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Methodology for Computational Fluid Dynamics Code Verification/Validation

William L. Oberkampf, Frederick G. Blottner, and Daniel P. Aeschliman
Aerodynamics Dept., Org. 1515
Sandia National Laboratories
Albuquerque, NM 87185-0825

Abstract

The issues of verification, calibration, and validation of computational fluid dynamics (CFD) codes has been receiving increasing levels of attention in the research literature and in engineering technology. Both CFD researchers and users of CFD codes are asking more critical and detailed questions concerning the accuracy, range of applicability, reliability and robustness of CFD codes and their predictions. This is a welcomed trend because it demonstrates that CFD is maturing from a research tool to the world of impacting engineering hardware and system design. In this environment, the broad issue of code quality assurance becomes paramount. However, the philosophy and methodology of building confidence in CFD code predictions has proven to be more difficult than many expected. A wide variety of physical modeling errors and discretization errors are discussed. Here, discretization errors refer to all errors caused by conversion of the original partial differential equations to algebraic equations, and their solution. Boundary conditions for both the partial differential equations and the discretized equations will be discussed. Contrasts are drawn between the assumptions and actual use of numerical method consistency and stability. Comments are also made concerning the existence and uniqueness of solutions for both the partial differential equations and the discrete equations. Various techniques are suggested for the detection and estimation of errors caused by physical modeling and discretization of the partial differential equations.

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I. Introduction

The issue of verification, calibration, and validation of computational fluid dynamics (CFD) codes has been receiving increasing levels of attention in the research literature and in discussions of engineering technology. Both CFD researchers and users of CFD codes are asking more critical and detailed questions concerning the accuracy and range of applicability of CFD code predictions. This is a welcomed trend because it shows that CFD is maturing from a research exercise to a useful tool that impacts engineering hardware and systems. The National Research Council committee chaired by Dr. Richard Bradley [1], summarized the pertinent stages of CFD development as: Stage IV, "Learning to Use Effectively"; and Stage V, "Mature Capability", as *Most analysis done without supporting experimental comparisons*. By this definition, most of us would agree that CFD is definitely not in Stage V.

A clear parallel can be drawn between the state-of-the-art in CFD today and the status of numerical simulation of electrical analog circuits of the past. Until twenty or thirty years ago, the response of complex analogue circuits was determined by bread-board experiments. Since that time, the numerical simulation capability, in both hardware and software, for solving ordinary differential equations has completely changed the technology. Designers now do little or no bread-board experiments, but numerically simulate the response of circuits. Ordinary differential equation (ODE) codes are clearly in Stage V. Today the key issues in circuit simulation are related to characterization of electrical components as a function of voltage, current, temperature, humidity, electric field, etc. Progress to Stage V for ODE solvers has been extremely rapid for two reasons. First, the mathematical complexity of solving ODEs is generally miniscule relative to partial differential equations (PDEs). Second, the complexity of fluid flow physics and the variety of geometries dwarf that of electrical circuits.

During the last few years new concepts and terminology have arisen that take advantage of the increased capability of numerical simulations. Terminology such as "virtual prototyping" and "virtual testing" is now being used by those in engineering development to describe numerical simulation for design, evaluation, and "testing" of new hardware and even entire systems. This trend is driven by increasing competition in many markets, such as aircraft, automobiles, engines, and consumer products. The need to decrease the time and cost of bringing products to market is intense. Another reason for this new trend is the high cost and time required for testing laboratory or field components and complete systems. An important, sometimes dominant, element of testing are the safety aspects of the product or system. The potential legal and liability costs of hardware failures can be staggering to a company, the environment, or the public. Examples of levels of impact are: wave induced structural failure of an offshore oil platform, fire spread in a high-rise office building or hotel, or pressure vessel failure of a nuclear power plant, detonation of a nuclear weapon in an accidental fire. On the opposite end of the spectrum consider the impact of an inaccurate or misleading numerical simulation in a research paper at a conference. The effect is typically nil because before the simulation information is used in engineering design or hardware, more correct results will become available.

The terminology, philosophy and methodology of building CFD code predictions is proving to be a very difficult and complex issue. The issues have been discussed and debated in the literature and among various engineering societies for several years. The Institute of Electrical and Electronics Engineers (IEEE) [2] and the American Nuclear Society [3] first studied the terminology of code verification and validation. A NASA ad hoc committee was formed and they produced a detailed definition of code calibration and validation [4]. In 1993 the International

Organization for Standardization (ISO)[5] and the American Institute of Aeronautics and Astronautics Committee on Standards also became involved in the debate. Because of the far reaching effects on hardware design, commercial software, government contracting, product liability, etc., this issue must be argued in these forums. (For a review of the history and perspectives on this issue, see Ref. [6])

The present paper avoids the debate on terminology and concentrates on the fundamentals of mathematical modeling of fluid dynamics and numerical solutions. For the purposes of the present discussion, the general terminology of code verification & validation (V&V) will be used. A wide variety of physical modeling errors and discretization errors are discussed. Here, discretization errors refer to all errors caused by conversion of the original partial differential equations to algebraic equations, and their solution. Boundary conditions for both the partial differential equations and the discretized equations will be discussed. Contrasts are drawn between the assumptions and actual use of numerical method consistency and stability. Comments are also made concerning the existence and uniqueness of solutions for both the partial differential equations and the discrete equations. Various techniques are suggested for the detection and estimation of errors caused by physical modeling and discretization of the partial differential equations.

Sources of Simulation Error

To build a logical, consistent and workable framework for the meaning of CFD quality assurance terminology, one must understand that CFD has a more diverse foundation and wider range of applications than analytical methods. Most researchers and users of CFD codes view CFD as an extension, or outgrowth, of traditional analytical methods in mathematical physics. Analytical methods, i.e., closed form, exact or approximate solutions to the equations of interest, are built on well defined, very reproducible, and rigorous methods of mathematical analysis. As is well known, the dominant shortcoming of analytical methods is that they address a much narrower range of fluid dynamics than computational methods. The accuracy of analytical predictions fundamentally depends on the accuracy of the mathematical model of the physics; the rigor of the mathematical methods is rarely an issue. CFD prediction accuracy, on the other hand, additionally depends on the equivalence of the discrete model to the continuum model and the accuracy of the solution to the discrete model.

To better understand the accuracy of CFD predictions, the fundamental sources of errors, or inaccuracies, must be identified and addressed. Error sources in numerically simulating physical phenomena described by partial differential equations can be grouped into four broad categories:

- Physical modeling errors
- Discretization errors
- Programming errors
- Computer round-off errors

The present paper delineates and discusses physical modeling and discretization errors, but omits a discussion of programming and computer round-off errors. The first two categories are

subdivided further in the following sections and each is discussed. The above categories are appropriate for *any* phenomena described by partial differential equations, e. g., heat conduction, solid dynamics, structural dynamics, electrodynamics, and neutron transport. The present discussion, however, will be limited to continuum fluid dynamics with emphasis on Newtonian fluids. Other approaches in fluid dynamics, such as molecular dynamics, direct simulation Monte Carlo, and lattice gas methods, are not considered in this paper.

Physical Modeling Errors

Physical modeling errors are those caused by inaccuracies in the mathematical model of the physics, completely separate of numerical issues. These errors are further subdivided into three additional categories associated with: the partial differential equations describing the flow; the auxiliary, or closure, physical models; and the boundary conditions for the partial differential equations. All three of these sub-categories are discussed to stress the evaluation of physical modeling limitations, as opposed to numerical solution limitations, when conducting a CFD simulation. Too often, difficulties in detecting and eliminating CFD simulation errors, whether in code V&V activities or in day-to-day simulations, are due to a failure to consider each error source.

Partial Differential Equations of Fluid Dynamics

The governing equations for fluid flow can be formulated with various assumptions and the analyst is usually interested in using the simplest form that is appropriate for the problem being solved. The starting point for the following discussion is the compressible form of the unsteady Euler equations and then the governing equations are expanded to include more physics. As the complexity of the physics increases, more information is required in the modeling. The following list is not comprehensive, but does address the more common areas of fluid dynamics.

Inviscid Flow: The partial differential equations that govern the flow of a compressible, inviscid, continuum fluid can be developed from the conservation laws of mass, momentum, and energy. The resulting equations are expected to be valid for all flows except when the size of the flow region of interest is of the same order as a characteristic length of the molecular structure, i. e., mean free path. These same equations can be developed with the Chapman-Enskog expansion method from the kinetic theory of gases [7]. The first term in the expansion gives the Euler equations while the second term in the expansion gives the Navier-Stokes equations. The Chapman-Enskog approach is valid for flows that are collision-dominated and is not appropriate for rarefied flows as previously indicated. These equations are completed with and limited by the models for the fluid thermodynamic properties and the equation of state employed.

Viscous Flow: The Navier-Stokes equations include the viscous and heat conduction properties of the fluid and require information on the transport property coefficients for the shear viscosity, bulk viscosity, and the thermal conductivity. These equations have the same limitations as the inviscid equations, in addition to limitations of the models for the transport properties. The Navier-Stokes equations can be used to determine the flow structure in weak shock waves where good agreement with experimental data has been obtained for low Mach numbers [8]. The Navier-Stokes equations for a liquid with no-slip boundary conditions can be used to determine the flow in small channels of height larger than approximately 10 molecular diameters [9]. For gases at low density, slip and temperature jump boundary conditions are required. At lower densities, the continuum approach becomes unsalvageable.

Incompressible Flow: This is a special case of the previously discussed governing equations where the fluid density is assumed approximately constant. There are many CFD codes that only include the incompressible form of the Navier-Stokes equations. In this case there is an additional restriction beyond those discussed above; the Mach number for fluid flows must be sufficiently small, typically $M < 0.2$ for less than 1% density change, such that density changes can be neglected. For liquids, the density changes are small as long as there are no large fluid temperature variations.

Gas with Vibrationally Excited Molecules: For gases at elevated temperatures the vibrational energy levels of the molecules becomes excited and this results in the specific heats of the gas becoming a function of temperature. This effect becomes important at temperatures above about 800K. This additional physics requires a vibrational rate equation if nonequilibrium effects are important or at high gas densities an equilibrium assumption can be used. For flow in a hypersonic wind tunnel nozzle, this additional physics is required for accurate flow predictions. A good example of this type of model is given in the paper by Canupp, Candler, Perkins, and Erickson [10].

Inert Gas Mixtures: The governing equations for a mixture of perfect gases are developed from the theory of gas kinetics [7] and these equations are well known. The gas mixture equations are nearly the same as the Navier-Stokes equations except a conservation of species equation is obtained for each species, the energy equation has an additional term due to diffusion of species, and the viscosity and thermal conductivity transport properties of the mixture are required. In addition, the diffusion velocity of the species is required. The complete theory accounts for diffusion due to concentration, temperature and pressure gradient in the flow. As this theory is rather complex and computationally expensive, most CFD codes use some approximations, such as; binary diffusion coefficients are used rather the multi-component diffusion coefficients, thermal and pressure diffusion are neglected, or approximate mixture rules for determining the viscosity and thermal conductivity of the gas mixture are employed. Significant errors can occur if the appropriate physics is not included; for example, expansion of gas mixtures in a rarefied jet [11] requires that pressure diffusion effects be included in the diffusion model.

Chemically Reacting Gas: For gas mixtures with chemical reactions, the inert gas mixture equations are appropriate when a production term is added to the conservation of species equations. The production terms are readily determined after the chemical model has been specified. The chemical model requires that the chemical species be determined and the chemical reactions must be identified. For each chemical reaction used in the model, the forward and backward reaction rates must be known. For air, a reasonable chemical model has been determined while for other gas mixtures the chemical models range from well established to poorly known. The chemically reacting gas model is required for air when the gas temperature is greater than approximately 2000K and the density is sufficiently low that the reaction rate times are less than the characteristic flow times. At higher densities the chemical equilibrium assumption can be employed and the conservation of species equations are replaced with conservation equations for the chemical elements if the element composition of the mixture varies spatially.

Turbulent/Transitional Flow: The previous flow models have assumed the Reynolds number is sufficiently low that the flow is laminar. The theory for predicting when the flow transitions to turbulent is an area of significant fluid dynamics research. Even reliable engineering techniques for predicting transition is lacking. A large number of turbulence models have been developed, with

the greatest effort devoted to the incompressible case. As a result of turbulence, the governing equations have additional terms. In the conservation of momentum equation, Reynolds stress terms are added. In the conservation of energy equation, a new term results from the diffusion of the total energy due to turbulent motion. In the conservation of species equation, a new term results from the turbulent mass transfer. The modeling of these additional turbulent correlation terms is performed at different levels of approximation which can require algebraic expressions to the solution of additional partial differential equations. For turbulent reacting flows, Probability Density Function (PDF) methods or other techniques appear to be required to obtain reasonable accuracy. The evaluation of accuracy and limitations of the various models is an ongoing activity of the turbulence modeling community.

Additional Physical Phenomena: There are additional physical phenomena of increasing complexity that can be included in flow models, such as; thermal nonequilibrium, ionized flows, radiative transfer in gases, and multi-phase mixtures. These areas are not addressed because they introduce an increased level of complexity with modeling questions in addition to those already discussed which are beyond the scope of this paper. This is not to say that present CFD simulations in these areas are useless; we simply recognize that the physical model unknowns and errors in these numerical simulations can dominate the discussion instead of complementing it.

The above list of physical modeling errors, or inaccuracies, deals with fluid physics. There are two other primary areas characterizing the partial differential equations; temporal nature and spatial dimensionality. Most CFD practitioners think of these as unrelated, but recent work is pointing out that they are more closely related than generally thought. It is common for a CFD analyst to presume that a steady-state solution exits, or that unsteady solution phenomena can be ignored. Of course, it is well known that above a critical Reynolds number some steady flows become unsteady. This behavior occurs for a test problem described by Pironneau[12] for a two-dimensional channel flow with an infinite periodic array of cylindrical obstructions where the critical Reynolds number based on the channel half-width is 150. Above this critical Reynolds number the flow becomes unsteady and remains laminar.

A classical flow that demonstrates both unsteady and steady behavior is low Reynolds number flow perpendicular to a long circular cylinder. For Reynolds numbers less than 49 the flow has been shown experimentally to be steady and two-dimensional [13]. For Reynolds numbers between 49 and 180, only two-dimensional, unsteady flow exists. For Reynolds numbers above 180, it has been suggested and argued that only three-dimensional, unsteady flow exists. Recent impressive computational work by Mittal and Balachnadar [14] has shed light on this issue. They computed the flow at a Reynolds number of 525 using both a two-dimensional and a three-dimensional simulation. They found that both solutions converged to a periodic solution, but the mean drag coefficient for the 2-D simulation was 1.44 and the 3-D simulation produced a value of 1.24. Experimental measurements yield a value very near their 3-D simulation value. The point of this example is two fold. First, a 2-D unsteady physical modeling assumption would seem to be appropriate and reasonable computational results are produced, but they have little relationship to nature. Second, be reminded this is a *very* simple flow lacking much of the complex flow physics discussed above. With the change of one parameter (Reynolds number), over a relatively small range, three fundamentally different flow fields, i. e., solutions to the Navier-Stokes equations, emerge.

For flow geometries that appear to be two-dimensional, the usual assumption is made that the two-dimensional form of the governing equations is appropriate. It has been shown by Rudy [15] that three-dimensional steady solutions are required for laminar, hypersonic flow over a two-

dimensional compression corner with a large deflection. In the test problem of Pironneau [12], at Reynolds numbers above the critical value the flow is unsteady and two-dimensional. However, at Reynolds numbers greater than 600 the flow becomes three-dimensional and remains unsteady. Knowledge of these steady/unsteady and 2-D/3-D boundaries is rarely known, especially for the unbounded variety of flow geometries that can be imagined. In fact, the following generalization is probably true: the vast majority of high Reynolds number flows encountered in engineering and technology are all unsteady, 3-D flows.

Auxiliary Physical Models

Auxiliary physical models complete the equation set needed to describe the flow of interest. These auxiliary models may be given by very simple algebraic equations, or by nonlinear partial differential equations.

Equation of State: The simplest equation of state is the relation for a perfect gas where the pressure is a function of the density, temperature, and molecular weight. The molecular weight is considered constant for this case. For air, this relation begins to become inaccurate at temperatures above approximately 700K, where vibrational excitation of the molecules begins. The perfect gas relation is valid at low pressures and becomes inaccurate at a pressure above approximately 10 atmospheres. For a gas mixture of ideal gases, the equation of state remains of the same form except the molecular weight is determined from the mass fraction and molecular weight of all of the species. If the gas model uses the species conservation equations, then the equation of state should provide accurate results. If the gas is assumed in chemical equilibrium, then errors can be introduced into the equation of state if the equilibrium assumption is not satisfied.

Thermodynamic properties: The thermodynamic properties of many individual chemical species have been calculated with the theory of statistical thermodynamics from a first principles approach. The specific heat at constant pressure, enthalpy, and internal energy are usually determined as a function of temperature. These results are tabulated for a large number of species over certain temperature ranges and the results are usually considered to be accurate for chemical species that have been studied. Errors can be introduced as these properties are approximated with curve fits. A review of the thermodynamic properties of an 11-species air model has been given by Gupta, et. al [16]. The mixture thermodynamic properties can be determined from the species thermodynamic properties and the gas mixture composition. If the gas is assumed to be in chemical equilibrium and the element composition fixed, then the composition is required to be determined only once for a range of temperatures and densities. Curve fits of the thermodynamic properties of equilibrium air have been developed by Tannehill [17] and Liu and Vinokur [18]. Again errors can be introduced with curve fit approximations. A difficulty occurs with the Tannehill curve fits as there are some discontinuities in these results which can result in numerical convergence problems.

Transport properties: The basic governing equations require a model for the stress tensor. For gases the stress tensor is the Newtonian form while the physical behavior of some liquids can be more complex and require a non-Newtonian stress model. For example, for polymeric liquids the non-Newtonian constitutive equations are reviewed in the article by Bird [19]. For the simplest Newtonian flow models the shear viscosity, bulk viscosity, and the thermal conductivity for the fluid are required. For a mixture of perfect monatomic gases, the bulk viscosity coefficient is zero and this is the usual assumption used in CFD codes. This assumption is not appropriate for acoustic motions and in the interior of shock waves. For air and a perfect gas assumption, the viscosity is usually approximated with the Sutherland law. The relation is appropriate for

temperatures between 100K and 2000K. At lower temperatures, Keyes' viscosity relation should be used. The thermal conductivity is typically obtained from the assumption of a constant Prandtl number and a constant specific heat. Errors in the thermal conductivity start to occur at temperatures above approximately 700K. For flows with a mixture of chemical species, the viscosity, frozen thermal conductivity, and binary diffusion coefficients are determined from the kinetic theory of gases. Curve fits for these properties for air species have been given by Gupta, et. al. [16]. These properties are assumed to be of reasonable accuracy but an estimate of the error in these results is not available. The transport properties of the gas mixture are usually determined from approximate mixture rules rather than the complete relation from the kinetic gas theory. For air with sublimation products of graphite, for example, Ryabov [20] has determined that the error in the mixture viscosity is less than 5%, while the error in the frozen thermal conductivity is less than 10%. Ryabov indicates that the Kendall approximation for binary diffusion coefficients gives errors less than 11.5%. The impact of these errors on flow results does not appear to have been evaluated.

Chemical model, reactions, and rates: The accuracy of chemical models is usually determined by the research devoted to the particular gas model. Also, many models for a gas or gas mixtures are a simplification of a more complete model in order to obtain reasonable computation times. For air, sufficient knowledge is available to decide the appropriate species to include and what reactions are necessary. There are generally large errors in the reaction rates for the various chemical reactions, but several models have evolved as standards for air. The accuracy of these chemical models decreases at the higher temperatures. When the flow of a new gas or gas mixture is being calculated, the chemical model needs careful evaluation to determine if reasonable results are being obtained.

Turbulence model: The accuracy of turbulence models must be determined with experimental results for a wide range of Reynolds numbers, shear layer geometries, and pressure gradients. Recently, direct numerical simulation (DNS) has provided useful information for model evaluation. The DNS results have been limited to low Reynolds number flows (< 1000) and to simple flow geometries. The evaluation of turbulence models requires a variety of experiments which test the ability of the model to simulate turbulent flows of increasing flow complexity. Presently, turbulence models can be best evaluated with the benchmark test cases developed at the Stanford Conferences on turbulent flows [21]. These experiments have been carefully picked as the best available as far as their accuracy and specification of flow conditions required to preform numerical simulations. Also, a variety of experiments are required to test gas models for different levels of complexity; for example, incompressible flow, compressible flow, hypersonic flow, multi-component gas mixtures, reacting gas mixtures, two-phase flow, etc. Many codes use wall functions to remove the requirement of a fine grid near walls, as the wall function approach can reduce the required number of mesh cells by a factor of two. For some flows, for example, near boundary layer separation, the velocity profile near a wall is not adequately represented with a logarithmic region. For this case, the wall function approach can introduce significant errors even if the first grid point away from the wall has been carefully located at an appropriate y-plus value. The evaluation of accuracy and limitations of turbulence models is a major research activity that involves the turbulence modeling community and experimentalists.

Boundary Conditions for the Partial Differential Equations

The boundary conditions required for the solution of the governing partial differential equations arising in fluid dynamics have not received the development and attention that is needed. As

pointed out by Oliger and Sundstrom [22] nearly twenty years ago, discretization of the boundary conditions have been studied before the appropriate boundary conditions have been established for the partial differential equations. Only after difficulties with computational boundary conditions have arisen has there been interest in understanding the appropriate boundary conditions that should be used. The paper by Oliger and Sundstrom is one of the few investigations that treat determination of the boundary conditions for fluid dynamics equations (mostly inviscid flows) to ensure a well-posed problem. As these authors point out, one can not expect reasonable numerical solutions unless the correct PDE boundary conditions have been approximated. It seems this lack of attention to what are the correct boundary conditions to the partial differential equations has worsened in the last twenty years; however, just recently the tide seems to be turning [23].

There are three types of boundaries that occur: wall boundaries, open boundaries, and free surfaces. The boundary conditions at these boundaries can take various forms.

Wall Boundary Conditions: These conditions generally have clear physical significance and the appropriate boundary conditions are easier to determine. For example, for continuum flow at a rigid wall, one could have the most common, and simplest conditions; the velocity components are zero and the gas and wall temperature are at the same specified value. One additional, slightly more complex boundary condition requires information from the flow solution, i. e., the interior of the solution domain. An example is zero pressure gradient at the wall. For near noncontinuum flows, there is velocity slip and temperature jump at a wall that must be modeled. It is more difficult to specify the appropriate wall boundary conditions for the chemical species equations as the heterogeneous chemical reactions of the gas species at the wall must be modeled. Some related questions are: What are the appropriate wall boundary conditions when vibrational nonequilibrium effects are included in the gas model with a separate vibrational temperature? How accurate does a porous wall have to be modeled? Can the flow through a porous wall be assumed to be continuous or at what size do the many individual jets have to be modeled?

Two additional error sources related to wall boundary conditions are, first, inaccurate wall geometry, and second, discontinuities or mathematical singularities. Inaccurate wall geometry refers to the difference between the actual physical geometry and its computational representation, i.e., fidelity of the computational to the physical geometry. Examples of these are the following: physical hardware not accurately fabricated to specifications; inaccurate CAD/CAM solid modeling; and lack of surface roughness knowledge for a turbulent flow simulation. Discontinuities in the boundary conditions occur, for example, where a wall can change from solid to porous with a step change in the surface normal velocity. There is also a discontinuity at the intersection of a sliding wall and a fixed wall, for example, the classic driven-cavity problem. The stagnation point on an axisymmetric blunt body is a mathematical singularity in the cylindrical coordinate system. For the partial differential equations these singularities can easily be written and understood; for the discrete form of the equations, such singularities can introduce numerical difficulties and errors if not handled correctly.

Open Boundary Conditions: These are conditions that are specified along a boundary, or portion of a boundary, where there is "free" (i. e., unrestricted) inflow and/or outflow. We describe this type of boundary as free, simply to distinguish it from inflow or outflow through a porous wall discussed above. These types of boundary conditions typically result from a requirement that numerical solutions be obtained over a limited region of the flow. In this sense, errors associated with these boundaries could be considered to be associated with boundary conditions for the discretized formulation. Even with this view, one can still ask the question; what

are the exact boundary conditions for the partial differential equations on an open boundary? Or, the inverse question: what errors are introduced by the physical model assumptions of specified conditions for the partial differential equations on an open boundary?

Even though these boundary conditions are commonly required by the finite size computational domain, this need not be the case. For example, if one were simulating the flow over a model in a wind tunnel, then the exact inflow boundary conditions must be given by a complete specification of all dependent variables in the partial differential equations and auxiliary equations at, say, the beginning of the test section. These specified flow quantities might not be consistent with the partial differential equations and rapid changes can occur in the computation of flow downstream from the inflow boundary. All of these variables would have to be measured spatially and possibly temporally if, for example, turbulence quantities were needed. This level of detailed knowledge, or calibration, of wind tunnels does not exist for the vast majority of facilities around the world.

It was recently stated by Sani and Gresho [23], and we fully agree, that boundary conditions at open boundaries are often the most difficult and elusive aspect of mathematical modeling. The number of physical boundary conditions required, and allowed, at an open boundary is determined from an evaluation of the characteristics of the governing partial differential equations. The number of physical boundary conditions must be the same as the number of characteristics of the governing equations entering the computational domain. If the flow is locally supersonic, there is no upstream influence and accurate boundary conditions can be specified without much difficulty. Inflow, more specifically upstream, boundary conditions can typically be much closer to the region of interest than outflow, or downstream, boundary conditions. For subsonic flow over an isolated body, the boundary conditions should be applied at infinity where the flow is uniform and known. If the downstream location of the computational boundary is not located sufficiently far downstream, some of flow may be entering the computational domain and the correct formulation is very nebulous. More will be said on this topic when discretization errors are discussed.

Free Surface Boundary Conditions: This is a more general case than the wall case and the development of the appropriate physical relations has been presented by Batchlor [24]. The general approach considers the relations that must be satisfied at the boundary between two media. At this interface the temperature of the two materials is the same and the heat flux normal to the boundary is equal on both sides. A balance of stress at the boundary with the effect of surface tension taken into account results in two transition relations. In addition, the tangential component of velocity is continuous across a material boundary separating a fluid and another media and there can be mass transport at the boundary. The boundary condition relations require a value of the surface tension for the materials involved. Also, these boundary conditions can become difficult to apply if the interface becomes unstable with large movement. For example, it is well known that the Rayleigh-Taylor instability occurs when a heavy fluid is above a light fluid in a gravitational field.

Discretization Errors

Discretization errors are those caused by the discretization of the partial differential equations, the auxiliary physical models, and the continuum boundary conditions, and the subsequent solution of these discrete equations. Errors generated by or associated with each of these sub-categories is now discussed. Techniques for detecting or quantifying some of these errors are discussed in the next section.

Discretization of the Partial Differential Equations

The reformulation of the partial differential equations into algebraic equations that accurately represent the original equations is a bigger, more problematic, mathematical step than is generally recognized. Formal mathematical analysis of the relationship of differential and difference equations (Lax equivalence theorem) states that if the numerical method is consistent and stable, then the solution to each system is equal [25, 26]. A discretization method is consistent if it can be analytically shown that as the discretization size approaches zero, the difference equations are equal to the differential equations. This can be written as

$$\text{Consistency Definition: } \lim_{\Delta \to 0} \delta_\Delta \Phi = \partial \Phi$$

where $\delta_\Delta \Phi$ represents the system of finite difference equations (which includes any method for discretizing the the partial differential equations), $\partial \Phi$ represents the original system of partial differential equations of the mathematical model, and Δ represents the size of all discretized independent variables. A numerical method is stable if it can be analytically shown that as the solution is marched in time, or is iteratively solved, the solution remains bounded. One can write this as

$$\text{Stability Definition: } \lim_{n \to \infty} \left| \Phi_\Delta^n - \Phi_\Delta^0 \right| < N$$

where Φ_Δ^n represents all dependent variables of the system of equations at time n for a fixed mesh size of Δ, Φ_Δ^0 represents arbitrary initial values of the dependent variables, and N is an arbitrary constant.

It can be proven mathematically that the above conditions are necessary and sufficient for the solution of the discretized system of equations to be identical to that of the partial differential equations. This proof is the foundation of the numerical solution of partial differential equations. If it were as simple as this, however, the state of the art in CFD would be further along than it is after thirty years of intensive research. The difficulties and hindrances to progress are diverse; some are mathematical in nature, some are practical issues, and some are implementation issues. In the following we attempt to categorize these issues.

Approximate Consistency and Stability Analyses: Consistency and stability proofs of numerical methods are predominantly developed for very simple model problems, never on a "real" problem. The model equations are always linearized equations and uncoupled from any other equations. For example, the most commonly used are the wave equation, the heat conduction equation, and the viscous Burger's equation in one spatial dimension. These simple, linearized, uncoupled, one dimensional equations do not exhibit the astounding spectrum of solutions exhibited by the Navier-Stokes equations (vortices cannot exist in one-dimension, for example). If additional complex physics such as gas mixtures, turbulence, and reacting flow are included, it is clearly seen that these model equations are far removed from real world problems. The reason for the elimination of these real world complexities, of course, is that the difference equations resulting from the analysis are nonlinear, just as the original partial differential equations, and can not be analyzed.

Additional, but related, simplifications of consistency and stability analyses are elimination of: mixed classification partial differential equations, non-uniform grids, and boundary conditions. Consistency and stability analyses are never done on differential, or difference, equations with

mixed classification, e. g., hyperbolic and elliptic. These mixed zones, however, very commonly exist. For example, in *every* supersonic flow problem modeled by the steady Navier-Stokes equations hyperbolic and elliptic regions exist adjacent to one another. In the extremely rare event that a multi-dimensional stability analysis is conducted, the structured grid is always assumed to be uniformly spaced. This assumption does not correspond to real world problems. Boundary condition type and geometry can influence the stability of numerical methods. Only those analyses that include the discrete boundary conditions along with the discrete equations can provide the correct behavior of the numerical scheme. See for example, the book by Morton and Mayers [27] for references to work on the effect of boundary conditions on stability.

Proof Applies Only in the Limit: The matching of solutions between difference and differential equations for consistent and stable methods applies only in the limit. The practical problem, of course, is that all numerical solutions obtained are *never* at the limit; they are always finite. Although this is obvious, it bears keeping in mind that the proof is a theoretical construct; equality is never attained. Examples of the mismatch between the two models are in order. The mathematical character of the difference equations can be very different from the differential equations. Consider inviscid supersonic flow; the numerical domain of dependence of the difference equations must include the domain of dependence of the differential equations. This mismatch can have varying effects in the discrete solution. As a second example, it has been found by Yee et al [28] that finite difference solutions can exhibit a much wider range of dynamical behaviour than their continuum counterparts. They have found that "the use of linearized analysis as a guide to studying strongly nonlinear PDE's is insufficient and can lead to misleading results." And finally, "In particular, when one tries to stretch the maximum limit of the linearized allowable time step for highly coupled...nonlinear systems, most likely all of the different types of spurious asymptotes (e.g. spurious steady states, periodic orbits, limit cycles, or chaotic phenomena) can be achieved in practice depending on the initial conditions."

For flow over slender bodies at angle of attack, the vortex patterns can be symmetric or asymmetric depending on the angle of attack and flow conditions. How the difference equations are written in discrete form can be important in determining what solution is obtained, as shown by Levy, Hesselink, and Degani [29]. These authors have shown that how the left hand side of each difference equation is formulated in the solution procedure impacts whether the steady-state result is symmetric or asymmetric. The left hand sides of the difference equations are zero when the steady-state solution is obtained but they can influence the solution obtained from the difference equations. These studies indicate that the steady-state solution is not unique and there are at least two solutions that can satisfy the right hand side of the difference equations. If the difference form of the left hand side is not symmetric, spurious asymmetric results can be obtained.

Conservation of mass, momentum and energy are so ingrained in us that we assume they are always true, whether a process occurs in nature or is simulated in a computer code. On any discretized grid, however, conservation cannot be assumed just because the original partial differential equations conserve mass, momentum and energy. Loss of conservation can be caused by a wide variety of inaccuracies and/or errors in the numerical simulation. For example, the following can cause loss of conservation: lack of iterative convergence either for a steady state solution or a time varying solution, numerical limiters in differences schemes, artificial diffusion schemes, skewness of the structured or unstructured grid, etc. A related question is: does the numerical simulation conserve mass, momentum, and energy regardless of the grid size? This test is rarely applied in the verification of computer codes. Control volume methods that are constructed properly are the only numerical schemes that have global conservation. Other schemes have

conservation only in the limit when step sizes go to zero; as a result, they never do in any actual solution.

Spatial and Temporal Resolution: This category of error is the most well recognized of the discretization errors and is unquestionably the most important. This error, also referred to as truncation error, is due to finite resolution in the spatial and temporal discretization. In the past, finite difference analyses rarely attempted to estimate the magnitude of this error on the results computed. Finite element methods seem to have a better record of addressing this issue. A strong initiative by individuals such as P. J. Roache, K. N. Ghia, F. M. White, C. J. Freitas and others has raised (forced) the importance of at least addressing the issue of grid convergence in CFD solutions. It is the opinion of the present authors that the enforced discipline was desperately needed for the maturation of numerical simulations. Because of the importance of this topic and because effective measures can be taken to control it, this matter will be addressed in detail in the following section on detection and quantification of errors.

Discretization of the Auxiliary Physical Models

If the auxiliary physical model equations are linear algebraic expressions, which can be solved directly, then the errors are of the computer round-off type and are very small. An example is the equation of state for a perfect gas. If the algebraic expressions are nonlinear in the unknowns, then some iterative technique is required and errors can occur if the iteration is not completely converged each time it is used. Equilibrium chemical composition requires iterative solution of nonlinear equations and errors result in the mass fraction of the chemical species if convergence is not adequate.

Thermodynamic and transport properties for real gases are approximated with table look-up or curve fits. The required accuracy of the approximations to these properties has not been established and, surprisingly, for many cases in the past, the approaches resulted in large errors. Clearly these errors can be reduced with more accurate techniques but the data storage requirements are significantly increased with possible increases in computer time. The errors in the approximation of the individual properties of the chemical species must be compatible with the errors being introduced in the techniques being used to approximate the gas mixture properties. Careful evaluation of accuracies required for thermodynamic and transport properties used in flow simulations and the impact on fluid dynamic predictions have not been performed. The standard approach is to use reasonable approximations that result in shorter computation time, but the impact on solution errors has not been determined.

Probably the most important auxiliary model used in CFD is the use of turbulence models. For algebraic models, the primary error source is the determination of some flow field feature needed in the calculation, e. g., the magnitude of a turbulent length scale. The reliable determination of the required flow field feature has proven to be difficult for a wide variety of shear layer geometries. By far the most difficult, however, is the calculation of turbulent transport variables using two-equation turbulence models. The discretization error of these type PDE's has been discussed above, and will be addressed again in the following section.

Discretization and Implementation of Boundary Conditions

The boundary conditions for the difference equations, whether they be for wall, open, or free surfaces, must provide the same independent information as provided for the PDE's. Over-

specification of the discrete boundary conditions (BC's) will cause divergence of the iterative, or temporal, solution. Under-specification of the BC's will cause the solution not to converge, i. e., wander about, or to converge to different solutions depending on arbitrary features, such as initial conditions, relaxation parameters, etc. This perfect balance between over- and under-specification of knowledge on boundaries is much more difficult to obtain for difference equations than it is for PDEs. We have not found a good explanation for this feature. We suggest the reason, however, is that in the continuum mathematics the PDE's are perfectly coupled to the boundaries; no discrepancy, inconsistency, or mismatch is tolerated. In the difference equations, however, the coupling is weak and it depends on a variety of numerical parameters, such as the numerical algorithm, differencing scheme, grid size, and smoothing parameters. Recent work in numerical boundary conditions, [23, 30], support our explanation.

Implementation of Dirichlet boundary conditions are usually straightforward. Neumann and mixed boundary conditions require that a difference method be used at the boundary. This method is usually of the same order accuracy as the PDE differencing method so that a globally consistent order scheme is obtained. However, only a grid refinement study will establish that the overall order of the complete numerical scheme is as expected. It should be noted that very few researchers have demonstrated the overall, or global, order of their simulation.

The most difficult type of boundary condition to implement is the open BC. The entire issue of inflow and outflow boundary conditions in now being studied in much more depth than in the past. An excellent summary, and we believe required reading on the subject, of open boundary conditions for incompressible Navier-Stokes equations is given by Sani and Gresho [23]. This paper shows that there are more questions than answers on the implementation of open boundary conditions, even for the relatively simple physics of steady, incompressible laminar flow. Concerning open boundary conditions, they state "Nature is usually silent, or in fact perverse, in not communicating the appropriate ones." Also, "The boundary conditions on such open portions of the boundary are a necessary evil ... We believe that there are no 'true' open boundary conditions, thus explaining Nature's silence. We also believe and may demonstrate herein that perhaps nowhere else do theory and practice seem to clash so much." Sani and Gresho also introduced the term "fuzzy boundary conditions" to suggest the existence of numerical BC's that produce good numerical solutions, but if one tries to take the limit as $\Delta \rightarrow 0$ of these BC's, one obtains unacceptable BC's for the PDE's.

If the inflow boundary condition is to represent undisturbed flow at infinity, then the inflow boundary conditions should be applied sufficiently upstream so that the flow in the region of interest is not significantly influenced by the inflow BC location. For subsonic outflow, the boundary condition location should be varied to determine the impact on the flow in the region of interest. For exterior flow over a body, the continuum freestream boundary conditions are imposed at infinity while the freestream conditions are imposed at a finite distance in numerical simulations which results in errors being introduced. Gresho has coined the phrase "manufactured boundary conditions" to clearly point out that the conditions specified at these locations are "dreamt-up" by the analysts and not provided by Nature.

The vast majority of effort in the formulation and implementation of numerical boundary conditions has been directed toward steady flow conditions. As CFD matures, the need for reliable and accurate unsteady boundary conditions will become more important in the prediction of real world flows. It is expected that the development of these type BC's will be even more challenging than the presently used steady BC's.

Solution of the Discrete Equations

The error in the solution of the discrete equations is referred to as the discrete solution error. The error associated with the solution can be defined as the difference between the exact solution to the discrete equations and the approximate solution obtained. An example of this type error is the difference between the exact and approximate iterative solution of the nonlinear discretized equations for the steady state Navier-Stokes equations. Often one reads in papers that the iteration procedure has been performed until there is a small change in the variables between the iterations. This type of test will not always produce accurate results as the convergence rate could be slowing down but the solution is not converged. The correct approach is to set each difference equation equal to a residual. At the start of the iteration, the dependent variables do not satisfy the difference equation and the residual is non-zero. As the iteration proceeds, the residual for all difference equations and at all spatial locations is driven to machine zero. Although this level of solution accuracy is probably not required for all simulations, it is highly recommended that this iterative convergence be demonstrated on coarse grid solutions.

For transient flow simulations, at each time step the difference equations must be iterated to convergence where the iterative error must be much smaller than the temporal discretization error. When the temporal and spatial step sizes are decreased, the iterative solution at each time step could require that more iterations be performed to obtain smaller iterative errors. Some numerical schemes can require no iterations when an ADI scheme is used, while many iterations are required when a Jacobi iterative solution is used. The solution technique used for the sparse matrix solver determines the iterations required. The iterative behavior at each time step also depends on how the governing equations are solved; for example, (1) with a segregated approach where each dependent variable is solved from a separate difference equation and is solved one at a time, (2) with a coupled approach where all dependent variables are solved for simultaneously from all of the difference equations. The behavior of the iterative solution technique at each time step must be understood so that no significant iterative errors are not introduced into the solution procedure.

Detection and Estimation of Errors

The following section discusses suggestions for methods to detect and quantify certain types of physical modeling, discretization, and programming errors. Some of these methods are similar to the types of error control methods incorporated in modern software packages for solving ordinary differential equations. Modern ODE solvers are extraordinarily adaptive at controlling accuracy and are very robust; a capability CFD code developers should strive to achieve also.

Physical Modeling Errors

To detect when an incompressible flow solution is beginning to deviate from the physical modeling assumption because of compressibility effects, a relatively simple test could be inserted into the code. For example, an average value of the speed of sound in the fluid analyzed could be an input parameter for the code. When the local fluid speed at any grid point became larger than say, 0.2, of the input speed of sound, then a warning would be issued to the user. Similar types of automatic error detection tests could be incorporated into a code to detect if the following types of physical modeling errors become larger than a specified input value at any point in the flow:

• Thermodynamic equilibrium assumption becomes in error

• If a chemically reacting gas model is required

• Thermodynamic and transport properties are evaluated outside their range of validity

Discretization and Programming Errors

Analytical solutions to the PDE's of interest provide an extremely valuable tool in demonstrating code verification. At the present time, use of analytical solutions in code verification seems to be distinctly out of favor in the CFD community. There are a surprisingly large number of exact and approximate analytical solutions to the Euler and Navier-Stokes equations [31-34]. Possibly the reason for lack of familiarity with analytical solutions among many CFD researchers and practitioners is the modern concentration on numerical solutions in graduate school training.

During the last several years a novel approach has been used to obtain exact solutions to the Navier-Stokes equations [35]. In their approach, a specific form of solution function is assumed to satisfy the PDE of interest. This function is inserted into the PDE and all the derivatives are analytically computed using symbolic manipulation software, such as MACSYMA™. The equation is simplified, and all remaining terms resulting in inequality between both sides of the equation are grouped into a forcing function term. This term is then considered to be simply added to the original PDE so that the assumed solution function satisfies the new PDE exactly. For example, in the Euler or Navier-Stokes equations this term can be considered to be a source term. The boundary conditions for the PDE are simply considered to be either the value of the solution function on the boundary (Dirichlet condition), or a Neumann condition that can be analytically computed from the solution function.

To verify the CFD code, the computed body force term and boundary conditions are programmed into the code and a numerical solution computed. This procedure verifies, albeit for a very narrow range of physical modeling, a large number of numerical features in the code, for example; numerical method, differencing technique, spatial transformation techniques, grid spacing technique, and coding accuracy. Shih, Tan and Hwang [36] have taken this approach a step further and applied it to the incompressible Navier-Stokes equations for laminar, two-dimensional flow. They have obtained an impressive exact solution to the classical lid-driven cavity problem for an arbitrary Reynolds number. It is highly recommended that incompressible Navier-Stokes codes be verified with this exact solution.

The largest contributor to numerical solution error, and the one that has caused the most unreliability and lack of confidence in CFD solutions, is that due to inadequate grid resolution. It is ironic that the quantification of this error is also the most straightforward. We believe the reason for this grid error/easy estimation paradox is simple: cost. The computer cost, and to a lesser extent personnel time cost, to carefully conduct the error estimation analysis is probably a factor of 4 for 2-D problems and a factor of 8 for 3-D problems beyond an "acceptable" solution. If one considers that the acceptable solution is usually at the limit of computer time or budgetary constraints already, it follows why these estimates are rarely done. We submit that our blunt assessment of the situation and the reason for its existence is supported by simply examining the state-of-the-art in ODE solvers. ODE solvers suffered the same paradox during their early years, but they are now the shining example for accuracy and reliability for numerical solutions. The reason they have progressed so rapidly in this regard is because the computer power required for their solution is usually minimal compared to the solution of PDE's. The initiatives of Roache, et. al., on

assessment of numerical error, as mentioned earlier, is forcing CFD to become more accountable.

Spatial discretization error is estimated using Richardson's classical method, also known as "deferred approach to the limit" and "iterated extrapolation" [37]. Using Richardson's extrapolation, one can write

$$\Phi_{exact} = \Phi_{\Delta} + \alpha\Delta^{p} + \text{higher order terms}$$

where Φ_{exact} is the exact solution to the PDE, Φ_{Δ} is the numerical solution obtained using a grid size of Δ, α is a constant that is determined from the numerical solution, and p is the order of the numerical method. It is important to note that Richardson's method applies not only to computed dependent variables at all grid points, but also to solution functionals. Solution functionals are integrated and differentiated quantities such as body lift and surface heat flux, respectively. At least two numerical solutions are required to estimate discretization error using Richardson's method. The fine grid solution need not be twice the number of grid points (in each coordinate direction) as the coarse grid, but this is common practice and it provides a more accurate estimate. Roache [38] has developed a Grid Convergence Index (GCI), based on Richardson's extrapolation, that converts error estimates obtained from any grid refinement ratio into an equivalent grid doubling estimate. He argues that using the GCI would help standardize the accuracy evaluation of grid refined solutions.

Careful use and estimation of error using Richardson's method has been documented only by a few researchers [39-42]. In most cases it has been found that two solutions are *insufficient* to properly use Richardson's method. The reason three or more solutions are required is that from the first two solutions it may be found that the demonstrated order of accuracy from the calculations does not match the formal accuracy of the method. This can be caused by one of two reasons. First, numerical difficulties or errors, such as excessive grid stretching, inaccurate implementation of boundary conditions, and coding errors, cause a degradation in the overall accuracy of the method. Second, it can be found that insufficient grid resolution was used on the first two, or more, solutions such that formal accuracy is not attained until finer grids are used. Until computed accuracy from two individual solutions matches previously demonstrated accuracy of the code, Richardson's method *cannot* be used to estimate error.

A final observation is made that has apparently not been pointed out in the literature concerning the use of Richardson's method. By examining the grid convergence plots of the researchers that have carefully used Richardson's method an interesting, but unsettling, feature is observed. Figures 1 and 2 are grid convergence plots taken from Blottner [41] and Walker & Oberkampf [42], respectively. Note that both of these plots demonstrate the numerical method is second order accurate. It is seen that the grid fineness required to obtain the demonstrated accuracy of the code is also a grid that produces relative errors on the order of 1% to 0.1%. In other words, to demonstrate accuracy using Richardson's method one must compute solutions that have relative errors on the order of 1% to 0.1%. This is a very sobering result if solutions of only ±10% are desired in production CFD solutions.

VI. Summary and Conclusions

A discussion of the sources of errors that result from the computational fluid dynamic approach is presented. The validation issue of determining the errors resulting from the governing partial

differential equations, boundary conditions, and auxiliary physical models has been addressed. From this discussion it is observed that the present approach in CFD is to use reasonable physical approximations in the modeling, but the impact of these assumptions on the errors introduced into CFD simulations is generally unknown. Also, modeling assumptions such as, two-dimensional steady flow are often made and in some cases are physically wrong. Confidence in the accuracy of the governing equations can be increased by using results from first principle physics solutions in validating the models being used. The validation of the governing equations requires carefully developed experiments to test the various modeling assumptions employed.

Verification of the numerical solution of the governing equations requires that the discretization errors be estimated and controlled. A discussion of the sources of discretization errors that result from the difference form of the governing equations, boundary conditions, and auxiliary physical models has been addressed. With attention to performing adequate grid refinement studies, one believes that accurate numerical solutions can be obtained to CFD governing difference equations if sufficient computer resources are available. However, one might obtain an accurate result but not the physically correct solution. The possibility of multi-solutions to the difference equations has not been adequately investigated in the CFD community.

Approaches for detection and estimation of errors are suggested. In many cases we know the limitation of the physical models, and codes could be used to tell the user when these limitations have been exceeded. We are strong supporters of careful grid refinement studies using the Richardson extrapolation method to estimate the errors in numerical solutions. These studies are very costly, especially for three-dimensional flows. It was pointed out that the grid resolution required for the valid use of Richardson's method produces results which are far beyond the accuracy needs of most engineering design requirements.

References

1. Bradley, R. G., 1986, "Current Capabilities and Future Directions in Computational Fluid Dynamics," National Research Council, National Academy Press, Washington, DC.

2. Institute of Electrical and Electronics Engineers, 1984, F. Jay, editor, "IEEE Standard Dictionary of Electrical and Electronics Terms," ANSI/IEEE Std. 100-1984.

3. American Nuclear Society, 1987, "Guidelines for the Verification and Validation of Scientific and Engineering Computer Programs for the Nuclear Industry," ANSI/ANS-10.4-1987.

4. Bradley, R. G., 1988, "CFD Validation Philosophy," AGARD Symposium on Validation of Computational Fluid Dynamics, Conf. Paper No. 1, Lisbon, Portugal.

5. International Organization for Standardization, 1993, "Quality management and quality assurance standards--Part 3: Guidelines for the application of ISO 9001 to the development, supply and maintenance of software," ISO 9000-3:1991(E).

6. Oberkampf, W. L., "A Proposed Framework for Computational Fluid Dynamics Code Calibration/Validation," 18th AIAA Aerospace Ground Testing Conf., Paper No. 94-2540, Colorado Springs, June 1994.

7. Hirschfelder, J. O., Curtiss, C. F. and Bird, R. B., Molecular Theory of Gases and Liquids, John Wiley & Sons, Inc., New York, 1954.

8. Vincenti, W. G. and Kruger, C. H. Jr., Introduction to Physical Gas Dynamics, John Wiley & Sons, Inc., New York, 1965. (see p. 412).

9. Koplik, J. and Banavar, J. R., Continuum Deductions from Molecular Hydrodynamics, Annual Review of Fluid Mechanics, Vol. 27, pp. 257-292,1995.

10. Canupp, P. W., Candler, G. V., Perkins, J. N., Erickson, W. D., "Analysis of Hypersonic Nozzles Including Vibrational Nonequilibrium and Intermolecular Force Effects," AIAA Journal, Vol. 31, PP. 1243-1249, July 1993.

11. Rothe, D. E., Electron Beam Studies of the Diffusive Separation of Helium-Argon Mixtures, Physics of Fluids, Vol. 9, PP. 1643-1658, Sept. 1966.

12. Pironneau, O. Summary and Conclusions for Test Case T2, in Numerical Simulation of Unsteady Flows and Transition to Turbulence, Edited by O. Pironneau, et al., Cambridge University Press, 1990.

13. Roshko, A., "Perspectives on Bluff Body Wakes," J. Wind Engr. and Industrial Aero., Vol. 49, 1993, pp. 79-100.

14. Mittal, R., and Balachandar, S., "Vortical Structures in Bluff Body Wakes," 33rd AIAA Aerospace Sciences Mtg., Paper No. 95-0867, Reno, NV, Jan. 1995.

15. Rudy, D. H., et al., "Computation of Laminar Hypersonic Compression-Corner Flows," AIAA Journal, Vol. 29, pp. 1108-1113, July, 1991.

16. Gupta, R. N., Yos, J. M., Thompson, R. A. and Lee, Kam-Pui, "A Review of Reaction Rates and Thermodynamic and Transport Properties for an 11-Species Air Model for Chemical and Thermal Nonequilibrium Calculations to 30,000K," NASA Reference Publication 1232, August 1990.

17. Tannehill, J. C., and Mugge, P. H., "Improved Curve Fits for the Thermodynamic Properties of Equilibrium Air Suitable for Numerical Computation Using Time-Dependent or Shock-Capturing Methods," Engineering Research Institute, Iowa State University, Ames, Iowa, Feb. 1974.

18. Liu, Yen and Vinokur, M., "Equilibrium Gas Flow Computations. I. Accurate and Efficient Calculation of Equilibrium of Equilibrium Gas Properties," AIAA-89-1736, 1989.

19. Bird, R. B., and Wiest, J. M., Constitutive Equations for Polymeric Liquids, Annual Review of Fluid Mechanics, Vol. 27, pp. 169-193,1995.

20. Ryabov, V. V., "Transfer Coefficient of Multicomponent Air with Sublimation Products of Graphite," Journal of Engineering Physics, Vol. 55, pp. 786-791, July 1988.

21. Bradshaw, P., Editor, Collaborative Testing of Turbulence Models - Collected Results of an

International Project, Mechanical Engr. Dept., Stanford University, Stanford, CA 94305-3030, August 1994.

22. Joseph Oliger, J. and Arne Sundstrom, A., "Theoretical and Practical Aspects of Some Initial Boundary Value Problems in Fluid Dynamics," SIAM J. Applied Math., Vol. 35, pp. 419-446, 1978.

23. Sani, R. L. and Gresho, P. M., "Resume' and Remarks on the Open Boundary Condition Minisymposium," Intl. J. Numerical Methods in Fluids, Vol. 18, 1994, pp. 983-1008.

24. Batchelor, G. K., "Introduction to Fluid Dynamics," Cambridge University Press, Cambridge, Great Britain, 1967.

25. Richtmyer, R. D. and Morton, K. W., "Difference Methods for Initial-Value Problems," Interscience Publ, 1967.

26. Anderson, D. A., Tannehill, J. C. and Pletcher, R. H., 1984, "Computational Fluid Mechanics and Heat Transfer," Taylor & Francis, 1984.

27. Morton, K. W. and Mayers, D. F., "Numerical Solution of Partial Differential Equations," Cambridge Univ. Press, Cambridge, Great Britain, 1994.

28. Yee, H., Sweby, P. and Griffiths, D., "Dynamical Approach Study of Spurious Steady-State Numerical Solutions of Nonlinear Differential Equation: 1. The Dynamics of Time Discretization and Its Implementations for Algorithm Development in Computational Fluid Dynamics," J. Comp. Phys., Vol. 97, No. 2, p. 249.

29. Levy, Y., Hesselink, L. and Degani, D., "Anomalous Asymmetries in Flows Generated by Algorithms that Fail to Conserve Symmetry," AIAA Journal, Vol. 33, pp. 999-1007, 1995.

30. Grinstein, F. F., "Open Boundary Conditions in the Simulation of Subsonic Turbulent Shear Flows," J. Comp. Phys., Vol. 115, 1994, pp. 43-55.

31. Karamcheti, K., "Principles of Ideal-Fluid Aerodynamics," Wiley, 1966.

32. Panton, R. L., "Incompressible Flow," Wiley, 1984,.

33. Hayes, W. D. and Probstein, R. F., "Hypersonic Flow Theory; Vol. 1, Inviscid Flows," Academic Press, 1966.

34. Wang, C. Y., "Exact Solutions of the Steady-State Navier-Stokes Equations," Annual Review of Fluid Mechanics, Vol. 23, 1991, pp. 159-177.

35. Steinberg, S. and Roache, P. T., "Symbolic Manipulation and Computational Fluid Dynamics," J. Comp. Phys., Vol. 57, No. 2., 1985, pp. 251-284.

36. Shih, T. M., Tan, C. H., and Hwang, B. C., "Effects of Grid Staggering on Numerical Schemes," Intl, J. Num. Methods in Fluids, Vol 9, 1989, pp. 193-212.

37. Richardson, L. F., "The Deferred Approach to the Limit," Trans. Royal Soc. of London, Ser. A, Vol. 226, pp. 299-361. "Part 1. Single Lattice." Part II. "Interpenetrating Lattices" by J. A. Gaunt.

38. Roache, P. J., "A Method for Uniform Reporting of Grid Refinement Studies," FED-Vol. 158, Quantification of Uncertainty in Computational Fluid Dynamics, ASME Fluids Engineering Conf., FED-Vol. 158, Washington, DC., 1993, pp. 109-120.

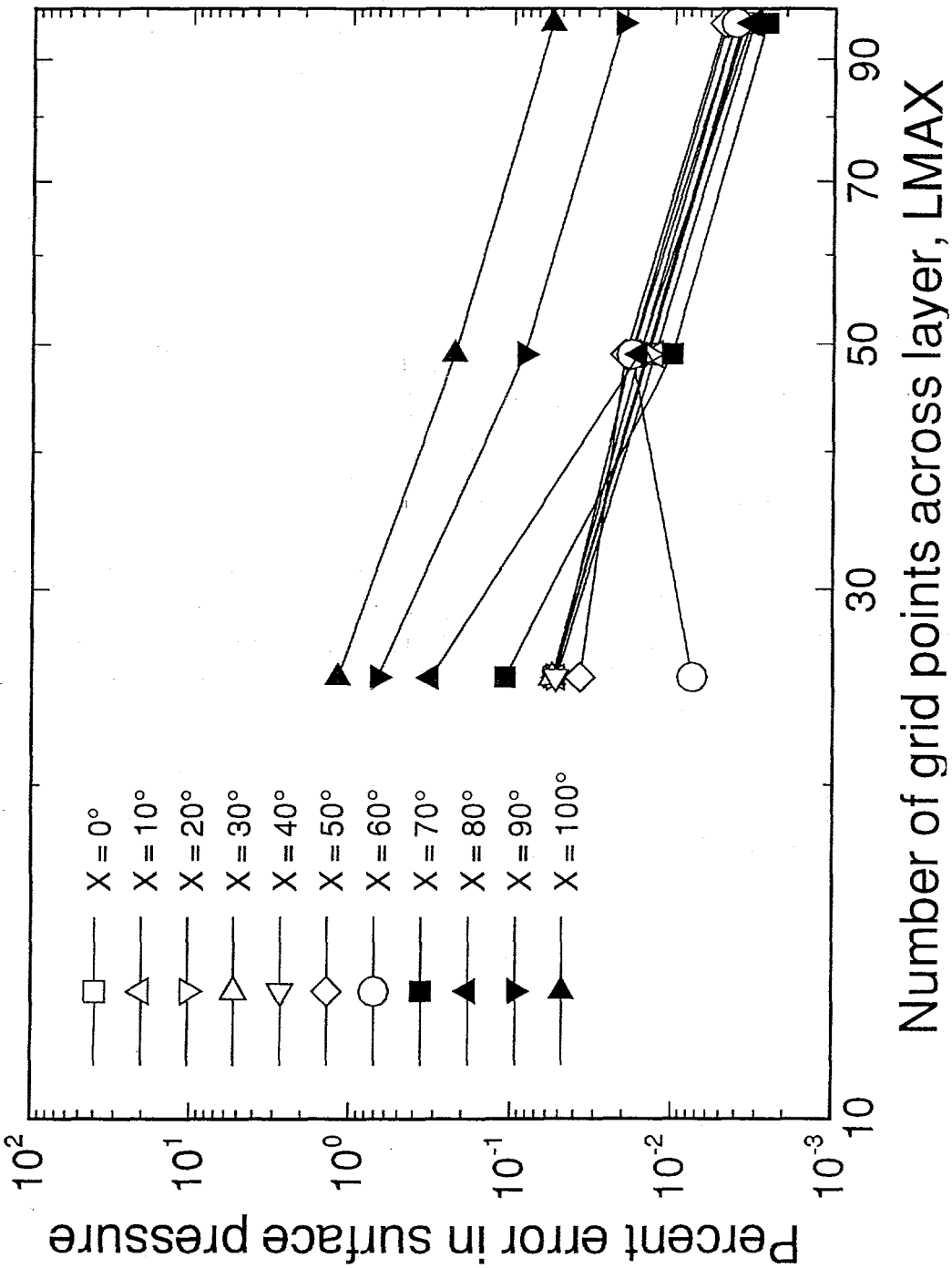
39. Roache, P. J., "Scaling of High-Reynolds-Number Weakly Separated Channel Flows," in Numerical Aspects and Physical Aspects of Aerodynamic Flows," T. Cebecci, Ed., Ch. 6, Springer-Verlag, NY, pp. 87-98.

40. Shirazi, S. A. and Truman, C. R., "Evaluation of Algebraic Turbulence Models for PNS Predictions of Supersonic Flow Past a Sphere-Cone," AIAA Journal, Vol. 27, No. 5, pp. 560-568.

41. Blottner, F. G., "Accurate Navier-Stokes Results for the Hypersonic Flow Over a Spherical Nosetip," J. of Spacecraft and Rockets, Vol. 27, No. 2, 1990, pp. 113-122.

42. Walker, M. A. and Oberkampf, W. L., "Joint Computational/Experimental Aerodynamics Research on a Hypersonic Vehicle: Part 2, Computational Results," AIAA Journal, Vol. 30, No. 8, 1992, pp. 2010-2016.

Fig. 1


Percent error in surface pressure
Number of grid points across layer, LMAX
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10
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50
70
90
X = 0°
X = 10°
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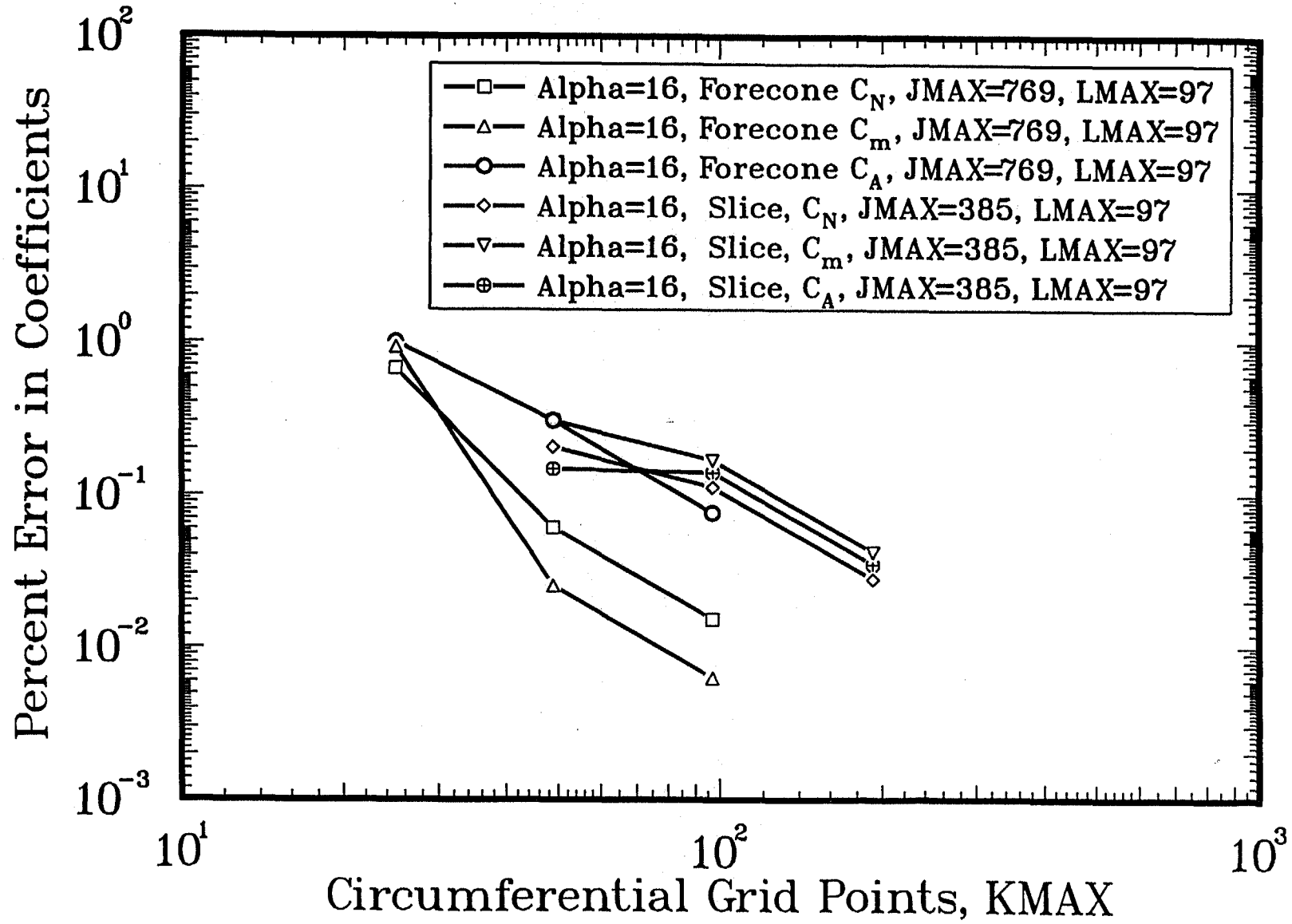
X = 80°
X = 90°
X = 100°

Fig. 2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Percent Error in Coefficients
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^1
10^2
10^3
Circumferential Grid Points, KMAX