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# Institute for Computational Mechanics in Propulsion (ICOMP)

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**INSTITUTE FOR COMPUTATIONAL MECHANICS  
IN PROPULSION (ICOMP)  
NINTH ANNUAL REPORT**

**1994**

**SUMMARY**

The Institute for Computational Mechanics in Propulsion (ICOMP) is operated by the Ohio Aerospace Institute (OAI) and funded under a cooperative agreement by the NASA Lewis Research Center in Cleveland, Ohio. The purpose of ICOMP is to develop techniques to improve problem-solving capabilities in all aspects of computational mechanics related to propulsion. This report describes the activities at ICOMP during 1994.

**INTRODUCTION**

The Institute for Computational Mechanics in Propulsion (ICOMP) was established at the NASA Lewis Research Center in September 1985, to improve problem-solving capabilities in all aspects of computational mechanics relating to propulsion. ICOMP provides a means for researchers with experience and expertise to spend time in residence at Lewis performing research to improve computational capability in the many broad and interacting disciplines of interest in aerospace propulsion.

The scope of the ICOMP program is to advance the understanding of aerospace propulsion physical phenomena and to improve computer simulation of aerospace propulsion systems and components. The specific areas of interest in computational research include: fluid mechanics for internal flows; CFD methods; turbulence modelling; and computational aeroacoustics.

This report summarizes the activities at ICOMP during 1994. It lists the resident and visiting researchers, their affiliations and educational backgrounds, followed by reports of RESEARCH IN PROGRESS, REPORTS AND ABSTRACTS published and SEMINARS presented. The agendas and overviews of two very fruitful workshops held in 1994 are also given. The first was a two-day "Industry-Wide Workshop on Computational Turbulence Modeling", held October 6-7, 1994. The second was a two-day "Workshop on Least-Squares Finite-Element Methods" held October 13-14, 1994.

### THE ICOMP STAFF OF VISITING RESEARCHERS

The ICOMP research staff for 1994 is shown in Table I. A total of fifty researchers were in residence at Lewis for periods varying from a few days to a year. The resident staff numbered twenty-four while the visiting staff, including one graduate student, numbered twenty-six. Table II shows the progression of ICOMP during its first nine years in terms of staff size and technical output as measured by the numbers of seminars, reports and workshops. The smaller number of seminars reflects, to a large extent, 1) the strong emphasis placed by the CMOTT turbulence modeling group and the aeroacoustics group on applying their existing capabilities for customer use in the industrial and user communities, and 2) the conducting of the two extensive workshops. These objectives were judged to be of higher priority than the seminars.

Figure 1 is a photograph of the ICOMP administrative and research staffs taken at a reception in August 1994. The next sections will describe the technical activities of the ICOMP researchers starting with reports of RESEARCH IN PROGRESS, followed by REPORTS AND ABSTRACTS, then SEMINARS, and finally, the overviews of the two workshops.

## RESEARCH IN PROGRESS

**KUMUD AJMANI**

My work for this year was performed in association with Meng-Sing Liou (Internal Fluids Mechanics Division) and Russell Claus (Interdisciplinary Technology Office). The thrust of the work was directed towards developing a parallel, three-dimensional, implicit CFD code capable of calculating flows in geometries of interest to NASA Lewis (inlets, nozzles, turbomachinery, etc.). The code development was initiated by introducing an implicit time-integration procedure into an existing multi-block, three-dimensional CFD code. This was done in order to enhance the convergence rate of the code, and hence improve upon the large processing times encountered in explicit time-integration of complex fluid flows.

The implicit time-integration scheme was based on a preconditioned Conjugate-Gradient algorithm, namely the GMRES algorithm. The code uses the Advection Upwind Splitting Method (AUSM) scheme for upwinding the convective fluxes, and a unique derivation of the AUSM flux-jacobians was programmed and validated for the code. The implicit code was then parallelized using domain-decomposition techniques and an SPMD (Single-Program Multiple-Data) approach, and tested on several distributed-memory parallel architectures. The architectures tested were an Intel Hypercube (32 nodes), a cluster of workstations (LACE cluster, 32 nodes) and a Cray-T3D machine (64 nodes). Several performance metrics were measured on the different machines, and comparisons were made regarding the pros and cons of the different architectures.

The parallel CFD code will be used as a kernel for a multiple-block code which uses the CHIMERA overset grid technique to compute flow in a variable-geometry inlet/nozzle and some turbomachinery configurations. The parallel implementation of the multiple-block code will also be ported to different architectures. The intent will be to evaluate the effect of parameters like file I/O, message-passing, and processor-speed on the actual productivity of a production-level CFD code in different parallel environments.

**ANDRE ARNONE**

During my visit to ICOMP, I continued working on the TRAF2D/3D codes. These are steady/unsteady viscous solvers under development in a joint project between the University of Florence and NASA Lewis. The goal is to develop and test efficient tools for the design, analysis, and comprehension of turbomachinery flows. Presently, activities are in two areas:

1) Unsteady rotor-stator interaction: A two-dimensional unsteady version of the TRAF code for multistage analysis is complete and under testing. A dual time stepping approach is used to achieve efficiency and realistic rotor to stator blade count ratios are handled by analyzing several blade passages. To check the capability of the method to predict natural unsteadiness, the multistage code has been adapted to study a wind tunnel configuration and has been applied to the shock buffeting on a biconvex airfoil. For this test case, measurements were available from NASA Ames. The computational results were in good agreement with experiments and with calculations by other authors. An AIAA Journal publication on this topic is in preparation.

2) Study of advanced compressor configurations: With Ali Ameri we participated in the ASME NASA Rotor 37 blind test case. This test case has shown how some work is still needed before we can accurately predict supersonic compressor flows with a high pressure ratio. In particular, a grid sensitivity analysis carried out in 1993 for rotor 67 proved to be very useful for rotor 37 also. We are presently examining both grid dependency (particularly leading edge resolution) and turbulence modeling in order to understand and learn more about the rotor 37 and 67 test cases. My collaboration with the Turbomachinery Fluid Physics Branch, where the TRAF codes are used for heat transfer and film cooling calculations, is continuing.

**THOMAS F. BALSA**

It is believed that in a small-disturbance environment in an incompressible boundary layer, the nonlinear interaction between a two-dimensional mode and two oblique modes, whose propagation angles are inclined at  $\pm 60^\circ$  to the streamwise direction, plays a very important role in the early stages (in the so-called parametric resonance stage) of the sequence of phenomena leading to transition. M.E. Goldstein and his colleagues have analyzed in detail the consequences of this, as well as of other types on mode interactions. Most of these analyses deal with pure modes (which may be slightly detuned though), rather than with slowly modulated wave trains arising from the forcing by the background disturbances which drift in time.

Goldstein's work is based on rational asymptotic methods applicable to high Reynolds numbers. In this case the wavenumber is *asymptotically* small, while in experiments the wavenumber is usually a numerically small number which is best considered as  $O(1)$  in an analysis. The purpose of the present activity is to extend heuristically the equations governing the interaction of modes, in the parametric regime, to modulated trains with finite wavenumbers. This is done by working with a realistic model problem. The boundary layer profile is represented as a linear profile plus a small perturbation, of  $O(\sigma)$ , representing the effects of the (small) second and higher derivatives of the Blasius profile near the wall.

The lowest order problem, essentially with  $\sigma=0$ , may be solved by elementary methods; the result is a neutral dispersive wave with a singular structure at the critical layer. In order to resolve this singularity, a slight unsteadiness (essentially an instability), a small nonlinearity, and a small amount of viscosity are introduced into the critical layer. Slow modulations in  $x, z$ , and  $t$  occur on long scales proportional to  $O(1/\sigma)$ . The critical layer is of the Hickernell-Goldstein type. The balance of these physical effects in the critical layer equations, and the matching of the flow in this layer with that in the external regions, lead to coupled equations for the amplitudes of the 2D and 3D modes. Work is in progress to extract interesting results from these equations and to obtain numerical results for various types of modulations.

**IAIN D. BOYD**

During my visit to ICOMP, I worked on computations of plume impingement from small rockets employed for spacecraft control and station-keeping. Recently, at NASA Lewis Research Center, static pressure measurements have been made on the surface of a  $50^\circ$  cone placed on the axis of a plume expanding from a nitrogen resisto-jet. I performed numerical simulations under identical flow conditions using a Monte Carlo technique. The results indicate that the measured pressures lie between those calculated using the theoretical limits of diffuse and specular reflection of the gas from the cone surface. The results of this preliminary study will be presented at the AIAA Joint Propulsion Conference, Indianapolis, June, 1994. Further experimental and numerical studies are planned to investigate this behavior in greater detail.

**GILES BRERETON**

In collaboration with Reda Mankbadi, I completed a paper on prediction of unsteady turbulent flows using rapid distortion closures, which has been submitted to the Physics of Fluids journal. I also worked on developing the rapid distortion approach to modeling heat transfer in unsteady flows. Though treating temperature as a passive scalar, this approach provides a way of predicting the unsteady component of a surface heat transfer coefficient or Nusselt number for constant wall-temperature heat transfer in unsteady duct flows. This advance is particularly significant since measurements of truly unsteady heat transfer coefficients are still beyond the capabilities of laboratory equipment and can only otherwise be estimated for quasi-steady changes in flow velocity. Upon completion, this work will also be submitted to a journal. I also consulted with R. Mankbadi, T.H. Shih, J. Trevor Stuart, T. Bui and others on issues related to the unsteady and acoustic aspects of turbulent fluid flow.

### TAWIT CHITSOMBOON

A High Speed Research (HSR) project is underway at the NASA Lewis Research Center to bring about the reality of profitable, commercial, supersonic flight that satisfies the U.S. government's regulations on noise and emission pollution. CFD has been identified as playing a key role in bringing about the completion of the project in a timely manner. In particular, the NPARC code has been used extensively to compute the flowfields around and inside the engine configurations, especially in the various noise-suppression nozzle configurations.

One shortcoming of NPARC (3D) was that it failed to give a converged solution when run with the two equation  $\kappa$ - $\epsilon$  turbulence model. The author collaborated with Nick Georgiadis of the Nozzle Technology Branch to make various corrections to the baseline turbulence model such that the model now works properly. In addition, we modified the baseline model such that it now becomes the Chien model [1]. In the various test cases performed, the Chien model gave better results than the baseline model.

The major effort in this reporting period has been directed toward implementing wall-function boundary conditions into the existing Low-Reynolds Number  $\kappa$ - $\epsilon$  turbulence model. These wall functions are needed to cut down the computation time. A major obstacle concerning the artificial viscosity has been identified and overcome, the detail of which is reported in reference 2. Six test cases are now being run to validate the implementation of the wall-functions. These cases are: (1) 2D flow over a flat plate; (2) 2D flow over a backward-facing step; (3) 2D flow in a mixer-ejector; (4) 2D flow in a diffuser; (5) 3D flow in a mixer-ejector (Pratt-Whitney); and (6) 3D flow in a mixer-ejector (G.E.)

1. N.J. Georgiadis; T. Chitsomboon; and J. Zhu: "Modification of the Two-Equation Turbulence Model in NPARC to a Chien Low Reynolds Number  $\kappa$ - $\epsilon$  Formulation", ICOMP 94-20, CMOTT 94-5, NASA TM 106710, 1994.
2. T. Chitsomboon: "Effect of Artificial Viscosity on the Accuracy of a High Reynolds Number  $\kappa$ - $\epsilon$  Turbulence Model", ICOMP 94-28, NASA TM 106781, 1994.

### JOONGKEE CHUNG

Subroutines developed and modified for Controls/CFD research have been incorporated into the latest versions of 2D and 3D NPARC. The modified version of 2D NPARC was provided to researchers at Indiana University and Purdue University-Indianapolis so that they could develop an efficient parallel version of the 2D code. Also for 3D NPARC, an initial version for coarse grain parallel computation was attempted, with the help of Suresh Khandelwal of NYMA, to produce some results for the Variable Diameter Centerbody (VDC) high speed engine inlet.

Meanwhile, 2D CFD results for the NASA 55-45 mixed compression inlet and VDC inlets were provided to the controls group for preliminary derivation and linearization of the 2D flow equations so that the model generation and reduction could be completed.

Inlet control design depends on a knowledge of both steady and unsteady flow-field behavior. The unsteady flow-field behavior predicted by a CFD simulation can be altered significantly, depending on the chosen exit boundary conditions (BC). As a part of an effort to further improve NPARC subroutines, a new type of compressor face BC was developed and time accurate computations were performed to study inlet transients caused by upstream and downstream disturbances. The new BC is imposed as a non-uniform static-pressure profile based on uniform corrected airflow (or Mach number). The static-pressure time histories calculated at various locations are less oscillatory when compared to results for other conventionally-used fixed pressure BCs. This suggests that the new BC is less reflective than the others. In particular, pressure responses to steps in the compressor face Mach number show no overshoot with the new BC, which is in good qualitative agreement with observed experimental data. 1D unsteady inviscid computational results calculated by the Large Perturbation Inlet analysis (LAPIN) code were in good agreement with those obtained with the 2D and 3D NPARC codes when applied to the NASA 55-45 mixed compression inlet and the VDC inlet. For 3D computations, a real geometry, which

has 3 supporting struts (120 degrees apart) blocking the passage of flow in the diffuser, was used and there was basically no change in the dynamic responses compared to 1D or 2D results.

### FREDERIC COQUEL

During my two months stay at ICOMP, I worked closely with Meng-Sing Liou on a NASA-ONERA cooperative program devoted to the development of the Hybrid Upwind Splitting (HUS) methods. These methods, which we have introduced earlier [1], are designed to combine the respective strengths of the classical FVS and FDS schemes in order to get stable and accurate solutions to the Euler and Navier-Stokes equations. An ICOMP report [2] completed during my stay, describes in full detail our hybridization procedure.

Our joint research effort has been focused on extending both the theoretical and numerical analysis of the HUS methods. The theoretical study was aimed at proving the entropy satisfying property. This property indeed turns out to be a crucial requirement for the nonlinear stability of a given numerical method (see [3] for instance) and therefore needs to be specifically investigated. We have proved that semi-discrete entropy inequalities can be derived for the HUS methods provided that the underlying FVS scheme is itself entropy-satisfying. Such inequalities hold true for either the Osher-Solomon or the Collela-Glaz path. Note that this latter approximate Riemann solver is entropy-violating. In this sense, entropy satisfaction for the HUS is directly inherited from the FVS scheme as was strongly expected. Our proof extends to the HUS methods some technical arguments due to Osher-Solomon. A comprehensive report devoted the complete derivation is currently under way.

The second part of our work has been focused on a numerical study of the stability of multidimensional discrete shock profiles. For a few years, it has been indeed recognized that, by contrast with the FVS schemes, several FDS methods, including the exact Riemann solver, may yield spurious steady solutions when capturing sufficiently strong shocks. The occurrence of such a failure, referred as to the carbuncle phenomena, heavily depends on the computational grid itself. HUS methods based on such approximate Riemann solvers turn out to suffer also from this difficulty even if the use of FVS fluxes makes them in practice much less sensitive than the pure underlying solver. Their associated path, used in the HUS methods under consideration, is obviously responsible for this difficulty. Our purpose was therefore to get a better understanding of this difficulty in order to derive suitable paths for the hybridization procedure. The numerical experiments we have carried out show that the so-called carbuncle phenomena is actually closely related with Quirk's problem. This observation allowed us to clearly point out the source of the failure. Equipped with these numerical evidences, we have undertaken an analytical study aimed at exhibiting the full dynamical system governing the odd-even decoupling observed in Quirk's problem. Such a study should explicitly determine the terms responsible for the breakdown of the discrete shock profile and therefore give a way for constructing suitable paths. Numerical evidences and the first part of our analysis will be presented in a forthcoming report.

1. F. Coquel and M.-S. Liou: "Field by Field Hybrid Upwind Splitting Methods", AIAA 93-3302-CP, 1993.
2. F. Coquel and M.-S. Liou: "Hybrid Upwind Splitting (HUS) Methods by a Field by Field Decomposition", ICOMP 95-2, NASA TM 106843, 1995.
3. F. Coquel and Ph. Le Floch: "Convergence of Finite Difference Schemes for Conservation Laws in Several Space Dimensions: A General Theory", SIAM J. Numer. Anal., vol. 30, 1993, pp 675-700.

### PETER DUCK

I have been investigating the interaction between the boundary layer located on a flat plate and freestream turbulence (joint work with A. Ruban Moscow of Lehigh University), using high Reynolds number asymptotic techniques. It is found that apart from the conventional viscous boundary layer of thickness  $O(\text{Re}^{-1/2})$ , a "vorticity deformation layer" of thickness  $O(\text{Re}^{-1/4})$  forms along the flat plate surface, in which the flow is to be determined by a solution of a form of the unsteady Euler

equations. Of particular interest is the apparent shock-like structure that appears to form in the vorticity distribution on the surface of the plate. This is likely to provoke abrupt transition in the boundary layer. If, on the other hand, a small roughness element (for example) is introduced to the plate surface sufficiently far ahead of the above breakdown, then it has been shown that Tollmien-Schlichting waves may be generated, and explicit formulae for the amplitude of these waves may be obtained.

I have had a number of interesting discussions with L. Hultgren of NASA Lewis regarding absolute instabilities; these have led to the investigation of the flow over moving walls/surfaces. In the first instance I studied the two-dimensional boundary-layer flow over a wall moving in a direction opposed to the freestream flow. In this case it can be shown that there is a critical wall velocity at which absolute instability can occur. This investigation has since been extended to three-dimensional situations and computations are continuing.

During my visit, following discussions with S. Leib, I also wrote a computer code to solve the unsteady "inviscid triple-deck" equations. As well being realizable as a limiting form of the triple-deck equations, these equations are also obtained at a crucial stage in transition processes involving both boundary layers and shear layers. The computations are based on a pseudo-spectral method, in which the solution is carried out partly in Fourier space and partly in physical space (the fast Fourier transform technique being used to transform between spaces). In the two-dimensional case, generally these computations appear to be able to be extended for all times. In the three-dimensional case (due largely to the much more demanding computational requirements) the situation is not quite so clear, and is currently under investigation.

#### **MAX GUNZBURGER**

Over the past year we have continued to work on least-squares finite element methods for incompressible viscous flows and, more generally, for systems of partial differential equations. Directly related to our association with ICOMP, we have been studying some issues that are often brought up in criticisms of these methods. These include the following issues: 1) the conditioning of the linear systems that one must solve as part of the solution process; 2) mixed boundary conditions, i.e., the velocity imposed on part of the boundary and other types of boundary conditions such as stress components on other parts of the boundary; 3) the accuracy of linear finite elements; 4) the effects on accuracy of singularities caused by corners in the boundary; 5) the imposition of velocity and other boundary conditions via the least-squares functional; and 6) loss of mass conservation. In each case, we have either determined that least-squares finite element methods perform optimally, or, if not, remedies have been developed. An ICOMP report on this work is currently being prepared.

#### **BERNARD GREENSPAN**

My work was focussed on the Space-Time Conservation Element and Solution Element method for solving the conservation laws. The basis of this method is to represent the solution as a piecewise polynomial on solution elements. The polynomial pieces are required to satisfy the differential form of the conservation laws up to a specified order and both local and global-flux conservation laws are also satisfied to a specified order. This method is also called the STS method. An abstract, "Energy Equation Solutions of Steady Incompressible Viscous Flow Using the STS Method" was submitted to the AIAA 26th Fluid Dynamics Conference. This work, coauthored with James R. Scott, will also be submitted as a NASA TM. An analysis of the stability and order of the adaptation of the STS method to ordinary differential equations was carried out and will appear in a joint work with James R. Scott.

#### **THOMAS HAGSTROM**

We have continued work with S.I. Hariharan on boundary conditions for hyperbolic systems based on progressive wave expansions. Our primary applications are the linearized compressible Euler equations and Maxwell's equations. The first order conditions based on this theory have been

implemented in a 2-4 MacCormack code and applied to the simulation of sound produced by a quadrupole source and propagated through a vortex dipole. We observe a halving of the error in comparison with a standard characteristic scheme (i.e., one defined by setting the incoming Riemann variables to their free stream values). We are currently implementing second order conditions and examining the stability theory. We have also studied high order conditions of the Engquist-Majda type and their application to the linearized Euler equations. From a theoretical viewpoint, we have developed a convergence theory which shows that for fixed times and sufficiently smooth solutions at the boundary, the Engquist-Majda approximations converge to the exact boundary operator. In collaboration with John Goodrich of NASA Lewis, we have looked at convenient implementations whose preliminary results are quite promising.

Work has also continued with K. Radhakrishnan of NYMA on an experimental high-order numerical algorithm for simulating unsteady reacting flows governed by the zero Mach number asymptotic limit of the governing equations. Recently, we have studied the acceleration of convergence to steady state for the purpose of quick and accurate flame speed computations. In particular, we have implemented the Recursive Projection Method, which involves the automatic detection of subspaces on which convergence is slow and the use of a projected Newton algorithm to accelerate convergence. Simplified (linearly implicit) time marching schemes which lead to significant speed-ups in the code have also been tested. The next step in the code's development will be extensions to two dimensions. The use of singular value decompositions to automatically reduce the dimension of nonlinear systems solved during simulations of reaction dynamics have been studied and methods explored for the rapid solution of linear systems arising in diffusion velocity calculations.

With E. Coutsias and D. Torres, we have developed fast methods for the solution of Galerkin spectral approximations to differential equations, using any of the classical orthogonal polynomial families and allowing general boundary and/or initial conditions. The basic idea behind the method is that certain integral operators are banded when expressed in these spectral families. Reformulating in terms of integral operators not only leads to banded matrices, but also yields well-conditioned linear systems. Mappings have been incorporated to resolve regions of rapid variation in the solution with only a slight increase in the bandwidth. Application of this method to the study of helical waves in pipe flow is currently under consideration.

### **S. I. HARIHARAN**

My work on boundary conditions for use in computational aeroacoustics is being carried out jointly with T. Hagstrom of The University of New Mexico. The work addresses model problems that can be used to check the effectiveness of computational aeroacoustics procedures. This includes the computation of the nonlinear Euler equations as well their linearized form that is standard for acoustics. The focus is on the prescription of accurate boundary conditions that are suitable for a given computational domain. Depending on the problem, these may be circular or rectangular domains in two dimensions or a sphere or a box in three dimensions. The procedures that have been developed for rectangular domains (or boxes) generally use a one-dimensional analysis, which does not, in general, translate to cylindrical (or spherical) geometries in a natural way. Enforcing the unidirectional principles is, in general, accurate for near normal incidence; however, at wider angles of incidence, they induce inaccuracies that often yield unacceptable reflections. These inaccuracies naturally lead to a build-up of errors in the solution. These errors are *a priori* errors independent of the errors due to the numerical schemes. In general they are functions of time and the location of the artificial boundaries. The goal of the work is to develop asymptotic boundary conditions for the linearized Euler equations. Several test problems are considered to validate the theory.

My work on the evaluation of numerical schemes for the analysis of sound generation by blade-gust interactions is being carried out jointly with J. N. Scott of the Ohio State University and R. Mankbadi of NASA Lewis. In this investigation several different numerical algorithms have been utilized to compute the flow about a flat plate in the presence of a transverse gust described by a sinusoidal disturbance. Since viscous effects are ignored in this problem, the governing equations

are the linearized Euler equations, which are also generally regarded as suitable for analyzing the propagation of acoustic disturbances. The schemes include: the MacCormack explicit finite difference scheme which is second order accurate in both time and space; the Gottlieb and Turkel modification of MacCormack's scheme, which is fourth order accurate in space and second order accurate in time (referred to as the 2-4 scheme); a two step scheme developed by Bayliss et. al., which has second order temporal accuracy and sixth order spatial accuracy (a 2-6 scheme); and the DRP scheme proposed by Tam and his coworkers. The flow field results are obtained with these schemes by using the same code with the only difference being the implementation of the respective solution algorithms. The computed results include the time histories of the acoustic pressures along grid lines five points away from the boundaries. In addition, the pressure distribution throughout the computational domain is monitored at various times. The numerical results are compared with an exact solution obtained by Atassi, Dusey, and Davis. The problem is set up so that the sinusoidal disturbance is imposed at the surface of the flat plate as a surface boundary condition. Thus the problem is treated as a scattering problem. At the outer boundaries, the computational procedure incorporates boundary conditions developed for far-field asymptotic expansions for the linearized Euler equations which are consistent with acoustic analyses. These formulations have been developed and demonstrated by Hariharan and Hagstrom. A study of the influence of grid refinement has been conducted and a report on these results is in preparation.

#### **M. EHTESHAM HAYDER**

The goal of my research is to compute jet flows and their associated noise both accurately and efficiently. The turbulent flow field was obtained by solving the full Navier-Stokes equations using a fourth order MacCormack scheme (Gottlieb and Turkel [1]) and large eddy simulation [2]. For accurate simulations, one needs to use a high order interior scheme and also an accurate boundary condition. In our recent studies, continued from last year, we evaluated a few boundary conditions and noted that the non-reflecting boundary conditions developed by Bayliss and Turkel, Hariharan and Hagstrom, and Tam and Webb are identical (see reference 3 for details). A version of our evaluations of boundary conditions has been submitted to the AIAA Journal [4]. We also developed a new outflow boundary condition for aeroacoustics computations. This work has been submitted for presentation in the upcoming ASME summer meeting [5]. One other sub-area of jet noise computation that we have examined is shock generated noise. The presence of sharp gradients associated with shocks and the relatively weak signals associated with acoustic waves make any accurate simulation very difficult. We have evaluated a few high order schemes to examine their effectiveness for simulations of nonlinear waves [6]. Further work in this area is in progress.

To solve the flow very efficiently, we examined our numerical model on various parallel computational platforms available at NASA Lewis. In particular, we concentrated our efforts on the Lewis Advanced Cluster Environment (LACE), the Cray YMP and the IBM SP2. The LACE is a cluster of RS6000 workstations. With the advent of powerful workstations, cluster computing is becoming a viable alternative to traditional super computing. We presented some of our results on the LACE at the ICASE/LaRC Industry Roundtable, Williamsburg, VA, October 1994. A comparative study of the Cray YMP, the LACE and the IBM SP2 will be presented at the AIAA meeting in January 1995 [7]. A scalability and communication study with our numerical model on parallel computers is being prepared for presentation at the Computational Aerosciences Workshop at Ames Research Center in March 1995 [8].

1. Gottlieb, D.; and Turkel, E.: "Dissipative Two-Four Methods for Time Dependent Problems", Math. Comp. Vol. 30, 1976, p703-723.
2. Mankbadi, R. R.; Hayder, M. E.; and Povinelli, L. A.: "The Structure of Supersonic Jet Flow and Its Radiated Sound", AIAA Journal, Vol. 32, No. 5, (1994), p 897-906.

## RESEARCH IN PROGRESS

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3. Hayder, M.E.; and Turkel, E.: "Boundary Conditions for Jet Flow Computations", ICOMP 94-13, NASA TM 106648, AIAA 94-2195, 1994.
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5. Hayder, M. E.; and Hagstrom, T.: "An Outflow Boundary Condition for Aeroacoustics Computations", Submitted for Presentation in the ASME Fluid Engineering Annual Summer Mtg., Hilton Head, SC, August, 1995.
6. Hayder, M. E.: "Evaluation of High Order Schemes for Nonlinear Wave Computations", Presented at the ICASE/LARC Workshop on Benchmark Problems in Computational Aeroacoustics, Hampton, Va, October, 1994.
7. Hayder, M. E.; Jayasimha, D. N.; and Pillay, S. K.: "Parallel Navier-Stokes Solutions on Shared and Distributed Memory Architectures", ICOMP 94-32, NASA TM 106823, AIAA 95-0577, 1995.
8. Hayder, M. E.; Jayasimha, D. N.; and Pillay, S. K.: "A Scalability and Communication Study on Parallel Computers for Jet Noise Computations", for the Computational Aerosciences Workshop, NASA Ames Research Center, Moffett Field, CA, 1995.

### DUANE RAY HIXON

My research is concerned with developing a noise prediction capability through the use of Computational Aero-Acoustics (CAA). For this purpose, an existing axisymmetric Large Eddy Simulation (LES) code was converted to compute the solution to the Linearized Euler Equations (LEE). This code was then validated by comparing calculated solutions with known analytic solutions for two test cases. Next, several different boundary conditions were implemented and evaluated. Since the goal of CAA is to accurately predict the long-term behavior of sound waves, it is important for the boundary conditions to allow waves to exit the computational domain without introducing spurious reflections that will degrade the accuracy of the solution. Three boundary conditions were tested, each representing a different theoretical approach for the specification of boundary conditions: (1) Characteristic-based (Thompson); (2) decomposition into Fourier modes (Giles); and (3) Asymptotic analysis of the governing equations at large distances (Tam and Webb). These boundary conditions were each applied to the test case of a monopole in a uniform freestream. The asymptotic boundary conditions showed a clear advantage in this case. The work will be presented at the 33rd AIAA Aerospace Sciences Meeting [1], and is currently being reviewed for journal publication. At this point, the code was applied to the computation of the noise radiated by a Mach 2.1 jet. This test case was chosen since both experimental data and analytical results were available. Along the boundary, the Thompson inflow, acoustic radiation, and Tam and Webb outflow boundary conditions were used where appropriate. The results of this work also will be presented at the 33rd AIAA Aerospace Sciences Meeting [2].

Future work proposed is to extend the LEE solver to 3D and combine it with the existing LES code in a zonal approach for predicting the noise from a 3-D jet. This will provide an important tool for evaluating proposed methods of reducing and controlling jet noise.

1. Hixon, R.; Shih, S.-H.; and Mankbadi, R. R.: "Evaluation of Boundary Conditions for Computational Aeroacoustics", ICOMP 94-11, NASA TM 106645, AIAA 95-0160, 1995.
2. Mankbadi, R. R.; Hixon, R.; Shih, S.-H., and Povinelli, L.: "On the Use of Linearized Euler Equations in the Prediction of Jet Noise", AIAA 95-0505, 1995.

### LIN-JUN HOU

My work was directed toward solving the time-dependent Navier-Stokes equations based on a velocity-pressure-vorticity formulation discretized by backward differencing in time. The time-accurate scheme is applied at each time step. Since the system is of first order, only the Dirichlet boundary conditions are needed. Numerical examples at low Reynolds numbers compared favorably with

steady state solutions. Recent efforts were directed at higher Reynolds number flows where periodic vortex shedding may exist and at a study of the effects of outlet boundary conditions.

#### **BO-NAN JIANG**

Work continued on the development and application of the least-squares finite element method (LSFEM) equations. This is a joint research with Sheng-Tao Yu (NYMA), Jie Wu (ICOMP) and Nan-Suey Liu (LeRC Internal Fluid Mechanics Division). We demonstrated that the LSFEM can simulate compressible viscous flows at low-Mach numbers without special treatments, such as operator splitting or preconditioning. This will open a new way to solve reacting flow problems in combustion chambers. We also demonstrated that the LSFEM can maintain the shape of a standing vortex in an inviscid fluid without loss of total kinetic energy. We showed that the LSFEM is perfectly suitable for solving Maxwell's equations in electromagnetics with divergence-free conditions satisfied easily. The least-squares method is also a theoretical tool for studying partial differential equations. By using this method we (in collaboration with Ching Y. Loh) rigorously derived all permissible non-standard boundary conditions for the Navier-Stokes equations.

#### **KAI-HSIUNG KAO**

Advanced algorithms exist, yet their limitations for complex flow fields are still not totally understood. It is known that the proper selection of a numerical algorithm is a key issue in order to resolve complicated mechanisms, such as shock wave/boundary layer interaction and high speed viscous flow, that occur with complex configurations. There are various methods and numerical schemes for solving the system equations. Many of them may display high accuracy and a fast convergence rate in simple geometries; however, for complex configurations, they may not be capable of resolving the complex flow as expected. A newly developed flux splitting scheme called AUSM+ has been developed by M-S. Liou [1] and has been incorporated into the Navier-Stokes code. The capability of the AUSM+ scheme for accurately predicting shock waves and viscous layers has been confirmed.

The grid construction for this work would initially seem tedious; however, a composite grid system was employed to greatly simplify the grid generation. Adoption of the Chimera scheme [2,3] allowed discretization of the volume about the complex configuration as a collection of structured grids. The overlapped grid approach was chosen over a patched scheme to reduce the labor time involved in domain decomposition. The overall philosophy behind the use of overlapped grids is that individual component grids can be generated easily if one does not have to match to other grids or pieces of geometry. This advantage greatly reduces the tedium of trying to generate a complex three-dimensional grid to define both external and internal flows. Recently, a hybrid grid technique was proposed for implementation into the Chimera overset grid. This maximizes the advantages of the Chimera scheme and adapts the strengths of the unstructured grid while at the same time keeping its weaknesses minimal. This new adaptation of the Chimera thinking is coined the DRAGON grid [4,5,6]. The DRAGON grid method has three important advantages: (1) preserving the strengths of the Chimera grid; (2) eliminating the difficulties sometimes encountered in the Chimera scheme; and (3) making grid communication in a fully conservative and consistent manner. Currently we are focusing on enhancements for unstructured grid generation and solvers for 3-D problems. Future work will emphasize the application of the present method for numerical simulations of various propulsion/airframe integration geometries. The entire procedure will provide a baseline for research into optimization of HSCT aerodynamics, propulsion integration, and sonic boom. By using the proposed numerical techniques, the preliminary design of complex bodies can be accelerated and made much more efficient. Design improvements will be suggested upon thorough examination of the computational results.

1. M.-S. Liou, "A Continuing Search for a Near-Perfect Numerical Flux Scheme, Part I: AUSM+", NASA TM 106524, 1994.

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2. J. A. Benek, J. L. Steger, F. C. Dougherty and P. G. Buning, "Chimera: A Grid Embedding Technique", AEDC-TR-85-64, April 1986.
3. N. E. Suhs and R. W. Tramel, "PEGSUS 4.0 User's Manual," AEDC-TR-91-8, November, 1991.
4. K. H. Kao and M. S. Liou, "Direct Replacement of Arbitrary Grid-Overlapping by Nonstructured Grid", ICOMP 94-07, NASA TM 106601, 1994.
5. M. S. Liou and K. H. Kao, "Progress in Grid Generation: From Chimera to DRAGON Grids", ICOMP 94-19, NASA TM 106709, 1994.
6. K. H. Kao and M. S. Liou, "An Advance in Overset Grids: From Chimera to DRAGON Grids," presented at the 2nd Overset Composite Grid and Solution Technology Symposium, Fort Walton Beach, FL, October 1994.

### BRIAN P. LEONARD

My research in 1994 centered on three related areas involving modelling of highly advective flows. First was the Flux Integral Method (FIM), a genuinely multidimensional approach, resulting in a flux-based, explicit, strictly conservative update. Control-volume face fluxes (for convection and diffusion) are estimated by integrating over characteristics --approximated by parallelograms (in 2D) based on local Courant numbers. The resulting algorithm depends on the form of the sub-cell interpolation adopted (given cell-average data). Multidimensional Nth-degree interpolation results in an (N+1)th-order accurate scheme (for constant coefficients). An interesting side issue of this study is that what are usually called "central" schemes are actually based on *downwind*- weighted sub-cell interpolation. Velocity-direction-independent interpolation results in "natural upwind" schemes. In other words, upwind schemes are inherently more natural than "central" schemes. Stated differently: a "central" scheme requires a velocity-dependent decision on the sub-cell interpolation. Because of geometric complexity, the FIM is restricted to Courant numbers less than  $O(1)$ . See ICOMP report 94-13, NASA TM 106679, August, 1994.

The second area was the Time-Split NIRVANA-1D scheme. The 1D NIRVANA scheme (nonoscillatory, integrally reconstructed, volume-averaged, numerical advection) represents the generalization of my ULTIMATE approach to arbitrarily large time steps. For "conventional" explicit schemes, stability restrictions on the time step result from a "short-sighted" view of sub-cell interpolation. When a global view is taken, *there are no time-step constraints*. I have been exploring multidimensional applications using the simple expedient of time-splitting. This introduces a problem I call "lumpiness": in a solenoidal (but strongly deformational) advection field, an initially constant transported scalar does not remain constant. Apart from this, the NIRVANA results are quite impressive--highly accurate and nonoscillatory, with little anisotropic distortion for moderate time-steps; Courant numbers can be significantly larger than 1. There are ways to fix the "lumpiness" problem that I will explore in future work.

The third area was the ENIGMATIC approach. The enigmatic problem of highly advective flow modelling requires an ENIGMATIC approach to its solution. In this case I mean Extended Numerical Integration for Genuinely Multidimensional Advective Transport Insuring Conservation. CFD researchers have been looking for such a scheme for many years. My FIM approach is conservative but restricted to Courant numbers less than  $O(1)$ . The very popular Semi-Lagrangian method has no stability restrictions on the time step, but it is not inherently conservative. ENIGMATIC combines the FIM with NIRVANA concepts to achieve both goals (i.e., conservation plus large time step). The resulting flux-based scheme consists of a one-dimensional flux component together with an "outrigger" flux representing the contribution of transverse advection. As with FIM and NIRVANA, the crucial step is sub-cell interpolation. Highly accurate, shape preserving schemes seem within reach. The explicit update is cost-effective in that it involves only point evaluations of the (multidimensional NIRVANA) integral variables. CFD applications may be far-reaching.

**WILLIAM W. LIU**

My research involves the development of turbulence models for incompressible/compressible flows and their validation/application in flows of engineering interest. During this reporting period, the following items were pursued.

Near-wall damping functions were included in the high Reynolds number compressible two-scale turbulence model (ICOMP 93-07, NASA TM 106072, Also Phys. Fluids, March 1995) to enable a direct integration of the model equations to a solid wall. This is accomplished by assuming Kolmogorov behavior of the near-wall turbulence, which was first proposed by Shih and Lumley (ICOMP 92-10, NASA TM 105663). The near-wall version of the two-scale model has been successfully developed and validated in compressible boundary layers and shock/turbulent boundary layer interaction ramp flows. The results will be reported in a NASA TM shortly.

Part of the effort was devoted to the establishment of a computational capability for turbulent compressible flow cases that are appropriate for the assessment of turbulence models. In addition to the already available compressible free shear layer and compressible boundary-layer flow capability, numerical platforms for four other types of compressible flows with a total number of ten cases are now completed. These include supersonic ramp flows, oblique shock wave/turbulent boundary layer interactions, and transonic bump flows. These cases were carefully selected so that they not only covered a wide range of physical phenomena typically encountered in real engine flow fields but also were thoroughly and creditably documented in the literature. Several new turbulence models developed at CMOTT have been successfully implemented. Some important results coming out of this effort have been submitted for presentation at ASME and AIAA conferences. They will also be reported in NASA TMs shortly. It is believed that this effort will help in building up the applicability envelope of turbulence models in compressible flow environments.

In cooperation with Andrew Norris of ICOMP, research in this period also included performing turbulent reacting flow calculations using probability density function methods and turbulence models developed at CMOTT. This project was initiated only recently.

**CHAOQUIN LIU**

The direct numerical simulation (DNS) method is still limited to only simple, low Reynolds number flows due to its extremely high CPU cost and thus, so far, it is not useful for real engineering applications. This effort is intended to develop a procedure to simulate the large scale motions in a flow by using rather coarse grids and then to apply it to engineering problems. After successfully simulating the whole process of flow transition in 3-D boundary layers last summer, we now use this code for fully-developed turbulent channel flow by using a 34 x 66 x 34 grid. We will compare the numerical results with the published DNS results obtained by Kim et. al. for a 192 x 129 x 160 grid. Although the detailed data collecting and comparisons are in progress, already a qualitative agreement has been observed.

**JAMES LOELLBACH**

My research is focused primarily on the generation of structured grids in support of flow analyses of turbomachinery components using the HAH3D flow solver, developed by Chunill Hah of NASA Lewis. Applications include compressible transonic flows through axial compressor and turbine stages, and incompressible flows through centrifugal pumps. I am also working (in cooperation with Chunill Hah and Fu-Lin Tsung of ICOMP) on developing a hybrid structured/unstructured flow solver.

Turbomachinery component geometries often consist of closely spaced blades at high pitch angles within a single blade row, as well as closely spaced blade rows in the axial direction. The requirements of establishing periodic boundaries between the blades and axial boundaries between the blade rows can produce high skewness in structured grids. Excessive grid skewness degrades both the accuracy and convergence rates of most flow solvers.

In an attempt to alleviate this problem, we are deviating from the H-grid topology often employed in the axial and blade-to-blade directions. Instead, we are using what is called an I-grid topology, which is essentially an H-grid centered about a blade with relaxed periodicity constraints on the interblade boundaries. Points are allowed to move along the curves defining these boundaries until the blade-to-blade grid lines intersect the boundaries at nearly right angles. Thus, while the curves defining the interblade boundaries of adjacent grids coincide with each other, they are discretized differently. The advantage to this approach is that the overall skewness of the grid can be greatly reduced. The disadvantage is that the flow solver must include additional logic to interpolate flow properties across the interblade boundaries.

I have been developing a set of programs and subroutines to simplify the generation of such grids for a wide range of configurations. The goal is not to develop a single, generalized grid generation package, but instead to create a set of routines which can be quickly combined into simple, easy-to-use programs for specific types of geometries. Eventually, some higher-level drivers may be written to link particular routines together for application to broader classes of configurations. The grid generation techniques that are used consist of both algebraic methods and elliptic differential equation methods.

The use of unstructured grids offers another approach to alleviating some of the problems caused by the complicated geometries of turbomachines. Unstructured grids, composed of tetrahedra or more general polyhedra, can be created using generalized methods for practically arbitrary configurations. Unstructured grid generation and flow solution techniques, however, are not fully mature, especially for three-dimensional viscous flows. Grid generation issues concerning cell aspect ratios and small cell sizes in boundary layers are being addressed by many different researchers. Flow solution issues related to the accuracy of viscous terms and turbulence modeling are also unresolved at this time. By developing a hybrid structured/ unstructured flow solver, we are attempting to take advantage of the strong points of both approaches. A structured grid will be used near solid walls where fine grids and accurate viscous modeling are required. Away from solid walls, the structured grid will mate with an unstructured grid. Preliminary results have been obtained, and the effectiveness of the scheme is being evaluated.

### SHERWIN A. MASLOWE

This year, I have continued to investigate resonant triad interactions in two-dimensional free shear layers. The goal is to describe vortex pairing and related phenomena that greatly influence the downstream evolution of mixing layers. In a recent paper coauthored with R. Mallier (J.F.M. 278, 1994), a number of features observed in experiments were duplicated by using a pair of oblique waves to model the subharmonic instability associated with vortex pairing. When these waves are inclined at  $\pm 60^\circ$  to the mean flow direction, their interaction with a plane neutral mode satisfies the resonance conditions exactly. By perturbing away from this state so that all modes were amplified, it was possible to formulate an analysis employing a non-equilibrium critical layer that is self-consistent as an asymptotic theory.

Various developments are possible depending on the initial amplitude of the oblique waves compared with that of the plane wave. Whereas these amplitudes were essentially all of the same order of magnitude in the paper by Maslowe and Mallier, a formulation more in accord with the experimental observations reported to date is presently being developed in collaboration with Lennart Hultgren of NASA Lewis. Specifically, if  $\epsilon$  is an amplitude parameter characteristic of the plane wave and  $\delta$  is the amplitude of the oblique waves, then the condition  $\delta \ll \epsilon^3$  ensures that the plane wave saturates before the onset of a stage in which the modes are fully coupled.

The approach of the plane wave toward equilibrium is described by the nonlinear, quasi-equilibrium analysis of Hultgren (J.F.M. Vol. 236, 1992) which includes viscous and nonparallel effects. At the same time, a parametric resonance leads to enhanced growth of the subharmonic oblique waves and their critical layer becomes thicker than that of the fundamental. Eventually a fully coupled stage is

reached and our results to date indicate a rapid amplification of the subharmonic. This may correspond with the increased rate of thickening observed in experiments near the sites of vortex pairing. We are making further comparisons with experiment and a paper is in preparation.

#### A. F. MESSITER

An asymptotic study of the long-wave instability of a supersonic shear layer has been completed. In the case considered, the disturbance is large enough that the amplitude is of the same order as the shear-layer thickness. Some of the main features were outlined in the 1993 ICOMP Annual Report. This year the work was extended in two ways: to describe the upstream behavior of this problem formulation; and to include consideration of certain other limiting cases, in an attempt to explain how the instability of a supersonic vortex sheet, with zero thickness, is related to the long-wave instability of a thin supersonic shear layer; the second extension is elaborated upon below.

If the spatial period is chosen as the reference length, the three primary nondimensional parameters are the disturbance amplitude, the shear-layer thickness, and the reciprocal of the Reynolds number. Each of these parameters is taken to be small, and different asymptotic representations can be obtained depending on the relative smallness of the three quantities. The parameter space can be reduced to a plane by introducing coordinates which are the logarithms of the amplitude and layer thickness divided by the logarithm of the Reynolds number. In one region of this plane (for small enough amplitude) the correct first approximation is the linear theory for disturbances to a shear layer; in another region (for large enough amplitude) the vortex-sheet representation is correct as a first approximation. Between these two regions there are various possibilities. It appears that there are three special points, corresponding to three specific limit processes and therefore three specific asymptotic descriptions involving various balances among effects of nonlinearity, diffusion, and slow diffusion. At each of these points the approximate equations contain more information than the equations obtained in any neighborhood of the point. The present case corresponds to one such limit, the case considered by T. F. Balsa to another, and there is a third that has not yet been considered in detail. A report is in preparation that may help to explain the relationships between the vortex-sheet limit and various shear-layer limits.

#### DAVID MODIANO

The goal of this project, which is being conducted in collaboration with E. Steinthorsson (ICOMP) and P. Colella (University of California at Berkeley and Lawrence Livermore National Laboratory), is to apply the Adaptive Mesh Refinement (AMR) method to the solution of the Navier-Stokes equations on mapped grids. Previous work by Colella, *et al.* produced an AMR algorithm for Cartesian meshes and a Godunov-based solver for the Euler equations on mapped grids. Work in 1994 involved the extension of the AMR algorithm to mapped grid systems. Extensive use was made of the AMR Library of C++ utility routines, developed at the Lawrence Livermore National Laboratory. E. Steinthorsson and I attended the Third AIAA Northern Ohio Mini-Symposium "Aerospace Today", held at the Cleveland State University, Cleveland, Ohio in May, 1994, where we presented papers on the adaptive refinement method and on the use of object-oriented programming. The complete implementation of the adaptive refinement algorithm using mapped grid systems was demonstrated at the ICASE/LaRC Workshop on Adaptive Grid Methods in November, 1994. The extension of the mapped grid AMR to arbitrary multiblock grid systems is under way and is expected to be completed shortly. Further work should involve the incorporation of viscous terms into the adaptive refinement procedure, and an extension to 3-D.

#### ANDREW T. NORRIS

My research is concerned with developing PDF methods for turbulent reacting flows. First, a comparison was made between combustion calculations performed by the laminar flame approximation (used in many conventional moment closure schemes) and the nodal PDF method used in the LPDF2D code [1]. It was shown that for turbulent combustion with a Damkohler number (defined as the ratio of

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turbulent to chemical time scales) of order one, the PDF method gives a far superior performance than the conventional approach. The flow used in this paper is the piloted CO/H<sub>2</sub>/N<sub>2</sub> - air diffusion flame of Masri et al. [2].

Second, the phenomenon of extinction was predicted by a velocity-dissipation scalar PDF model. Very good agreement was shown between the experimentally determined extinction conditions and those predicted by the PDF model. Again, the flow used in this paper was the piloted CO/H<sub>2</sub>/N<sub>2</sub> - air diffusion flame of Masri et al. [2]. Thermochemistry was modeled by a 3-scalar simplification of the full mechanism, obtained by the ILDM method of Maas and Pope [4]. This paper was selected for publication in a special edition of the Combustion and Flame journal.

Third, at the industry-wide turbulence workshop, organized by CMOTT, the LPDF2D 1.2 code was released. This code contains several new features not present in the 1.0 version. They are: a) A new time averaging scheme was developed to reduce statistical error and save memory. Details of this scheme were presented at the AIAA Reno Conference [5]; b) Several new combustion models have been added, including adaptive lookup tables and CHEMKIN compatibility; and c) The code has been ported to a workstation environment, and also implemented in a parallel cluster, using PVM message passing.

Finally, a collaborative effort was initiated with Pratt and Whitney to provide a series of post-processing tools for combustion calculations based on the PDF transport equation. The first stage, a NO<sub>x</sub> prediction tool for 2D structured meshes, has been written and tested on a Pratt and Whitney experimental combustor. Further development will occur extending this tool for 3D unstructured meshes with arbitrary chemical species.

Next year's focus will be on developing the Pratt and Whitney post processors and on extending the LPDF2D code to 3D, both tasks involving the use of parallel and massively parallel machines.

1. A.T. Norris and A.T. Hsu: "Comparison of PDF and Moment Closure Methods in the Modeling of Turbulent Reacting Flows", ICOMP 94-9, CMOTT 94-3, NASA TM 106614, AIAA 94-3356, 1994.
2. A. R. Masri; R. W. Dibble; and R. S. Barlow: "The Structure of Turbulent, Pilot Stabilized Flames of CH<sub>4</sub>/CO/H<sub>2</sub>/N<sub>2</sub> Fuel Mixtures", Combustion and Flame, 1993. (in Press.)
3. A.T. Norris and S.B. Pope: "Modeling of Extinction in Turbulent Diffusion Flames by the Velocity-Dissipation-Composition PDF Method", In Twenty-Fifth Symposium (International) on Combustion, 1994, (In Press).
4. U. A. Maas and S. B. Pope: "Simplifying Chemical Kinetics: Intrinsic Low-Dimensional Manifolds in Composition Space", Combustion and Flame, 88(3/4) ,1992, p239-264.
5. A. T. Hsu; M. S. Raju; and A. T. Norris: "Application of a PDF Method to Compressible Turbulent Reacting Flows", In AIAA 32nd Aerospace Sciences Meeting and Exhibit, Reno, Nevada, AIAA 94-0781, 1994.

### CHRISTOPHE PIERRE

The purpose of this research is the development of computational tools for understanding and predicting the effects of unavoidable blade-to-blade dissimilarities, or mistuning, on the dynamics of nearly cyclic bladed-disk assemblies. This topic is of importance as mistuning has been shown to increase the forced response amplitudes of some blades significantly, and even to lead to single blade failure. Furthermore, the trend toward high performance propulsion turbomachinery designed for finite service life demands an accurate prediction of system performance and dynamics.

This past year, research supported by ICOMP has focused on two areas. First, the applicability of the transfer matrix method to the study of mode and wave localization in mistuned assemblies has been examined and demonstrated, resulting in the compact characterization of the effects of mistuning by scalar *localization factors*. Second, these localization factors have been utilized in the formation of an optimization constraint which would allow one to prevent damaging mistuning effects at the design stage, based solely on tuned system information and anticipated mistuning strength. One paper [1] and one technical note [2] have been written and accepted for journal publication.

1. Ottarson, G.; and Pierre, C.: "A Transfer Matrix Approach to Free Vibration Localization in Mistuned Blade Assemblies", ICOMP 93-10, NASA TM 106112, 1993, also, Journal of Sound and Vibration, 1994, in print.
2. Murthy, D.; Pierre, C.; and Ottarson, G.: "An Efficient Design Constraint Accounting for Mistuning Effects in Engine Rotors", AIAA Journal, in print.

#### **RICHARD H. PLETCHER**

Work was continued with Philip Jorgenson on the simulation of internal viscous flows using unstructured grids. Some of the early results were reported in a paper presented at the 1994 Aerospace Sciences meeting (Jorgenson and Pletcher, "An Implicit Numerical Scheme for the Simulation of Internal Viscous Flows on Unstructured Grids", AIAA 94-0306, ICOMP Report 93-48). Recently, improvements have been made in the grid generation scheme to permit representation of more complex geometries. Work is also underway to improve treatment of viscous effects, increase the efficiency of the algebraic equation solver, and to incorporate turbulence modeling.

With graduate student Tom Ramin, both explicit and implicit versions of the two-dimensional cell-centered unstructured viscous flow code have been developed and implemented on parallel machines including the nCube2s at Iowa State University and the LACE workstation cluster at the NASA Lewis Research Center. An implicit upwind version of the unstructured scheme has been extended to three dimensions and is running on the nCube, LACE cluster, and the Cray YMP. Work is continuing on the three-dimensional scheme to improve algorithm efficiency and to reduce memory requirements. A paper on the development of the three-dimensional scheme and the implementation on parallel machines is in preparation. Work on unstructured grid schemes for combustion applications has also been initiated with graduate student Rob Cupples.

In the area of low Mach number preconditioning, the results reported in AIAA 93-3368-CP, ICOMP Report 93-43, are being supplemented with additional calculations to establish the time-accuracy of a preconditioned compressible Navier-Stokes solution scheme over a range of Mach numbers including the incompressible limit. The combined results to date will be reported in an article being prepared with K. H. Chen.

#### **ROBERT RUBINSTEIN**

My research is concerned with renormalization group theory of Bolgiano scaling in Boussinesq turbulence. Boussinesq turbulence is the simplest problem with coupled fluctuating fields. As such, the understanding of the possible scaling regimes in Boussinesq turbulence will be useful in other problems as well.

Application of the Kolmogorov scaling theory of hydrodynamic turbulence to Boussinesq turbulence suggests two regimes. The simpler possibility is that the gravitational coupling can be neglected. Then the temperature is a passive scalar and the velocity and temperature fluctuations have Kolmogorov spectra. The Kolmogorov regime is characterized by a constant flux of kinetic energy. Bolgiano identified a second possibility in which there is a constant flux of temperature variance. This leads to scaling exponents distinct from the usual Kolmogorov indices.

Bolgiano scaling in Boussinesq turbulence was analyzed by applying the Yaghot-Orszag renormalization group to an isotropic model problem. Scaling exponents were calculated by forcing the temperature equation so that the temperature variance flux is constant in the inertial range. Universal amplitudes associated with the scaling laws were computed by expanding about a logarithmic theory. Connections between this formalism and the direct interaction approximation were discussed. The Yaghot-Orszag theory yields a lowest order approximate solution of a regularized direct interaction approximation which can be corrected by a simple iterative procedure.

This work has been reported in "Renormalization Group Theory of Bolgiano Scaling in Boussinesq Turbulence", ICOMP 94-8, CMOTT 94-2, NASA TM 106602, 1994.

**JAMES N. SCOTT**

In a collaborative effort with S. I. Hariharan of The University of Akron and R. R. Mankbadi of NASA Lewis, an investigation was conducted to assess the application of several numerical schemes to the analysis of noise production and propagation in an unsteady flow. In particular, four different numerical algorithms have been utilized to compute the flow about a flat plate in the presence of a transverse gust described by a sinusoidal disturbance. This is described as Problem Category 6 in the CAA Benchmark problem description. Since viscous effects are ignored in this problem, the governing equations are the linearized Euler equations, which are also generally regarded as suitable for analyzing the propagation of acoustic disturbances.

The four schemes include: the MacCormack explicit finite difference scheme which is second order accurate in both time and space; the Gottlieb and Turkel modification of MacCormack's scheme which is fourth order accurate in space and second order accurate in time, (referred to as a 2-4 scheme); the fourth order Dispersion Relation Preserving (DRP) scheme of Tam and Webb; and a two step scheme developed by Bayliss et. al. which has second order temporal accuracy and sixth order spatial accuracy (a 2-6 scheme). The flowfield results are obtained with these schemes by using the same code with the only difference being the implementation of the respective solution algorithms. The computed results include the time history of the acoustic pressure along grid lines five points away from the boundaries. In addition, the pressure distribution throughout the computational domain is monitored at various times. The numerical results are compared with an exact solution obtained by Atassi, Dusey, and Davis.

The problem is formulated so that the sinusoidal disturbance is imposed at the surface of the flat plate as a surface boundary condition. Thus the problem is treated as a scattering problem. At the outer boundaries, the computational procedure incorporates boundary conditions developed for far field asymptotic expansions for the linearized Euler equations which are consistent with acoustic analyses. These formulations have been developed and demonstrated by Hariharan and Hagstrom. It should be noted that while the grid, boundary conditions, and general overall procedure are the same for all schemes, a smaller time step was required for the DRP scheme in order to achieve stable solutions. The MacCormack schemes and the 2-6 scheme utilize a time step size of .25 while the DRP scheme utilizes an optimized time step of 0.596. The grid is comprised of 200 points in both the x and y directions and the grid spacing is equal in both directions. This gives a uniform spatial step size of 1 in both the x and y directions. A study of the influence of grid size has been conducted by increasing the size of the grid to 600 points in both the x and y directions and the results indicate that substantial improvement can be achieved by increasing the extent of the computational domain. In addition, the computation run time for this case was increased substantially and good agreement with the analytical results of Atassi and his associates was achieved.

**AAMIR SHABBIR**

In last year's report I briefly described my work aimed at developing a two equation model for the scalar turbulence in which transport equations for the scalar variance and its dissipation rate are used to calculate the turbulent eddy diffusivity. The work toward the development of a new model equation for the thermal dissipation equation for wall-free flows had already been completed at that time. This model has now been extended to calculate the wall bounded flows. The diffusion term in the thermal dissipation equation has been modeled using the gradient diffusion hypothesis, similar to its counterpart in the mechanical dissipation equation. The model equation balances the log-layer of a flat plate boundary layer which has a constant surface temperature. The newly developed model for the constitutive relation for the scalar flux also gives the correct level of thermal diffusivity for a log-layer. The complete model has been successfully applied to several benchmark cases of homogeneous scalar turbulence. The model has also been successfully applied to the flat plate boundary layer with a constant surface temperature using wall functions. The results compare favorably with the experimental data of Gibson et al. The future work for this project will involve assessing the model for other wall boundary conditions for the thermal/scalar field and extending the model for integration down to

the wall. This will require providing the damping functions for the thermal variance and thermal dissipation rate.

Some of the effort was directed toward developing and assessing the performance of a new two equation k-epsilon model in a joint effort with the other CMOTT researchers and is reported in a paper by Shih et al. The model performs reasonably well for a host of benchmark flows which include: rotating homogeneous shear flow; various flat plate boundary layers; mixing layers; and jets.

An industry-wide workshop on computational turbulence modeling was also organized in collaboration with local researchers as well as with industry researchers. The objective of the workshop was twofold; to discuss the current needs of the industry in turbulence modeling and to transfer the technology developed at ICOMP. The details of the workshop are given in a separate section of this ICOMP Annual Report.

1. M. M. Gibson, C. A. Verriopoulos and Y. Nagano: "Measurements in the Heated Turbulent Boundary Layer on a Mildly Curved Convex Surface". In Turbulent Shear Flows 3 (Edited by L.J. S. Bradbury et al.) pp. 80-89. Springer, Berlin (1982).
2. T.-H. Shih, W. W. Liou, A. Shabbir, Z. Yang and J. Zhu: "A New k- $\epsilon$  Eddy Viscosity Model for High Reynolds Number Turbulent Flows". To appear in Computers and Fluids.

#### SHYUE-HORNG SHIH

The present research is a part of the continuing effort for developing noise prediction capabilities using Computational Aero-Acoustics techniques. Large eddy simulation (LES) of the unsteady, compressible Navier-Stokes equations is applied to a round jet to obtain the time-dependent flow and acoustic fields. During the past year, work was done in the following areas:

1. In simulating a round jet, the centerline ( $r=0$ ) is a boundary of the computational domain. Spurious modes can be generated near the centerline unless special attention is given to the behavior of the 3D structure near the centerline. Three approaches to the centerline treatment are considered, namely, asymptotic, averaging, and interior points approaches. Computational results were obtained for a Mach 1.5 supersonic jet with a pair of helical mode excitations. The results clearly showed the helical nature of the flow structure in a circular jet. This work will be presented at the 33rd AIAA Aerospace Sciences Meeting [1].

2. The second work consisted of a direct computation of both the flow and acoustic fields for the axisymmetric jet. Existing experimental data were surveyed and those from a Mach 2.1 jet experiment were selected for comparison with results from the analytical solutions. Various boundary conditions, including Thompson, Giles, Tam & Webb, and radiation boundary conditions are implemented into the code. These results will be presented at the 33rd AIAA Aerospace Sciences Meeting [2].

Future directions for this research are as follows. (1) A zonal approach for prediction of three-dimensional jet noise. In this work, large eddy simulation will be limited to the nearfield and the linearized Euler equations will be used for extension to the far field. (2) Control of jet noise via inflow excitation, which in turn controls the subsequent development of the coherent structure, the spreading of the mean flow, and the radiated sound. The following excitation patterns will be considered: (a) single frequency excitation with various frequencies and amplitudes; (b) bi-modal excitation at the fundamental and subharmonic frequencies; and (c) resonant triad which consists of a pair of oblique waves at the subharmonic frequency and a fundamental axisymmetric frequency.

1. Shih, S. H., Hixon, D. R. and Mankbadi, R. R., "Three-Dimensional Structure in a Supersonic Jet: Behavior Near Centerline", AIAA Paper 95-0681, January, 1995.
2. Mankbadi, R. R., Shih, S. H., Hixon, D. R. and Povinelli, L. A., "Large-Scale Simulation of Flow and Acoustic Fields of A Supersonic Jet", AIAA Paper 95-0680, January, 1995.

### **TSAN-HSING SHIH**

As technical leader of the CMOTT group, I have been involved in all CMOTT's turbulence modeling research activities. There has been a major, intensive effort this year by the CMOTT research group to incorporate new and physically correct turbulence models into the working CFD codes, such as NPARC, used at NASA Lewis. This is an ongoing effort to demonstrate the value of improved turbulence models to user groups. In addition to the NPARC work, are propulsion-related projects to achieve improved combustion codes, inlet/nozzle flow codes and a turbomachinery code that will be tested against detailed experimental data from NASA Lewis' Rotor 37 studies. Early results from this work already point to the merits of this objective.

In a related activity, I was responsible for organizing the 1994 Industry-Wide Workshop on Computational Turbulence Modeling, sponsored by ICOMP/CMOTT and held at the Ohio Aerospace Institute on October 6-7, 1994. An overview of this workshop is given in a separate section of this report. In addition, I have been developing improved two-equation and Reynolds stress transport equation models.

### **WEI SHYY**

A pressure-based multi-block computational method has been developed for solving the incompressible Navier-Stokes equations in a general curvilinear grid system. For the momentum equations, the pressure fields between two adjacent blocks allow an arbitrary jump, which can be adjusted by conserving the total momentum fluxes across the block interface. The importance of maintaining local mass flux conservation across the interface with certain accuracy is illustrated through a series of numerical experiments. Specifically, without conservative measure for the mass flux at the interface, the linear and quadratic interpolations cannot lead to the desired solution even for very fine grids. Linear interpolation with global correction for mass flux does not improve the solution either. The piecewise constant treatment can improve the solution accuracy due to its conservative nature, but it creates artificial pressure oscillations due to the non-smooth mass flux distribution in the fine grid block. Nevertheless, it illustrates the importance of local mass flux conservation across the interface. Both linear and quadratic interpolations, with local conservative correction, prove to be good choices. The fact that their solutions are of very comparable accuracy indicates that (1) the interface treatment does not need to be of higher formal order of accuracy than the interior schemes, and (2) the local conservative mass flux treatment at the interface holds a key for composite grid computations.

### **ERLENDUR STEINTHORSSON**

As in the previous year, my research has been conducted on two fronts; the continued development of TRAF3D.MB, a multiblock/multigrid flow solver for flows in complex geometries, and the development of solution-adaptive mesh refinement (AMR) methodology that can be used effectively in structured body-fitted grid systems. The objective of both research projects is to develop methodologies that will allow detailed and accurate simulations of flows in complex geometries, such as coolant passages of turbine blades, with efficient use of computing resources.

This year, the TRAF3D.MB code was enhanced by adding a capability to simulate flows in rotating reference frames, and by refining the central differencing scheme for the inviscid flux terms of the governing equations. Also, in cooperation with Ali Ameri (Resident research associate, NASA LeRC), the ability to handle grid systems with non periodic branch cuts was added. The formulation adopted to enable simulations of flows in rotating reference frames was proposed by Chima and Yokota (NASA TM 100878). The central differencing scheme in the code was modified to make it more compatible with the use of multiblock grid systems. In particular, the artificial dissipation terms were modified to ensure conservation of fluxes at block boundaries, and to ensure minimal dissipation at all solid-wall boundaries. At the same time, solid wall boundary conditions were tuned to minimize artificial entropy generation at solid wall surfaces.

With the above enhancements, the TRAF3D.MB code was used in the study of tip heat transfer in a SSME turbine cascade. The code proved capable of accurately matching available experimental data for the cascade and the computed solution provided new insights into the behavior of the flow in the clearance between the tip and the shroud. The results are discussed in a forthcoming paper (Ameri, A., and Steinthorsson, E., "Prediction of Unshrouded Rotor Blade Tip Heat Transfer," to be presented at the ASME International Gas Turbine Conference and Exposition, Houston, Texas, June, 1995). The code is currently being applied in the study of coolant flows in turbomachinery.

Solution-adaptive mesh refinement (AMR) in body-fitted grid systems has been studied in collaboration with David Modiano, ICOMP, and Phillip Colella, Univ. of California, Berkeley. The AMR algorithm of Berger and Colella (*J. of Comp. Physics*, Vol. 87, pp. 171-200, 1990) was applied to curvilinear, body fitted grid systems and implemented in a flow solver for unsteady, two-dimensional inviscid flows. The algorithm was implemented using mixed language programming, with a driver module written in C++, and routines executing computationally intensive parts of the flow solver written in FORTRAN. The implementation builds on a library of C++ routines developed at Lawrence Livermore National Laboratory to facilitate implementation of the AMR scheme of Berger and Colella (W. Y. Crutchfield and M. Welcome, "Object Oriented Implementation of Adaptive Mesh Refinement Algorithms", *Scientific Programming*, vol. 2, no. 4, winter 1993.). The current implementation of the AMR algorithm for curvilinear grid systems is described in ICOMP 94-17 (NASA TM 106704 and AIAA-94-2330).

#### **J. T. STUART**

During my visit to ICOMP, I worked with Reda Mankbadi on problems connected with sound radiation from jets. In particular, I studied Green's Functions and the Kirchhoff surface with a view to the creation of a simplified procedure for calculation of the sound radiation from a finite cylindrical source with end faces. I also considered another aspect of this subject, namely the appropriate formulation of viscous flow problems leading to transition to turbulence, the latter being a source of sound. Of growing importance is a better knowledge of the role of boundary conditions and their specification and this has been under consideration.

#### **TIMOTHY W. SWAFFORD**

As in the prior year, my activities centered around investigations into reducing the generation of entropy near impermeable walls with regard to numerically solving the two-dimensional Euler equations. Although the primary interest is in obtaining unsteady solutions, the present effort concentrated on obtaining steady-state solutions while minimizing the entropy generation near solid surfaces for test cases involving non-viscous, non-heat conducting flows (i.e., flows which should be isentropic throughout).

The numerical scheme employed is Whitfield's so-called 'm-pass' scheme, as used in the program NPHASE [1], with the exception that the left-hand side implicit operator is constructed using Jacobians computed numerically from the first-order Roe fluxes [2], as opposed to that reported in reference 1, where Steger-Warming flux vector splitting (FVS) was used to form the implicit operator. The approach taken in the present investigation was centered around the observation that computed static pressures at the wall appear to agree very well with corresponding solutions ensuing from codes in which the entropy is, by definition, zero (e.g., LINFLO, ref. 3). Therefore, if the assumption is made that pressures computed by the present method are 'correct', then perhaps adjustments can be made to the dependent variables within phantom cells (which are used to enforce a given boundary condition, in this case, no flux at the wall) which will tend to minimize entropy generation in this region.

Using the relation for the total energy of a fluid particle and the perfect gas equation of state, static pressure can be expressed in terms of density, velocity (two components), and total energy. This expression can be expanded into a Taylor series which results in a relationship that describes how the pressure at any field point changes from some initial state (supposedly entropy free) to another

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state as a function of changes in the above mentioned variables. The intent of this effort was to try and quantify how and to what extent these changes take place in a region of the flow field where entropy generation occurs (i.e., within cells where significant turning of the flow takes place, e.g., the leading edge). The particular geometry used was a planar version of the so-called 'waisted body of revolution', where the Mach number was subsonic ( $=0.6$ ). Solutions were executed until residuals reached machine zero (about 150 time steps at CFL=100). Within the leading edge cell, the computed value of density was 12.135% above the initial state, whereas the density required for isentropic flow is 12.935% above the initial value, assuming that the computed pressure is 'correct'. The relatively small difference between these values of density can often result in solutions containing unacceptably high entropy levels. How these observed changes in density are related to corresponding changes in velocity and energy (computed using the Taylor series expansion) remains under investigation.

1. Swafford, T.W.; Loe, D.H.; Huff, D.L.; Huddleston, D.H.; and Reddy, T.S.R.: "The Evolution of NPHASE: Euler/Navier-Stokes Computations of Unsteady Two-Dimensional Cascade Flow Fields", AIAA 94-1834-CP, June, 1994.
2. Whitfield, D.L.; and Taylor, L.K.: "Discretized Newton-Relaxation Solution of High Resolution Flux-Difference Schemes", AIAA 91-1539, June, 1991.
3. Verdon, J.M.; and Hall, K.C.: "Development of a Linearized Unsteady Aerodynamic Analysis for Cascade Gust Response Predictions", NASA CR 4303, 1990.

### CHRISTOPHER K. W. TAM

My work at ICOMP concerned the outflow conditions for instability and dispersive waves. It is well-known, within linear theory, that the growth rate and wave propagation characteristics of instability waves are controlled locally by the mean flow. Unlike acoustic waves, instability waves are generally slightly dispersive, that is, the wave speed varies slightly with wave number or frequency. This dependence can be found from the wave dispersion relation. Another distinct characteristic of instability waves which sets them apart from acoustic, vorticity or entropy waves is that a flow can support more than one mode of instability waves. Each mode of an instability wave has a distinct dispersion relation. For instance, a two-dimensional jet flow has two families of instability waves, namely, the varicose and the sinuous modes. For a circular jet, there are the axisymmetric mode, the helical/flapping mode and numerous high-order Fourier modes. In a recent work on supersonic jet noise, Tam and Chen showed that for cold jets the helical/flapping mode was the single dominant instability wave mode. It alone accounts for most of the turbulent mixing noise generated by the jet. But for jets at higher temperature, the noise from the axisymmetric instability wave mode is also important. In this case, there are two dominant modes. For very hot jets, it turns out that the contributions from as many as the first five azimuthal instability wave modes must be included in the calculations to provide good agreement with experiments. Jet noise is broadband. It is generated by a broad spectrum of instability waves. In this work, the slightly dispersive nature and the multi-mode as well as broadband spectral characteristics of instability waves are all taken into consideration in formulating the proposed outflow boundary conditions.

### GRETAR TRYGGVASON

Work continued on the development and application of the Tracked, Immersed Boundary (TIB) technique to simulate multifluid flows. The basic method is described in Unverdi and Tryggvason: "A Front Tracking Method for Incompressible Flows" (J. Comput. Phys., Vol.100, (1992), pp. 25-37). The specific work done at ICOMP has focused on drop collisions.

Some work was done on a three-dimensional topology change algorithm to make it more robust, but most of my time was devoted to the development of an axisymmetric version of the code with adaptive grid refinement. As for many flows, our simulations generally involve regions where the flow has relatively fine scales and a fine resolution is required and regions where the flow is smooth and we can

use much coarser grid. Furthermore, often one is interested in the behavior of drops far from walls or boundaries and a large computational domain is necessary to avoid effects of the boundaries of the computational domain. In both cases adaptive gridding is called for. In the method implemented this summer, I used a relatively simple stretched mesh to focus the resolution on the region where the drops collide. This code also includes heat transfer, and will eventually be extended to handle evaporation of drops. Both the adaptive gridding as well as the heat transfer part will also be implemented into our fully three-dimensional code.

Although our front tracking method is both robust and accurate, it is relatively complex for three-dimensional flow. In many cases, particularly for short time evolution, it is likely that simply capturing the front may be sufficiently accurate. Although several methods exist that claim to do so, most suffer from inaccuracy in implementing the proper interface stress boundary conditions, in maintaining a sharp boundary, and in conserving mass. I spent some of my time here this summer on an effort to devise a technique to overcome these problems. For the relatively simple test case of advection of a cylinder in a uniform flow, I was only partially successful in that while the interface is kept sharp, there are still grid effects that distort the cylinder.

Two manuscripts: "The Flow Induced by the Coalescence of Two Initially Stationary Drops" (ICOMP 94-24, NASA TM 106752) and "Numerical Simulations of Drop Collisions" (ICOMP 94-23, NASA TM 106751, AIAA 94-0835) describing work done in part during my earlier stay here have been issued as ICOMP reports.

#### **FU-LIN TSUNG**

A 3-D, unstructured, Navier-Stokes flow solver has been coupled with a 3-D structured code to allow structured-unstructured hybrid calculations. The two codes are loosely coupled and interact only through boundary conditions. The structured solver is a center-differenced finite-difference scheme and the unstructured solver is an upwind-differenced finite volume scheme. The hybrid procedure has been tested for a transonic wing and an annular cascade, and good results have been obtained. The flow properties across the boundary between the structured and unstructured portions of the grid are smooth and well behaved. The results show that two distinct discretization techniques can be coupled together with little effect on the solution accuracy, as long as both are of the same order.

Detailed and extensive testing of the stress terms and  $k-\epsilon$  turbulence model for the unstructured solver is currently underway; the test cases include turbine stators, axial compressor rotors, and centrifugal compressors. Once the unstructured solver is judged accurate and reliable in a highly viscous region, it will be used to calculate complex flows over a rim seal cavity geometry.

#### **ELI TURKEL**

Work continued in collaboration with Etesham Hayder, on developing and comparing boundary conditions to be used at the inflow and outflow boundaries for jet acoustic problems. A series of radiation boundary conditions developed by; 1) Bayless and Turkel; 2) Giles; 3) Tam and Webb; and 4) Hariharan and Hagstrom were compared for both subsonic and supersonic jets. Both inflow and outflow boundaries were considered. The results were published in ICOMP Report 94-12 (NASA TM 106648, AIAA Paper 94-2195) and presented at the AIAA 25th Fluid Dynamics Conference in Colorado Springs, CO, June, 1994.

Another project was the development of preconditioning matrices for both compressible and incompressible flows. Work is just beginning with A. Arnone (ICOMP and the University of Florence) to implement these conditions into his compressible code. It was incorporated in his incompressible code earlier. The method will also be useful to other internal fluid dynamics codes employed at Lewis.

#### **BRAM VAN LEER**

Multi-dimensional advection schemes that include independent updates of several moments of the distribution of the state variable inside a computational cell were investigated. For instance, a second-

order scheme with third-order evolutionary error can be obtained using a linear distribution with least squares-fit gradient in each cell (van Leer, 1977) There is renewed interest in such schemes since they yield high accuracy on very compact stencils, a desirable feature when implementing these on a massively computer. The three dimensional version of this scheme was derived; this had not been done previously. Compact schemes in general were discussed with Hung T. Huynh (LeRC) and Robert Lowrie (doctoral student at the University of Michigan, visiting ICOMP).

**DAVID WHITFIELD**

In the numerical solution of the unsteady Euler and Navier-Stokes equations, the formal linearization of the equations sometimes includes the time derivative as part of the residual vector in order to ensure time accuracy. This approach can be viewed as a Newton formulation for the numerical solution of the equations although the linear subsystem of equations is sometimes solved iteratively rather than directly [refs.1,2]. When this Newton formulation approach is used to obtain steady state solutions, one frequently does not update the residual vector because time accuracy is not of interest when proceeding to a steady state. However, my work centered on following the same numerical approach for solving steady state problems as for unsteady problems with the exception of using local time stepping for steady state problems. This requires updating the residual vector when going from time level  $n$  to  $n+1$ . The results of this exercise were interesting in that it was found that the CFL number could be increased tremendously by using Newton iterations compared to what could be used without Newton iterations if the linear subsystems were solved rather accurately. Even when the extra CPU time was invested in the Newton iterations and the improved iterative solution of the subsystems, it was possible to save up to a factor of three in CPU time to comparable levels of convergence ( in this case, machine zero in 64 bit arithmetic). The approach used to obtain the steady state is the discretized Newton-relaxation (DNR) method, described in references 1-3, that has been used for unsteady solutions of the Euler and Navier-Stokes equations.

1. Vanden, K.J.; and Whitfield, D.L.: "Direct and Iterative Algorithms for the Three-Dimensional Euler Equations", AIAA 93-3378, July, 1993.
2. Whitfield, D.L.; and Taylor, L.K.: "Discretized Newton-Relaxation Solution of High-Resolution Flux-Difference Split Schemes", AIAA 91-1539, June, 1991.
3. Whitfield, D.L.; and Taylor, L.K.: "Numerical Solution of the Two-Dimensional Time Dependent Incompressible Euler Equations", Engineering and Industrial Research Station Report MSSU-EIRS ERC 93-14, Mississippi State University, Mississippi State, MS, April. 1994.

**DANIEL WINTERSCHIEDT**

My research has involved the application of unstructured methods to the problem of transient, compressible flow. In particular, I have concentrated on the solution of the Euler equations in two dimensions. Upwind methods on structured grids have been developed which are capable of handling the discontinuous nature of the Euler equations. These schemes include flux vector splitting, where the flux terms are split and discretized directionally according to the sign of the associated propagation speeds, and flux difference splitting, where an approximate local solution of the Euler equations is introduced in the discretization. Most finite element researchers have been reluctant to use these types of upwinding methods, preferring instead to use either Petrov-Galerkin methods or Galerkin methods with some type of artificial dissipation added. Only recently have the above mentioned upwind schemes been incorporated into finite element formulations for the Euler equations.

A common finite element approach for these types of problems involves an explicit Taylor-Galerkin formulation which is basically a finite element implementation of the Lax-Wendroff method. Linear elements are generally used because of the discontinuous nature of the solution and for the simplicity of element computations. This method was implemented in two dimensions using triangular elements. Although the method does yield some high frequency dissipation, additional dissipation terms

are necessary to control strong shocks. The basic scheme is second order accurate although higher temporal accuracy can be achieved using a multi-step method. In an effort to better resolve strong shocks, a method was developed which uses upwinding rather than artificial dissipation. The 'upwinded' flux values were only used in elements with extremely large solution gradients. In smooth regions, the standard Taylor-Galerkin finite element method was used to compute the flux values. The method is therefore second order accurate except in the vicinity of discontinuities. The approach was implemented on a mesh of triangular elements and successfully tested on flow past a NACA 0012 airfoil at several Mach numbers.

Although unstructured methods easily accommodate complex geometry, the resulting spacial discretization is, at best, second order accurate. Typically an extremely fine mesh is required to properly resolve the flow solution. Several high-order flux interpolation methods were investigated in an effort to improve the spacial accuracy. Unstructured meshes composed of triangular or quadrilateral elements were used. High-order flux interpolation was achieved by the use of an expanded stencil. The method was successfully implemented, but the high-order interpolation on the unstructured mesh was found to be computationally intensive. The h-p version of the finite element method is an alternative approach which may prove to be more efficient.

#### JIE WU

Since I joined ICOMP in March 1994, I have been working on the development of a complete multi-disciplinary analysis package for engineering problems related to propulsion systems. This is a joint effort with Bo-Nan Jiang (ICOMP), Nan-Suey Liu (LeRC Internal Fluid Mechanics Division) and Sheng-Tao Yu (NYMA Setar Team). The whole effort involves introducing the correct formulations for the problems of interest, developing and validating the general computer code, and implementing and validating the necessary models (such as the turbulence models and the chemical reaction models). In the past year I was mainly responsible for the code development and part of the code validation work.

The methodology of the least-squares finite element method (LSFEM) is chosen as the basis for this package. The reasons for this choice are: (1) that LSFEM has proved to be a simple and unified method for many different types of problems, and (2) that LSFEM operates on totally unstructured grids. The latter is of great importance when complicated geometries such as those in propulsion systems are in consideration.

To date, a general LSFEM computer code has been developed for solving three-dimensional fluid flows and conjugate heat transfer problems, for both time-dependent and steady-state situations. This code uses linear and quadratic unstructured elements and incorporates the following:

1. velocity/vorticity/flux component (normal or tangential) specification on complex geometries (e.g., on symmetric, slippery and adiabatic boundaries);
2. non-reflecting boundary conditions (e.g., at the outlet);
3. interfacing conditions of both temperature and heat fluxes for conjugate heat transfer problems.

This code uses a matrix-free preconditioned conjugate gradient (PCG) method to solve the algebraic equation systems which requires much less computer memory than other approaches and enables large problems to be solved in moderate computer systems. The code has been extensively tested on two-dimensional incompressible fluid flow problems. By performing numerical tests on a standing vortex problem, we demonstrated that the present scheme introduces no additional numerical dissipation by showing that the kinetic energy of a inviscid fluid in a closed system is totally conserved. We also showed that the non-reflecting boundary condition enables a vortex to propagate out of the domain without being reflected back or distorted by the existence of the artificial outflow boundary. The code has also been tested on the problem of vortex shedding by a circular cylinder and flow around a NACA 0012 airfoil. Very accurate results have been obtained for all test cases.

This code has also been extensively tested on two-dimensional low-Mach-number fluid flow problems (this work was mostly carried out by S. T. Yu). The code has also been tested on three-dimensional lid-driven cavity flow and fully developed channel flow. Several meshes and rotated

coordinate systems have been used to ensure that the solution is mesh-independent. Some other tests have also been performed, including a 2D demonstrative test to show the ability of the package in handling the complex geometry of a combustion chamber. Some preliminary tests have also been carried out on 2D conjugate heat transfer problems. Comparisons have been made with analytical or other numerical solutions where possible.

The nature of LSFEM makes it possible to develop a general computer code framework in such a way that, with modifications in a few subroutines which describe the governing equations and the associated boundary conditions, it can be used to solve completely different problems. An example of this is the modification of the flow/conjugate thermal code to solve electro-magnetic scattering problems. These problems are governed by the time-dependent Maxwell's equations. Numerical tests carried out here further confirmed the excellent performance of the time-accurate LSFEM formulation and the non-reflecting boundary conditions.

### ZHIGANG YANG

In the past year, my research activity has been focused on the development of a  $k-\epsilon$  two-equation turbulence model and its applications to flows in propulsion systems. The  $k-\epsilon$  two-equation turbulence model is the most widely used turbulence model in engineering flow calculations; however, current two-equation models are inadequate for the complex flows in propulsion systems which contain complex flow phenomena including mixing, pressure gradient effects, shock wave-turbulent boundary layer interaction, and separation. In addition, the geometries involved in propulsion systems are often very complex, and it is very difficult to use any turbulence model which depends on the coordinate information.

A new  $k-\epsilon$  two equation model has been developed. No geometry information is used in constructing the near wall corrections so that the final model form is Galilean and tensorially invariant. Thus the model could be easily incorporated into a CFD code with unstructured grids and used for flows with complex geometry. For wall bounded flows, it captures accurately the effect of the pressure gradient on the skin friction. For mixing in free-shear flows, it is free from the round jet/plane jet spreading rate anomaly, which is associated with most turbulence models. Preliminary results were reported in the 1994 Industry-Wide Workshop on Computational Turbulence Modeling, sponsored by ICOMP/CMOTT and held on Oct. 6-7 at the Ohio Aerospace Institute. A paper detailing the model is in preparation.

The purpose of turbulence models is to predict flows in engineering and in nature. In this regard, the NPARC code, a general purpose code widely used in the propulsion systems community, is used as a base code. Two-equation turbulence models are incorporated into the NPARC code via a separate turbulence subprogram written by Jiang Zhu of CMOTT. Different turbulence models have been tested against typical flows in propulsion systems. A paper containing these model applications has been submitted to the 1995 AIAA-ASME-SAE-ASEE Joint Propulsion Conference.

### AKIRA YOSHIZAWA

Some of the difficulties with the familiar representation of turbulent-viscosity, based on the turbulent kinetic energy and its dissipation rate, arise from its equilibrium character. As a method of alleviating these difficulties, the inclusion of the  $D/Dt$ -related nonequilibrium effect has already been proposed and its validity has been confirmed in highly nonequilibrium flows like homogeneous-shear flow with a large initial shear rate [refs. 1,2].

During my stay at ICOMP, this concept was developed further to introduce a model transport equation for the nonequilibrium turbulent viscosity with the aid of a result from a two-scale direct-interaction approximation (TSDIA). The resulting model consists of three equations for: 1) the turbulent kinetic energy; 2) its dissipation rate and; 3) the nonequilibrium turbulent viscosity. The first two equations are used to calculate the equilibrium part of the turbulent viscosity. The application of this model to some typical turbulent flows subject to strong nonequilibrium effects is in progress.

1. Yoshizawa, A. and Nisizima, S.: "A Nonequilibrium Representation of the Turbulent Viscosity Based on a Two-Scale Turbulence Theory", Phys. Fluids A, Vol. 5,(1993), pp 3302-3304.
2. Yoshizawa, A.: "Nonequilibrium Effect of the Turbulent-Energy Production Processes on the Inertial-Range Energy Spectrum", Phys. Rev. E, Vol. 49,(1994), pp 4065-4071.

### SHAYE YUNGSTER

My research for the 1994 year has focused on two different areas. First, we are implementing the "chimera" domain decomposition method into the allspeed CFD code. This method allows a system of relatively simple grids, each describing a component of a complex configuration, to be combined into a composite grid to yield solutions for complex flow fields. It is expected that the chimera scheme will greatly increase the range of combustor flows that can be addressed by the allspeed CFD code. We are currently writing the subroutines that will be incorporated into the allspeed code, and we expect to begin testing in January 1995.

Second, we are conducting time accurate CFD studies of flow establishment in pulsed hypersonic facilities, in support of experimental model studies. One of the major stumbling blocks to ground testing of hypersonic propulsion systems is, of course, the relatively short test times available at realistic flight conditions. In many cases, the test time may be shorter than the non-reacting flow establishment time. The addition of reaction (especially in the boundary layer and in recirculation zones) will certainly increase the time necessary for full flow establishment. Time accurate CFD analysis can provide detailed information on reacting flow establishment, a critical issue in pulse facility tests, and provide general support to experimental programs such as the Scramjet and Premixed Shock-Induced Combustion (PM/SIC) Engines. In addition, we believe that our capability with detailed chemistry will be crucial for understanding the effects of contaminants upon the combustion processes.

The time accurate computation of chemically reacting flows remains a challenging research topic. In many cases, existing methods are not efficient enough to allow time accurate, viscous computations of reacting flows involving a large number of chemical species. In addition, standard features in ODE solvers, such as error control and automatic time step determination, are lacking in current CFD codes. This investigation, in collaboration with Krish Radhakrishnan, is aimed at developing more efficient time-accurate methods for solving chemically reacting flows involving a large number of species. We are trying to implement some of the proven techniques utilized by stiff ODE solvers (such as LSODE) into a CFD code. We have studied several possible algorithms, and developed a new relaxation method that is used with an implicit TVD scheme to solve the fully coupled chemically reacting flow equations. The algorithm is based on successive backward and forward Gauss-Seidel relaxation sweeps, and includes automatic time stepping and error control (currently being implemented). The inversion of large matrices is avoided by partitioning the system into reacting and nonreacting parts, but still maintaining a fully coupled interaction.

To illustrate the applicability of the new algorithm, we conducted a series of numerical simulations of the periodic combustion instabilities observed in ballistic-range experiments of blunt projectiles flying at subdetonative speeds through hydrogen-air mixtures. The frequencies of the computed oscillations were in excellent agreement with experimental data. The results of this work were presented at the 30th Joint Propulsion Conference, Indianapolis, IN, June, 1994 (ICOMP-94-18, NASA TM 106707, AIAA-94-2965).

In recent computations, we have simulated the motion of a slug of hydrogen-air expanding into an evacuated test chamber, and its subsequent interaction with a conical projectile. The chemistry was modeled with a detailed hydrogen-air reaction mechanism. The temporal evolution of the reacting flow was studied until steady-state conditions were established; thus the flow establishment time was determined. We are also simulating the temporal evolution of the shock-induced combustion processes in a ram accelerator. In particular, we are investigating the transition from the launch tube into the ram accelerator section, or the transition from one ram accelerator section into another containing a dif-

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ferent gas mixture. These computations will allow us to follow the development and establishment of the shock-induced combustion, and monitor the change in thrust force as a function of time.

### JIANG ZHU

The work this year has been mainly concerned with developing a turbulence sub-program that will effectively bridge the gap between turbulence model developers and CFD users. The sub-program has been written in a self-contained way so that the user can use any turbulence model in the sub-program without worrying about how it is implemented and solved. Great care has been taken to ensure both numerical stability and accuracy, and to make the code user-friendly. The inputs to the sub-program are the mean flow variables, and the boundary and geometric information which are to be provided by a mean flow program. The output of the sub-program is the turbulent diffusivity and relevant turbulent source terms which are needed for the mean flow calculation. The interaction between the mean flow program and the turbulence sub-program will give the final turbulent flow solution.

Two particular versions of the sub-program have been written, one for compressible and the other for incompressible flows. The compressible version has been applied to NPARC - a CFD code that has a widespread use in the propulsion community and the incompressible version has been applied to FAST2D which serves as a research code at CMOTT. Both versions were released at the 1994 Industry-Wide Workshop on Computational Turbulence Modeling, sponsored by ICOMP/CMOTT and held at the Ohio Aerospace Institute.

Currently, this work is being extended by generating a turbulence sub-program for the VSTAGE code that will permit the accurate simulation of turbomachinery flows.

## 1994 REPORTS AND ABSTRACTS

**Feiler, Charles E., Compiler and Editor:** "Institute for Computational Mechanics in Propulsion (ICOMP), Eighth Annual Report - 1993", ICOMP Report 94-1, NASA TM 106542, April, 1994, 91 pages.

The Institute for Computational Mechanics in Propulsion (ICOMP) was established at the NASA Lewis Research Center in Cleveland, Ohio to develop techniques to improve problem-solving capabilities in all aspects of computational mechanics related to propulsion. This report describes the activities and accomplishments during 1993.

**Ajmani, Kumud (ICOMP); and Taylor, Arthur C. (Old Dominion University):** "Discrete Sensitivity Derivatives of the Navier-Stokes Equations with a Parallel Krylov Solver", ICOMP Report 94-2, NASA TM 106481, AIAA 94-0091, January, 1994, 12 pages.

This paper solves an 'incremental' form of the sensitivity equations derived by differentiating the discretized thin-layer Navier-Stokes equations with respect to certain design variables of interest. The equations are solved with a parallel, preconditioned Generalized Minimal RESidual (GMRES) solver on a distributed-memory architecture. The 'serial' sensitivity analysis code is parallelized by using the Single Program Multiple Data (SPMD) programming model, decomposition techniques, and message-passing tools. Sensitivity derivatives are computed for low and high Reynolds number flows over a NACA 1406 airfoil on a 32-processor Intel Hypercube and found to be identical to those computed on a single processor Cray Y-MP. It is estimated that the parallel sensitivity analysis code has to be run on 40-50 processors of the Intel Hypercube in order to match the single-processor processing time of a Cray Y-MP.

**Shih, Tsan-Hsing (ICOMP); Zhu, Jiang (ICOMP); and Lumley, John L. (Cornell University):** "Modeling of Wall-Bounded Complex Flows and Free Shear Flows", ICOMP Report 94-3, CMOTT 94-1, NASA TM 106513, February, 1994, 10 pages.

Various wall-bounded flows with complex geometries and free shear layers have been studied with a newly developed realizable Reynolds stress algebraic equation model. The model development is based on the invariant theory in continuum mechanics. This theory enables us to formulate a general constitutive relation for the Reynolds stresses. Pope (1975) was the first to introduce this kind of constitutive relation to turbulence modeling. In our study, realizability is imposed on the truncated constitutive relation to determine the coefficients so that, unlike the standard  $\kappa$ - $\epsilon$  eddy viscosity model, the present model will not produce negative normal stresses in any situations of rapid distortion. The calculations based on the present model have shown an encouraging success in modeling complex turbulent flows.

**Jiang, Bo-nan (ICOMP); Loh, Ching Y. (NASA Lewis) ; and Povinelli, Louis A. (NASA Lewis) :** "Theoretical Study of the Incompressible Navier-Stokes Equations by the Least-Squares Method", ICOMP Report 94-4, NASA TM 106535, March, 1994, 46 pages.

Usually the theoretical analysis of the Navier-Stokes equations is conducted via the Galerkin method which leads to difficult saddle-point problems. This paper demonstrates that the least-squares method is a useful alternative tool for the theoretical study of partial differential equations since it leads to minimization problems which can often be treated by an elementary technique. The principal part of the Navier-Stokes equations in the first-order velocity-

pressure-vorticity formulation consists of two div-curl systems, so the three-dimensional div-curl system is thoroughly studied at first. By introducing a dummy variable and by using the least-squares method, this paper shows that the div-curl system is properly determined and elliptic, and has a unique solution. The same technique then is employed to prove that the Stokes equations are properly determined and elliptic, and that four boundary conditions on a fixed boundary are required for three-dimensional problems. This paper also shows that under four combinations of non-standard boundary conditions the solution of the Stokes equations is unique. This paper emphasizes the application of the least-squares method and the div-curl method to derive a high-order version of differential equations and additional boundary conditions. In this paper an elementary method (integration by parts) is used to prove Friedrichs' inequalities related to the div and curl operators which play an essential role in the analysis.

**Yungster, Shaye (ICOMP); and Trefny, Charles J. (NASA Lewis):** "Computational Study of Single-Expansion-Ramp Nozzles with External Burning", ICOMP Report 94-5, NASA TM 106550, AIAA-94-0024, April, 1994, 28 pages.

A computational investigation of the effects of external burning on the performance of single expansion ramp nozzles (SERN) operating at transonic speeds is presented. The study focuses on the effects of external heat addition and introduces a simplified injection and mixing model based on a control volume analysis. This simplified model permits parametric and scaling studies that would have been impossible to conduct with a detailed CFD analysis. The CFD model is validated by comparing the computed pressure distribution and thrust forces, for several nozzle configurations, with experimental data. Specific Impulse calculations are also presented which indicate that external burning performance can be superior to other methods of thrust augmentation at transonic speeds. The effects of injection fuel pressure and nozzle pressure ratio on the performance of SERN nozzles with external burning are described. The results show trends similar to those reported in the experimental study, and provide additional information that complements the experimental data, improving our understanding of external burning flowfields. A study of the effect of scale is also presented. The results indicate that combustion kinetics do not make the flowfield sensitive to scale.

**Ibraheem, S.O.; and Demuren, A.O.:** "On Bi-Grid Local Mode Analysis of Solution Techniques for 3-D Euler and Navier-Stokes Equations", ICOMP Report 94-6, NASA TM 106749, October, 1994, 51 pages.

A procedure is presented for utilizing a bi-grid stability analysis as a practical tool for predicting multigrid performance in a range of numerical methods for solving Euler and Navier-Stokes equations. Model problems based on the convection, diffusion and Burger's equation are used to illustrate the superiority of the bi-grid analysis as a predictive tool for multi-grid performance in comparison to the smoothing factor derived from conventional von Neumann analysis. For the Euler equations, bi-grid analysis is presented for three upwind difference based factorizations, namely Spatial, Eigenvalue and Combination splits, and two central difference based factorizations, namely LU and ADI methods. In the former, both the Steger-Warming and van Leer flux-vector splitting methods are considered. For the Navier-Stokes equations, only the Beam-Warming (ADI) central difference scheme is considered. In each case, estimates of multigrid convergence rates from the bi-grid analysis are compared to smoothing factors obtained from single-grid stability analysis. Effects of grid aspect ratio and flow skewness are examined. Both predictions are compared with practical multigrid convergence rates for 2-D Euler and Navier-Stokes solutions based on the Beam-Warming central scheme.

**Kao , Kai-Hsiung (ICOMP); and Liou, Meng-Sing (NASA Lewis):** "Direct Replacement of Arbitrary Grid-Overlapping by Non-Structured Grid", ICOMP Report 94-7, NASA TM 106601, May, 1994, 17 pages.

A new approach that uses non-structured mesh to replace the arbitrarily overlapped structured regions of embedded grids is presented. The present methodology uses the Chimera composite overlapping mesh system so that the physical domain of the flowfield is subdivided into regions which can accommodate easily-generated grid for complex configuration. In addition, a Delaunay triangulation technique generates non-structured triangular mesh which wraps over the interconnecting region of embedded grids. It is designed that the present approach, termed DRAGON grid, has three important advantages, (1) eliminating some difficulties of the Chimera scheme, such as the orphan points and/or bad quality of interpolation stencils, (2) making grid communication in a fully conservative way, and (3) implementation into three dimensions is straightforward. A computer code based on a time accurate, finite volume, high resolution scheme for solving the compressible Navier-Stokes equations has been further developed to include both the Chimera overset grid and the non-structured mesh schemes. For steady state problems, the local time stepping accelerates convergence based on a Courant-Friedrichs-Leury (CFL) number near the local stability limit. Numerical tests on representative steady and unsteady supersonic inviscid flows with strong shock waves are demonstrated.

**Rubinstein, Robert (ICOMP):** "Renormalization Group Theory of Bolgiano Scaling in Boussinesq Turbulence", ICOMP Report 94-8, CMOTT 94-2, NASA TM 106602, May, 1994, 19 pages.

Bolgiano scaling in Boussinesq turbulence is analyzed using the Yakhot-Orszag renormalization group. For this purpose, an isotropic model is introduced. Scaling exponents are calculated by forcing the temperature equation so that the temperature variance flux is constant in the inertial range. Universal amplitudes associated with the scaling laws are computed by expanding about a logarithmic theory. Connections between this formalism and the direct interaction approximation are discussed. It is suggested that the Yakhot-Orszag theory yields a lowest order approximate solution of a regularized direct interaction approximation which can be corrected by a simple iterative procedure.

**Norris, Andrew T. (ICOMP); and Hsu, Andrew T. (NYMA):** "Comparison of PDF and Moment Closure Methods in the Modeling of Turbulent Reacting Flows", ICOMP Report 94-9, CMOTT 94-3, NASA TM 106614, AIAA 94-3356, May, 1994, 12 pages.

In modeling turbulent reacting flows, PDF(Probability Density Function) methods have an advantage over the more traditional moment closure schemes in that the PDF formulation treats the chemical reaction source terms exactly, while moment closure methods are required to model the mean reaction rate. The common model used is the laminar chemistry approximation, where the effects of turbulence on the reaction are assumed negligible. For flows with low turbulence levels and fast chemistry, the difference between the two methods can be expected to be small. However, for flows with finite rate chemistry and high turbulence levels, significant errors can be expected in the moment closure method. In this paper, the ability of the PDF method and the moment closure scheme to accurately model a turbulent reacting flow is tested. To accomplish this, both schemes were used to model a CO/H<sub>2</sub>/N<sub>2</sub>-air piloted diffusion flame near extinction. Identical thermochemistry, turbulence models, initial conditions and boundary conditions are employed to ensure a consistent comparison can be made. The comparison reveals that the PDF method provides good agreement with the experimental data, while the moment closure scheme incorrectly shows a broad, laminar-like flame structure.

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**Cole, Gary L. (NASA Lewis); Melcher, Kevin J. (NASA Lewis); Chicatelli, Amy K. (U. of Akron); Hartley, Tom T. (U of Akron); and Chung, Joongkee (ICOMP):** "Computational Methods for HSCT-Inlet Controls/CFD Interdisciplinary Research", ICOMP Report 94-10, NASA TM 106618, AIAA 94-3209, May, 1994, 13 pages.

A program aimed at facilitating the use of computational fluid dynamics (CFD) simulations by the controls discipline is presented. The objective is to reduce the development time and cost for propulsion system controls by using CFD simulations to obtain high-fidelity models for control design and as numerical test beds for control system and validation. An interdisciplinary team has been formed to develop analytical and computational tools in three discipline areas--controls, CFD, and computational technology. The controls effort has focused on specifying requirements for an interface between the controls specialist and CFD simulations and a new method for extracting linear, reduced-order control models from CFD simulations. Existing CFD codes are being modified to permit time accurate execution and provide realistic boundary conditions for controls studies. Parallel processing and distributed computing techniques, along with existing system integration software, are being used to reduce CFD execution times and to support the development of an integrated analysis/design system. This paper describes: the initial application for the technology being developed, the high speed civil transport (HSCT) inlet control problem; activities being pursued in each discipline area; and a prototype analysis/design system in place for interactive operation and visualization of a time-accurate HSCT-inlet simulation

**Hixon, R. (ICOMP); Shih, S.-H. (ICOMP); and Mankbadi, R.R. (NASA Lewis):** "Evaluation of Boundary Conditions for Computational Aeroacoustics", ICOMP Report 94-11, NASA TM 106645, AIAA 95-0160, December, 1994, 31 pages.

The performance of three acoustic boundary condition formulations are investigated. The effect of implementation differences are also studied. Details of all implementations are given. Results are shown for the acoustic field of a monopole in a uniform freestream.

**Hayder, M.E. (ICOMP); and Turkel, E. (ICOMP):** "Boundary Conditions for Jet Flow Computations", ICOMP Report 94-12, NASA TM 106648, AIAA 94-2195, June, 1994, 18 pages.

Ongoing activities are focused on capturing the sound source in a supersonic jet through careful LES. One issue that is addressed herein is the effect of the boundary conditions, both inflow and outflow, on the predicted flow fluctuations, which represent the sound source. In this study, we examine the accuracy of several boundary conditions to determine their suitability for computations of time-dependent flows. Various boundary conditions are used to compute the flow field of a laminar axisymmetric jet excited at the inflow by a disturbance given by the corresponding eigenfunction of the linearized stability equations. We solve the full time dependent Navier-Stokes equations by a high order numerical scheme. For very small excitations, the computed growth of the modes closely corresponds to that predicted by the linear theory. We then vary the excitation level to see the effect of the boundary conditions in the nonlinear flow regime.

**Leonard, B.P.(ICOMP); and MacVean,M.K. (U. K. Meteorological Office); and Lock, A. P. (U. K. Meteorological Office):** "The Flux-Integral Method for Multidimensional Convection and Diffusion", ICOMP Report 94-13, NASA TM 106679, August, 1994, 29 pages.

The flux-integral method is a procedure for constructing an explicit, single-step, forward-in-time, conservative, control-volume update of the unsteady, multidimensional convection-

diffusion equation. The convective-plus-diffusive flux at each face of a control-volume cell is estimated by integrating the transported variable and its face-normal derivative over the volume swept out by the convecting velocity field. This yields a *unique* description of the fluxes, whereas other conservative methods rely on nonunique, arbitrary pseudoflux-difference splitting procedures. The accuracy of the resulting scheme depends on the form of the *sub-cell interpolation* assumed, given cell-average data. Cellwise constant behavior results in a (very artificially diffusive) first-order convection scheme. Second-order convection-diffusion schemes correspond to cellwise linear (or bilinear) sub-cell interpolation. Cellwise quadratic sub-cell interpolants generate a highly accurate convection-diffusion scheme with excellent phase accuracy. Under constant-coefficient conditions, this is a uniformly third-order polynomial interpolation algorithm (UTOPIA).

**Shih, Tsan-Hsing (ICOMP); and Shabbir, Aamir (ICOMP);** "Methods of Ensuring Realizability for Non-Realizable Second Order Closures", ICOMP Report 94-14, CMOTT 94-7, NASA TM 106681, August, 1994, 15 pages.

Several methods of ensuring realizability for non-realizable second order closure models are discussed. The well known isotropization of production (IP) model and the Launder, Reece, and Rodi (LRR) model are particularly studied for their wide application in engineering calculations. Ensuring realizability for these models will extend their applicability to more critical flow situations and reduce the numerical difficulties caused by the non-realizability of the original models. Different methods of ensuring realizability are tested for several extreme flow situations. The suggested realizability modifications not only make the models realizable but also maintain the performance of the original models for realistic flows. The methods discussed in this paper can be straightforwardly applied to other non-realizable models.

**Shih, Tsan-Hsing (ICOMP); Zhu, Jiang (ICOMP); and Lumley, John L. (Cornell University);** "A New Reynolds Stress Algebraic Equation Model", ICOMP Report 94-15, CMOTT 94-8, NASA TM 106644, August, 1994, 30 pages.

A general turbulent constitutive relation (Shih and Lumley, *Mathematical Computer Modelling*, Vol. 18, No. 2, (1993), pp 9-16) is directly applied to propose a new Reynolds stress algebraic equation model. In the development of this model, the constraints based on rapid distortion theory and realizability (i.e., the positivity of the normal Reynolds stresses and the Schwarz' equality between turbulent velocity correlations) are imposed. Model coefficients are calibrated using well-studied basic flows such as homogeneous shear flow and the surface flow in the inertial sublayer. The performance of this model is then tested in complex turbulent flows including the separated flow over a backward-facing step and the flow in a confined jet. The calculation results are encouraging and point to the success of the present model in modeling flows with complex geometries.

**Huang, P.G. (Eloret Institute); and Liou, W.W. (ICOMP);** "Numerical Calculations of Shock Wave/Boundary Layer Flow Interactions", ICOMP Report 94-16, CMOTT 94-4, NASA TM 106694, August, 1994, 14 pages.

This paper presents results of calculations for 2-D supersonic turbulent compression corner flows. The results seem to indicate that the newer, improved  $\kappa$ - $\epsilon$  models offer limited advantages over the standard  $\kappa$ - $\epsilon$  model in predicting the shock wave/boundary layer flows in the 2-D compression corner over a wide range of corner angles and flow conditions.

**Steinthorsson, E. (ICOMP); Modiano, D.(ICOMP); and Colella, P. ( U. of California, Berkeley);** "Computations of Unsteady Viscous Compressible Flows Using Adaptive Mesh Refinement in Curvilinear Body-Fitted Grid Systems", ICOMP Report 94-17, NASA TM 106704, AIAA 94-2330, August, 1994, 14 pages.

A methodology for accurate and efficient simulation of unsteady, compressible flows is presented. The cornerstones of the methodology are a special discretization of the Navier-Stokes equations on structured body-fitted grid systems and an efficient solution -adaptive mesh refinement technique for structured grids. The discretization employs an explicit multidimensional upwind scheme for the inviscid fluxes and an implicit treatment of the viscous terms. The mesh refinement technique is based on the AMR algorithm of Berger and Colella ( J. Comp. Phys., Vol. 82, pp64-84, 1989). In this approach, cells on each level of refinement are organized into a small number of topologically rectangular blocks, each containing several thousand cells. The small number of blocks leads to small overhead in managing data, while their size and rectangular topology means that a high degree of optimization can be achieved on computers with vector processors.

**Yungster, Shaye (ICOMP); and Radhakrishnan, Krishnan ( NYMA, Inc.):** "A Fully Implicit Time Accurate Method for Hypersonic Combustion: Application to Shock-Induced Combustion Instability", ICOMP Report 94-18, NASA TM 106707, AIAA 94-2965, August, 1994, 16 pages.

A new fully implicit, time accurate algorithm suitable for chemically reacting, viscous flows in the transonic-to-hypersonic regime is described. The method is based on a class of Total Variation Diminishing (TVD) schemes and uses successive Gauss-Seidel relaxation sweeps. The inversion of large matrices is avoided by partitioning the system into reacting and nonreacting parts, but still maintaining a fully coupled interaction. As a result, the matrices that have to be inverted are the of same size as those obtained with the commonly used point implicit methods. In this paper, we illustrate the applicability of the new algorithm to hypervelocity unsteady combustion applications. We present a series of numerical simulations of the periodic combustion instabilities observed in ballistic-range experiments of blunt object projectiles flying at subdetonative speeds through hydrogen-air mixtures. The computed frequencies of oscillation are in excellent agreement with experimental data.

**Liou, Meng-Seng (NASA Lewis); and Kao, Kai-Hsiung (ICOMP):** "Progress in Grid Generation: From Chimera to DRAGON Grids", ICOMP Report 94-19, NASA TM 106709, August, 1994, 28 pages.

Hybrid grids, composed of structured and unstructured grids, combines best features of both. The chimera method is a major stepstone toward a hybrid grid from which the present approach is evolved. The chimera grid composes a set of overlapped structured grids which are independently generated and body-fitted, yielding a high quality grid readily accessible for efficient solution schemes. The chimera method has been shown to be efficient to generate a grid about complex geometries and has been demonstrated to deliver accurate aerodynamic prediction of complex flows. While its geometrical flexibility is attractive, interpolation of data in the overlapped regions-which in today's practice in 3D is done in a nonconservative fashion, is not. In the present paper we propose a hybrid grid scheme that maximizes the advantages of the chimera scheme and adapts the strengths of the unstructured grid while at the same time keeps its weaknesses minimal. Like the chimera method, we first divide up the physical domain by a set of structured body-fitted grids which are separately generated and overlaid throughout a complex configuration. To eliminate any pure data manipulation which does not necessarily

follow governing equations, we use non-structured grids only to directly replace the region of the arbitrarily overlapped grids. This new adaptation to the chimera thinking is coined the DRAGON grid. The nonstructured grid region sandwiched between the structured grids is limited in size, resulting in only a small increase in memory and computational effort. The DRAGON method has three important advantages: (1) preserving strengths of the chimera grid, (2) eliminating difficulties sometimes encountered in the chimera scheme, such as the orphan points and bad quality of interpolation stencils, and (3) making grid communication in a fully conservative and consistent manner insofar as the governing equations are concerned. To demonstrate its use, the governing equations are discretized using proposed flux scheme, AUSM+, which will be briefly described herein. Numerical tests on representative 2D inviscid flows are given for demonstration. Finally, extension to 3D is underway, only paced by the availability of 3D unstructured grid generator.

**Georgiadis, Nicholas J. (NASA Lewis); Chitsomboon, Tawit (ICOMP); and Zhu, Jiang (ICOMP):** "Modification of the Two-Equation Turbulence Model In NPARC to a Chien Low Reynolds Number  $k$ - $\epsilon$  Formulation", ICOMP Report 94-20, CMOTT 94-5, NASA TM 106710, September, 1994, 19 pages.

This report documents the changes that were made to the two-equation  $k$ - $\epsilon$  turbulence model in the NPARC (National-PARC) code. The previous model, based on the low Reynolds number of Speziale, was replaced with the low Reynolds number  $k$ - $\epsilon$  model of Chien. The most significant difference was in the turbulent Prandtl numbers appearing in the diffusion terms of the  $k$  and  $\epsilon$  transport equations. A new inflow boundary condition and stability enhancements were also implemented into the turbulence model within NPARC. The report provides the rationale for making the change to the Chien model, code modifications required, and comparisons of the performances of the new model with the previous  $k$ - $\epsilon$  model and algebraic models used most often in PARC/NPARC. The comparisons show that the Chien  $k$ - $\epsilon$  model installed here improves the capability of NPARC to calculate turbulent flows.

**Shih, T. H. (ICOMP); Liou, W. W. (ICOMP); Shabbir, A. (ICOMP); Yang, Z. (ICOMP); and Zhu, J. (ICOMP):** "A New  $\kappa$ - $\epsilon$  Eddy Viscosity Model for High Reynolds Number Turbulent Flows--Model Development and Validation", ICOMP Report 94-21, CMOTT 94-6, NASA TM 106721, August, 1994, 32 pages.

A new  $\kappa$ - $\epsilon$  eddy viscosity model, which consists of a new model dissipation rate equation and a new realizable eddy viscosity formulation, is proposed in this paper. The new model dissipation rate equation is based on the dynamic equation of the mean-square vorticity fluctuation at large turbulent Reynolds number. The new eddy viscosity formulation is based on the realizability constraints; the positivity of normal Reynolds stresses and Schwarz' inequality for turbulent shear stresses. We find that the present model with a set of unified model coefficients can perform well for a variety of flows. The flows that are examined include: (i) rotating homogeneous shear flows; (ii) boundary free shear flows including a mixing layer, planar and round jets; (iii) a channel flow, and flat plate boundary layers with and without a pressure gradient; and (iv) backward facing step separated flows. The model predictions are compared with available experimental data. The results from the standard  $\kappa$ - $\epsilon$  eddy viscosity model are also included for comparison. It is shown that the present model is a significant improvement over the standard  $\kappa$ - $\epsilon$  eddy viscosity model.

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**Hariharan, S. I. (ICOMP); and Johnson, D. K. (University of Akron):** "Boundary Conditions for Unsteady Compressible Flows", ICOMP Report 94-22, NASA TM 106737, September, 1994, 27 pages.

This paper explores solutions to the spherically symmetric Euler equations. Motivated by the work of Hagstrom and Hariharan and Geer and Pope, we modeled the effect of a pulsating sphere in a compressible medium. The literature on this suggests that an accurate numerical solution requires artificial boundary conditions which simulate the propagation of nonlinear waves in open domains. Until recently, the boundary conditions available were, in general, linear and based on reflection. Exceptions to this are the nonlinear nonreflective conditions of Thompson, and the nonlinear reflective conditions of Hagstrom and Hariharan. The former are based on the rate of change of the incoming characteristics; the latter rely on asymptotic analysis and the method of characteristics and account for the coupling of incoming and outgoing characteristics. Furthermore, Hagstrom and Hariharan have shown that, in a test situation in which the flow would reach a steady state over a long time, Thompson's method could lead to an incorrect steady state. The current study considers periodic flows and includes all possible types and techniques of boundary conditions. The technique recommended by Hagstrom and Hariharan proved superior to all others considered and matched the results of asymptotic methods that are valid for low subsonic Mach numbers.

**Nobari, M.R.H. (University of Michigan); and Tryggvason, G. (ICOMP):** "Numerical Simulations of Drop Collisions", ICOMP Report 94-23, NASA TM 106751, AIAA 94-0835, October, 1994, 11 pages.

Three-dimensional simulations of the off-axis collisions of two drops are presented. The full Navier-Stokes equations are solved by a Front-Tracking/Finite-Difference method that allows a fully deformable fluid interface and the inclusion of surface tension. The drops are accelerated towards each other by a body force that is turned off before the drops collide. Depending on whether the interface between the drops is ruptured or not, the drops either bounce or coalesce. For drops that coalesce, the impact parameter, which measures how far the drops are off the symmetry line, determines the eventual outcome of the collision. For low impact parameters, the drops coalesce permanently, but for higher impact parameters, a grazing collision, where the drops coalesce and then stretch apart again is observed. The results are in agreement with experimental observations.

**Nobari, M.R.H. (University of Michigan); and Tryggvason, G. (ICOMP):** "The Flow Induced by the Coalescence of Two Initially Stationary Drops", ICOMP Report 94-24, NASA TM 106752, October, 1994, 27 pages.

The coalescence of two, initially stationary drops of different size is investigated by solving the unsteady, axisymmetric Navier-Stokes equations numerically, using a Front-Tracking/Finite Difference method. Initially, the drops are put next to each other and the film between them ruptured. Due to surface tension forces, the drops coalesce rapidly and the fluid from the small drop is injected into the larger one. For low nondimensional viscosity or Ohnesorge number, little mixing takes place and the small drop fluid forms a blob near the point where the drops touched initially. For low Ohnesorge number, on the other hand, the small drop forms a jet that penetrates far into the large drop. The penetration depth also depends on the size ratio of the drops and we show that for a given fluid of sufficiently low viscosity, there is a maximum penetration depth for intermediate size ratios.

**Coutsias, Evangelos A. (University of New Mexico); Torres, David (University of New Mexico); and Hagstrom, Thomas (ICOMP):** "An Efficient Spectral Method for Ordinary Differential Equations with Rational Function Coefficients", ICOMP Report 94-25, NASA TM 106762, October, 1994, 28 pages.

We present some relations that allow the efficient approximate inversion of linear differential operators with rational function coefficients. We employ expansions in terms of a large class of orthogonal polynomial families, including all the classical orthogonal polynomials. These families obey a simple 3-term recurrence relation for differentiation, which implies that on an appropriately restricted domain the differentiation operator has a unique banded inverse. The inverse is an integration operator for the family, and it is simply the tridiagonal coefficient matrix for the recurrence. Since in these families convolution operators (i.e. matrix representations of multiplication by a function) are banded for polynomials, we are able to obtain a banded representation for linear differential operators with rational coefficients. This leads to a method of solution of initial or boundary value problems that, besides having an operation count that scales linearly with the order of truncation  $N$ , is computationally well conditioned. Among the applications considered is the use of rational maps for the resolution of sharp interior layers.

**Balsa, Thomas F. (ICOMP):** "On the Behavior of Three-Dimensional Wave Packets in Viscously Spreading Shear Layers", ICOMP Report 94-26, NASA TM 106770, November, 1994, 50 pages.

We consider analytically the evolution of a three-dimensional wave packet generated by an impulsive source in a mixing layer. The base flow is assumed to be spreading due to viscous diffusion. The analysis is restricted to small disturbances (linearized theory). A suitable high-frequency ansatz is used to describe the packet; the key elements of this description are a complex phase and a wave action density. It is found that the product of this density and an infinitesimal material volume convecting at the local group velocity is *not* conserved: there is a continuous interaction between the base flow and the wave action. This interaction is determined by suitable mode-weighted averages of the second and fourth derivatives of the base-flow velocity profile. Although there is some tendency for the dominant wavenumber in the packet to shift from the most unstable value toward the neutral value, this shift is quite moderate. In practice, wave packets do not become locally neutral in a diverging base flow (as do instability modes), therefore, they are expected to grow more suddenly than pure instability modes and do not develop critical layers. The group velocity is complex; the full significance of this is realized by analytically continuing the equations for the phase and wave action into a complex domain. The implications of this analytic continuation are discussed vis-a-vis the secondary instabilities of the packet; very small-scale perturbations on the phase can grow very rapidly initially, but saturate later because most of the energy in these perturbations is convected away by the group velocity. This remark, as well as the one regarding critical layers, has consequences for the nonlinear theories

**Balsa, Thomas F. (ICOMP):** "A note on the Wave Action Density of a Viscous Instability Mode on a Laminar Free-Shear Flow", ICOMP Report 94-27, NASA TM 106771, November, 1994, 15 pages.

Using the assumptions of an incompressible and viscous flow at large Reynolds number, we derive the evolution equation for the wave action density of an instability wave traveling on top of a laminar free-shear flow. The instability is considered to be viscous; the purpose of the present work is to include the cumulative effect of the (locally) small viscous correction to the wave, over the length and time scales on which the underlying base flow appears inhomogeneous owing to its viscous diffusion. As such, we generalize our previous work for inviscid waves. This

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generalization appears as an additional (but usually non-negligible) term in the equation for the wave action. The basic structure of the equation remains unaltered.

**Chitsomboon, Tawit (ICOMP):** "Effects of Artificial Viscosity on the Accuracy of High Reynolds Number k- $\epsilon$  Turbulence Models", ICOMP Report 94-28, NASA TM 106781, November, 1994, 20 pages.

Wall functions, as used in the typical high Reynolds number k- $\epsilon$  turbulence model, can be implemented in various ways. A least disruptive method (to the flow solver) is to directly solve for the flow variables at the grid point next to the wall while prescribing the values of k and  $\epsilon$ . For the centrally-differenced finite-difference scheme employing artificial viscosity (AV) as a stabilizing mechanism, this methodology proved to be totally useless. This is because the AV gives rise to a large error at the wall due to too steep a velocity gradient resulting from the use of a coarse grid as required by the wall function methodology. This error can be eliminated simply by extrapolating velocities at the wall, instead of using the physical values of the no-slip velocities (*i.e.*, the zero value). The applicability of the technique used in this paper is demonstrated by solving a flow over a flat plate and comparing the results with those of experiments. It was also observed that AV gives rise to a velocity overshoot (about 1%) near the edge of the boundary layer. This small velocity error, however, can yield as much as 10% error in the momentum thickness. A method which integrates the boundary layer up to only the edge of the boundary (instead of to  $\infty$ ) was proposed and demonstrated to give better results than the standard method.

**Hagstrom, Thomas, (ICOMP):** "On the Convergence of Local Approximations to Pseudodifferential Operators with Applications", ICOMP Report 94-29, NASA TM 106792, November, 1994, 12 pages.

We consider the approximation of a class of pseudodifferential operators by sequences of operators which can be expressed as compositions of differential operators and their inverses. We show that the error in such approximations can be bounded in terms of the  $L_1$  error in approximating a convolution kernel, and use this fact to develop convergence results. Our main result is a finite time convergence analysis of the Engquist- Majda (B. Engquist and A. Majda, Absorbing boundary conditions for the numerical simulation of waves, *Math. Comp.* 31 (1977), 629-651.) Padé approximants to the square root of the d'Alembertian. We also show that no spatially local approximation to this operator can be convergent uniformly in time. We propose some temporally local but spatially nonlocal operators with better long time behavior. These are based on Laguerre and exponential series.

**Shabbir, Aamir(ICOMP), Compiler:** "Industry-Wide Workshop on Computational Turbulence Modeling", ICOMP Report 94-30, CMOTT 94-9, NASA CP 10165, February, 1995.

This publication contains the presentations made at the Industry-Wide Workshop on Computational Modeling, which was hosted by ICOMP/OAI, and took place on October 6-7, 1994 at the Ohio Aerospace Institute. The purpose of the workshop was to initiate the transfer of technology developed at Lewis Research Center (LeRC) to industry and to discuss the current status and the future needs of turbulence models in industrial CFD.

**Tsung, F.-L (ICOMP); Loellbach, J. (ICOMP); Kwon, O. (NYMA); and Hah, C. (NASA Lewis):** "A Three-Dimensional Structured/Unstructured Hybrid Navier-Stokes Method for Turbine Blade Rows", ICOMP Report 94-31, NASA TM 106813, AIAA 94-3369, December, 1994, 12 pages.

A three-dimensional viscous structured/unstructured hybrid scheme has been developed for numerical computation of high Reynolds number turbomachinery flows. The procedure allows an efficient structured solver to be employed in the densely clustered, high aspect ratio grid around the viscous regions near solid surfaces, while employing an unstructured solver elsewhere in the flow domain to add flexibility in mesh generation. Test results for an inviscid flow over an external transonic wing and a Navier-Stokes flow for an internal annular cascade are presented.

**Hayder, M. Ehtesham (ICOMP); Jayshima, D. N. (Ohio State University); and Pillay, Sasi Kumar (NASA Lewis):** "Parallel Navier-Stokes Computations on Shared and Distributed Memory Machines", ICOMP Report 94-32, NASA TM 106823, AIAA 94-0577, January, 1995, 15 pages.

We study a high order finite difference scheme to solve the time accurate flow field of a jet using the compressible Navier-Stokes equations. As part of our ongoing efforts, we have implemented our numerical model on three parallel computing platforms to study the computational, communication, and scalability characteristics. The platforms chosen for this study are a cluster of workstations connected through fast networks (the LACE experimental testbed at NASA Lewis), a shared memory multiprocessor (the Cray YMP), and a distributed memory multiprocessor (the IBM SP1). Our focus in this study is on the LACE testbed. We present some results for the Cray YMP and the IBM SP1 mainly for comparison purposes. On the LACE testbed, we study: (a) the communication characteristics of Ethernet, FDDI and the ALLNODE networks and (b) the overheads induced by the PVM message passing library used for parallelizing the application. We demonstrate that clustering of workstations is effective and has the potential to be computationally competitive with supercomputers at a fraction of the cost.

## 1994 SEMINARS

**Pletcher, Richard H. (ICOMP):** "Simulation of Viscous Flows: Some Recent Results for Free Surface Flows, Large Eddy Simulation, and Unstructured Grids"

Progress on three studies under way at Iowa State University will be discussed. The first involves the simulation of three-dimensional free surface flows. Two approaches to dealing with the free surface have been employed in this research over the last several years, surface fitting and surface capturing. The key features of the two approaches will be described and computational results compared. Developments in a new study on the application of large eddy simulation methods to flows with heat transfer will be presented. Aspects of algorithms and subgrid-scale modeling will be considered. Preliminary results for several flows being used to validate the approach (a coupled compressible formulation with a dynamic subgrid-scale model) will be presented. As time permits, experiences gained implementing two and three-dimensional cell-centered unstructured grid schemes on parallel machines will be shared.

**Tam, Christopher (ICOMP):** "Computation of Nonlinear Acoustic Waves"

High-order finite difference schemes are generally less dispersive, less dissipative and more isotropic than low-order schemes. For these reasons, they are well-suited for solving linear acoustic wave propagation problems. However, for nonlinear problems, high-order schemes invariably generate spurious spatial oscillations in regions with steep gradients and shocks. The presence of these spurious oscillations renders the computed solution totally unacceptable. The origin and the dominant wavelengths of these spurious oscillations are investigated. Based on the results of this investigation, a method to eliminate the spurious oscillations is proposed. The effectiveness of the proposed method is discussed and illustrated by numerical experiments.

**Turkel, Eli (ICOMP):** "Preconditioning the Fluid Dynamic Equations"

We consider the Euler equations for inviscid flow. We modify the physical equations by multiplying the time derivative by a matrix. We then show how to decompose this modified system into a sum of canonical forms that consist of scalar convective equations and wave equations. These preconditioned equations also have different wave speeds than the physical equations. By choosing the preconditioning properly, one can guarantee that all the wave speeds are equal for low Mach numbers. This enables us to remove the stiffness that occurs when using the compressible equations for low Mach flows. We use the pressure as the main variable instead of density. One can then show that the compressible equations approach the incompressible equations as the Mach number goes to zero also on the numerical level. With these improvements we can improve both the convergence rates and accuracy. Results are presented for both inviscid and viscous flows.

# 1994 Industry-Wide Workshop on Computational Turbulence Modeling October 6-7, 1994

## Objective and Scope

The purpose of this workshop is to initiate the transfer of turbulence modeling technology, developed within the institute for Computational Mechanics in Propulsion (ICOMP), located at the Lewis Research Center (LeRC), to industry and to discuss the current status and future needs of turbulence models in industrial applications. Over the past several decades, various turbulence models have been developed and applied to a variety of turbulent flows. It is urgent to assess their performance and to identify their capabilities, as well as their deficiencies, when applied to complex problems. This process should help to improve the capability of Computational Fluid Dynamics (CFD) in industrial design applications.

This workshop will emphasize the exchange of ideas, and enhance collaboration between ICOMP/NASA LeRC, industry, and universities. It should be noted that a Technology Transfer session is arranged for releasing a self-contained turbulence sub-program and a pdf solver to industry users.

The turbulence sub-program was developed at ICOMP. It has its own solver for the various built in turbulence model equations. The inputs for this sub-program are the mean flow variables and boundaries. This information can be provided by a mean flow program. The outputs of this sub-program are the turbulent diffusivity and the relevant turbulent source terms which are needed for the mean flow calculations. The interaction between the mean flow program and the turbulence sub-program will give the final turbulent flow solution. As an illustration, applications of this turbulence sub-program to the NPARC code will be demonstrated during the session. Some interface programs may be needed for this turbulence sub-program to match the other mean flow codes. Help will be available from within ICOMP to assist industry users. Those interested in the application of this turbulence sub-program can initiate a follow up program during the workshop.

Version 1.1 of the LPDF2D code, a Monte Carlo pdf solver for turbulent combustion, will also be released during the technology transfer session. The new features of this version of LPDF2D include: look-up tables for chemistry; new averaging schemes; and other improvements to reduce memory requirements. A version of this LPDF2D, which can be run on a workstation, will also be released.

The afternoon of October 7 is also reserved for those who might be interested in testing or discussing the use of the turbulence subprogram with their codes. A few workstations will be available for this purpose. Those wishing to test their codes are requested to contact CMOTT representatives on the workshop organizing committee at least two weeks prior to the work shop so that proper arrangements (computer accounts, etc.) can be made. Since some interface program may be needed to run the turbulence subprogram with a given mean flow code, a longer stay by a user may be needed.

## Organizing Committee

### WORKSHOP CHAIRMAN

L.A. Povinelli (NASA LeRC)

### INDUSTRY

C. Prakash (GE)  
M. Sindir (RocketDyne)  
S. Syed (P&W)

### UNIVERSITY

J.Y. Chen (UC Berkeley)  
J.L. Lumley (Cornell Univ.)

### NASA

D.R. Reddy (LeRC)  
P. Richardson (HQ)  
R.J. Shaw (LeRC)

### ICOMP

T. Keith (OAI/Univ. of Toledo)  
A. Shabbir (CMOTT)  
T.-H. Shih (CMOTT)

## Workshop Agenda

### Welcome by

Theo Keith  
Louis Povinelli  
Pamela Richardson

### Turbulence Modeling at NASA LeRC/COMP

Chairman: J. L. Lumley

Turbulence Program for Propulsion Systems by T.-H. Shih

### Turbulence Modeling and Applications in Industry

Chairman: M. Sindir

Turbulence Model Development and Application at Lockheed Fort Worth Company by B.R. Smith

A Summary of Computational Experience at GE Aircraft Engines for Complex Turbulent Flows in Gas Turbines by R. Zerkle

The Applicability of Turbulence Models to Aerodynamic and Propulsion Flow Fields at McDonnell Douglas Aerospace by L.D. Kral, J.A. Ladd, and M.Mani

Experience with  $k - \epsilon$  Turbulence Models for Heat Transfer Computations in Rotating Cooling Passages by P. Tekriwal(GE-CRD)

### Turbulent Combustion Modeling in Industry

Chairman: S. Syed

Turbulence Models for Gas Turbine Combustors by A. Brankovic (P&W)

Combustion System CFD Modeling at GE Aircraft Engines: Current Capabilities and Future Directions by D. Burrus, H. Mongia, A. Tolpadi, S. Correa, and M. Braaten

Recent Progress in the Joint Velocity-Scalar PDF by M.S. Anand (Allison Engine Co.)

Overview of Turbulence Model Development and Applications at Rocketdyne by A.H. Hadid and M.M. Sindir

Recent Advances in PDF Modeling of Turbulent Reacting Flows by A.D. Leonard and F. Dai (CFD Research Corporation)

### Turbulence Modeling Needs of Commercial CFD Codes

Chairman: C. Prakash

Turbulence and Turbulence-Chemistry Interaction Models in FLUENT by D. Choudhury, S.E. Kim, D. Tselepidakis, and M. Missaghi (Fluent Inc.)

Experiences with Two-Equation Turbulence Models by A.K. Singhal, Y.G. Lai, and R.K. Awra (CFD Research Corp.)

Progress in Modeling Industrial Flows using Two-Equation Models: Can More Be Achieved with Further Research? by V. Haroutunian (Fluid Dynamics International., Inc.)

Turbulence Modeling Needs by Commercial CFD Codes: Complex Flows in the Aerospace and Automotive Industries by B. Befrui (ADAPCO)

Turbulence Modeling Requirements of a Commercial CFD Code by J.P. van Doormaal, C.M. Mueller, and M. Raw (ASC)

**Turbulence Modeling at Universities**

Chairman: T. Keith

Second-Order Closures for Compressible Turbulence by J.L. Lumley

Modeling of Turbulent Chemical Reaction by J.Y. Chen

**Technology Transfer**

Chairman: L.A. Povinelli

Introduction by T.-H. Shih

Description of Turbulence Sub-Program by J. Zhu

Introduction by D.R. Reddy

PDF Method for Reactive Flows by A. Hsu

Improvements and New Features in the PDF Module by A. Norris

**Panel Discussion and Concluding Remarks**

**1994 Least-Squares  
Finite-Element Methods Workshop  
October 13 - 14 1994**

**Objective**

The Galerkin finite element method for selfadjoint elliptic differential equations has proved to be extremely successful, and has become a dominating computational technique in solid mechanics. However, attempts to apply the Galerkin approach to non-selfadjoint equations in fluid dynamics and other transport problems encounter serious difficulties, including oscillations and instabilities. The least-squares finite element method (LSFEM) is based on simply minimizing the  $L_2$  norm of the residuals of the first-order system of differential equations. The LSFEM is a unified method for the numerical solution of all types of partial differential equations in engineering and science without introducing special treatments, such as upwinding, non-equal elements, staggering grids, operator-splitting, etc. The LSFEM produces symmetric positive-definite algebraic systems which can be solved efficiently by iterative methods for use on large-scale problems.

The purpose of this workshop is to bring together researchers working in these areas to discuss the current status, to exchange new ideas and to identify research opportunities that would benefit existing and emerging application areas.

**Organizing Committee**

**WORKSHOP CHAIRMAN**  
L.A. Povinelli (NASA LeRC)

**ADVISOR**  
George J. Fix (U. of Texas-Arlington)

**INDUSTRY**  
Vijay Sonnad (IBM at Austin)

**ICOMP**  
T.Keith (OAI/Univ. of Toledo)  
Bo-nan Jiang (ICOMP)

**UNIVERSITY**  
Max D. Gunzburger (Virginia Polytechnic Institute and State University)

Steve McCormick (University of Colorado-Boulder)  
Tate T.H. Tsang (University of Kentucky-Lexington)

**GOVERNMENT**  
Thomas A. Manteuffel (Los Alamos National Labs)  
Nan-Suey Liu (NASA LeRC)  
Robert M. Stubbs (NASA LeRC)

**Workshop Agenda**

**Welcome by**

Theo Keith  
Louis Povinelli

Why Least-Squares by Bo-nan Jiang (ICOMP)

Analysis of Least-Squares Methods for the Navier-Stokes Equations by Max D. Gunzburger (Virginia Polytechnic Institute and State Univ.)

First-Order System Least-Squares: Algorithms and Applications by Steve McCormick (University of Colorado)

Simulation of Immiscible Displacement Using Least-Squares Methods by Tsu-Fen Chen (UT- Arlington)

Least-Squares Finite Element Methods for Fluid Dynamics and Transport Processes by Tate T.H. Tsang (University of Kentucky)

Development of Multi-disciplinary Analysis of Aeropropulsion Devices by using the LSFEM by Nan-Suey Liu (NASA LeRC)

The LSFEM for Chemically Reacting Flows by Sheng-Tao Yu (NYMA SETAR Team)

Time-Accurate LSFEM for Fluid Flows and Electromagnetic Scattering Problems by Jie Wu (ICOMP)

Analysis of Least Squares Finite Element Method for the Navier-Stokes Equations with Nonstandard Boundary Conditions by P. Bochev (UT Arlington)

Computation With Sobolev Gradients by John Neuberger (U. of North Texas)

First-Order System Least-Squares for the Stokes Equations by Zhiqiang Cai (University of Southern California)

The Application of the LSFEM on Inelastic Deformations by Ying-Kuo Lee (Georgia Institute of Technology)

Three-Dimensional Rayleigh-Benard Convection and Laminar Flow through a 90 degree Square Bend by L.Q. Tang (University of Kentucky)

Minimal Memory Solution Techniques in Computational Fluid Dynamics using the P-Version of LSFEM by Vijay Sonnad (IBM)

Implementation of a Parallel LSFEM using Quadratic and Spectral Elements by Daniel Chan (RocketDyne)

Steepest Descent, Nonlinear Boundary Conditions and Optimal Sobolev Embedding Constants by W. Richardson (UT San Antonio)

Numerical Studies of Optimal Grid Construction by T.F. Chen, George J. Fix, and H.D. Yang (UT Arlington)

Panel Discussion - Future Direction of LSFEM

TABLE I. The ICOMP Research Staff-1994

A. Resident Staff.

Kumud Ajmani, Ph.D., Mechanical Engineering, Virginia Polytechnic Institute and State University, 1991. Development of Codes for Parallel Processing. January, 1992--Present.

Tawit Chitsomboon, Ph.D., Mechanical Engineering, Old Dominion University, 1986. Code Development for Mixer-Ejector Nozzle Flows. January, 1990--Present.

Joongkee Chung, Ph.D., Mechanical Engineering, University of California, Berkeley, 1991. Code Development for Unsteady Inlet Flows Using Parallel Processing. May, 1992--Present.

Bernard Greenspan, Ph.D., Applied Mathematics, Cornell University, 1981. New Solution Methods for PDE's Using Conservation Laws in Both Time and Space. December, 1992--December, 1994.

Ehtesham Hayder, Ph.D., Mechanical and Aerospace Engineering, Princeton University, 1988. Computation of Jet Noise in the Source Region Near the Nozzle Exit. February, 1991--Present.

Duane R. Hixon, Ph.D., Aerospace Engineering, Georgia Institute of Technology, 1993. Numerical Calculation of Jet Noise from First Principles. October, 1993--Present.

Lin-Jun Hou, Ph.D., Engineering Science and Mechanics. Georgia Institute of Technology, 1992. Flow Applications of the Least-Squares Finite Element Method. July, 1992--September, 1994.

Bo-nan Jiang, Ph.D., Engineering Mechanics, University of Texas, Austin, 1986. Team Leader, Flow Applications of the Least-Squares Finite Element Method. October, 1987--Present.

Kai-Hsiung Kao, Ph.D., Aerospace Engineering Sciences, University of Colorado, 1989. Chimera Overset Grid Scheme with Time-Accurate 3D Compressible Finite Volume Navier-Stokes Flow Solver. November, 1992--Present.

William W. Liou, Ph.D., Aerospace Engineering, Pennsylvania State University, 1990. Modeling and Calculation of Compressible Turbulent Flows. November, 1990--Present.

James M. Loellbach, Ph.D. expected 1995, Aeronautical and Astronautical Engineering, University of Illinois. Development of 3D Structured Grid Generation Codes for Turbomachinery. May, 1992 -- Present.

David Modiano, Ph.D., Computational Fluid Dynamics, Massachusetts Institute of Technology, 1993. Application of Adaptive Mesh Refinement to Improve the Accuracy of Heat Transfer Calculations in Turbine Cooling Passages. February, 1993--Present.

Andrew Norris, Ph.D., Mechanical and Aerospace Engineering, Cornell University, 1993. Computation of Turbulent Reacting Flows by a Compressible Hybrid PDF Model. June, 1993--Present.

Robert Rubinstein, Ph.D., Mathematics, Massachusetts Institute of Technology, 1972. Theory and Modeling of Turbulence. May, 1993--November, 1994.

Aamir Shabbir, Ph.D., Mechanical Engineering, State University of New York, Buffalo, 1987. Modeling of the Scalar Field of Turbulent Flow and Model Assessment. June, 1991--Present.

Shyue-Horng Shih, Ph.D., Aerospace Engineering, University of Cincinnati, 1993. Near-Field Calculation of Axisymmetric and 3D Supersonic Jet Noise. June, 1993--Present.

Tsan-Hsing Shih, Ph.D., Aerospace Engineering, Cornell University, 1984. Technical Leader, CMOTT Group. Developing, Validating and Implementing Improved Turbulence Models for Propulsion Systems. March, 1990--Present.

Erlendur Steinthorsson, Ph.D., Mechanical Engineering, Carnegie Mellon University, 1992. Code Development for Flows in Complex Geometries such as Turbine Blade Coolant Passages. January, 1992-- Present.

Fu-Lin Tsung, Ph.D. expected 1995, Aerospace Engineering, Georgia Institute of Technology. Development of 3D Structured/Unstructured Hybrid Navier-Stokes Solver for Turbomachinery. March, 1993--Present.

Daniel Winterscheidt, Ph.D., Mechanical Engineering, University of Kansas, 1992. Finite Element Methods for Incompressible and Compressible Flows Involving Fluid-Structure Interactions. September, 1992--September, 1994.

Wu, Jie, Ph.D., Civil Engineering, University College of Swansea, 1993. Development of Finite Element Methods for Fluid Mechanics and Electromagnetics. March, 1993--Present.

Zhigang Yang, Ph.D., Mechanical and Aerospace Engineering, Cornell University, 1989. Modeling of Bypass Transition and Stability Analysis of Swirling Flows. July, 1990--Present.

Shaye Yungster, Ph.D., Aeronautics and Astronautics, University of Washington, 1989. Development of CFD Codes for High Speed Combustion and Detonation Waves. November, 1989--Present.

Jiang Zhu, Ph.D., Mechanics, Institut National Polytechnique de Grenoble, 1986. Development of Efficient, Robust Codes for Propulsion System Flows that Can Accomodate Various Turbulence Models. April, 1992--Present.

#### B. Visiting Staff/Consultants.

Andrea Arnone, Ph.D., Computational Fluid Dynamics, University of Bologna, Bologna, Italy, 1989. Assistant Professor, Department of Energy Engineering, University of Florence, Florence, Italy.

Thomas F. Balsa, Ph.D., Aerospace and Mechanical Engineering, Princeton University, 1970. Professor, Department of Aerospace and Mechanical Engineering, University of Arizona.

Iain Boyd, Ph. D., Aeronautics and Astronautics, Southampton University, Southampton, United Kingdom, 1988. Assistant Professor, Department of Aerospace Engineering, Cornell University.

Brereton, Giles, Ph.D., Mechanical Engineering, Stanford University, 1987. Assistant Professor, Department of Mechanical Engineering and Applied Mechanics, University of Michigan.

Frederic Coquel, Ph.D., Numerical Analysis, Ecole Polytechnique, Palaiseau, France, 1994. Researcher, Centre National de la Recherche Scientifique, Numerical Analysis Dept., Pierre et Marie Curie University, Paris VI, and Scientific Consultant, Theoretical Aerodynamics Branch I, ONERA, Chatillon, France.

Peter W. Duck, Ph.D., Fluid Mechanics, Southampton University, Southampton, United Kingdom. Reader, Department of Mathematics, University of Manchester, Manchester, United Kingdom.

Max D. Gunzburger, Ph.D., Mathematics, New York University, 1969. Professor, Department of Mathematics and Interdisciplinary Center for Applied Mathematics, Virginia Polytechnic Institute and State University.

Thomas Hagstrom, Ph.D., Applied Mathematics, California Institute of Technology, 1983. Associate Professor, Department of Mathematics and Statistics, University of New Mexico.

S. I. Hariharan, Ph.D., Applied Mathematics, Carnegie Mellon University, 1980. Professor, Department of Mathematical Sciences, University of Akron.

Brian P. Leonard, Ph.D., Aerospace Engineering, Cornell University, 1965. Professor, Department of Mechanical Engineering, University of Akron.

Chaoqun Liu, Ph.D., Applied Mathematics, University of Colorado, Denver, 1989. Scientist, Front Range Scientific Computations, Inc. and Associate Professor (adjunct), University of Colorado, Denver.

Sherwin A. Maslowe, Ph.D., Fluid Mechanics, University of California, Los Angeles, 1970. Professor, Department of Mathematics and Statistics, McGill University, Montreal, Canada.

Arthur F. Messiter, Ph.D., Aerodynamics and Mathematics, California Institute of Technology, 1957. Professor, Department of Aerospace Engineering, University of Michigan.

Christophe Pierre, Ph.D., Mechanical Engineering, Duke University, 1985. Associate Professor, Department of Mechanical Engineering and Applied Mechanics, University of Michigan.

Richard H. Pletcher, Ph.D., Mechanical Engineering, Cornell University, 1966. Professor, Department of Mechanical Engineering, Iowa State University.

James N. Scott, Ph.D., Aeronautical and Astronautical Engineering, Ohio State University, 1977. Associate Professor, Department of Aeronautical and Astronautical Engineering, Ohio State University.

Wei Shyy, Ph.D., Mechanical Engineering, University of Michigan, 1982. Professor, Department of Aerospace Engineering, University of Florida.

J. Trevor Stuart, Ph.D., Applied Mathematics, Imperial College of Science and Technology, University of London, 1951. Professor, Department of Applied Mathematics, Imperial College, London, United Kingdom.

Timothy W. Swafford, Ph.D., General Engineering, Mississippi State University, 1983. Associate Professor, Engineering Research Center for Computational Field Simulation, Mississippi State University.

Christopher K. W. Tam, Ph. D., Applied Mechanics, California Institute of Technology, 1966. Professor, Department of Mathematics, Florida State University.

Gretar Tryggvason, Ph.D., Engineering, Brown University, 1985. Associate Professor, Department of Mechanical Engineering and Applied Mechanics, University of Michigan.

Eli Turkel, Ph.D., Applied Mathematics, New York University, 1970. Professor, Department of Mathematics, Tel Aviv University, Tel Aviv, Israel.

Bram van Leer, Ph. D., Theoretical Astrophysics, Leiden University, Leiden, The Netherlands, 1970. Professor, Department of Aerospace Engineering, University of Michigan.

David L. Whitfield, Ph.D., Aerospace Engineering, University of Tennessee, 1971. Professor and Director, Computational Fluid Dynamics Laboratory, Mississippi State University.

Akira Yoshizawa, Sc. D., Physics, University of Tokyo, Tokyo, Japan, 1970. Professor, Institute of Industrial Science, University of Tokyo.

C. Graduate Students.

Scott A. Dudek, Department of Mechanical Engineering, University of California, Berkeley.

	1986	1987	1988	1989	1990	1991	1992	1993	1994
RESEARCHERS	23	43	50	46	47	49	58	64	50
SEMINARS	10	27	39	30	37	26	32	46	3
REPORTS	2	9	22	32	25	29	27	51	32
WORKSHOP/LECT. SERIES	1	0	2	1	1	1	1	1	2
NO. OF PRESENTATIONS	7	0	21	14	15	21	15	33	40

TABLE II. - ICOMP STATISTICS (1986 TO 1994)

ORIGINAL PAGE  
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Figure 1.- ICOMP Research and Administrative Staff in August, 1994. First row: Isaac Greber; Jie Wu; Karen Balog; Arthur Messiter; Andrea Arnone; William Liou. Second row: Peter Duck; Robert Rubinstein; Akira Yoshizawa; T.H. Shih; Fu-Lin Tsung. Third row: James N. Scott; M. E. Hayder; Jiang Zhu; Bo-Nan Jiang. Fourth row: Michael Salkind; Marvin Goldstein; David Modiano; S.H. Shih; Tawit Chitsomboon; Shaye Yungster. Fifth row: J.K. Chung; Bernard Greenspan; Daniel Winterscheidt; Andrew Norris; Kumud Ajmani. Sixth row: Theo Keith; Gretar Tryggvason; Erlendur Steinthorsson; James Loellbach; Charles Feiler; Aamir Shabbir; Zhigang Yang.

# REPORT DOCUMENTATION PAGE

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13. ABSTRACT (Maximum 200 words)  The Institute for Computational Mechanics in Propulsion (ICOMP) is operated by the Ohio Aerospace Institute (OAI) and funded under a cooperative agreement by the NASA Lewis Research Center in Cleveland, Ohio. The purpose of ICOMP is to develop techniques to improve problem-solving capabilities in all aspects of computational mechanics related to propulsion. This report describes the activities at ICOMP during 1994.			
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