnic Institute & State University "Stochastic Methods for Fluid Mechanics — An Introduction"	September 12
Phil Hall, Imperial College, United Kingdom "Transition in Stokmes Layers and Other Unsteady "Boundary Layers"	September 17

Name/Affiliation/Title	Date
George Haller, Brown University "Lagrangian Coherent Structures and Their Control"	September 17
Robert Walters, Virginia Polytechnic Institute & State University "Stochastic Methods for Fluid Mechanics — An Introduction"	September 20
David Thomas, The Pragmatic Programmers, LLC ICASE Series on Modern Programming Practices:"Advances in Scripting"	September 21
Alan Morris, Cranfield University, United Kingdom Distributed MDO: The Way of the Future"	September 24

Satish Kumar, Georgia Institute of Technology
  "Films, Fibers, and Coatings from Carbon Nano Tubes, Nano Fibers, and Their
  Composites with Polymers"
	September 25

ICASE SUMMER ACTIVITIES

VISITOR and AREA OF RESEARCH	AFFILIATION	DATE OF VISIT
Abarbanel, Saul *Applied & Numerical Math*	Tel Aviv University, Israel	6/18 – 8/10
Avihar, Edan *Fluid Mechanics*	Tel Aviv University, Israel	7/30 – 9/14
Bai, Dov *Applied & Numerical Math*	Wright Patterson Air Force Base	6/19 – 6/26
Beskok, Ali *Fluid Mechanics*	Texas A&M University	8/20 – 8/24
Bijl, Hester *Applied & Numerical Math*	Delft University of Technology, The Netherlands	7/23 – 8/24
Bodas-Salcedo, Alejandro *Atmospheric Sciences*	University of Valencia, Spain	9/01 – 11/30
Bogacki, Przemyslaw *Applied & Numerical Math*	Old Dominion University	6/25 – 6/29
Brandt, Achi *Applied & Numerical Math*	The Weizmann Institute of Science, Israel	6/18 – 6/29 9/23 – 10/05
Camanho, Pedro *Structures and Materials*	University of Portugal	9/10 – 9/28
Cao, Yanzhao *Applied & Numerical Math*	Florida A&M University	6/18 – 6/21
Chen, Yu *Computer Science*	The University of Tokyo, Japan	8/06 – 8/17
Criminale, William *Fluid Mechanics*	University of Washington, Seattle	6/05 – 6/23

VISITOR and AREA OF RESEARCH	AFFILIATION	DATE OF VISIT
Day, Nancy *Computer Science*	University of Waterloo, Canada	7/16 – 7/20
Dinar, Nathan *Applied & Numerical Math*	The Weizmann Institute of Science, Israel	6/18 – 6/28
Filliatre, Jean-Christophe *Computer Science*	Universite Paris Sud, France	8/12 – 8/25
Fleuriot, Jacques *Computer Science*	University of Edinburgh, Scotland	7/09 – 8/03
Gottlieb, David *Applied & Numerical Math*	Brown University	7/09 – 7/11 8/20 – 8/22
Hafez, Mohamed *Applied & Numerical Math*	University of California, Davis	8/06 – 8/10
Hall, Philip *Fluid Mechanics*	Imperial College, England	9/10 – 9/21
Hardin, Therese *Computer Science*	Universite Paris VI, France	10/22 – 11/02
Hesthaven, Jan *Applied & Numerical Math*	Brown University	5/21 – 5/25
Hussaini, M. Yousuff *Applied & Numerical Math*	Florida State University	6/18 – 6/21
Inoue, Yasuhiro *Computer Science*	The University of Tokyo, Japan	8/06 – 8/17
Jameson, Antony *Applied & Numerical Math*	Stanford University	6/18 – 6/29
Jeong, Eunhwan *Fluid Mechanics*	Texas A&M University	6/18 – 7/27

VISITOR and AREA OF RESEARCH	AFFILIATION	DATE OF VISIT
Jothiprasad, Giridhar *Applied & Numerical Math*	Cornell University	5/21 – 6/20 7/20 – 8/24
Kaiser, Andreas *Computer Science*	Wilhelm Schickard Institute for Computer Science, Germany	8/13 – 8/24
Kalvala, Sara *Computer Science*	University of Warwick, England	9/10 – 10/16
Kesner, Delia *Computer Science*	Universite Paris Sud, France	8/20 – 8/31
Kim, Jaehwan *Structures and Materials*	Inha University, Korea	6/20 – 8/28
Kirchner, Florent *Computer Science*	Ecole Nationale de l'Aviation Civile, France	7/23 – 8/17
Krafczyk, Manfred *Fluid Mechanics*	Technical University Munchen, Germany	6/11 – 6/18
Ladd, Anthony *Applied & Numerical Math*	University of Florida, Gainesville	8/06 – 8/10
Lallemand, Pierre *Computer Science*	Universita Paris Sud, France	6/04 – 6/22
Lewis, Michael *Applied & Numerical Math*	The College of William & Mary	5/16 – 8/24
Li, Wu *Applied & Numerical Math*	Old Dominion University	5/06 – 5/31 6/10 – 6/14 7/22 – 7/26 8/12 – 8/16
Lindner, Douglas *Structures and Materials*	Virginia Polytechnic Institute & State University	5/21 – 6/01
Llorente, Ignacio *Applied & Numerical Math*	Universidad Complutense, Spain	7/02 – 7/13

VISITOR and AREA OF RESEARCH	AFFILIATION	DATE OF VISIT
Loh, Ken *Fluid Mechanics*	NASA Glenn Research Center	8/13 – 8/17
Luettgen, Gerald *Computer Science*	The University of Sheffield, England	7/02 – 8/03 9/17 – 9/28
Mayero, Micaela *Computer Science*	INRIA - Rocquencourt, France	6/25 – 7/06
Milder, Seth *Computer Science*	George Mason University	5/14 – 5/18 8/06 – 8/31
Mizukaki, Toshiharu *Fluid Mechanics*	Tohoku University, Japan	4/24 – 7/24
Montero, Ruben *Applied & Numerical Math*	Universidad Complutense, Spain	7/02 – 7/27
Nordstrom, Jan *Applied & Numerical Math*	The Aeronautical Research Institute of Sweden	9/10 – 9/28
Parikh, Stavan *Computer Science*	University of Virginia	5/29 – 8/18
Prieto-Matias, Manuel *Applied & Numerical Math*	Universidad Complutense, Spain	7/02 – 7/27
Qi, Dewei *Fluid Mechanics*	Western Michigan University	5/07 – 5/18 6/04 – 6/18
Ronzheimer, Arno *Applied & Numerical Math*	German Aerospace Center	6/04 – 8/31
Ryaben'kii, Viktor *Applied & Numerical Math*	Russian Academy of Sciences	7/09 – 8/06
Ryan, Jennifer *Applied & Numerical Math*	Brown University	8/13 – 8/31

VISITOR and AREA OF RESEARCH	AFFILIATION	DATE OF VISIT
Seifert, Avi *Fluid Mechanics*	Tel Aviv University, Israel	6/13 – 6/21 7/02 – 8/31
Shu, Chi-Wang *Applied & Numerical Math*	Brown University	8/16 – 8/25
Sidilkover, David *Applied & Numerical Math*	Soreq Nuclear Research Center, Israel	9/17 – 10/12
Sinz, Carsten *Computer Science*	Wilhelm Schickard Institute for Computer Science, Germany	8/13 – 8/24
Smith, Natasha *Applied & Numerical Math*	Vanderbilt University	6/25 – 8/24
Tarafdar, Arijit *Computer Science*	Old Dominion University	6/08 – 8/24
Thatipelli, Shiva *Computer Science*	Old Dominion University	5/16 – 8/15
Tsynkov, Semyon *Applied & Numerical Math*	North Carolina State University and Tel Aviv University, Israel	5/14 – 6/08 7/09 – 8/03
Tufo, Henry *Fluid Mechanics*	University of Chicago	5/08 – 5/25
Turkel, Eli *Applied & Numerical Math*	Tel Aviv University, Israel	7/16 – 9/30
Walters, Robert *Applied & Numerical Math*	Virginia Polytechnic Institute & State University	5/14 – 8/17
Weaver, Paul *Structures and Materials*	University of Bristol, England	7/16 – 9/21
Wu, Xuesong *Fluid Mechanics*	Imperial College, England	3/12 – 4/04 9/01 – 9/28

VISITOR and AREA OF RESEARCH	AFFILIATION	DATE OF VISIT
Xu, Kun *Applied & Numerical Math*	The Hong Kong University of Science and Technology	8/06 – 8/24
Yom-Tov, Jonathan *Fluid Mechanics*	Tel Aviv University, Israel	7/30 – 8/31

OTHER ACTIVITIES

On April 24, 2001, ICASE and NASA Langley Research Center co-sponsored the Fourth Biennial Theodorsen Lectureship Award. Professor Robert W. MacCormack, Stanford University, was presented this award for his lifetime contributions in the field of aeronautical sciences and engineering. His award lecture entitled "Reflections on 30 Years in Computational Fluid Dynamics (CFD)" was presented at the Pearl Young Theater with over 100 in attendance.

ICASE STAFF

I. ADMINISTRATIVE

Manuel D. Salas, Director, M.S., Aeronautics and Astronautics, Polytechnic Institute of Brooklyn, 1970. Fluid Mechanics and Numerical Analysis.

Linda T. Johnson, Office and Financial Administrator

Barbara A. Cardasis, Administrative Secretary

Etta M. Morgan, Accounting Supervisor

Emily N. Todd, Conference Manager/Executive Assistant

Shannon K. Verstynen, Information Technologist

Gwendolyn W. Wesson, Contract Accounting Clerk

Shouben Zhou, Systems Manager

J. Ryan Cresawn, Systems Manager for Coral and the ICASE Computational Grid/Assistant Systems Manager (Through October 12, 2001)

II. SCIENCE COUNCIL

David Gottlieb, (Chair) Professor, Division of Applied Mathematics, Brown University.

Ilhan Aksay, Professor, Engineering Quad, Princeton University.

Lee Beach, Professor, Department of Physics, Computer Science & Engineering, Christopher Newport University.

Jack Dongarra, Distinguished Professor, Department of Computer Science, University of Tennessee.

Joseph E. Flaherty, Amos Eaton Professor, Departments of Computer Science and Mathematical Sciences, Rensselaer Polytechnic Institute.

Forrester Johnson, Aerodynamics Research, Boeing Commercial Airplane Group.

John C. Knight, Professor, Department of Computer Science, School of Engineering and Applied Science, University of Virginia.

Robert W. MacCormack, Professor, Department of Aeronautics and Astronautics, Stanford University.

Stanley G. Rubin, Professor, Department of Aerospace Engineering and Engineering Mechanics, University of Cincinnati.

Manuel D. Salas, Director, ICASE, NASA Langley Research Center.

III. RESEARCH FELLOWS

Dimitri Mavriplis - Ph.D., Mechanical and Aerospace Engineering, Princeton University, 1988. Applied & Numerical Mathematics [Grid Techniques for Computational Fluid Dynamics]. (February 1997 to August 2003)

Josip Lončarić - Ph.D., Applied Mathematics, Harvard University, 1985. Applied & Numerical Mathematics [Multidisciplinary Design Optimization]. (March 2001 to August 2002)

IV. SENIOR STAFF SCIENTISTS

Brian G. Allan - Ph.D., Mechanical Engineering, University of California at Berkeley, 1996. Applied & Numerical Mathematics [Multidisciplinary Design Optimization]. (February 1996 to November 2003)

Maria Consiglio - M.S., Computer Science, University of Illinois-Urbana, 1982. Computer Science [Crew Systems Research for Aviation Capacity and Safety]. (June 2001 to June 2003)

Thomas M. Eidson - Ph.D., Mechanical Engineering, University of Michigan, 1982. Computer Science [Distributed Computing]. (October 2000 to September 2003)

Alfons E. Geser - Ph.D., Computer Science, University of Passau, Germany, 1991. Computer Science [Formal Methods]. (January 2001 to December 2002)

Vasyl M. Harik - Ph.D., Mechanical Engineering, University of Delaware, 1997. Structures & Materials [Composites and Failure Mechanics]. (October 2000 to October 2002)

Roger C. Hart - Ph.D., Physics, University of Tennessee, 1991. Fluid Mechanics [Measurement Science and Technology]. (December 1998 to October 2001)

Guowei He - Ph.D., Theoretical and Applied Mechanics, Northwestern Polytechnic University, Xian, China, 1991. Fluid Mechanics [Turbulence Modeling and Direct Numerical Simulation]. (July 2000 to June 2003)

Navin Jaunky - Ph.D., Mechanical Engineering, Old Dominion University, 1995. Structures & Materials [Composite Structural Damage Tolerance and Residual Strength Methodologies]. (January 2001 to December 2002)

Li-Shi Luo - Ph.D., Physics, Georgia Institute of Technology, 1993. Computer Science [Parallel Algorithms]. (November 1996 to August 2002)

Zoubeida Ounaies - Ph.D., Engineering Science and Mechanics, The Pennsylvania State University, 1995. Structures & Materials [Characterization of Advanced Piezoelectric Materials]. (March 1999 to November 2002)

Alexander Povitsky - Ph.D., Mechanical Engineering, Moscow Institute of Steel and Alloys Technology (MISA), Russia, 1988. Computer Science [Parallelization and Formulation of Higher Order Schemes for Aeroacoustics Noise Propagation]. (October 1997 to December 2001)

74

V. SCIENTIFIC STAFF

Scott C. Beeler - Ph.D., Applied Mathematics, North Carolina State University, 2000. Applied & Numerical Mathematics [Nonlinear Suboptimal Feedback Control]. (March 2001 to February 2003)

Theodorus Dingemans - Ph.D., Organic Chemistry, University of North Carolina at Chapel Hill, 1998. Structures & Materials. (September 2000 to August 2002)

Boris Diskin - Ph.D., Applied Mathematics, The Weizmann Institute of Science, Israel, 1998. Applied & Numerical Mathematics [Convergence Acceleration]. (July 1998 to September 2004)

Alicia M. Dwyer - M.S., Mechanical Engineering, Aerospace Track, The George Washington University, 2001. Applied & Numerical Mathematics [Planetary Exploration]. (July 2001 to July 2003)

Sarah-Jane V. Frankland - Ph.D., Chemistry (Physical), The Pennsylvania State University, 1997. Structures & Materials [Computational Nanotechnology]. (June 2001 to June 2003)

Hanne Gottliebsen - Ph.D., Computer Science, University of St. Andrews, Scotland, 2001. Computer Science [Formal Methods]. (August 2001 to August 2003)

Jill L. Hanna - M.S., Aerospace Engineering (Astronautics), The George Washington University, 2001. Applied & Numerical Mathematics [Planetary Exploration]. (July 2001 to July 2003)

Luc Huyse - Ph.D., Civil Engineering, Structures, University of Calgary, Canada, 1999. Applied & Numerical Mathematics [Managing Uncertainties in Multidisciplinary Research]. (October 1999 to November 2001)

Ronald Krueger - Ph.D., Aerospace Engineering, University of Stuttgart, Germany, 1996. Structures & Materials [Analysis of Composite Delamination of Structures]. (August 2000 to August 2003)

Mark E. Little - Ph.D., Physics, Ohio University, 2001. Structures & Materials [Intelligent Optics]. (April 2001 to April 2003)

Edward P. Locke - Ph.D., Synthetic Organic Chemistry, University of Virginia, 2000. Structures & Materials [Advanced Aircraft and Space Materials]. (March 2001 to September 2001)

César A. Muñoz - Ph.D., Computer Science, University of Paris 7, 1997. Computer Science [Formal Methods Research for Safety Critical Systems]. (May 1999 to April 2002)

Lee M. Nicholson - Ph.D., Materials Science, University of Cambridge, United Kingdom, 1997. Structures & Materials [Computational Nanotechnolgy]. (May 2000 to June 2001)

Cheol Park - Ph.D., Macromolecular Science and Engineering, The University of Michigan, 1997. Structures & Materials [Electro-active Materials]. (November 2000 to October 2002)

Jason H. Rouse - B.S., Chemistry, Lehigh University, 1995. Structures & Materials [Molecular Self-Assembly]. (May 2001 to May 2003)

Kent A. Watson - Ph.D., Organic/Polymer Chemistry, Virginia Commonwealth University, 1998. Structures & Materials [Nanocomposites]. (April 2001 to March 2003)

David W. Way - Ph.D., Aerospace Engineering, Georgia Institute of Technology, 2001. Applied & Numerical Mathematics [Planetary Exploration]. (August 2001 to August 2003)

Won J. Yi - Ph.D., Electrical Engineering, University of Nebraska, 1997. Structures & Materials [Smart Materials and Flow Control]. (February 2001 to August 15, 2001)

VI. VISITING SCIENTISTS

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REPORT DOCUMENTATION PAGE		Form Approved OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*	2. REPORT DATE February 2002	3. REPORT TYPE AND DATES COVERED Contractor Report

4. TITLE AND SUBTITLE
Semiannual Report
April 1, 2001 through September 30, 2001

5. FUNDING NUMBERS

C NAS1-97046
WU 505-90-52-01

6. AUTHOR(S)

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
ICASE
Mail Stop 132C
NASA Langley Research Center
Hampton, VA 23681-2199

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
National Aeronautics and Space Administration
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Hampton, VA 23681-2199

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
NASA/CR-2002-211436

11. SUPPLEMENTARY NOTES
Langley Technical Monitor: Dennis M. Bushnell
Final Report

12a. DISTRIBUTION/AVAILABILITY STATEMENT

Unclassified–Unlimited
Subject Category 59
Distribution: Nonstandard
Availability: NASA-CASI (301) 621-0390

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*
This report summarizes research conducted at ICASE in applied mathematics, computer science, fluid mechanics, and structures and material sciences during the period April 1, 2001 through September 30, 2001.

14. SUBJECT TERMS
applied mathematics, multidisciplinary design optimization, fluid mechanics, turbulence, flow control, acoustics, computer science, system software, systems engineering, parallel algorithms, structures and material science, smart materials, nanotechnology

15. NUMBER OF PAGES 90
16. PRICE CODE A05

17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT