Institute for Computational Mechanics in Propulsion (ICOMP)
Fourteenth Annual Report—1999

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May 2001
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INSTITUTE FOR COMPUTATIONAL MECHANICS IN PROPULSION (ICOMP)

FOURTEENTH ANNUAL REPORT

1999

SUMMARY

The Institute for Computational Mechanics in Propulsion (ICOMP) was formed to develop techniques to improve problem-solving capabilities in all aspects of computational mechanics related to propulsion. ICOMP is operated by the Ohio Aerospace Institute (OAI) and funded via numerous cooperative agreements by the NASA Glenn Research Center in Cleveland, Ohio. This report describes the activities at ICOMP during 1999, the Institute's fourteenth year of operation.

INTRODUCTION

The Institute for Computational Mechanics in Propulsion (ICOMP) was established at the NASA Glenn Research Center in September 1985. The overall purpose was 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 Glenn 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 1999.

The following sections of this report provide lists of the resident and visiting researchers, their affiliations and educational backgrounds. Individual sections are provided which briefly describe reports of RESEARCH IN PROGRESS, the REPORTS AND ABSTRACTS published over the past year.
THE ICOMP STAFF OF VISITING RESEARCHERS

The ICOMP research staff for 1999 is shown in Table I. A total of twenty researchers were in residence at ICOMP for periods varying from a few days to a year. The resident staff numbered sixteen while the visiting staff numbered four.

As usual, the resident researchers were very productive. Table II provides a numerical summary of ICOMP during its fourteen years of operation in terms of research staff size and technical output as measured by the numbers of seminars, reports and workshops.
JOONGKEE CHUNG
Research Area: Code Development for Unsteady Inlet Flows Using Parallel Processing, Iced Airfoils

1. Natural Laminar Flow airfoil (NLF 0414) experiment numerical analysis

An experiment using a NLF 0414 airfoil was conducted in the Low Turbulence Pressure Tunnel (LTPT) at the NASA Langley Research Center in October through November, 1998 for a 5 week time period. Measurements of the aerodynamic properties of an iced and a clean airfoil in a two-dimensional configuration were taken to obtain lift, drag, moment, pressure distributions.

Two codes (NPARC and WIND) were used for the evaluation of various flow properties to aid the direction of the experiment, and extensive computations were performed after the experiment for code validation and improvements. The final experimental and computational results led to two papers that were presented at the 38th AIAA conference in January 2000 in Reno, Nevada.

2. Code evaluation

The WIND code was applied to several different airfoils including NLF-0414, GLC-305, and several NACA series foils. This was done in order to compare to existing experimental results and computational results obtained from the NPARC code. It was found that for the selected problems, WIND predicts generally slightly higher lift than the NPARC code when the same turbulence model was used. The code did not show any instability due to the packing of grid in the inviscid region and was a little more stable at relatively high angles of attack or near stall. CPU time requirement was generally comparable or longer than that of the NPARC code. One advantage over the NPARC code was the capability of applying a Chimera-type overset grid for simplicity of grid generation.

3. Aeroperformance degradation comparison between the LEWICE-generated ice shapes and experimental ice shapes.

Aerodynamic calculations were performed using the WIND code on 10 experimental ice shapes and the corresponding 10 ice shapes predicted by the LEWICE 2.0 code. The difference in aerodynamic results between the experimental ice shapes and the LEWICE shapes were compared qualitatively. Correlations were generated to determine the geometric features which have the greatest effect on performance degradation. The results of this research led to a conference paper that was presented at the 38th AIAA conference in January 2000.

4. Cooperative research in automated grid generation for iced-airfoil aerodynamic performance analysis

Technical assistance was provided to Mississippi State University (MSU) researchers by supplying grids and NPARC subroutines and necessary files to evaluate the aerodynamic properties of iced airfoils to help develop an automated grid generation code 'ICEG2D'. This code was delivered to the NASA Glenn Icing Branch and the evaluation is underway for efficient aerodynamic performance degradation calculations.

THOMAS HAGSTROM
Research Areas: Algorithms for Boundary Layer Value Problems, Domain Decomposition

1. Radiation Boundary Conditions for Computational Aeroacoustics

The construction and implementation of accurate radiation boundary conditions continues to be a fundamental stumbling block to the development of reliable and efficient tools for jet and fan noise prediction. For simpler problems in wave propagation, such as electromagnetism, we along with other researchers have found an essentially complete solution of the boundary condition problem. The main issue is to what extent these successful ideas can be carried over to the linearized compressible flow equations.

i. With J. Goodrich of the Acoustics Branch, we continued work on high-order approximate conditions for periodic and duct flows. In particular we developed and tested high-order discretizations, and also developed a simply solved yet relevant model problem for quick comparisons of different approximate sequences. An extensive article including a complete theoretical analysis and comprehensive experiments is under preparation.
i. With S. I. Hariharan of ICOMP, we have continued work on boundary conditions for external problems based on the generalization of progressive wave expansions to the convective wave equation. In three dimensions, these are exact for solutions described by finitely many spherical harmonics. However, they are only defined on an elliptical boundary whose aspect ratio is determined by the free stream Mach number. We have looked at a few formulations using auxiliary functions, and are in the process of testing them.

ii. We have started to look at boundary conditions for the Euler equations linearized about parallel flows. In this important case, detailed representations of the exact condition are unavailable or difficult to use. Alternatives under consideration include high-order expansions of the symbol of the boundary operator derived from factoring the problem into incoming and outgoing pieces, and proper generalizations of sponge layer methods.

2. High-Order Methods for Hyperbolic Problems in Complex Geometry

Although the superior efficiency of high-order methods for simulating difficult wave propagation problems is well-known, their application to problems in engineering is hampered by the need to deal with physical boundaries. It has been difficult to define stable and accurate boundary closures near complicated boundaries. One source of difficulty, which has been the primary focus of our work, is the so-called Runge phenomenon, which suggests that one must cluster points near the boundary. One way around this problem, which we have worked on with J. Goodrich and R. Dyson of the NASA Glenn Acoustics Branch, is to use derivative data rather than stencil enlargement to attain high accuracy. This approach skirts the Runge phenomenon completely. A second approach, focused on the scalar wave equation, involves integral equation reformulations. Discretizing these leads to methods with adaptive stencils which we've found to be stable independent of CFL number. This allows us to use a clustered mesh without decreasing the time step. Collaborators on this project are B. Alpert of NIST and L. Greengard of the Courant Institute.

3. High-Order Simulations of Unsteady Combustion Phenomena with Complex Physical Models

In collaboration with K. Radhakrishnan of ICOMP and R. Zhou, a graduate student of UNM, we have continued work on an accurate code for simulating unsteady combustion phenomena employing complex models. This year, high order time stepping based on a linearly implicit method with a simple preconditioner combined with deferred correction has been successfully implemented and tested. In concert with a new mesh adaption algorithm, the code has been used to simulate quenching of a flame impinging onto a cold wall. Simulations of a number of other problems, including flame ignition, pulsating instabilities, and spherically expanding flames are under way.

DUANE R. HIXON
Research Area: Aeroacoustics

Work continued on the development and application of high-accuracy numerical schemes for the computational prediction of supersonic jet noise. The sixth-order compact code has been parallelized using MPI, and is running on a distributed workstation cluster as well as on an SGI Origin 2000. The first preliminary results from a coarse-grid Large Eddy Simulation with a round nozzle geometry in the computational domain were obtained, and are very promising.

Some steps towards the computation of arbitrary geometry nozzles have been taken. Wall boundary conditions for 3-D unsteady viscous flows were formulated [1], and an investigation of the cylindrical coordinate centerline singularity showed that the curvilinear equations accurately calculate the flow in this region [2]. In a step towards dynamic grid adaption, the effect of a moving grid on an unsteady solution was investigated, and a numerically conservative and consistent set of unsteady metrics was derived for the strong conservation equations [3].

The code was validated for nonlinear flows with shocks as well as for complex-geometry airfoils in blind tests for the 3rd CAA Workshop for Benchmark Problems [4,5]. The solutions for these cases agreed very well with the exact solutions, and more work is currently being done on the airfoil gust problem.

Also in 1999, journal papers were published which dealt with numerical methods [6-7], nonlinear jet flow physics [8], boundary conditions [9], and numerical treatment of centerline singularities without coordinate transformations [10].

Work will continue in two directions: application and improvement of the curvilinear code. Further 3-D LES nozzle + jet applications will be run in 2000, and improvements in the accuracy, speed, and robustness of the compact scheme will be investigated.

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References


FOLUSO LADEINDE

Research Area: Parallel Implementation of Compact, Curvilinear High-Order Formulas

High-order formulas are required for differencing and filtering the Navier-Stokes equations in order to obtain the needed accuracy for a variety of CFD applications. Furthermore, the computational load associated with the solution of realistic fluid dynamic systems mandates code execution on supercomputers, to take advantage of massive parallelization in such systems. The parallel performance issues relevant to the AFRL code, FDL3DI, which is based on the compact formulas and developed for general curvilinear systems, was studied in this investigation with emphasis on the associated implicit operators. These operators usually lead to low-efficiency parallel codes. In our search for an efficient parallel procedure, three methods were investigated: the one-sided method, the Parallel Diagonal Dominant method (PDD), and the Parallel Thomas Algorithm method (PTA). These parallel procedures were implemented in the AFRL code, FDL3DI. Kernel codes were also developed to extract some inherent performance features of these methods. Some of the calculations combine the methods for compact differencing and filtering. In general, the procedures based on the one-sided schemes produced accurate results and good parallel performance (efficiency, speedup, and scalability). The procedures that combine the one-sided schemes and PDD also performed well. However, parallel calculations that use the PDD method for both compact differencing and filtering produced the wrong results for low-order filters. On the other hand, high-order filters cause PDD to be very expensive. The one-sided method leads to superscalable calculations when the number of processors is few. For PDD, increasing the number of grid points in the derivative-difference direction leads to better speedup, as does an increase in the number of right-hand side (RHS) columns. In standard implementation (i.e., without engaging the processors during the idle time), the PTA procedure has a very poor parallel performance in comparison to PDD and the one-sided formulations. However, the procedure tends to be more accurate.

The relevance of aeroacoustics to the aerospace industry is well recognized. The requirement for very high-order accurate procedure and massive parallelization makes this topic a target for the application of the capability developed in this project. Numerical procedures based on the dispersion relation-preserving (DRP) technique have been proposed for aeroacoustic computation. However, the application of this technique to realistic aerodynamic systems has not received enough attention. Also, the performance of the method on general curvilinear coordinate formulation has not been reported. Preliminary work that compares DRP with the
compact procedures was initiated in this project. The objectives were three-fold: 1) to compare accuracy of DRP and the sixth-order compact differencing scheme (CD6), 2) to investigate far-field boundary treatments by the two methods, and 3) to investigate relative performance under curvilinear coordinate transformation. The AFRL code, FDL2Di, was used for the studies, meaning that the DRP procedure was implemented inside this code. The results of the preliminary studies can be summarized as follows: For the rectangular aeroacoustic Benchmark Category 1 Problem 2 (1997) test, both DRP and CD6 performed very well. For the Benchmark Category 4 Problem 1 (1995) test involving the scattering of acoustic pulse from a cylinder, which involved the implementation of DRP in curvilinear coordinate, we observed that CD6 was easier to implement. The time-dependent acoustic pulse problem posed some difficulties for DRP in a curvilinear coordinate formulation.

STEWART LEIB

Research Area: The Effect of Finite Nozzle Length on Sound Radiation from Turbulent Flows

The use of mixer-ejector nozzles to improve mixing and reduce the exit velocity of aircraft engine exhaust jets has focussed attention on the problem of predicting the sound field due to sources located within the nozzle. Clearly such sources are profoundly influenced by the presence of the nozzle, but current jet noise prediction schemes do not incorporate its influence on the far-field sound.

During the past year work has been done on the development of a theoretical prediction scheme for the far-field sound radiated by internal sources which includes the effect of a finite length nozzle. The scheme is based on a high-frequency, geometric acoustics, solution to the acoustic analogy of Lilley. This solution was used to evaluate the sound radiated by a turbulent flow within the nozzle by assuming the turbulence to be axisymmetric about the mean flow direction. The general analysis was applied to the case of a circular duct with an axisymmetric mean flow for both hard and acoustically treated walls.

The solution requires the computation of many ray trajectories, which can be a time consuming process. However, since each ray path is completely independent of all the others, the calculations lend themselves to parallel-processing techniques. A code for parallel computation of ray trajectories on a cluster of personal computers has been developed, and calculations are being performed for the case of a rectangular duct -- the geometry envisioned for the high speed mixer-ejector.

Publications


JAMES LOELLBACH

Research Area: 3D Structured Grid Generation Codes for Turbomachinery

During 1999, research tasks were performed relating to numerical analysis of turbomachinery components. The work was performed in cooperation with Chunill Hah of NASA Glenn Research Center.

One project, performed in conjunction with the U.S. Navy, and currently ongoing, concerns the design of the exit volute of a centrifugal compressor for a refrigeration system. The goal of this program is to couple a numerical flow solver with an optimization program to obtain a diffuser and volute geometry that minimizes total pressure loss and maximizes static pressure recovery. Numerical simulations were performed using an unstructured Navier-Stokes solver originally developed at NASA Langley Research Center (USM3D) and later modified by Fu-Lin Tsung of ICOMP for turbomachinery flows (TUSM). The optimization programs were developed by the U.S. Navy. The contribution during 1999 consisted of developing grid-movement programs that modify an existing computational grid to conform to a new shape prescribed by the optimization program. These programs link the flow solver to the optimization program and allow automation of the entire process. Work is continuing on integrating all of the component programs with the goal of performing an optimization of the vaneless diffuser and possibly the volute in 2000.

In addition research tasks were initiated in support of the Ultra Efficient Engine Technology (UEET) Program. The goal of this work, which continues through 2000, is to simulate the effect of secondary flow jets on the performance of the UEET compressor rotor. Numerical simulations for this program are being performed using the unstructured Navier-Stokes solver mentioned above. During 1999, work was devoted to generating an unstructured computational mesh for the numerical solution. Flow simulations with and without secondary jets will be performed in 2000.

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Other work during 1999 involved grid generation and post processing tasks for numerical simulations of turbomachinery components in support of various NASA programs and industry collaborations. These simulations were performed using a structured Navier-Stokes solver developed by Hah and grid generation codes developed by Loellbach. One such study examined the effects of various circumferential groove configurations around the casing of an axial compressor operating near stall. In another study, numerical solutions of NASA’s Rotor 35 were examined to identify details of the tip clearance flow structure in transonic axial compressors. In late 1999, work was begun on the simulation of a centrifugal compressor stage (including inlet guide vane, rotor, and vaned diffuser) in cooperation with NASA Marshall Research Center.

ROBERT W. MACCORMACK

Research Area: Numerical Algorithm Research for Magneto-Aerodynamics

The application of a magnetic field on the hypersonic flow about a body was observed experimentally, more than forty years ago, to have a strong effect on displacing the surrounding bow shock wave away from the body. Early analysis confirmed this observation and indicated that surface pressure falls more rapidly away from the nose of the body and velocity gradients are reduced near the body surface with an applied magnetic field. This also indicates potential drag and heat transfer reduction from magneto-fluid dynamics interaction and possible favorable effects for propulsion. Recent Russian studies have renewed considerable interest in this subject area. The purpose of the present effort was to develop a numerical procedure for simulating the flow about a body traveling at hypersonic speeds with and without magnetic field interaction.

A computer program was written for solving the equations of magneto-fluid dynamics with boundary conditions suitable for simulating the flow about a hypersonic body traveling within an imposed magnetic field. Preliminary results are in agreement with both the earlier experimental observation and analysis. However, under the conditions of the present study, for both adiabatic and isothermal wall boundary conditions and with zero gradient wall boundary conditions for the magnetic field components, the drag is actually increased when the magnetic-fluid stresses also acting on the body are included. In some cases there is a small heat transfer reduction. Additional cases, with other wall boundary conditions for the magnetic field components, are to be studied for, perhaps, a more realistic simulation of the physical flow.

REDA MANKBADI

Research Area: Aeracoustics

1. Very Large Eddy Simulations for Jet Noise (VLES): Several turbulence models were identified for use in VLES of the jet noise prediction code. These models are the Smagornisky model, the dynamical model and the Yoshizawa and Horiuti one-equation model. The Smagornisky model run with no excitation and the results showed no real spreading due to lack of resolution near lip. A coarse-grid k-epsilon VLES is currently running (but not quite completed). The preliminary results indicate that the k-epsilon model is causing the jet to spread in a steady manner. The next series of runs will focus on running a finer grid. To keep the CPU time reasonable, the time stepping method needs to be improved.

2. Noise Produced by Nonlinear Instability Wave: In collaboration with Dahl and Lee critical-layer theory was used to obtain the nonlinear development of an oblique wave in compressible shear layers. This solution could be used to obtain the resulting sound field using either asymptotic analysis or Kirchhoff’s Method.

3. Collaboration: Work was initiated with R. Hixon to develop fast-running axisymmetric version of the jet noise code based on the split-compact scheme.

4. Inflow Treatment: A paper was written on the performance of various subsonic inflow treatments for jet flow. The paper was presented as an AIAA paper in the 1999 Aeroacoustics Conference.
James H. Miller  
Research Area: Fluid Dynamics and Lasers

Work was performed on the computational COIL (Chemical Oxygen Iodine Laser) initiative using the 2nd-order accurate (in time and space) codes FDL3DIP and Cobalt. Validation test cases were completed in September of 1999. Cobalt was chosen over FDL3DIP as the baseline code to incorporate COIL chemistry.

Two-dimensional flow through converging-diverging nozzle geometries were simulated using Cobalt and FDL3DIP. Superior parallel performance was demonstrated using Cobalt for a grid consisting of 158,000 points. Nearly linear speedup was observed up to 60 processors on the IBM SP2 and 120 processors on the SGI T3E. Because of the parallel performance and expected ease of implementation, Cobalt was chosen to implement the COIL chemistry.

The COIL utilizes a three-dimensional supersonic converging-diverging nozzle with sonic injection occurring upstream of the nozzle throat. The complexity of the injector/core flow interaction may be a source of flow unsteadiness or turbulent flow. The question of unsteadiness or turbulence will be answered by rigorously examining results obtained from numerical simulations using time-accurate methods and a k-ω turbulence model available in the Cobalt code.

Near the end of September, experiments were performed at Kirtland Air Force base to help provide better understanding of the fluid dynamic phenomena inside the COIL nozzle. In these experiments high pressure helium flow was injected into subsonic helium flow via sonic normal injection. Computations were then performed to compare with experimental data. The computed steady-state results were obtained using laminar assumptions. The computed results are in excellent agreement with the measured mass flow rates and measured pressures. These results will be presented at the 31st AIAA Plasmadynamics and Lasers Conference.

Philip E. Morgan 
Research area: Computational Research in Multidisciplinary CFD and CEM

Research was performed using a parallel version of the FDL3DI code. The parallel version of the FDL3DI code is a three-dimensional second-order time accurate, Navier-Stokes solver based on an implicit approximate-factorization Beam-Warming algorithm. The parallel scheme decomposes the grid using two-dimensional multi-partitioning to evenly distribute the work across multiple processors with parallel communication via Message-Passing Interface (MPI) library.

The parallel version of the code was validated and its performance was assessed on two supercomputers, the IBM SP2 and the Silicon Graphics Origin 2000. The solver was validated for Couette flow, and both steady and unsteady flow over a circular cylinder. The parallel version of the solver was able to maintain 50% efficiency for up to 64 processors on both supercomputers. The solutions from FDL3DI code were shown to be independent of the number of processors and computer platform.

In August, the code successfully passed beta testing. Preparation for the beta test consisted of detailed parallel performance, development of code documentation and a graphical user interface.

The code was upgraded to be second order accurate in time and boundary conditions were modified to investigate direct numerical simulation (DNS) for two and three dimensional flow over a stationary and a rotationally oscillating circular cylinder. The code solved grids ranging from 0.5 to 8.5 million grid points at rates up to 10 times faster than capable by a sequential vector-based supercomputer version of the code.

Results from the above work were presented in a paper [1] at the AIAA 38th Aerospace Science Meeting & Exhibit at Reno, NV in January 2000.


Andrew T. Norris  
Research Area: Aerothermochemistry

1. ILDM Work

Two different activities were proposed for the development of the ILDM method, and one task from 1998 was resumed.
i. Jacobian Evaluation of Manifolds.

For this task, the development of an adaptive tabulation scheme was accomplished. How this differs from the existing version is that the new method allows full point-refinement, rather than requiring the sequential partial refinement of all points. The code for this is currently being verified. In addition, an existing Jacobian ILDM code has been obtained, and its suitability evaluated.

ii. Interactive Tabulation.

For this task, the first requirement is point-refinement adaptive tabulation scheme, and this was developed in conjunction with the previous task. Details of how this code should be altered for parallel computer architectures are currently being considered.

iii. Neural Network Reaction Storage.

Preliminary work was resumed on this task, which is currently being carried out in conjunction with Albert Huntington of Virginia Tech. He has been working closely with AbTech in developing neural models from data supplied by NASA. In turn, these neural models will be returned to NASA to be tested.

2. NCC work

Three main areas of work were performed in the development of the NCC.

i. PDF models

Development of the PDF model was accomplished, with the standardization of the combustion modules, and physical properties. In addition a new convection scheme was coded, along with new time averaging and random number generation.

ii. User Interface

The chemistry user interface for NCC has been streamlined, with the new input automatically assigning properties from the NASA thermodynamic database. In addition, significant portions of the chemistry routines have been re-written to accommodate the new method. Also a dedicated one-step global chemistry option has been added as an additional chemistry model.

iii. Validation

Validation has been confined to testing the chemistry and input routines, and so has focused on simple flame problems.

3. Publications


KRISH RADHAKRISHNAN

Research Area: Improved Numerics for Reacting Flow Application

Introduction

The ability to perform computational fluid dynamic (CFD) computations of turbulent chemically reacting flowfields is very important to the success of the Smart Green Engine, Fire Safety, and Pulse Detonation Engine programs at the NASA Glenn Research Center. The chemical kinetics of practical fuels typically involves numerous chemical reactions among a large number of species. However, at present, it is not practicable to include all species and all reactions in a CFD calculation, because of prohibitive memory and computer time (i.e., computational cost) requirements. It is therefore common practice to use "simplified" reaction mechanisms, which typically consider only a few species participating in reactions thought to be essential to the simulation.
An alternate approach is to simplify the geometry and fluid dynamic considerations and then solve the full set of chemical kinetic rate equations. This approach enables one to understand the impact of the complete set of chemical reactions and species on the process of interest (e.g., pollutant formation and destruction). It also permits judgment of the efficiency of a simplified mechanism used in CFD simulations, by comparisons of the results with those produced from detailed mechanisms. At the same time, analyses with the full mechanism helps to identify reactions and species that must be included in the CFD simulation; that is, the minimal set of species and reactions is identified that is needed to study the process of interest.

To make possible calculations using detailed combustion chemistry, the NASA-Lewis kinetics and sensitivity code, LSENS was developed by Radhakrishnan. This code, which has been widely distributed, solves a variety of reaction models, and has been continually updated to both enhance its utility by including new options and convenience features and improve computational efficiency.

In addition to using codes like LSENS, which can handle only static problems (i.e., no diffusion of matter of energy), to assess utility of reduced mechanism, calculations of flame speed and species distributions are reasonable choices. One drawback of currently available flame codes is the lack of robustness. In addition they were developed in the 1970's and do not exploit some of the recent advances in the numerical solution of pde's. Consequently, to ensure reliability of computed results, a large number of grid points have to be used, and so current flame codes can be expensive to run. In collaboration with Professor Thomas Hagstrom of the University of New Mexico a new flame code that uses very high-order accurate methods is being developed. This one-dimensional reaction/diffusion code, which uses complex models for the combustion chemistry and species transport, is being updated to make it time accurate and enable simulation of two-dimensional problems.

These codes are useful for studying low speed phenomena, in order to better understand flow physics and help with the elucidation and reduction of complex chemical reaction pathways. However, many practical devices, such as ram accelerators and pulse detonation engines, involve chemically reacting gas mixtures that flow at very high speeds (typically at hypersonic velocities). In order to simulate/study the physics of high speed flows encountered in hypersonic applications, Dr. Shaye Yungster of ICOMP and I developed a fully implicit (for computational efficiency) time-accurate reacting flow code, capable of simulating of two-dimensional or axisymmetric, viscous (or turbulent), reacting flows, using detailed chemistry. Accuracy of this research code has been established by calculating several benchmark test cases, for which experimental data are available.

**Progress**

**Smart Green Engine Program**

For the Smart Green Engine program, the LSENS code has been modified to incorporate several new features, as follows: (1) The ability to handle several new rate coefficient expressions that are being increasingly used were included. (Previously only the so-called modified Arrhenius expressions could be used.) (2) At the request of Dr. Viet Nguyen of the Combustion Branch, the automatic calculation of sensitivity coefficients (i.e., partial derivatives) of the heat release rate with respect to initial condition values and rate coefficient parameters for both static and inviscid, one-dimensional chemically reacting flow problems was incorporated. For example, these sensitivity coefficients are required for performing linear stability analysis of combustion-acoustic interactions using detailed reaction mechanisms. This new option can be utilized to examine the effects of perturbations in the fuel-air ratio due to fluctuations in the fuel system and/or the air line. Thus effects of fluctuations in fuel-flow rate due to fluctuations in the fuel line can be separated from those caused by fluctuations in the air stream. (3) Recently, several methods have been proposed to automatically reduce a given mechanism, producing a simplified mechanism. One such method, involving the ranking of a mechanism to discard species and reactions considered unimportant according to criteria provided by the user, was incorporated into LSENS. (4) The rewrite of LSENS to make it more user friendly by simplifying input data file preparation was initiated last year. Also, the options included in the code are being expanded by enabling the user to perform reflected shock calculations and detonations and to use global reaction (i.e., simplified) mechanisms. The required coding to perform these calculations has been completed and will be included once the format-free version of the code has been completed. The present version of LSENS was presented at the '99 AIAA/SAE/ASEE Joint Propulsion Conference. It was subsequently revised for publication as a NASA CR and is being further revised for submission to the AIAA Journal.

Also for the Smart Green Engine Program, the collaboration with Prof. Thomas Hagstrom, that is, the implementation and testing of new numerical methods for solving the equations of low Mach number reactive gas mixtures including detailed reaction mechanisms and diffusion models, continued Zero Mach number limiting equations, rather than the full compressible equations, are solved. These equations do not support sound waves. The relatively fast sound waves, when treated explicitly, create severe stability problems due to CFL restriction, while when treated implicitly lead to systems with nearly imaginary large eigenvalues, creating problems for iterative solvers. Their absence allow us to employ more efficient time-stepping strategies. As many flame propagation problems involve rather small Mach numbers, these equations have a wide range of applicability. Acoustic effects can be included in a perturbative framework, although we have not as yet experimented with such an approach.
Explicit and compact spatial differencing of order up to six has been used. The use of higher order methods allows us to use fewer mesh points. The overhead associated with high order differencing is overwhelmed by the costs associated with evaluating the complex reaction and diffusion models. A form of grid staggering is used to ensure the parabolicity of the discrete diffusion operators. We have experienced some stability difficulties with sixth order explicit methods near boundaries. We believe these are associated with the Runge phenomenon, and can be alleviated via mesh clustering.

A linearly implicit time-stepping strategy is used. It is centered around the use of a (preferably simple) preconditioner in the implicit step. We do not iterate, hence the method is fully implicit. We have found that a preconditioner based on low order discretizations of simplified (Fickian) diffusion models combined with the full linearization of the reaction mechanisms is effective. Indeed, we have found that the time step is restricted only by accuracy.

For the direct computation of plane flames and their speeds, the time-stepping strategy is combined with a novel control strategy to determine the stabilizing inlet velocity while enforcing a phase condition. Final convergence is accelerated by Newton’s method. In our experiments so far, the method has never failed to converge despite the use of a generic and quite inaccurate initial guess.

Spatial mesh adaptation is based on the equidistribution of scaled first and second derivatives of a monitor function. In our experiments so far we have always used the temperature in this role. We also adapt in time. Temporal error estimates are readily available as part of the deferred correction procedure.

We have carried out a number of experiments with the code. For the steady code, we have considered hydrogen-air, methane-air, and propane-air mixtures at a variety of temperatures and pressures. This work was presented at the HBCU Conference at OAI, NASA Glenn and at the 1998 and 1999 AIAA/ASME/SAE/ASEE Joint Propulsion Conferences, and is appearing as a NASA CR. Another NASA CR is under preparation, and we expect to submit in the near future two or three journal publications dealing with the numerical methods and applications.

Finally for the Smart Green Engine Program, a two page summary of the findings and recommendations of the Trace Chemistry Group at the Aerosols and Particulates Workshop hosted by NASA Glenn in summer 1997 was prepared. (I was the co-chairman of this group and the summary was prepared for a NASA publication.)

**Aircraft Safety Program**

For the Fire Safety Program, the goal for the past year was the identification of models and computational fluid dynamic (CFD) computer codes that can be used for analyzing the three-dimensional flow field and temperature and composition distribution in the central fuel tank of a commercial aircraft, given heat fluxes to the tank. The ability to simulate the processes occurring inside the fuel tank during flight, given the flight path, is crucial to minimizing, or even eliminating, highly flammable regions inside the tank, thereby minimizing possibility of an in-flight explosion. Because of the complexity of the modeling work involved it had been envisioned that development of this capability will be a long-term effort. The goal for the first year was to identify/locate submodels and computer codes that enable one to study the flow field and temperature and composition distributions within a simple, stationary rectangular tank containing a single volatile liquid and subject to a known heat flux profile. Several meetings were held with personnel at the Boeing Aircraft Company in order to obtain data that are good approximations for the heat and to better understand the flow physics inside the fuel tank, including especially the experience gained from their simple, one-dimensional modeling of a fuel tank. Based on these meetings and a comprehensive review of the literature, the following obstacles to successful modeling of the fuel tank were identified: (1) The physics of evaporation and condensation are not well understood. In particular, the interfacial boundary conditions, which include discontinuities in thermodynamic properties and velocity, are not well understood. (2) The flow inside the tank can transition from laminar flow to turbulent flow, because of the high Grashof numbers. The turbulent transport modeling poses another problem, because of the difficulty in constructing computationally efficient models that capture the flow physics. In light of these obstacles to modeling, after discussions with Bryan Palaszewski, the current goals were modified to: (1) Develop a one-dimensional code to test physics of evaporation, (2) Adapt existing laminar two component code to include turbulent transport, and (3) Identify minimal component set that simulates aircraft fuel and develop correlations for their thermodynamic and transport properties.
High-Speed Research Program

For the High-Speed Research Program, help was provided to Dr. Shaye Yungster in using the equilibrium routines built into LSENS and which were rewritten last year for use with a 1-D CFD code for analyzing the "independent ramjet stream" (IRS) cycle, in which the rocket and ramjet streams do not mix. Work with Dr. Yungster continued with the testing/validating of our two-dimensional CFD code developed for studying flow physics of high-speed chemically reacting flows. In particular, the code was used to study the reacting flow establishment and development around projectiles in an expansion tube, for which some published experimental data were located. The temporal evolution of combustion flow fields established by wedge-shaped bodies and explosive hydrogen-oxygen-nitrogen mixtures accelerated to hypersonic speeds in an expansion tube was investigated. Two kinds of flow phenomena were observed experimentally. In the first the interaction between the shock wave and the explosive mixture resulted in either a stable shock-induced combustion, wherein the flame front was decoupled from the oblique shock, or in a steady-state situation with combustion only in the boundary layer, especially within the separated flow region created by the shock wave/boundary layer interaction. In the second type of phenomenon, flow unstart and the generation of an upstream-propagating detonation wave were observed. Our CFD simulations were able to capture all these phenomena, thereby reinforcing the accuracy and reliability of our code. More importantly, our simulations showed that experimental data for one set of conditions had been obtained before the reacting flow had been fully established; that is, before steady state conditions. This lack of test times sufficiently long to fully establish the flow field is one of the main difficulties associated with modern pulse facilities. CFD simulations can complement experimental work by answering important questions, such as the existence of a steady state and time required for its establishment time, because they do not have test time limitations. Also, CFD can be used to extrapolate test results to the high pressures where propulsion systems will actually operate and which cannot currently be attained in the laboratory. This work was presented at the 1999 AIAA/ASME/SAE/ASEE Joint Propulsion Conference. It is also appearing as a NASA CR, and we have submitted a revised version to the journal "Shock Waves."

Presentations/Publications


Research Area: Modeling Metabolic Pathways and Dynamics in the Human Body

Introduction

Coronary heart disease remains the leading cause of death in the United States, with approximately 1.5 million new and recurrent cases of myocardial infarction per year. A severe coronary artery occlusion may result in myocardial ischemia (decreased blood flow.
to heart) or cardiac arrest, causing global ischemia and consequent interruption of brain blood flow. In both myocardial and cerebral ischemia oxygen delivery does not match the energetic demands of the underperfused tissue/organ, resulting in profound metabolic derangements, energy loss, and acidosis. Some of the deleterious effects of ischemia may be reversed by successful resuscitation with organ reperfusion, but unwanted consequences may arise from this abrupt increase in organ blood flow. A better understanding of the underlying mechanisms regulating tissue pH and substrate oxidation under ischemic conditions would lead to the development of new pharmacological therapies that reduce tissue acidosis, increase carbohydrate oxidation, or inhibit fatty acid oxidation. These "metabolic strategies" could act by direct or indirect manipulation of (1) enzyme levels, (2) enzyme activities, or (3) concentrations of metabolites affecting the metabolic pathways altered by the ischemic insult. Specifically, we do not currently know the physiological events that lead to the pathology of reperfusion injury. Cell death in reperfusion injury can be tied to metabolic-stress-induced cellular apoptosis and necrosis. During ischemia and reperfusion, the redox state of the cytoplasm is changed, as is the phosphorylation potential. However, we do not know the impact of these changes on enzyme activity in key metabolic pathways and on the activation/inhibition of control proteins.

The last several decades have witnessed an immense increase in biomedical information, mainly due to application of reductionism in biomedical research. In metabolism, this approach has made possible: (1) discovery of the functional pathways of metabolic processes and the component reactions in the pathways; (2) characterization of the enzymes that catalyze the reactions; and (3) identification of the genes that encode the enzymes. However, accumulated knowledge of the components of a metabolic system at all levels of complexity has not led to an understanding of the factors determining material fluxes in different pathways, nor of how the rates of production and utilization of metabolites are maintained at specific steady states, based on the tissue's metabolic, redox, and energy states. To understand the significance of molecular events and their role in controlling metabolic processes in complex physiological systems, it is necessary to link the molecular level with the system level by means of quantitative physiological models and appropriate numerical simulations.

In collaboration with Professor Joseph LaManna of Case Western Reserve University School of Medicine, Cleveland, OH and Professor Marco Cabrera of Rainbow Babies and Children's Hospital, Cleveland OH a previously developed mathematical model of the human bioenergetic system that integrates metabolic pathways and cellular processes to organ and whole body responses was recently extended to include sensitivity analysis. This model had been validated with published experimental data of metabolite concentrations across various tissue beds and from skeletal muscle biopsies collected in response to ischemia, hypoxia (reduction in oxygen delivery), and exercise. Our next step is to extend this model to include other metabolites, develop detailed models for other tissues/organs, and simulate metabolic responses to various stimuli.

Progress

During this year, analytical models and a computer code were developed that extend the work of Cabrera, who developed a model for studying energy metabolism and its regulation in the human body. Specifically, the improvements include more efficient solution methods for solving the ordinary differential equations that arise in modeling biological systems (see below) and the inclusion of the ability to perform a systematic sensitivity analysis, which provides the basic methodology for studying parameter sensitivities (i.e., changes in model behavior due to parameter variation). Sensitivity analysis establishes relationships between the predictions of a model and the parameters of the problem (i.e., initial conditions, rate coefficient parameters, etc.). It permits studying the effects of variations in tissue oxygenation and parameters controlling cellular respiration on glycolysis, lactate production, and pyruvate oxidation. An important application of this capability would be the examination of the results of defects (e.g., genetic and pathological states) in a metabolic pathway, as well as the effects of pharmaceutical intervention. This capability may also prove to be important in optimizing experimental design, thereby reducing use of animals.

In the modeling approach adopted by us, cellular processes are lumped together to provide tissue and organ, and in turn whole body, responses to stimuli. Indeed, the whole body is described as a bioenergetic system consisting of metabolically distinct organ/tissue subsystems that exchange materials with the blood (i.e., the circulatory subsystem). These materials include the species involved in both the production and utilization of ATP (adenosine triphosphate, the universal "energy currency" of living things). Examples of such species are glycogen, glucose and its breakdown products (e.g., pyruvate), alanine, fatty acids, oxygen, and carbon dioxide. Thus the species list includes the major fuels, the oxidizer, and the waste products of respiration.

In our initial collaborative studies, following Cabrera's work, the human body was subdivided into the following four subsystems: (1) cardiopulmonary gas exchanger (i.e., the lungs and heart as a pump), (2) splanchnic (i.e., visceral) tissues, (3) skeletal muscles, (4) all other tissues. The advantage of this modular approach is that additional tissue systems can be included as details concerning their metabolic rates become available. Each subsystem was modeled as a perfectly mixed compartment; communication/interaction among the subsystems was by means of the circulating blood. This problem was selected, because results of previous simulation and experimental data are available, thereby permitting evaluation of the new computer code. In addition, results generated by systematic sensitivity analysis (which is a relatively new tool in the study of metabolic pathways) can be evaluated more readily on a relatively small model. Experience gained from this exercise has led to increased confidence in both the numerical approach and the computer
In order to study the dynamic behavior of each subsystem, the metabolic pathways and transport processes were coupled within each subsystem. The species' conservation equations then reduce to a system of first order, nonlinear ordinary differential equations. Dependent variables are the concentrations of various metabolites relevant to energy (i.e., ATP) metabolism and regulation. The independent variable is time and the input parameters include anatomical (e.g., tissue volume), physiological (e.g., inspiration rate), and chemical (e.g., reaction rates) details of each subsystem.

To solve the stiff system of ordinary differential equations resulting from the different relaxation times for different species, numerical techniques (and FORTRAN subroutines) were adapted from the NASA Glenn kinetics and sensitivity analyses code, LSENS, written by Radhakrishnan. Suitable modifications were made to LSENS for application to biological systems, to incorporate nonstandard rate expressions that arise from the coupling of the diffusion and reaction terms. A major advantage of LSENS is the efficient procedures supporting systematic sensitivity analysis.

During the first year of the project, a FORTRAN subroutine package giving us the ability to model the dynamics of energy metabolism and regulation was developed. To illustrate the predictive value of our code, we applied it, in conjunction with the above model of bioenergetics, to study effects of skeletal muscle ischemia (i.e., of reduced oxygen transport), and compared the computed results with experimental observations from human occlusion studies. For a skeletal muscle blood flow rate of 0.3 l/min (normal flow rate is 0.9 l/min), the computed changes over 30 minutes in muscle glycogen, glucose, pyruvate, lactate, and phosphocreatine concentrations closely corresponded to those observed experimentally.

To illustrate the utility of sensitivity analysis, we examined the effects of various parameters, such as initial skeletal muscle and arterial oxygen and glucose levels and rates of oxidative phosphorylation. Among the species examined, those that had the largest effect were skeletal muscle adenosine diphosphate (ADP) and phosphocreatine. However, the effects of reduced oxidative phosphorylation rate were far more significant. Indeed, this parameter was found to be much more important than the concentration of oxygen in the tissue. Our conclusion is that, in agreement with previous observations, although tissue oxygen concentration has to be extremely low (near its critical value) to reduce the rate of oxygen consumption by one-half, changes in oxygen delivery that result in a reduction in the tissue oxygen consumption rate by as little as 1% can significantly affect lactate metabolism through the effects on ADP and nicotinamide adenine dinucleotide (NADH). These results are in good agreement with those previously obtained by actually changing the values of model parameters to study their effects on the computed solution.

Results summarizing the above findings were presented by Radhakrishnan (by invitation as a paper) at the 27th Annual Meeting of the International Society on Oxygen Transport to Tissue, Dartmouth Medical School, Hanover, NH, 28 August - 2 September, 1999. Subsequently, the paper has been submitted for publication in *Advances in Experimental Biology and Medicine*.

Presentations/Publications


AAMIR SHABBIR

*Research Area: Turbulence Modelling*

Simulations of Low Speed Axial Flow Compressor (LSAC) were carried out using APNASA, which is a viscous three dimensional solver for multistage turbomachines. LSAC is nine blade-row compressor. The flow leakage arising from the leakage path beneath the stator-foot-rings was accounted in these simulations. The results of the simulation agreed well with the experimental data of Wellborn and Okiishi (1996). Comparisons included the overall performance parameters as well as the detailed axisymmetric profiles. These results lend confidence to the closure scheme used for calculating the deterministic stresses in APNASA.

References

TSAN-HSING SHIH

Research Area: Achievements in ASCOT Engine Component Flow Physics and Modeling

1. Refinement of a non-linear Reynolds stress turbulence model for aircraft engine component flows.

   - Model coefficients are dynamically determined by the evolving mean flow field so that the turbulence model can be applied to a broader range of turbulent flows.

   - The model is further developed fully realizable to enhance the robustness of CFD codes.

   - Improved results against experimental data have been obtained for several benchmark flows: boundary layer flows, mixing and jet flows, swirling pipe flows, backward facing-step flows, etc.

2. Development and evaluation of a generalized turbulent wall function for complex flows with acceleration, deceleration and separation, for which the standard wall function is not valid.

   - Using the theory of singular perturbation, an asymptotic solution for surface flow at large Reynolds numbers under various pressure gradients, including separation and re-attachment, is obtained. This solution can be used as the boundary condition to bridge the near wall turbulence, hence no fine grids near the wall are needed for CFD applications. Furthermore, using the near wall behavior of turbulence, this asymptotic solution can be extended down to the wall to form a unified wall function valid for the whole region of surface flows, from the viscous sub-layer, the buffer layer to the inertial sub-layer. So that in the CFD applications, this new wall function will allow us to put the first grid point anywhere away from the wall in the surface layer. This will create a great convenience for CFD applications.

   - The theoretical results have been developed. Validations and applications have been carried out for National Combustion Code Program.

   - The achievements have partially been published in the following papers:

GERALD TRUMMER

Area: System Administration

- Maintained and upgraded the operating system software for the software for the AFRL/VAA workstation cluster. This included installing new software, software patches and editing and configuring files to bring new machines into the network cluster and making the machines secure. Performed other system administration duties such as archiving user accounts, adding/removing users, backing up file systems, installing new hardware, etc.

- Installed, maintained and upgraded visualization plotting packages used by the VAA division. This included new packages requiring configuration of license servers and script files and editing existing software at users' request to add or improve features.

FU-LIN TSUNG

Research Area: Development of 3D Structured/Unstructured Hybrid Navier-Stokes Solver for Turbomachinery

- The purpose of the current research is to improve axial compressor capabilities by modifying and controlling the compressor stall-line characteristics. A passive flow-control system consisted of casing flow-injectors is being designed to alter the compressor tip flow features to improve the compressor stall performance. The goal of the current study is to optimize the geometry of the injection system in order to maximize its effectiveness. The injection system consists of the tip injector, the flow intake nozzle, and the flow return channel.

- Since the injection system contains secondary flow and includes unusual geometries, an unstructured grid method was first used to quickly generate computational domains and solutions to understand the flow fields and identify any unexpected flow features. For this purpose, a version of the unstructured-grid solver USM3D was obtained from LaRC. In order to apply the solver to internal flows, a total condition inlet and static pressure exit boundary conditions using Riemann-Invariants based characteristic waves has been incorporated into the solver. The new boundary conditions allow different inlet and exit conditions to be specified at multiple inlet and multiple exit boundaries.
A preprocessor has been written to extract inlet face positions to allow variable total conditions (as opposed to remaining constant) be specified at various locations. In addition to the injection system, with the above modifications to the solver, the solver is currently being used to analyze other internal flow fields in geometries with extreme topological complexities.

Once a geometry has been narrowed to an approximate shape where only fine tuning of the geometry is necessary, and where several conditions are needed to be applied to each shape, an efficient structured solver is used to compute the matrix of flow cases. For this purpose, the multi-block solver, Glenn-HT, is used in combination with the grid generator GridPro.

Several design iterations have been computed and an injector tip geometry has been finalized. Currently, the geometries of the intake nozzle and the return channel are being optimized to perform with the injector tip. Once the injection system design is selected, the system will be fabricated and tested in a wind tunnel. Experimental test and CFD simulations will then be used to evaluate the concept to determine its effectiveness and explore any unanticipated flow features.

ELI TURKEL
Research Area: Matrix Viscosity and Preconditioning Techniques for Rotating Turbomachinery

We consider the solution of the compressible Navier-Stokes equations for the solution of flow in both stationary and rotating turbomachinery. These equations are supplemented by a $k$ turbulence model. We only consider steady state flow. Hence, in order to account for rotation effects it is necessary to consider the equations in a rotating frame of reference. However, in order to simplify the imposition of boundary conditions it is easier to base the dependent variables on the absolute velocity components. Furthermore, also to simplify the imposition of boundary conditions it is easiest to use generalized coordinates starting from cylindrical coordinates.

We solve these equations by marching the time dependent equations in pseudo-time. A Runge-Kutta scheme is used for the marching technique coupled with local time-stepping and residual smoothing. The original algorithm of Jameson, Schmidt and Turkel was based on a scalar coefficient to this artificial viscosity. This coefficient was proportional to the largest eigenvalue of the Jacobian matrices in each direction. In recent years this has been improved by the addition of both a matrix valued coefficient in the artificial viscosity and low speed preconditioning. The purpose of the matrix viscosity is to mimic upwind schemes within a framework of a central difference method. This allows the artificial viscosity to vary based on the wave speeds of individual waves at a mesh point. This is done dimension by dimension. The preconditioning is introduced to both improve the rate of convergence to a steady state and to improve the accuracy for low Mach number flows. Both the artificial viscosity and the preconditioning techniques are based on the inviscid equations. Hence, our analysis will be based on the Euler equations even though the results use the Navier-Stokes equations.

We consider applications of these improvements to both stators and rotors for low speed and transonic flows. In particular we have applied the method to both Rotor 37 and Rotor 35 and compared the original algorithm and the improvements to experimental data. To test the effectiveness of the preconditioner on low-speed flows, the IGV and first rotor of the Glenn low speed axial compressor (LSAC) were simulated as isolated blade rows. All the calculations show that the matrix viscosity improves the accuracy of the steady state solution. Also the preconditioning improves the convergence rate by a factor of four and also improves the accuracy for low speed flow.

MICHAEL D. WHITE
Research Area: Electromagnetics and Fluid Dynamics

Work was performed on CHARGE, an Electromagnetic Grand Challenge Project utilizing a second order Runge-Time integrator and 3rd order Van-Leer flux vector splitting.

Multiple validation runs comparing computed RCS (Radar Cross Sections) of a finned missile with experimental range data were presented as part of a paper for the 1999 AIAA summer conference in Norfolk, VA[1]. Enhancements were made to the code and documentation in preparation for the beta testing of the code, which was successfully passed last August. Detailed performance evaluation of the parallel capabilities on a number of platforms was studied over a variety of platforms showing the efficient use of caching in the cell based architecture of the code[2].

Collaboration with Dr. Jianming Jin, of the Department of Electrical and Computer Engineering at the University of Illinois at Urbana-Champaign resulted in a modeling methodology to accommodate patch antennas into CHARGE. Implementation and testing shows early promise in this area. This area is being continued as well as further general enhancement of the capabilities of CHARGE.
A related effort of a jet code utilizing a high order accurate acoustic formulation of the Navier Stokes equations in a Cylindrical coordinate system was investigated. Work on the codes modeling and accuracy was presented at the 1999 AIAA summer conference in Norfolk, VA[3]. The code was further developed for parallel processing during this time. This code was used to assess the usefulness and assist the beta testing of a semi-automatic parallelization tool (CAPTools) developed by the University of Greenwich with enhancements made at NASA Ames[4]. As a result of this work, significant input was given towards the improvement of CAPTools functionality.

References


DAVID WUNDROW
Research Area: Boundary Layer Transition and Aeroacoustics

An investigation of boundary-layer transition in the presence of free-stream turbulence was completed. This work was primarily concerned with the secondary instability of Klebanoff modes (and other quasi-steady vortex structures) on an otherwise two-dimensional boundary layer and how such instabilities can lead to a local (and thus turbulent-spot like) breakdown of the flow[11]. A computer code for determining the discrete and continuous spectra of normal modes for the generalized Rayleigh stability problem was developed. The computer code was used to show how, in most circumstances, the highly localized Rayleigh instabilities that exist in the long spanwise wavelength limit evolve into growing discrete mode solutions to the generalized Rayleigh problem as the characteristic spanwise length scale of the base flow becomes order one.

An investigation of high-frequency sound convected by a parallel mean flow through a semi-infinite duct was completed. This work focused on the diffracted radiation produced at the exit lip of the duct. The analysis was done in the context of the high-frequency geometric-acoustics approximation and required generalizing the geometrical theory of diffraction developed by Keller[21] to acoustic waves propagating in a uni-directionally transversely sheared mean flow. The analysis shows how the diffraction effects are accounted for by a higher-order correction to the high-frequency approximation of the Green's function for Lilley's equation. This result was used to develop a computer code that can determine the direct, reflected and diffracted radiation due a point source in a circular duct with an axi-symmetric mean flow. Using this code it was shown that the dominant effect of diffraction on the far-field directivity pattern comes from the diffracted rays in the vicinity of the shadow boundaries.

References


SHAYE YUNGSTER
Research Area: High Speed Combustion and Detonation Waves

The research work for the 1999 year focused on two different areas described below:

1. CFD Analysis of Rocket-Based Combined Cycle (RBCC) propulsion systems at low speed
The NASA Glenn Research Center is conducting research and development of a reusable, single-stage to orbit launch vehicle known as "GTX" (formerly known as "Trailblazer") that is based on a Rocket-Based Combined-Cycle (RBCC) propulsion system. This vehicle will operate in four modes from lift-off to orbit: 1) ejector-ramjet, 2) ramjet, 3) scramjet, and 4) all-rocket.

The research work focused on the low speed operation mode, that is the ejector-ramjet, which covers the Mach number range from takeoff to approximately Mach 3.

In the conventional ejector-ramjet operation mode, a fuel-rich rocket exhaust is mixed and burned with air captured by the inlet. The rocket provides all of the fuel needed for combustion with the entrained air. The internal flowpath is designed to produce thermal choking where mixing is complete. The main disadvantage of this concept is the relatively long duct required to achieve complete mixing of the air and rocket streams. In order to overcome this difficulty, a variation of the conventional ejector-ramjet was proposed in which the requirement for complete mixing of the two streams is removed. In this new "Independent Ramjet Stream" (IRS) cycle, the airstream is fueled independently using the ramjet and scramjet mode fuel injectors. The rocket serves as a pilot for the fueled airstream. At the point of ignition, a flame propagates across the combustor duct forming a thermal throat. The fuel injectors provide the means to control the location of the thermal choke by adjusting the amount and penetration distance of the fuel injected into the airstream.

Calculations have focused on the analysis of the IRS cycle. Two approaches have been taken; 1) development of a quasi-one dimensional CFD code for fast analysis of the performance of the IRS cycle, and 2) application of an axisymmetric CFD code to provide a more detailed analysis of the flow and combustion processes.

**Quasi-one dimensional CFD calculations of the IRS cycle**

The objective of this work is to develop an analysis tool for the IRS cycle, and investigate the performance of this propulsion mode over its operating flight range (0<M<3). An additional objective is to generate performance maps for trajectory optimization.

**Approach**

The ramjet and rocket streams are solved simultaneously using a TVD MacCormack time-marching scheme. A quasi-one dimensional approximation is used to model both streams. Combustion in the ramjet stream is modeled by a prescribed distribution of hydrogen fuel along the combustor duct. Equilibrium chemistry is used to model the combustion process utilizing the LSENS kinetics code of Radhakrishnan. The two streams are coupled using a pressure matching auxiliary equation.

**Accomplishments**

Performance maps for the GTX vehicle were generated for the Mach number range 0<M<3, and rocket chamber pressures range of 100<p/p0<350, where p0 is the free-stream pressure. The effects of varying the airstream fuel-air ratio was investigated, and performance comparisons were made between the IRS cycle and the conventional ejector ramjet (SMC) cycle. A summary of this work was presented at the 35th Joint Propulsion Conference (S. Yungster and C.J. Trefny, "Analysis of a New Rocket-Based Combined Cycle Engine Concept at Low Speed," AIAA 99-2393, ICOMP-99-05, NASA/TM 1999-209393).

**Axisymmetric CFD calculations**

This research effort, which focuses on the IRS cycle, analyzes axisymmetric configurations that closely model the GTX vehicle. The goal is to understand the flow and combustion physics, study the effects of airstream fuel-air ratio, mixture distribution, geometric configuration, and rocket chamber pressure and O/F ratio on engine performance.

**Approach**

The analysis of the IRS cycle is carried out using a specialized CFD code developed in-house for computing reacting flows. This code has been used in the past to accurately model combustion phenomena in high-speed propulsion applications. It solves the Navier-Stokes equations with finite-rate chemistry and real gas effects using an implicit, total variation diminishing (TVD) algorithm. It includes a generalized detailed chemistry capability, various options for turbulence models, and steady-state or time accurate marching algorithms. In particular, the Spalart-Allmaras one-equation turbulence model was implemented into this code, and used in all the calculations. The hydrogen-air combustion is modeled with a 7-species, 8-step reaction mechanism.
Accomplishments

Calculations that demonstrate stable operation of the IRS cycle under thermal choked conditions have been carried out for various axisymmetric configurations. The investigation examined the effects of airstream fuel-air ratio, mixture distribution, and rocket chamber pressure on flame propagation and stability. These calculations have revealed many interesting features related to the thermal choke process. Comparisons between axisymmetric and quasi-one-dimensional calculations have also been performed (using the same heat release distribution obtained in the axisymmetric calculations). A report summarizing these results is in preparation.

2. Detonation Wave Modeling

Work on detonation wave modeling continued in two main areas; code validation and application to pulse detonation-wave engines (PDE). In the validation area (carried out in collaboration with K. Radhakrishnan), we investigated high-speed, time-dependent, reacting flowfields for which experimental data has been recently reported. In particular, we studied the flow of hydro-gen-air mixtures over two different projectile configurations in an expansion tube. The computed solutions were compared with experimental OH PLIF data. These computational studies complement experimental work by providing detailed information about combustion initiation, flow structure and flow establishment time, a critical parameter in pulse facilities, in which the available test time may be too short to establish fully the reacting flowfield. Such calculations are also appropriate benchmark cases for evaluating numerical models for flow and combustion chemistry. Results of this work were presented at the 35th Joint Propulsion Conference (S. Yungster and K. Radhakrishnan, "Simulation of Unsteady Hypersonic Combustion Around Projectiles in an Expansion Tube, "AIAA 99-2640, ICOMP-99-06, NASA/CR 1999-209304), and submitted to the Journal "Shock Waves". The second research effort (started in the last quarter of 1999) consists of an investigation of a PDE in an ejector configuration. The goal of this work is to study single and multiple detonation wave cycles in axisymmetric ducts using various H2-O2 mixtures. Parametric studies on mixture ratio, pressure ratio, duct length, duct fueling, etc., will be performed. Nitrogen oxide formation in these PDE configurations will also be investigated (in collaboration with K. Radhakrishnan). Initial results have demonstrated excellent prediction of detonation wave speeds for several initial pressures of up to 50 psi.
1999 REPORTS AND ABSTRACTS


The Institute for Computational Mechanics in Propulsion (ICOMP) was formed to develop techniques to improve problem-solving capabilities in all aspects of computational mechanics related to propulsion. ICOMP is operated by the Ohio Aerospace Institute (OAI) and funded via numerous cooperative agreements by the NASA Glenn Research Center in Cleveland, Ohio. This report describes the activities and accomplishments during 1998, the Institute’s thirteenth year of operation.


In September 1997 the National Transportation Safety Board (NTSB) requested assistance from the NASA Glenn Research Center (GRC) Icing Branch in the investigation of an aircraft accident that was suspected of being caused by ice contamination. In response to the request NASA agreed to perform an experimental and computational study. The main activities that NASA performed were GRC Icing Research Tunnel (IRT) testing to define ice shapes and 2-D Navier-Stokes analysis to determine the performance degradation that those ice shapes would have caused. An IRT test was conducted in January 1998. Most conditions for the test were based upon raw and derived data from the Flight Data Recorder (FDR) recovered from the accident upon the current understanding of the Meteorological conditions near the accident. Using a two-dimensional Navier-Stokes code, the flow field and resultant lift and drag were calculated for the wing section with various ice shapes accreted in the IRT test. Before the final calculations could be performed extensive examinations of geometry soothing and turbulence were conducted. The most significant finding of this effort is that several of the five-minute ice accretions generated in the IRT were found by the Navier-Stokes analysis to produce severe lift and drag degradation. The information generated by this study suggests a possible scenario for the kind of control upset recorded in the accident. Secondary findings were that the ice shapes accreted in the IRT were mostly limited to the protected pneumatic boot region of the wing and that during testing, activation of the pneumatic boots cleared most of the ice.


An analytical study was performed as part of the NASA Glenn support of a National Transportation Safety Board (NTSB) aircraft accident investigation. The study was focused on the performance degradation associated with ice contamination on the wing of a commercial turbo-prop-powered aircraft. Based upon the results of an earlier numerical study conducted by the authors[1], a prominent ridged-ice formation on the subject aircraft wing was selected for detailed flow analysis using 2-dimensional (2-D), as well as, 3-dimensional (3-D) Navier-Stokes computations. This configuration was selected because it caused the largest lift decrease and drag increase among all the ice shapes investigated in the earlier study. A grid sensitivity test was performed to find out the influence of grid spacing on the lift, drag, and associated angle-of-attack for the maximum lift (Cmax). This study showed that grid resolution is independent of the grid. The 2-D results suggested that a severe stability and control difficulty could have occurred at a slightly higher angle-of-attack (AOA) than the one recorded by the Flight Data Recorder (FDR)[3]. This stability and control problem was thought to have resulted from a decreased differential lift on the wings with respect to the normal loading for the configuration. The analysis also indicated that this stability and control problem could have occurred whether or not natural ice shedding took place. Numerical results using an assumed 3-D ice shape showed an increase of the angle at which this phenomena occurred of about 4 degrees. As it occurred with the 2-D case, the trailing edge separation was observed but started only when the AOA was very close to the angle at which the maximum lift occurred.
REPORTS AND ABSTRACTS


NPARC v3.1 is a modification to the NPARC v3.0 computer program which expands the capabilities for time-accurate computations through the use of a Newton iterative implicit method, time-varying boundary conditions, and planar dynamic grids. This document discusses some of the changes from the NPARC v3.0, specifically: changes to the directory structure and execution, changes to the input format, background on new methods, new boundary conditions, dynamic grids, new options for output, usage concepts, and some test cases to serve as tutorials. This document is intended to be used in conjunction with the NPARC v3.0 user’s guide.


An analysis of the Independent Ramjet Stream (IRS) cycle is presented. The IRS cycle is a variation of the conventional ejector ramjet, and is used at low speed in a rocket-based combined-cycle (RBCC) propulsion system. In this new cycle, complete mixing between the rocket and ramjet streams is not required, and a single rocket chamber can be used without a long mixing duct. Furthermore, this concept allows flexibility in controlling the thermal choke process. The resulting propulsion system is intended to be simpler, more robust, and lighter than an ejector ramjet. The performance characteristics of the IRS are analyzed for a new single-stage-to-orbit (SSTO) launch vehicle concept, known as the “Trailblazer.” The study is based on a quasi-one-dimensional model of the rocket and air streams at speeds ranging from lift-off to Mach 3. The numerical formulation is described in detail. A performance comparison between the IRS and ejector-ramjet cycles is also presented.


The temporal evolution of combustion flowfields established by the interaction between wedge-shaped bodies and explosive hydrogen-oxygen-nitrogen mixtures accelerated to hypersonic speeds in an expansion tube is investigated. The analysis is carried out using a fully implicit, time-accurate, computational fluid dynamics code that we developed recently for solving the Navier-Stokes equations for a chemically reacting gas mixture. The numerical results are compared with experimental data from the Stanford University expansion tube for two different gas mixtures at Mach numbers of 4.2 and 5.2. The experimental work showed that flow unstart occurred for the Mach 4.2 cases. These results are reproduced by our numerical simulations and, more significantly, the causes for unstart are explained. For the Mach 5.2 mixtures, the experiments and numerical simulations both produced stable combustion. However, the computations indicate that in one case the experimental data were obtained during the transient phase of the flow, that is, before steady state had been attained.

Hagstrom, Thomas (University of New Mexico and ICOMP); Radhakrishnan, K. (ICOMP); Zhou, Ruhai (University of New Mexico): “Computation of Steady and Unsteady Laminar Flames: Theory”, ICOMP Report 99-7, NASA CR 209305, October, 1999, 23 pages.

In this paper we describe the numerical analysis underlying our efforts to develop an accurate and reliable code for simulating flame propagation using complex physical and chemical models. We discuss our spatial and temporal discretization schemes, which in our current implementations range in order from two to six. In space we use staggered meshes to define discrete divergence and gradient operators, allowing us to approximate complex diffusion operators while maintaining ellipticity. Our temporal discretization is based on the use of preconditioning to produce a highly efficient linearly implicit method with good stability properties. High order for time accurate simulations is obtained through the use of extrapolation or deferred correction procedures. We also discuss our techniques for computing stationary flames. The primary issue here is the automatic generation of initial approximations for the application of Newton’s method. We use a novel time-stepping procedure, which allows the dynamic updating of the flame speed and forces the flame front towards a specified location. Numerical experiments are presented, primarily for the stationary flame problem. These illustrate the reliability of our techniques, and the dependence of the results on various code parameters.

The asymptotic solutions, described by Tennekes and Lumley (1972), for surface flows in a channel, pipe or boundary layer at large Reynolds numbers are revisited. These solutions can be extended to more complex flows such as the flows with various pressure gradients, zero wall stress and rough surfaces, etc. In computational fluid dynamics (CFD), these solutions can be used as the boundary conditions to bridge the near-wall region of turbulent flows so that there is no need to have the fine grids near the wall unless the near-wall flow structures are required to resolve. These solutions are referred to as the wall functions. Furthermore, a generalized and unified law of the wall which is valid for whole surface layer (including viscous sublayer, buffer layer and inertial sublayer) is analytically constructed. The generalized law of the wall shows that the effect of both adverse and favorable pressure gradients on the surface flow is very significant. Such an unified wall function will be useful not only in deriving analytic expressions for surface flow properties but also bringing a great convenience for CFD methods to place accurate boundary conditions at any location away from the wall. The extended wall functions introduced in this paper can be used for complex flows with acceleration, deceleration, separation, recirculation and rough surfaces.
1999 SEMINARS

Ito, Takashi (Institute of Space and Astronautical Science): “Computation of Axisymmetric Plug Nozzle Flow”

Plug nozzle flow is analyzed using numerical simulation. The method of characteristics is used to design the plug contour and several types of plug nozzles are considered by truncating the length of the nozzle at various locations. Plug nozzles altitude compensating features are confirmed by the computed results. Also, the base pressure is shown to play an important role in maintaining the thrust performance of the nozzle for high truncation configurations. The altitude clearly influences the base pressure distribution under the assumption that the chamber pressure is constant during ascent. The computed thrust difference between contoured and conical nozzles linearly increases as a function of the pressure ratio. The thrust performance of the contoured plug nozzle is estimated to be about 5-6% higher than the conical plug nozzle. Various conditions of external flow over the plug nozzle are also imposed and the results demonstrate that the external flow does not influence the pressure distribution on the nozzle surface for pressure ratios higher than the design point value.

Oldfield, Martin and Moss, Roger (University of Oxford): “The Use of High Frequency Pressure Transducers and Fast Traversing to Measure Hot Combustor Exit Turbulence”

This lecture will covered a number of topics including:

1. The importance of knowing the turbulence level and length scale of the flow leaving a hot combustor
2. The difficulties in making such measurements
3. The theory of deriving turbulence from high frequency pitot data
5. The use of high speed traverses to ensure survival of the probe.
6. Signal processing and data acquisition considerations (anti-aliasing filtering, effect of time-domain windowing on spectra, ensemble averaging of spectra, definitions of length-scale, measuring Kulite temperature).
7. Results from Oxford measurements in a hot combustor.
8. Proposed experiments in an ENEL (Pisa) combustor.
9. Traverse requirements.
10. Preliminary NASA funded experiments.

[Martin Oldfield discussed 1, 2, 8, 9 and Roger Moss discussed 3 - 7].


An improved method for performing measurements of turbulent quantities and spectra in hypersonic flows using a miniature pitot probe was presented. The probe is equipped with a high-frequency silicon pressure transducer, capable of withstanding the impact pressure and stagnation point heat flux realized by arc-driven or shock-driven hypersonic facilities. Turbulent velocity fluctuations are derived using a linearized hypersonic pitot relation, in the case of small turbulence intensity and assuming that the Strong Reynolds Analogy holds exactly. A discussion of the fundamental assumptions was provided, together with experimental and theoretical consideration of applicability and limits of the proposed method. An extensive investigation of velocity fluctuation spectra has been performed in the weakly compressible, decaying turbulent field established in the test section of a small scale hypersonic wind tunnel. The measured one-dimensional spectra exhibits a non-Kolmogorov power-law behavior over a significant wavenumber range, with a -11/3 exponent which is not predicted by available scaling relations for compressible turbulence. On the other hand,
such power-law exponent is in agreement with recent EDQNM and LES results for the irrotational component of velocity fluctuations in weakly compressible flows. Based on these results, a new dimensionally-based scaling relation is obtained for the compressible energy spectrum, which is in agreement with the numerically observed radiative behavior for weakly compressible turbulence.

Carpenter, Mark H. (NASA Langley Research Center): “Recent Developments in Finite Difference Methodology”

Several topics of current interest were presented, beginning with a discussion on the relative merits of high-order shock capturing schemes. Several different discretization techniques are used to show that all high-order schemes revert to first-order accuracy downstream of a shock, unless special provision is made to account for the shock position. Thus, it is necessary to use both H- and P-refinement in problems having discontinuous solutions. A new approach to deal with complex geometries using multi-domain high-order finite-difference techniques was presented. Special treatments at zonal boundaries guarantee stability, conservation and design accuracy between domains. Several test cases were presented that highlight the new techniques. Finally, some new low-storage explicit Runge-Kutta schemes that show promise in cases where temporal accuracy is extremely important were presented.

Tam, Christopher (Florida State University): “Applications of Computational Aeroacoustics Methods to Airframe Noise and Acoustic Liner Technology”

Development of Computational Aeroacoustics (CAA) Methods has made steady progress in recent years. This presentation emphasizes the application of these methods to realistic aeroacoustic problems. Two examples were discussed, one related to the generation of tones in airframe noise and the other simulating the dissipation mechanisms of acoustic liners. These examples strongly suggest that CAA methods are now sufficiently advanced that they can make a significant impact on aeroacoustic technology.


A Domain Decomposition (DD) method is developed for parallel computation of time-harmonic aerodynamic-aeroacoustic problems. The computational domain is decomposed into subdomains, and the aerodynamic-aeroacoustic boundary-value problem is solved independently for each subdomain. Impedance-type transmission conditions are imposed on the artificially introduced subdomain boundaries to ensure the uniqueness of the solution. A Dirichlet-to-Neumann map is used as a nonreflecting radiation condition along the outer computational boundary. Subdomain problems are then solved using the finite element method and an iterative scheme updates the transmission conditions to recover the global solution.

The present algorithm is implemented for two model problems. First, the sound radiated from a surface simulating a two-dimensional monopole is calculated using an unstructured mesh. Second, the flow of a thin airfoil in a transverse gust is computed using a structured mesh. The accuracy of the numerical scheme is validated by comparison with existing solutions for both the near-field unsteady pressure and the far-field radiated sound. The convergence and the computational time and memory requirements of the present method are investigated. It is shown that by combining the subdomain direct solvers with global iterations, this DD method significantly reduces both the computational time and memory requirements.
35th AIAA/ASME/SAE/ASEE JOINT PROPULSION CONFERENCE

Session 39-ACT-3
Institute for Computational Mechanics in Propulsion (ICOMP)

Tuesday, June 22, 1999

8:00 a.m.  AIAA-99-2390
Extended ILDM Method for NCC
A. Norris, Institute for Computational Mechanics in Propulsion (ICOMP), Cleveland, OH

8:30 a.m.  AIAA-99-2391
Numerical Treatment of Cylindrical Coordinated Centerline Singularities
R. Hixon and S.-H. Shih, Institute for Computational Mechanics in Propulsion (ICOMP), Cleveland, OH; R. Mankbadi, Cairo University, Cairo, Egypt

9:00 a.m.  AIAA-99-2392
Turbulent Surface Flows and Wall Function
T.-H. Shih, Institute for Computational Mechanics in Propulsion (ICOMP), Cleveland, OH; J. Lumley, Cornell University, Ithaca, NY; N.-S. Liu and M. Potapczuk, NASA Glenn Research Center, Cleveland, OH

9:30 a.m.  AIAA-99-2393
Analysis of a New Rocket Based Combined Cycle Engine Concept at a Low Speed
S. Yungster, Institute for Computational Mechanics in Propulsion (ICOMP), Cleveland, OH; C. Trefny, NASA Glenn Research Center, Cleveland, OH

10:00 a.m. AIAA-99-2394
LSENS, The NASA Lewis Kinetics and Sensitivity Analysis Code
K. Radhakrishnan, Institute for Computational Mechanics in Propulsion, Cleveland, OH

10:30 a.m. AIAA-99-2395
Curvilinear Wall Boundary Conditions for Computational Aeroacoustics
R. Hixon, Institute for Computational Mechanics in Propulsion (ICOMP), Cleveland, OH

11:00 a.m. AIAA-99-2396
Aero-Thermal Simulation of Secondary Flow Systems Using Grid-Overset Methodology
K. Ajmani, T. Tech and M.-S. Liou, NASA Glenn Research Center, Cleveland, OH

11:30 a.m. AIAA-99-2397
Simulations of Unsteady Combustion Phenomena Using Complex Models
R. Zhou, T. Hagstrom, and S. Steinberg, University of New Mexico, Albuquerque, NM; K. Radhakrishnan, Institute for Computational Mechanics in Propulsion (ICOMP), Cleveland, OH
A. Resident Staff.

Michael White, Ph.D., Mechanical Engineering, University of California, Davis. October, 1997–Present.

B. Visiting Staff/Consultants.

Thomas Hagstrom, Ph.D., Applied Mathematics, California Institute of Technology, 1983. Professor, Department of Mathematics and Statistics, University of New Mexico.
Foluso Ladeinde, Ph.D., Mechanical and Aerospace Engineering, 1968. Associate Professor, Department of Mechanical Engineering, SUNY Stony Brook.
Eli Twel, Ph.D., Applied Mathematics, New York University, 1970. Professor, Department of Mathematics, Tel Aviv University, Tel Aviv, Israel.
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Table II. - ICOMP STATISTICS (1986 TO 1999)
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