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Credible Computational Fluid Dynamics Simulations

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This summary presents the motivation for the Special Section on the credibility of computational fluid dynamics (CFD) simulations, its objective, its background and context, its content, and its major conclusions. Verification and validation (V&V) are the processes for establishing the credibility of CFD simulations. Validation assesses whether correct things are performed, and verification assesses whether they are performed correctly. Various aspects of V&V are discussed. Progress is made in verification of simulation models. Considerable effort is needed for assessing the validity of simulated reality.

Introduction

EARLY in the 20th century, computational fluid dynamics (CFD) technology came into being with the publication of Richardson's *Weather Prediction by Numerical Process.*[1] Thom[2] was the first to solve a substantial fluid dynamics problem in aerodynamics by using discrete formulas. He solved the Navier–Stokes equations by replacing them with finite difference equations for simulating the flow past a circular cylinder at a Reynolds number of 10. Since then, CFD technology has advanced tremendously. As we approach the end of the 20th century, CFD technology is an extensively used tool in advancing science and technology in aeronautics and other fields, in understanding various phenomena, and in designing, operating, and investigating systems or processes. Advances in this technology are made for realistic modeling of phenomena and for incorporating CFD tools into development programs. This summary presents the motivation for the Special Section on the credibility of CFD simulations, its objective, its background and context, its content, and its major conclusions.

Motivation and Objective

The developers and users of CFD simulations, those affected by the decisions based on these simulations, and buyers of CFD software are justly concerned with whether the simulations are credible or whether the level of credibility of the simulations is acceptable for the purposes for which they are being used. This concern has been the principal issue from the inception of numerical simulations technology.[3] Although significant advances have been made in improving the accuracy of numerical simulations and of the simulated reality, there is still little agreement on how to systematically assess and report the credibility of simulated reality. This lack of a consensus on the appropriate treatment of the CFD credibility-assessment issue is the reason for this Special Section.

During the past three decades, there have been numerous efforts to deal with the CFD credibility issue. It has been dealt with in various sessions and panel discussions at conferences, JANNAF-sponsored workshops, and other related activities within organizations such as AGARD, the Gesellschaft für Angewandte Mathematik und Mechanik, the Fluids Engineering Division of the American Society of Mechanical Engineers, and the AIAA. All of these efforts attempted to identify and address various facets of the credibility issue. The objective of this Special Section is to do just that, by presenting some recent contributions and perspectives. It is hoped that these efforts will facilitate the development of a consensus regarding methods for measuring credibility.

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Background and Context

Whenever simulations are presented, a statement regarding their credibility is essential; it must also be shown that the achieved level of credibility is acceptable for the purposes for which simulations are being used. The burden of proof lies with the presenter of the simulations.

The first serious attempt to define a few terms for assessing CFD credibility was made, as stated in Ref. 4, in 1987 with the introduction of the phrases *CFD code validation* and *CFD code calibration.* The definitions of these phrases have shortcomings, however, and the phrases have been used with different meanings. For example, code validation and simulation validation are different. The bottom line is the validation of simulation.

The word *calibration* means the act or process of calibrating simulations or the act of tuning a computational (numerical) model or fluid dynamics model. The calibration of simulations or the appropriateness of model adjustments requires the establishment of the credibility of the simulations. Calibration is not the process of determining the credibility of simulations; it is the process of obtaining correction factors for adjusting simulated results or for adjusting models, respectively, thus causing calibration to follow validation or making calibration an integral part of modeling.[5]

In 1988, the AIAA's Standards Program approved a project called "Guidelines for Presentation of Numerical Simulations from Computational Fluid Dynamics."[6] This project was initiated by the AIAA CFD Committee on Standards that was formed in 1987. Guidelines were not developed, however, and by 1989 this committee was inactive. The development of a standard for assessing CFD simulation credibility was first recommended in 1989.[7] (The word *standard* is used in a broad sense to mean standard, guide, or procedure, as done by standard organizations.)

In January 1993, the present author informed William H. Heiser, a member of the AIAA Publication Committee, that the credibility of CFD simulations in publications is a serious issue. He saw fit to seek action from this Committee that led to the development of the AIAA Editorial Policy Statement on Numerical Accuracy and Experimental Uncertainty by the AIAA Fluid Dynamics Technical Committee.[8] This policy is a good beginning, but it is a halfway measure for establishing the credibility of simulations. The policy addresses only verification of simulations.

The editorial policy states, "The appropriateness of the governing equations for modeling the physical phenomena and [of] comparison with experimental data is not part of this evaluation." The wisdom of making this statement is questionable. A policy statement for validation of simulations is highly desirable. CFD encompasses two disciplines, computational analysis (numerical analysis) and fluid dynamics. The distinction between computational modeling and modeling of physics is essential for developing, understanding, and assessing CFD simulations.[9] The numerical accuracy is not the same as simulated-reality accuracy. The AIAA uses simulations principally for making reality-related decisions, that is, fluid-dynamics decisions. Simulations with improper fluid dynamics and simulation-credibility assessments based on inappropriate comparisons with experimental data are questionable.

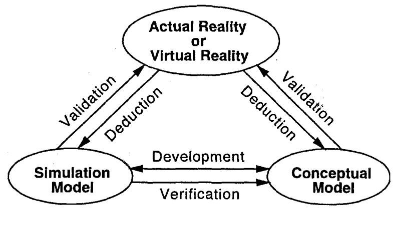

Fig. 1 CFD simulation paradigm.

Since the formulation of the AIAA Editorial Policy, AGARD Working Group 15 on Quality Assessment for Wind Tunnel Testing[10] and the Standards Subcommittee of the AIAA Ground Testing Technical Committee[11] have produced documents that are applicable to the vast majority of engineering testing. These documents provide engineering uncertainty-assessment methods for large-sample tests and for most single-sample tests. They are less complex than the "Guide to the Expression of Uncertainty in Measurement" by the International Organization for Standardization.[12]

Recently, the Fluid Dynamics Panel of AGARD recommended a selection of experimental test cases for validating CFD models. The following is a key conclusion of that panel concerning the overall assessment of test cases: "From an experimental point of view, it can be remarked that it is difficult to judge the validity and accuracy of the presented data sets."[13] The value of those sets is limited for the intended purposes. Such data are frequently used by persons other than the developers of the data sets. "If data from other workers are used, they require no uncertainty."[8] If this instruction of the AIAA Editorial Policy is followed for validation activities, the outcomes of these activities may be questionable.

In 1992, James E. French, Standards Specialist (AIAA), resurrected the AIAA CFD Committee on Standards. This Committee has restarted the aforementioned project of the Standards Program and has embarked on a new effort: the development of a guide for assessing the credibility of CFD simulations. The first draft and the second draft of this guide were prepared in June 1996 and January 1998, respectively.

Modeling and simulation are done also in other fields. Because of the criticality of simulations in defense efforts (principally using operations research) and in nuclear engineering, extensive efforts have been made to define, develop, and systematize processes and practices for establishing the credibility of simulations. The U.S. Department of Defense developed the "Verification, Validation and Accreditation (VV&A) Recommended Practices Guide,"[14] and the American Nuclear Society has outlined "Guidelines for the Verification and Validation of Scientific and Engineering Computer Programs for the Nuclear Industry."[15]

Considering the efforts in operations research and nuclear engineering and in the context of CFD, the CFD simulation paradigm was formulated (Fig. 1, from Ref. 5). In Fig. 1, reality is called virtual reality when a majority of the critical, quality measurements for confirming the simulated quantities and features that are of interest are not available; verification and validation are the processes for measuring the credibility of simulations.

Verification assesses the credibility of a simulation model by estimating the degree to which this model is an accurate representation of the conceptual model from the perspective of the intended uses of the simulations.[5] Validation assesses the credibility of a simulation model by estimating the degree to which this model is an accurate representation of reality from the perspective of its intended uses.[5] Validation assesses whether correct things are performed, and verification assesses whether they are performed correctly.

Recently, Paul E. Rubbert expressed what CFD code V&V is and is not. He concluded that, in the eyes of an experienced airplane designer, CFD comparisons with archival-quality test cases do not provide a feasible or accepted means of establishing trust in the results produced by a code. This conclusion is supported mainly by the following observations: 1) Generalizations cannot be trusted for (computer or wind-tunnel) simulation practices; 2) CFD models and codes and test techniques cannot be fully verified and validated ahead of time; 3) computer simulations should not be expected to be the same as wind-tunnel data; 4) archived data usually do not improve with age; and 5) the assessment of simulation credibility needs to be done for every new problem. Rubbert suggests replacing the concept of CFD code validation based on archived, wind-tunnel data by a process of uncertainty management. This suggestion is in agreement with Mehta's recommendation of using uncertainty analysis.[5]

In mathematics, the word *error* is defined as the difference between an observed or calculated value and a true value. When the true value is uncertain or unknown, the error in the observed or calculated value cannot be determined. The word *uncertainty* is defined as an estimate of error. In a number of endeavors, uncertainty analysis is used for measuring credibility of simulations. Because of the responsibility placed on computer simulations in nuclear engineering, a systematic effort was made beginning in the early 1970s to develop a practical uncertainty method.[16]

The credibility of wind-tunnel data must be known whenever they are used to establish the credibility of computer-simulated reality. With regard to the appropriateness of comparing computer simulations with wind-tunnel data, Coleman[17] shows that the uncertainties should set the scale at which comparisons for validation should be made, discusses misconceptions regarding the effects of bias uncertainties in comparative tests for validating computer-simulated trends or increments, and explains the need for accounting for uncertainties resulting from the incorporation of previous wind-tunnel data, including fluid property values, into the conceptual (fluid-dynamics) model.

Most of the uncertainty methods available prior to the AGARD/AIAA standard[10,11] were not well suited for application to large, complex measurement systems, making the uncertainty analysis of test data a black art. The two major sources of error in wind-tunnel data are the measurements of the model attitude and of the aerodynamic loads acting on the model. As a result of having this standard, the significance of the experimental errors is realized and efforts are instituted to reduce the uncertainties associated with data. Cahill[18] and Belter[19] have discussed their experiences with the application of this standard. The AIAA standard[11] is appropriate for including in the AIAA Editorial Policy Statement as a recommendation.

The only certain aspect of a wind-tunnel or computer simulation is that it is uncertain. Generally, fluid-dynamics systems cannot be wind-tunnel tested at conditions within their operational envelope to obtain the data necessary for validation. Simulation capabilities, costs, and timeliness are other limiting factors. The importance of sensitivities and uncertainties in computer simulations becomes paramount. Only through uncertainty analysis can the issues related to obtaining credible simulations be determined.[5] This analysis is the primary method used in validating simulated virtual realities; it is also the method used when design and analysis tools have shortcomings.

Van Wie[20] presented an example of the use of uncertainty analysis for an analysis of a hypersonic airbreathing engine. To provide a framework for the accuracy requirements for the measurements and for the CFD simulation validation, sample engine calculations were used to estimate the sensitivity of engine performance to uncertainties in the performances of engine components. These requirements were used to select an inlet performance measurement technique. The propagation of the uncertainties in wind-tunnel data to those in computed results was also demonstrated. Van Wie concluded by listing a few tenets that include the following: 1) Uncertainties are not useful, if one is uncertain of them, and 2) pursuit of absolute knowledge is a noble cause, but validation of CFD simulation should be at the level required for the problem at hand. The essence of the latter tenet is applicable to verification of CFD simulation models.

The foregoing discussion sets the stage for introducing this Special Section. Most of the papers in this section were presented as invited papers in two sessions that the author organized at the AIAA 27th Fluid Dynamics Conference.

Content

The Special Section presents 1) different perspectives on establishing the credibility of CFD simulations and 2) discussions of the various aspects of this task. The presented papers are organized in four groups: overviews, verification issues, experimental perspectives, and experiences in validation of simulation.

The first three papers compose the overview group: They present perspectives toward establishing the credibility of CFD simulations.

Rizzi and Vos outline essential steps toward assessing credibility, present lessons learned from a few collective credibility exercises, and suggest a vision for the process of systematic collaborative validation that is open to public scrutiny by means of the Internet. Jameson and Martinelli present a perspective on verification and validation for analysis and design. They identify principal sources of error and give examples of verification and validation. Oberkampf and Blottner resurrect many fundamental issues and questions concerning sources of errors that affect the validation of conceptual models and the verification of simulation models. They also suggest the use of analytical solutions and of Richardson's extrapolation for verification of simulations.

Issues of verification are addressed in the next three papers. Roache discusses terminology for credibility assessment, error taxonomy, and methods for verification. These methods are the grid convergence index, the cumulative area fraction error curves, and surrogate single-grid error indicators. Habashi et al. present an efficient and generic mesh-optimization approach for controlling the numerical accuracy. Anisotropic mesh adaptation is used with triangular meshes, and the method is illustrated with simulations of laminar flows past airfoils. Yee and Sweby reveal some causes of spurious phenomena resulting from numerics in time marching to the steady-state numerical simulations. They provide a few guidelines for overcoming spurious phenomena.

Two papers on wind-tunnel simulations are presented next. Dolling discusses examples of wind-tunnel simulations of shock-induced turbulent separated flows to underscore the importance of understanding what time-averaged data represent physically. This understanding is essential for ensuring that a proper conceptual model is used for desired CFD simulations. Aeschliman and Oberkampf outline and demonstrate a method for designing wind-tunnel simulations with the objective of validating CFD models.

Experiences with validations of CFD simulations are reported in the last three papers. Reed et al. report on laminar–turbulent transition simulations conducted to date with the nonlinear parabolized stability equations and with the direct numerical simulation approach. Barber focuses on the issues of accuracy and robustness when CFD codes are used in support of the design process. He illustrates the difficulty in relying on benchmark studies for validating a code for design use. Benek et al. examine validation issues associated with the use of CFD in the engine/airframe integration method.

Conclusions

The motivation for and the objective of this Special Section are addressed. The contributed papers demonstrate that a consensus on an appropriate treatment of the credibility-assessment issue is beginning to form. Verification and validation are processes of choice for measuring the credibility of simulations. The authors of the papers that comprise the Special Section discuss various aspects of the credibility issue; their major conclusions are presented next.

The principal conclusions of the papers on perspectives toward measuring credibility are the following: 1) A systematic and collaborative validation that is open to public scrutiny by means of the Internet is recommended; 2) validation of simulations requires first the validation of the conceptual model, then the verification of the simulation model, and, at the end, the credibility assessment of simulated reality with wind-tunnel data; and 3) a great deal of caution must be exercised in claiming confidence in simulations involving nonlinear physics that are highly coupled.

The verification-issue papers make the following conclusions: 1) Techniques are already available to convincingly verify the numerical accuracy of CFD codes and calculations; 2) not only is numerical accuracy controllable by using mesh adaptation, but optimal meshes can be automatically determined; and 3) knowledge of the nonlinear behavior of numerical schemes can help in minimizing sources of spurious solutions.

The experimental papers show that 1) when unsteadiness plays a critical role in obtaining time-averaged quantities, accurate simulations will be elusive without modeling the unsteadiness and 2) wind-tunnel simulations specifically conducted for CFD validation are the recommended source of data for CFD validation.

Lessons learned from validation activities include the following: 1) The nonlinear parabolized stability equations and the direct numerical simulations approach provide simulations that agree quantitatively with wind-tunnel data, provided the environment and operating conditions can be modeled and input correctly; 2) benchmark studies are unreliable; they need to be augmented with numerical experiments and design calibrations; and 3) procedures for using CFD simulations for test facility corrections are well developed, but validation efforts are ad hoc. The unreliability of benchmark studies confirms Paul Rubbert's conclusion stated earlier.

Progress is made in verification of simulation models. Considerable effort is needed for assessing the validity of simulated reality. The issue of making this assessment in the absence of relevant wind-tunnel or flight-test data is critical; it is receiving little attention. The present author believes that all of those interested in credible simulated realities do prefer a process of continuous improvement.

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