Towards A Generalized Computational Fluid Dynamics Technique for all Mach Numbers

S8-34

R. W. Walters, D. C. Slack and A. G. Godfrey

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Statement of the Problem

Currently there exists no single unified approach for efficiently and accurately solving computational fluid dynamics (CFD) problems across the Mach number regime, from truly low speed incompressible flows to hypersonic speeds. There are several CFD codes that have evolved into sophisticated prediction tools with a wide variety of features including multi-block capabilities, generalized chemistry and thermodynamics models among other features. However, as these codes evolve, the demand placed on the end user also increases simply because of the myriad of features that are incorporated into these codes. In order for a user to be able to solve a wide range of problems, several codes may be needed requiring the user to be familiar with the intricacies of each code and their rather complicated input files. Moreover, the cost of training users and maintaining several codes becomes prohibitive.

Objective of the Work

The objective of the current work is to extend the compressible, characteristic-based, thermochemical nonequilibrium Navier-Stokes code GASP to very low speed flows and simultaneously improve convergence at all speeds. Before this work began, the practical speed range of GASP was Mach numbers on the order of 0.1 and higher. In addition, a number of new techniques have been developed for more accurate physical and numerical modeling.

Approach Used

The primary focus has been on the development of optimal preconditioning techniques for the Euler and the Navier-Stokes equations with general finite-rate chemistry models and both equilibrium and nonequilibrium thermodynamics models. We began with the work of Van Leer, Lee, and Roe for inviscid, one-dimensional perfect gases and extended their approach to include three-dimensional reacting flows. The basic steps required to accomplish this task were a transformation to steam-aligned coordinates, the formulation of the preconditioning matrix, incorporation into both explicit and implicit temporal integration schemes, and modification of the numerical flux formulae. In addition, we improved the convergence rate of the implicit time integration schemes in GASP through the use of inner iteration strategies and the use of the GMRES (General Minimized RESisual) which belongs to the class of algorithms referred to as Krylov subspace iteration. Finally, we significantly improved the practical utility of GASP through the addition of mesh sequencing, a technique in which computations begin on a coarse grid and get interpolated onto successively finer grids.

Conclusions Relevant to Rocket Propulsion

The fluid dynamic problems of interest to the propulsion community involve complex flow physics spanning different velocity regimes and possibly involving chemical reactions. This class of problems results in widely disparate time scales causing numerical *stiffness*. Even in the absence of chemical reactions, eigenvalue stiffness manifests itself at transonic and very low speed flows which can be quantified by the large condition number of the system and evidenced by slow convergence rates. This results in the need for thorough numerical analysis and subsequent implementation of sophisticated numerical techniques for these difficult yet practical problems. As a result of this work, we have been able to extend the range of applicablity of compressible codes to very low speed inviscid flows (M=.001) and reacting flows. Our work now centers on the extension to viscous flows.

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Workshop for CFD Applications in Rocket Propulsion
Marshall Space Flight Center
April 20-22, 1993

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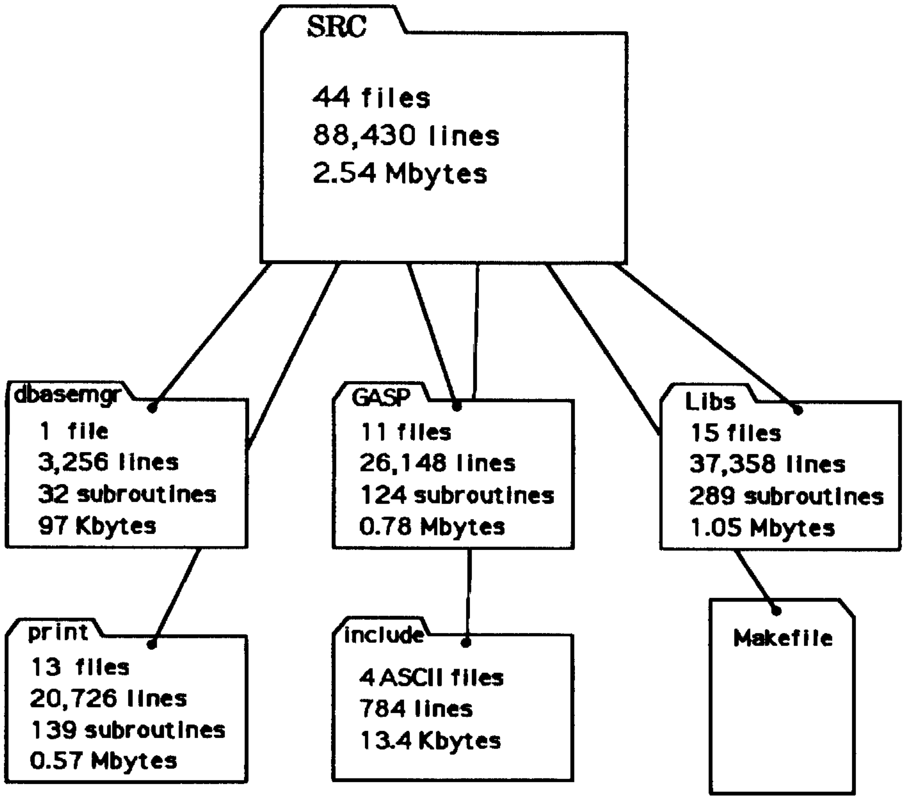
Outline

- Phase I Objectives
- Recent improvements and enhancements
- Results
- Phase II Objectives and schedule

Source Code File Structure



SRC
44 files
88,430 lines
2.54 Mbytes

dbasemgr
1 file
3,256 lines
32 subroutines
97 Kbytes

GASP
11 files
26,148 lines
124 subroutines
0.78 Mbytes

Libs
15 files
37,358 lines
289 subroutines
1.05 Mbytes

print
13 files
20,726 lines
139 subroutines
0.57 Mbytes

include
4 ASCII files
784 lines
13.4 Kbytes

Makefile

GASP Version 2.2 Extended Features

Basic Features

- Solves steady and unsteady 3-D, Reynolds-Averaged, Navier-Stokes Equations (RANS) and subsets:
  - Thin-layer Navier-Stokes (TLNS)
  - Parabolized Navier-Stokes (PNS)
  - Euler equations
- Fully conservative, cell-centered, upwind, finite volume code
  - 3D, 2D, axisymmetric
  - Multiple grids
- Explicit & implicit time integration of primitive variables
- Finite-rate, frozen, & equilibrium chemistry, mixtures
- Equilibrium and nonequilibrium thermodynamics models

Fluxes and Jacobians

- Roe, Van Leer, and Steger-Warming flux splittings
- Approximate Roe linearization, complete Van Leer Jacobian
- Full flux with Vigneron technique and complete linearization

Chemistry

- Fully coupled finite-rate chemistry
- Species and Reaction databases for thermochemical properties
  - stand alone database manager
- Extended rate equations curve fits
- Complete reaction sets for existing chemistry models

Thermodynamics

- Equilibrium and non-equilibrium thermodynamics models
- NASA LeRC extended curve fit option
- Equilibrium curve fits
  - Tannehill TGAS routines
  - Liu and Vinokur curve fits

Time Integration

- m-stage Runge-Kutta integration
- 3-Factor Approximate Factorization (AF)
- 2-Factor AF/Relaxation in third direction
  - supports all (i,j,k) combinations
- Option to freeze LU elements

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GASP Version 2.2 Extended Features

Boundary Conditions
- User-selectable list of explicit and implicit boundary conditions:
  - Inflow/Outflow
  - Solid surface
  - Zonal boundaries

Turbulence Models
- Fully-coupled two-equation models
  - Characteristic-based treatment of the convective terms
  - Sarkar's compressibility correction
- Baldwin-Lomax algebraic model in any two logical directions
  - Option for Goldberg's backflow model

Graphical User Interface
- Implemeted as a FAST module
- Contains On-line documentation
- Performs consistency and error checks
- Graphical display of boundary conditions
- Constructs syntactically correct input

Mesh Sequencing
- Requires a single input deck per zone
- Refinement may be performed in any or all of the logical directions (i,j,k)
- Restart files contain solutions on all grids for convergence studies

Space-Marching
- Valid for many:
  - supersonic, inviscid flows (Euler)
  - high speed viscous flows (PNS)
- March in any logical (i,j,k) direction
- Use the same grid for PNS, TLNS, and RANS calculations

Post-Processing
- Integrated quantities, e.g. lift & drag
- Improvements & enhancements to the GASP 1.x output utilities
- Support for PLOT3D, FAST, and TECPLOT TM
- English and SI units

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Phase I Objectives

- Preconditioning for Inviscid Flows
- Mesh Sequencing
- GMRES and Jacobi inner iterations
- 3 Factor AF, Jacobi & Gauss Seidel solvers
- Documentation

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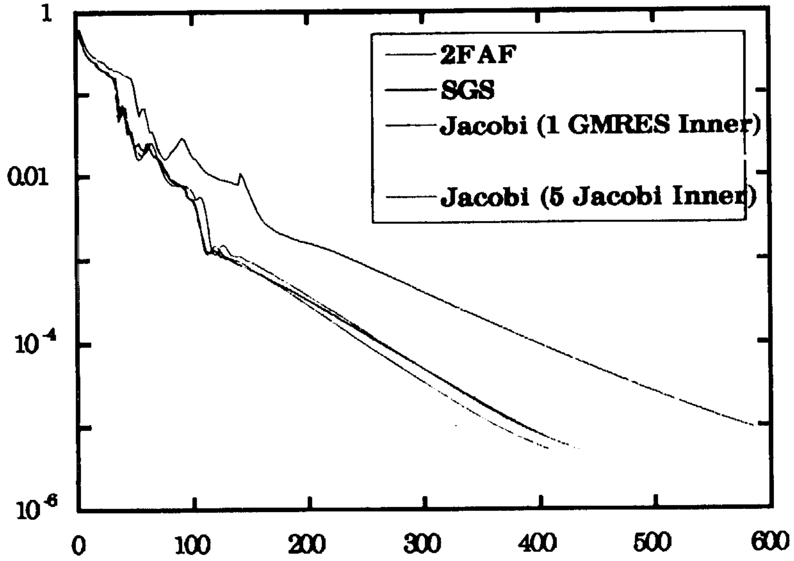
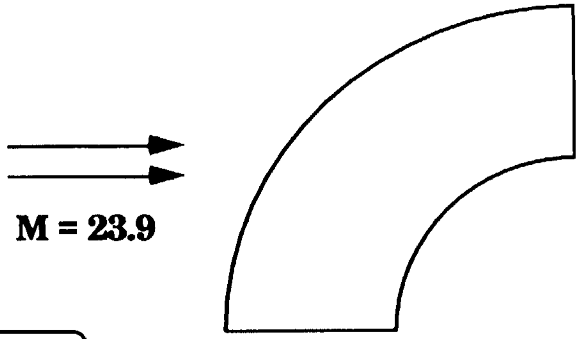
GASP 2.0

Inner Iterations

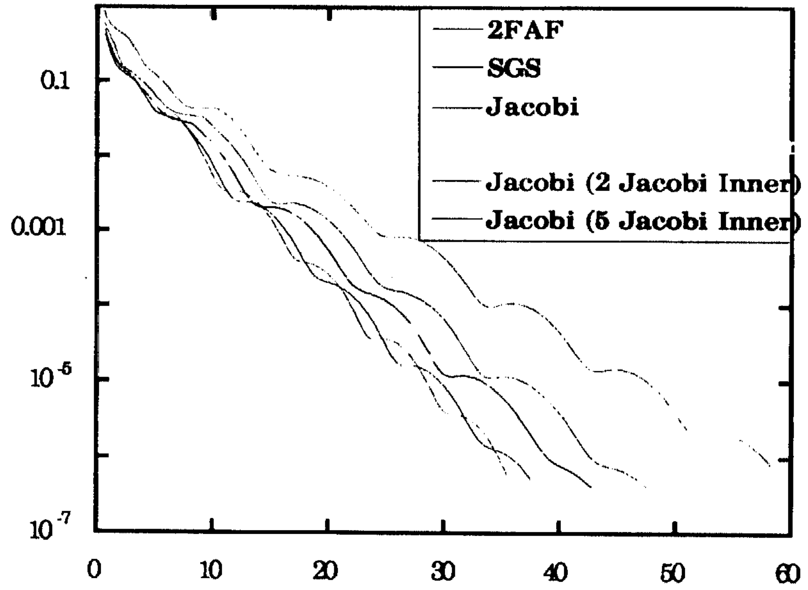
- Improve Update Vector Δq
- Approaches Exact Solution of Linear Problem
- Relatively Inexpensive
- Most Useful with Block Jacobi Time Integration

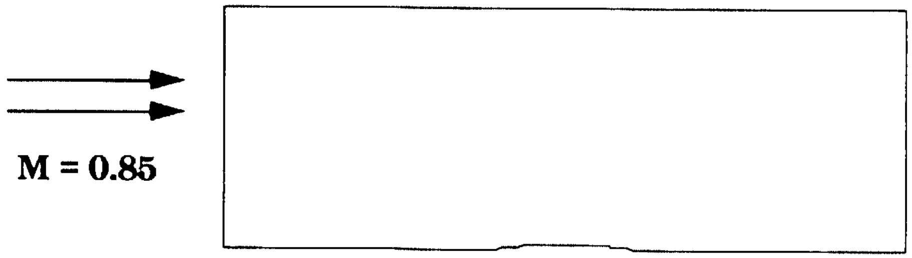
RamIIc Blunt Body





Transonic Flow over Circular Arc





Basic Steps in Preconditioning Analysis

- Transformation of governing equations to stream-aligned coordinates
- Formulation of the Preconditioning Matrix
- Incorporation into explicit and implicit time integration schemes
- Modification of the numerical flux formula (Roe's scheme)

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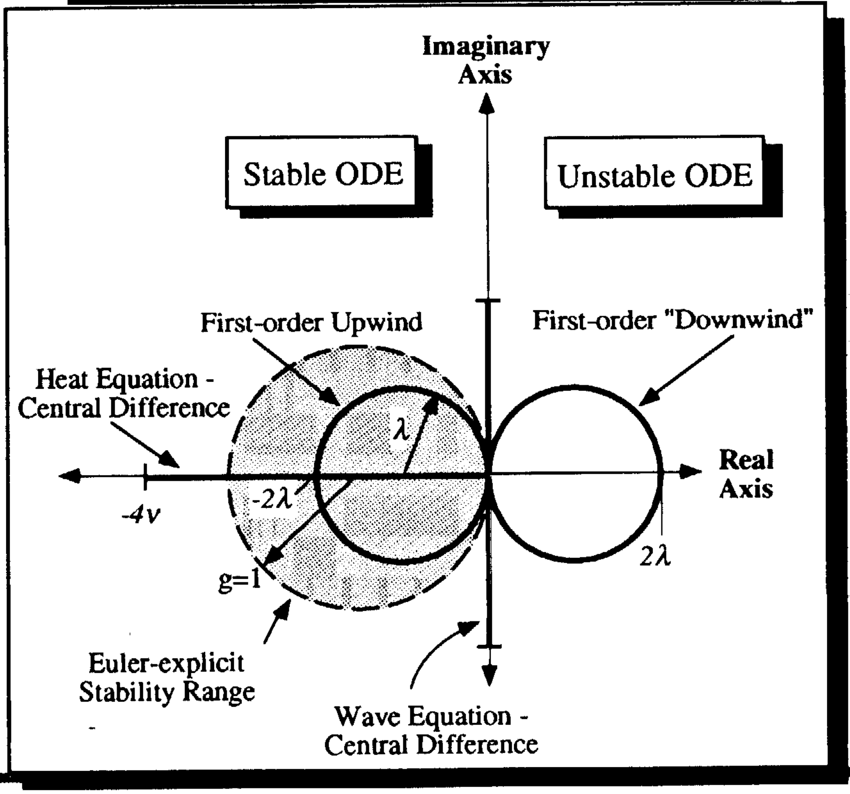
Preconditioned 2-D Euler Equations

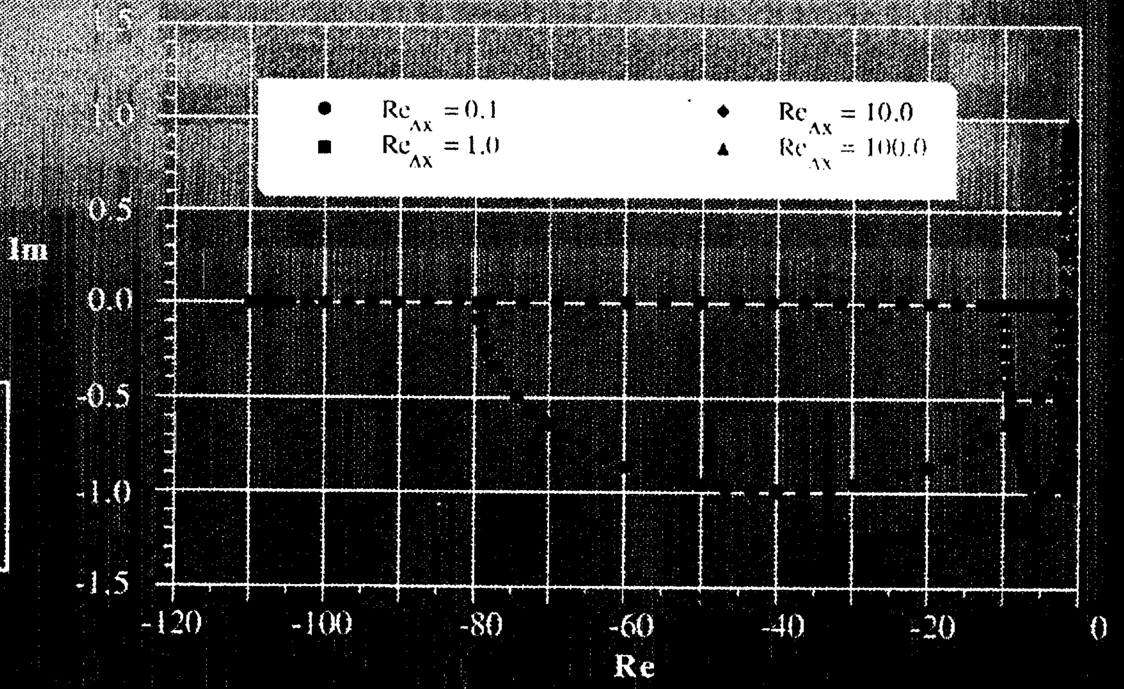
Euler equations: $$\frac{\partial Q}{\partial t} = -P\left(\frac{\partial F}{\partial x} + \frac{\partial G}{\partial y}\right)$$

Steady state: $\frac{\partial Q}{\partial t} = 0$ **implies** $R(q) = 0.$

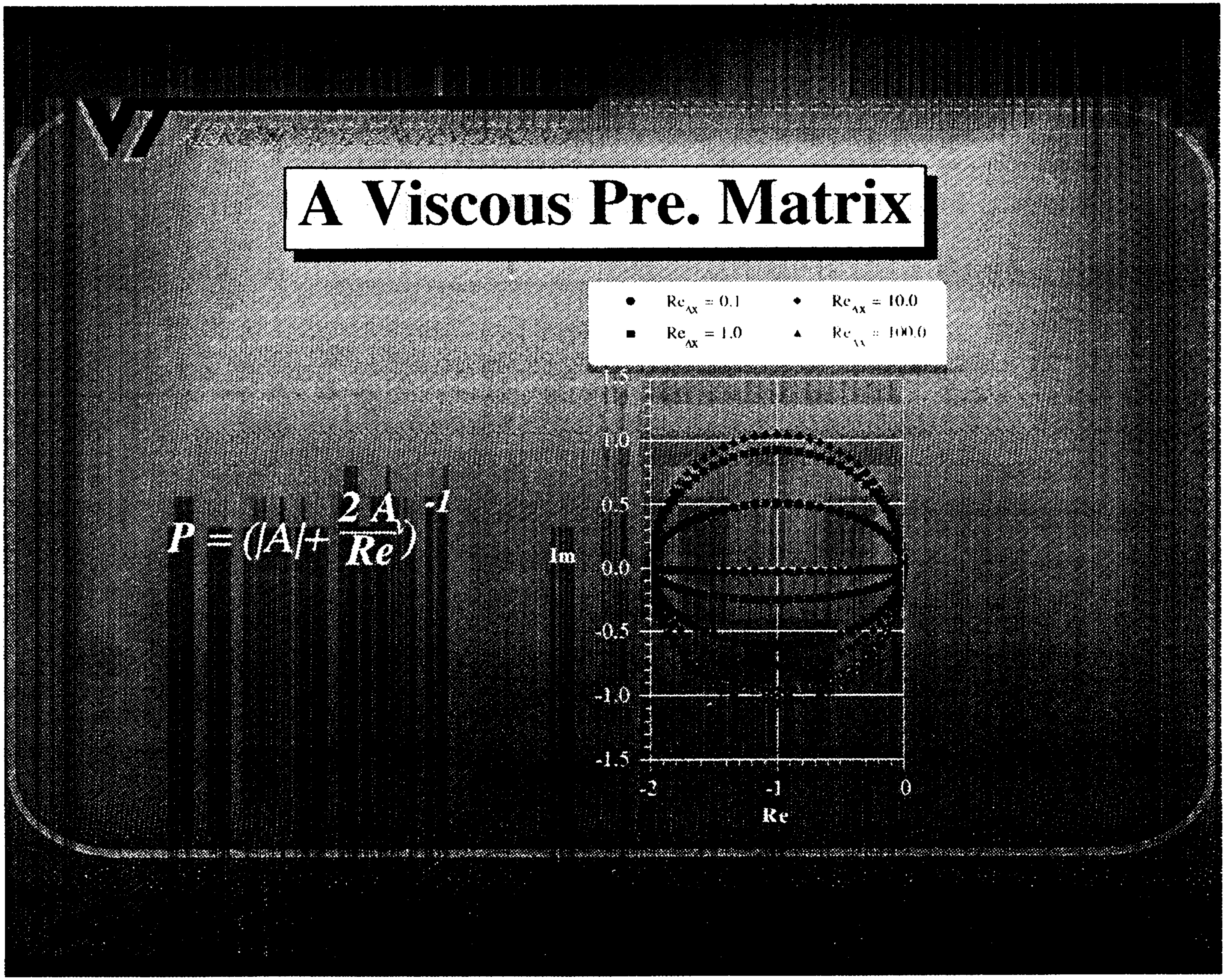
Fourier Footprints



Viscous Preconditioning



Inviscid 1-D P with $\tau = 1$



A Viscous Pre. Matrix

$$P = \left(|A| + \frac{2A}{Re}\right)^{-1}$$

GASP Version 2.2 *New* Features

- **Improved turbulence modeling**
    - All algebraic and Two-equation models more accurate
      See Figure 1.
    - New k-ε minimization routine
    - Sarkar's compressibility correction
    - Goldberg's backflow extension to the Baldwin-Lomax model
- **Graphical User Interface - Version 1.1**
    - FAST™ Module (requires Silicon Graphics workstation)
- **New limiters**
    - Venkat's limiter with the improved convergence property
      See Figure 2. Reference AIAA-93-0880
    - The highly compressive Superbee limiter
    - Characteristic-based limiting option for all limiters

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GASP Version 2.2 *New* Features

- **Improved implementation of the Vigneron Technique**

  See Figure 3. Reference AIAA-92-0189
- **New Binary Conversion Utility**
  - Convert Grid and Solution 'C' Binary files between architectures

    Cray, IEEE
- **Miscellaneous Improvements**
  - Entropy fix for Roe's numerical flux function
  - Extended Residual file format
  - CFL / Time Step ramping
- **Revised User Manual**
  - New chapter on theoretical formulation
  - Revised Quick Reference Cards

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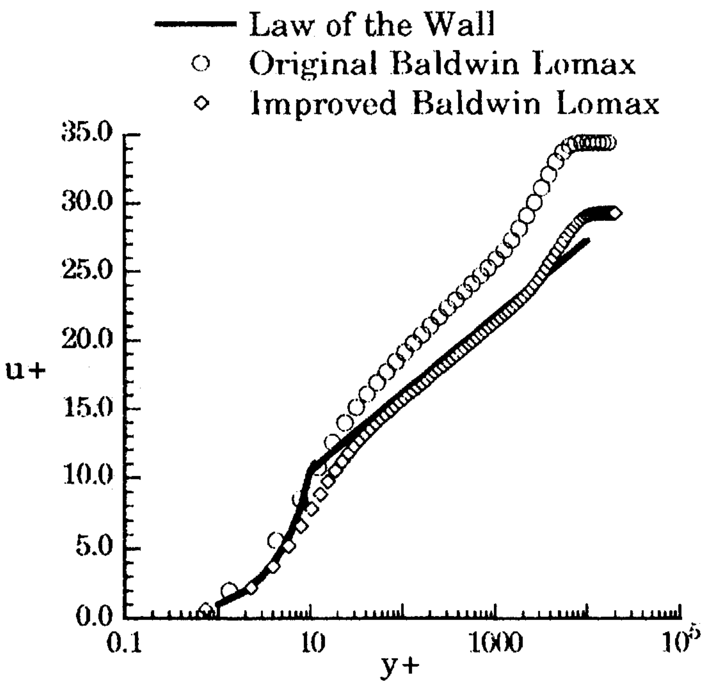
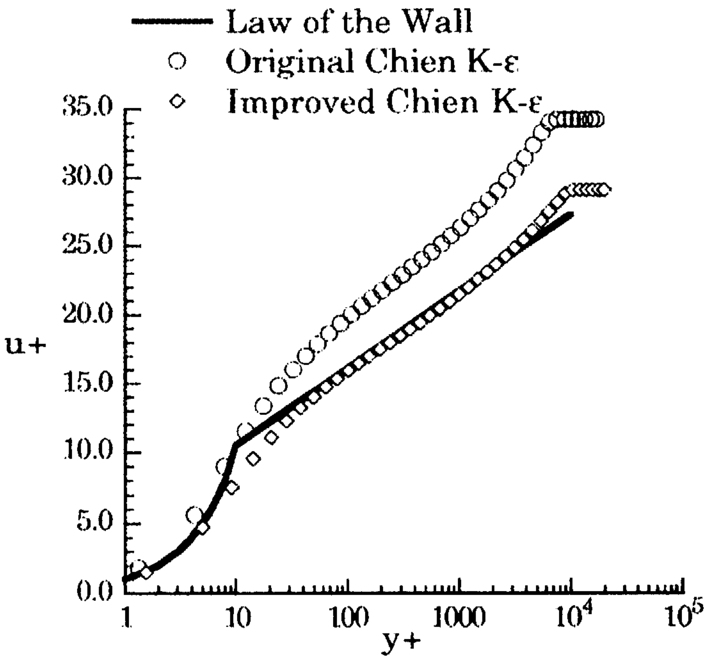
Recent Improvements Made to Turbulence Models





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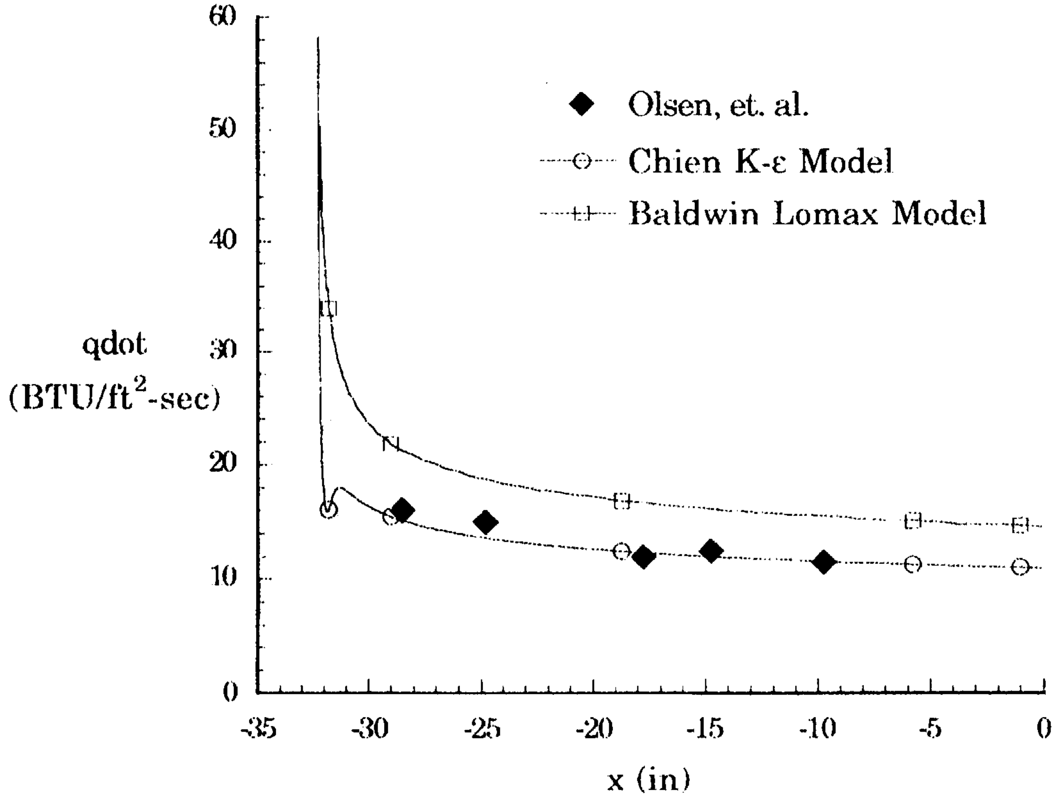
Mach 6.5, Flow Over a Flat Plate, Comparison to Data



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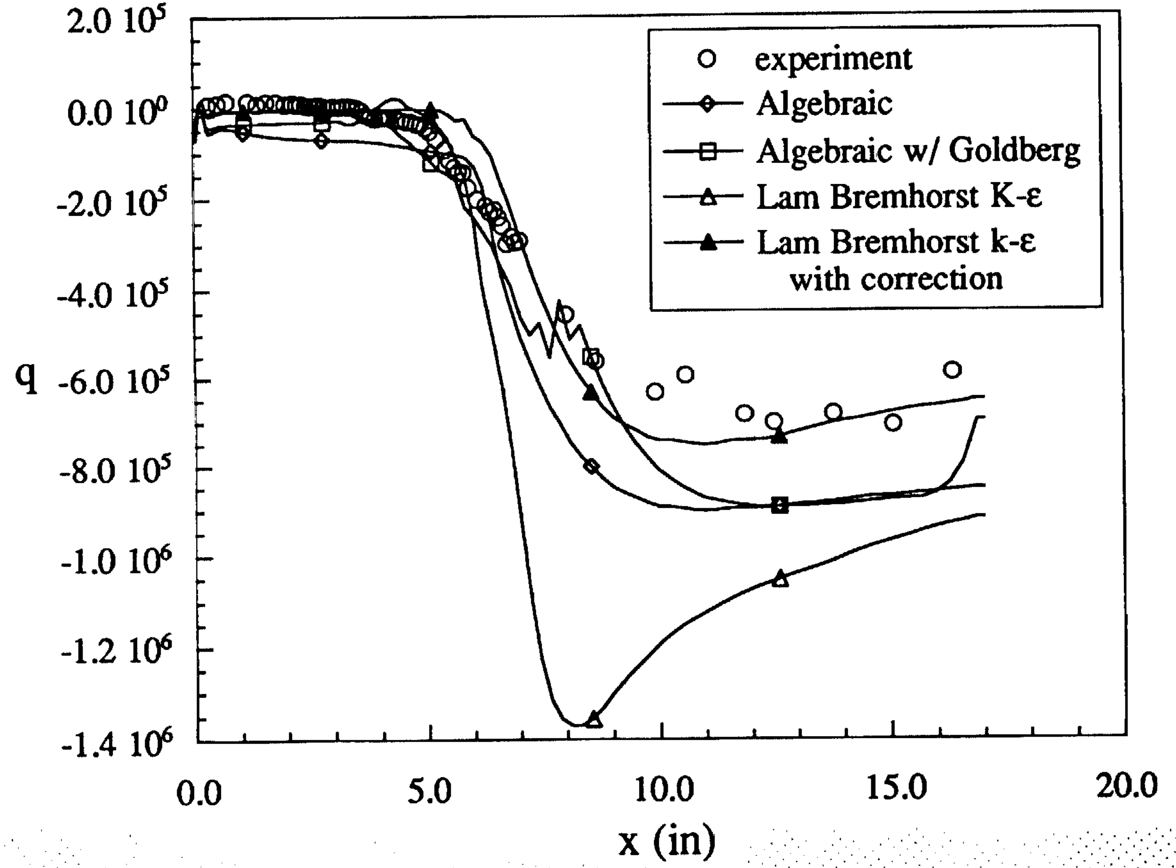
Tangential Injection of Helium into Air with Shock/Boundary Layer Interaction



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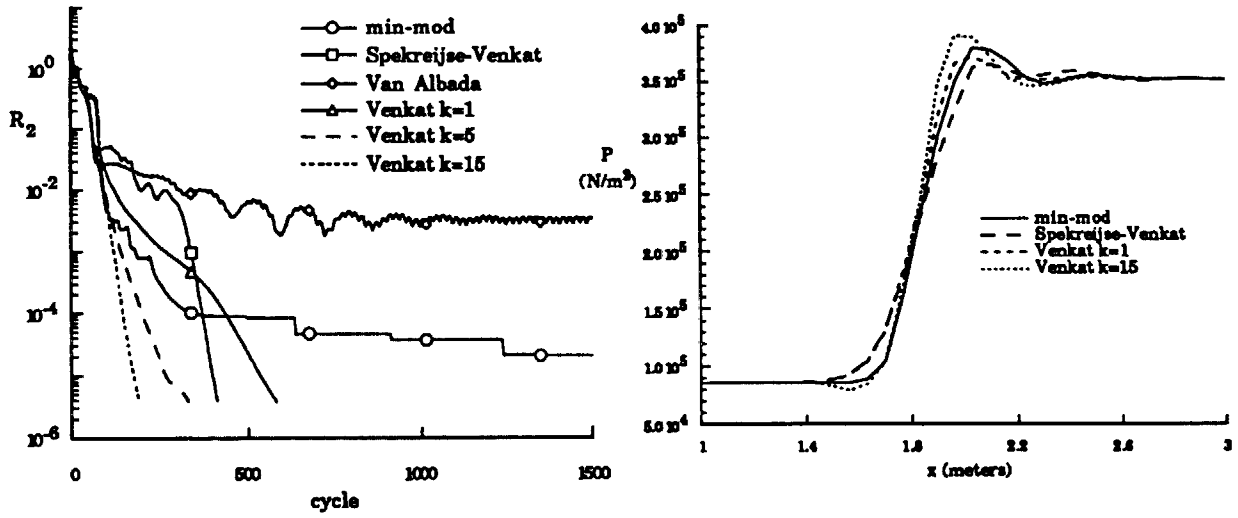
Limiter comparison for the Shock Reflection problem



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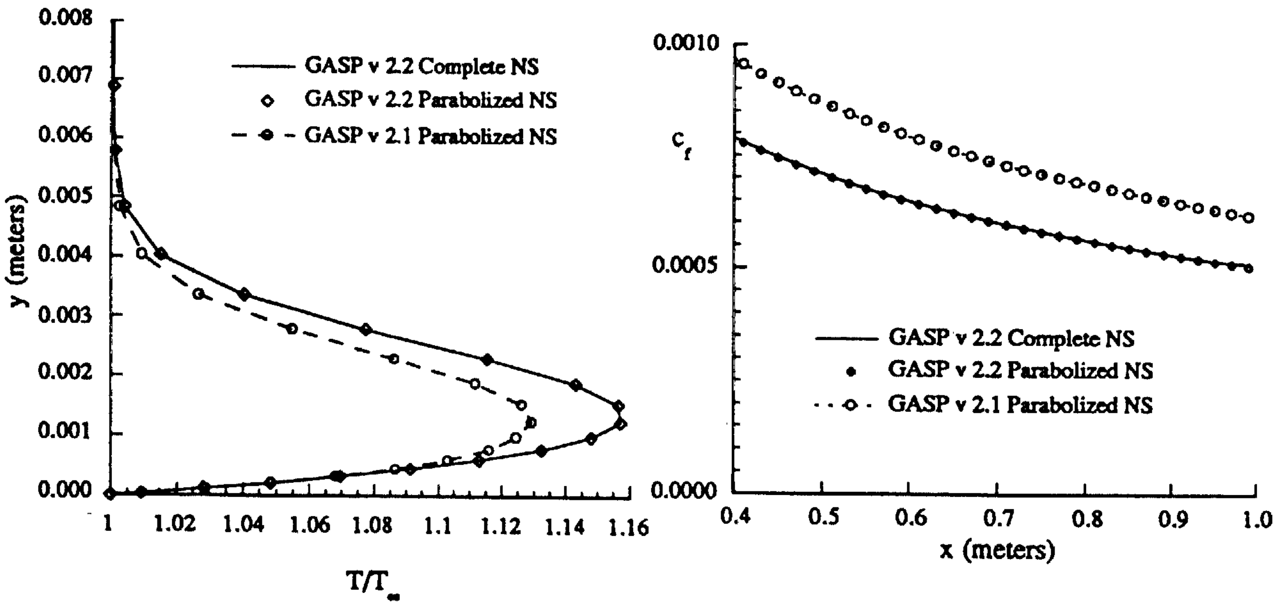
Improved PNS results for the Mach 2 flow over a flate plate



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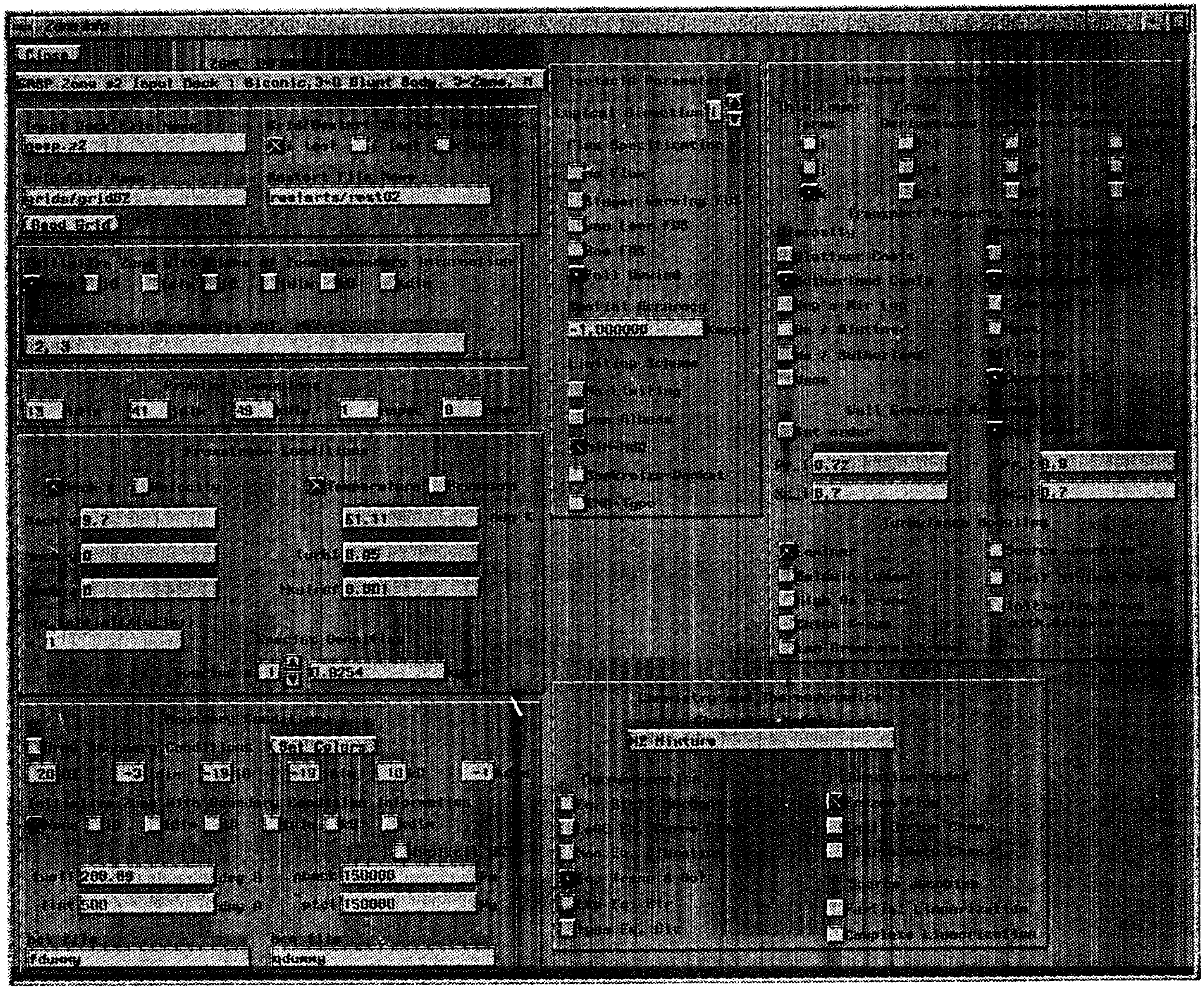

CASP Zone #2 Input Deck 1 Biconic,3-D Blunt Body, 2-Zone, N

casp.z2

grids/grid02

restarts/rest02

2, 3

13 41 49 1 0

9.2

0

0

61.11

0.05

0.001

1

1 3.0254

20 -3 -19 -19 10 -1

288.89

500

150000

150000

fdummy

gdummy

-1.000000

0.72

0.7

0.9

0.7

Support for GASP v2 GUI

- ➤ Use of Motif User Interface as well as FAST
  - ◆ Motif GUI supported on many Unix platforms
  - ◆ Motif widget set offers features not found in FAST
- ➤ Support for pointwise boundary conditions
  - ◆ Create boundary condition specification file graphically
- ➤ Refinement of the zonal boundary definition
  - ◆ Current implementation guarantees proper range
  - ◆ New implementation will also guarantee proper orientation

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Unstructured Technology

Support for GASP v2 GUI (cont.)

- Refinement of the mesh sequencing definition
  - Rules checking will be extended to include pointwise boundary conditions and zonal boundaries
- Access to the GASP thermo-chemical database
  - Interface will be able to calculate all freestream quantities
  - Interface will only allow the selection of valid chemistry models subject to current database.

Expected GASPv3.0 Features

- ➤ **More General Zonal Interpolation**
  - ◆ Allow for mesh point discontinuities at zonal boundaries
  - ◆ Correct fluxes to maintain global conservation
- ➤ **Improved Time Integration Algorithms**
  - ◆ Multi-Grid
  - ◆ Preconditioning
  - ◆ Inner Iteration techniques
  - ◆ Dual Time Stepping
- ➤ **Extended Mesh Sequencing**
  - ◆ More capabilities for multi-zone problems
  - ◆ Make it compatible to run with Multi-Grid

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GASP v3

Expected *GASP*v3.0 Features

- ➤ **Chemistry Modeling**
  - ◆ Option for loosely OR fully coupled chemistry
  - ◆ New equilibrium chemistry solution technique
    - – Law of mass action
    - – Steffenson acceleration for Newton's method
- ➤ **Turbulence Modeling**
  - ◆ Option for loosely OR fully coupled turbulence
  - ◆ Possible new models
    - – Wilcox's k-ω model
- ➤ **Implicit Boundary Conditions**
  - ◆ Library of linearized boundary conditions built-in

Months after start of contract -------->	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
Preconditioning																									
Improve Robustness of Inviscid Preconditioner	▨	▨	▨	▨	▨	▨																			
Deliver Completed Inviscid Preconditioning												△													
Perform Research for Viscous Preconditioning	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨										
Deliver Formulation of Viscous Preconditioning															△										
Code Complete Preconditioning Matrix																▨	▨	▨	▨	▨	▨				
Deliver GASP with New Preconditioning																								△	
Chemistry																									
Restructure Code for Chemistry Algorithms				▨	▨	▨																			
Implement Loosely Coupled Chemistry							▨	▨	▨																
Implement Equilibrium Chemistry Algorithm										▨	▨	▨													
Deliver GASP with New Chemistry												△													
Code Diagonalization of Fluid Dynamic Terms																▨	▨	▨	▨	▨	▨				
Deliver GASP with Diagonalization																								△	
Miscellaneous																									
Implement Wall Functions for Turbulence	▨	▨	▨																						
Deliver Wall Function Results			△																						
Improve Mesh Sequencing				▨	▨	▨																			
Deliver GASP with Improved Sequencing												△													
Implement Mesh Embedding Techniques													▨	▨	▨	▨	▨	▨							
Deliver GASP with Mesh Embedding																								△	
Vigorously Validate New GASP Code																						▨	▨	▨	
Deliver GASP and Validation Results																								△	
Reporting																									
Deliver Quaterly Reports			△			△			△			△			△			△			△			△	
Prepare Final Report																									▨
Deliver Final Report																									△

Table 1: AeroSoft Phase II Timetable

Unstructured Flow Solver Technology

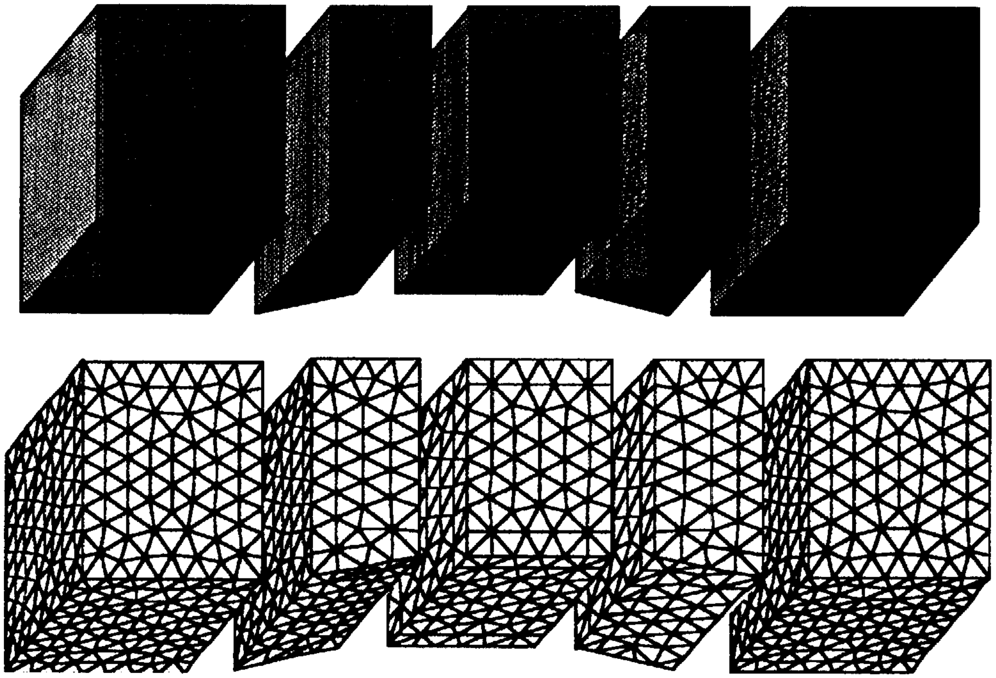
➤ **The Best of GASP**

- ◆ Generalized thermodynamics and chemistry models
- ◆ Finite volume, flux splitting algorithms
- ◆ Full Navier-Stokes physical model with appropriate turbulence models
- ◆ Space marching, including PNS
- ◆ Multi-zone capabilities

Unstructured Flow Solver Technology (cont.)

- ➤ **The Best of Current Unstructured Flow Solver Technology**
  - ◆ k-exact reconstruction for higher-order spatial accuracy and accurate modeling of viscous terms
  - ◆ Implicit relaxation methods for efficient time integration
  - ◆ Support for multiple control volume types including triangles, quadrilaterals, tetrahedra, prisms, and hexahedra

3-D Space Marching
Discretization 2



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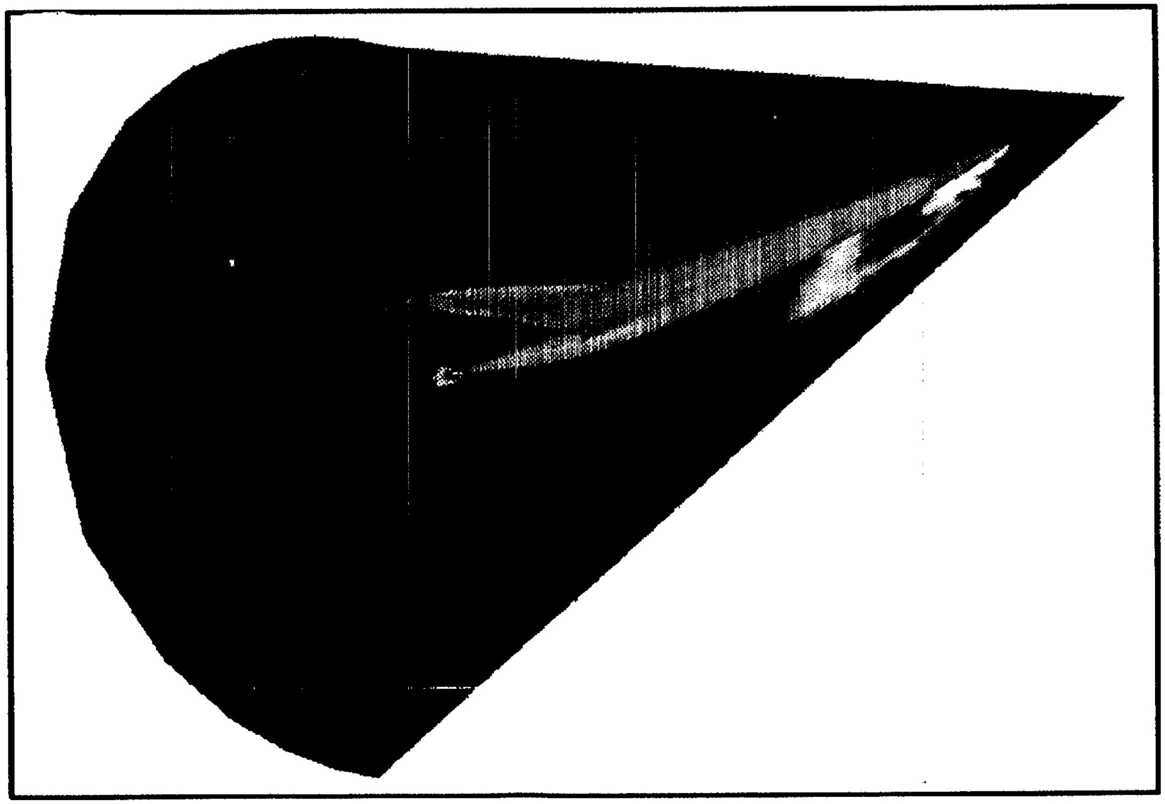
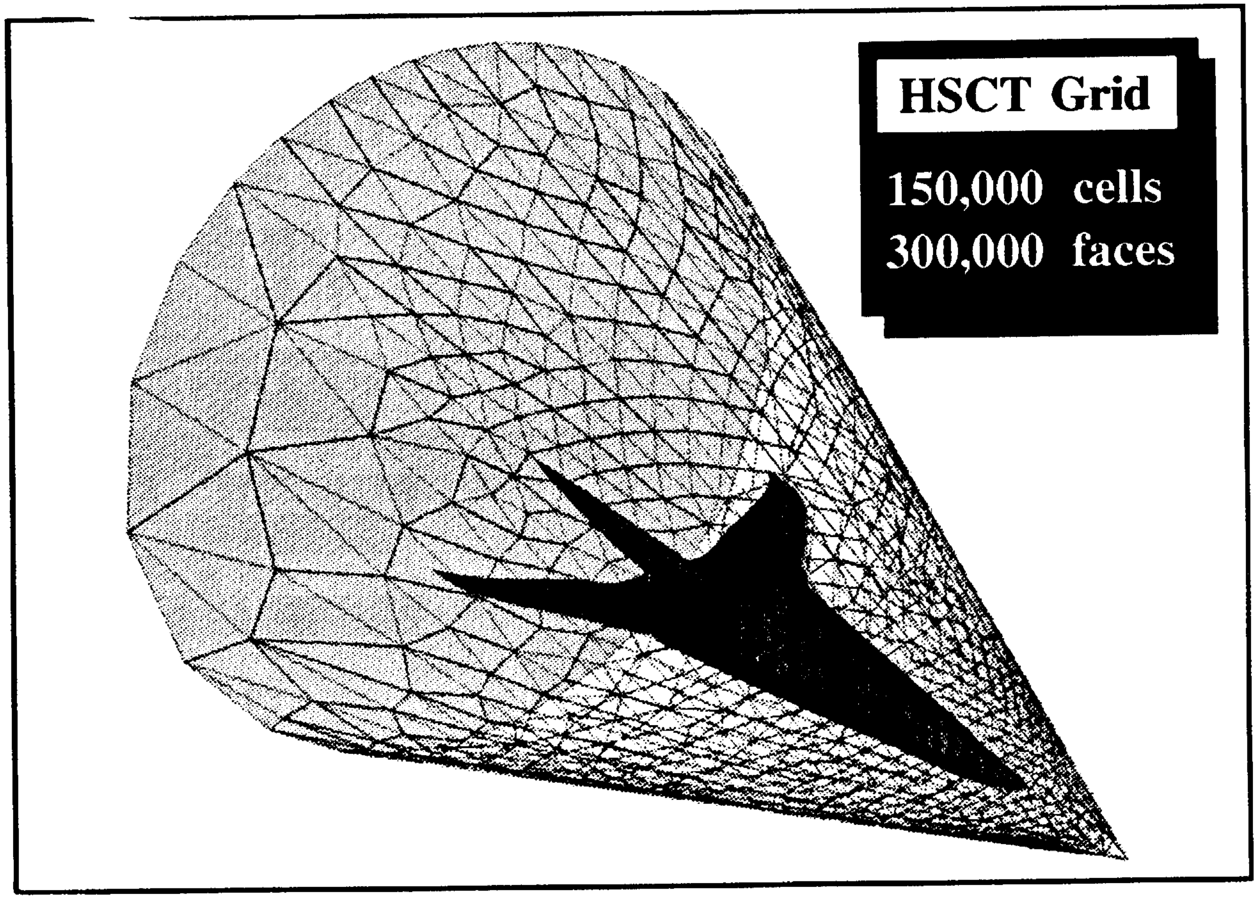
Unstructured Technology

Pressure Contours




HSCT Grid
150,000 cells
300,000 faces