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Guide to Credible Computer Simulations of Fluid Flows

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The significance of computer simulations depends solely on their credibility. A user of computer products, simulations and software, expects that these products are credible for the intended use. Because no standards exist for fluid-flow simulations by which to establish this credibility, a guide is presented here. The credibility is established by conducting verification and validation of simulation models and certification of simulations and of simulation software. Verification assesses whether the problem is solved correctly and estimates the level of computational accuracy of simulations; validation determines whether the right problem is solved and assesses the level of the validity of the simulation model by estimating the degree to which simulations accurately represent reality. These processes are achieved by identifying the intended uses of the simulations and the sources of uncertainties in them and by conducting sensitivity-uncertainty analyses. Certification determines 1) whether a software in terms of its logic, conceptual and computational models, procedures, rules, and documentation and 2) whether the simulations derived from the software are in compliance with specified requirements.

Introduction

SIMULATION of reality on a computer is done to design, operate, or investigate existing or proposed processes (or systems) and to determine their performance under various conditions. Simulations are conducted when these processes do not exist or cannot be used for experimentation or when explicit analytical solutions are not available. Simulation results are used in problem solving and to aid in decision making. The practitioners and users of simulation results, the decision makers arriving at decisions based on these results, and those affected by these decisions are all justly concerned with whether the results are credible or whether the level of credibility of the results is acceptable for the purposes for which they are being used. Credibility assessment is a key part of any simulation activity; it is a difficult subject about which there is a wide range of opinions. No consistent approach is being used for assessing systematically and uniformly the credibility of fluid-flow simulations. To address this situation, concepts, terminology, framework, principles, and guidelines are presented.

A need for guidelines may be illustrated by the fact that the U.S. General Accounting Office reported, concerning the multibillion dollar simulation business in the Department of Defense (DoD), that "while DoD officials agree that credibility is important, DoD generally has not in fact established the credibility of its simulations systematically and uniformly."[1] Observe that the emphasis is on simulations, not on simulation codes.

A few archival journals have formulated editorial policies on the control of numerical accuracy in fluid-flow simulations for publications in these journals.[2–6] However, the numerical accuracy is not the same as the simulated–reality accuracy. When simulations are used for making reality-related (rather than numerical-methods) decisions, the simulated–reality uncertainty is the issue. Furthermore, there are also uses, other than publication, of these simulations. A guide is presented herein to control the simulated–reality uncertainty for all uses of simulations.

The editorial policies presented in Refs. 3, 5, and 6 principally deal with archival publications. These policies provide some guidance for conducting verification and limited guidance for carrying out validation. Unlike the policies stated in Refs. 5 and 6, the policy articulated in Ref. 3 for verification requires that numerical methods must be at least second-order accurate in space, except when methods are based on switching or blending strategies between first- and second-order methods. This criterion is unnecessary, because another criterion requires that the effect of inherent artificial diffusion be assessed and minimized. Comparisons of simulations with test data for validation are accepted, provided experimental uncertainty is established. However, reasonable agreement with test data is not, in general, sufficient justification for acceptance of simulations, when adjustable simulation-parameters are involved. These policies provide limited guidance for assessing the credibility of simulations under such conditions.

The policy of the AIAA for archival publications deals with verification. This policy does not address the issue of validation, because of the following statement. "The appropriateness of the governing equations for modeling the physical phenomena and [of] comparison with experimental data is not part of this evaluation."[4]

An assessment of computational [the word computational is used instead of the word numerical to be consistent with the use of computational in the phrase computational fluid dynamics (CFD)] accuracy is a necessary, but a halfway measure, for establishing the accuracy of simulated reality. As the phrase indicates, CFD encompasses two disciplines, computational analysis (i.e., numerical analysis) and fluid dynamics. Together, these disciplines are used to simulate the real fluid dynamics through modeling. Such simulations are acceptable if they accurately reproduce the reality. However, this can almost never be done because either the computational methods or the fluid dynamics modeling, or both, contain errors that affect the computed results. Computation errors and modeling errors may be viewed, respectively, as precision and bias errors, analogous to precision errors and bias errors in measurements. The reason for the existence of errors in simulations is obvious: simulation attempts to describe reality, but by definition simulation is not reality.

Experimental data lack credibility unless their uncertainties are known. Likewise, a simulation lacks credibility unless its

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uncertainty is known. Note that standards are available for quantifying measurement errors and assessing wind-tunnel data uncertainties.[7–11] As first recommended in Ref. 12, a credibility–assessment standard is needed for all uses of fluid-flow simulations.

In the sections that follow, a guide is developed for establishing the credibility of simulations. The concepts and terminology used in this guide are presented, a process of conducting the sensitivity–uncertainty analysis is outlined, principles for developing and assessing simulation models are suggested, and guidelines for conducting verification, validation, and certification are recommended. The guide presented here provides a foundation for practitioners and developers of simulation tools and for users of simulations. Most of this guide is equally appropriate for establishing the credibility of other computational physical–chemical sciences simulations, such as computational structural dynamics (CSD) simulations.

Concepts and Terminology

Science may be viewed as a hypothetical–deductive activity (Fig. 1). Empirical observations are put together into a model. If observations can be simulated by this model, then the model is confirmed. It is possible that more than one model can simulate a given set of observations and that future observations might call the model into question, because "[w]hat we observe is not nature itself, but nature exposed to our method of questioning."[13]

The simulation model is the conceptual model manipulated with computational models and a set of computational or logical associations for creating simulations based on these conceptual and computational models (Fig. 2). Both computational models and conceptual models essentially have structures and parameters. All such structures and parameters are modeling inputs to the simulation model. Using these structures and parameters, the set of computational or logical associations simulate, on a computer, raw and processed (derived) quantities for specified flow conditions.

The simulation uncertainty is ubiquitous (Fig. 3). The only certain aspect of the simulation model is that it is uncertain (except possibly when the conceptual model is trivial). It is difficult to evaluate the degree of validity of the simulation model and improve its credibility without knowing the model uncertainty. The analysis of the effect of uncertainties (which is involved in all stages of a simulation), on the simulated reality determines the credibility of the simulation.

Any one of the following terms, calibration, verification, validation, or certification, can be found in the literature relating to CFD in discussions of the accuracy or credibility of CFD simulations, the CFD code, or of CFD. These terms denote processes or acts of calibrating, verifying, validating, or certifying. But they, and the words from which they derive, mean different things to different people.[12,19–21] As done in Ref. 12 for interpreting the word certify, the definitions of these words are used considering their meaning as provided in *Webster's Third New International Dictionary of the English Language Unabridged*.[22] Also consideration is given to the usage of words verification and validation in operations research and in nuclear engineering.

The term calibration is "the act or process of calibrating"[22] or the act of tuning a computational or fluid dynamics model, that is, a simulation model, somewhat without scientific justification. A confirmation of reality with a calibrated model may be fortuitous, when it is used for simulations under conditions different from those present during calibration. Calibration is not the process of determining the level of accuracy or credibility, but is the process of obtaining correction factors.

In this guide, verification and validation are used to connote the processes for establishing the credibility of simulations.[23] This choice is made because there are two aspects of credibility assessment: 1) computational accuracy and 2) fluid-dynamics accuracy, and these two aspects are assessed by two

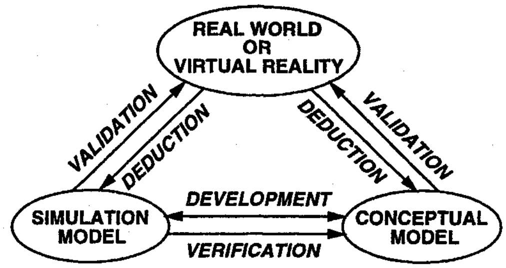

Fig. 1 Simulation paradigm (cf. Refs. 14 and 15). Whether a majority of the critical, quality measurements for describing the real world, in terms of confirming simulated quantities and features that are of interest, is available or not, the simulation is either of real world or of virtual reality, respectively.

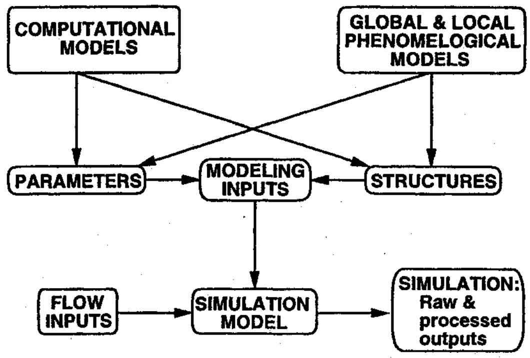

Fig. 2 Simulation model characteristics.

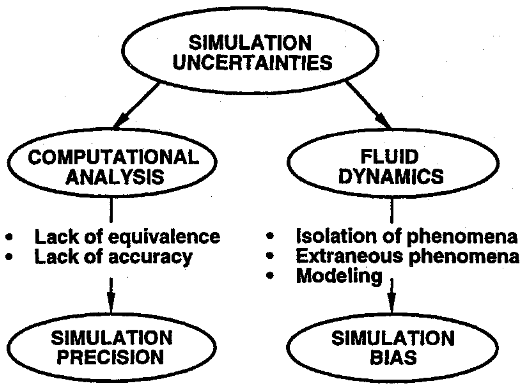

Fig. 3 Sources of uncertainties in simulations.[16–18]

different processes. Validation assesses whether right things are done and verification assesses whether they are done right. Validation and verification deal with the semantics and the syntax, respectively, of the simulation model. Verification and validation activities are done to assess the credibility of the computational model and the simulation model, respectively (Fig. 1). Verification and validation are used solely to determine the degree of veracity and the level of validity, respectively. In an open system, the veracity or validity of the model cannot be declared, even though a high degree of veracity or validity may have been achieved.[24]

Verification is defined as the process of assessing the credibility of a computational model by determining whether the conceptual model is solved correctly and by estimating the level of computational accuracy from the perspective of the intended uses of the simulations.

Validation is defined as the process of assessing the credibility of the simulation model, within its domain of applicability, by determining whether the right simulation model is developed and by estimating the degree to which this model is an accurate representation of reality from the perspective of its intended uses.

Emphasis is purposely placed on computational models and on simulation models rather than on codes or on conceptual models. Modeling, rather than coding, is significant for simulation of reality. Further, codes by themselves are useless, unless they have been verified and validated as defined in software engineering related to coding and unless procedures for correctly utilizing them are available. Conceptual models indirectly go through validation (Fig. 1). Validation establishes the credibility of the simulation model, whereas verification establishes the credibility of the computational model. Only if the credibility of the computational model is very high, can the level of credibility of the conceptual model be essentially the same as that of the simulation model. When this if-condition is not achieved through verification (which is often the case), then the credibility of the simulation model (determined through validation) is the only thing that matters. The credibility of the simulation model is established in terms of the degree of agreement between the simulation and (measured) reality or virtual (assumed) reality. If the computational model has gone through verification, but if the simulation model has not gone through validation, then the corresponding code is primarily acceptable for further study of the computational model, but not for simulating reality or virtual reality.

Accredit means "to give official authorization to or approval of" or "to vouch for officially: recognize or clear officially as bona fide, approved, or in conformity with a standard."[22] Certify means "to inform with certainty," "to guarantee," "to designate as having met the requirements ..." or "to attest especially authoritatively or formally."[22] A developer of a software cannot accredit, but he can certify that it is acceptable for a specific purpose. In operations research, accreditation is an official determination that a simulation model or software is acceptable for a specific purpose (cf. Ref. 25). In the context of the credibility of CFD simulations, certification is viewed as a process that combines verification and validation related to the computational and fluid dynamics accuracy, respectively,[12,23] and also deals with the credibility of software.

Certification is defined as the process of evaluating software in terms of its logic, conceptual and computational models, procedures, rules, and documentation, and in terms of the simulations derived from it to ensure compliance with specific requirements from the perspective of the intended uses of the software (cf. Ref. 12).

Certification assesses whether the right things are done and whether they are done right. Note that certification is concerned with CFD software rather than only that of a CFD code. The same code or simulation model may result in a more or less credible simulation depending on how it is used.

Software is defined as an intellectual creation comprising the programs, procedures, rules, and any associated documentation pertaining to the operation of a computer system and fulfilling specific needs of a user (adapted from Ref. 26). This is a definition of an application software, for example, a CFD simulation software, which is different from system software and support software. In software engineering, code is defined as computer instructions and data definitions expressed in a programming language or in a form output by an assembler, compiler, or other translator.[27]

The credibility of a simulation is determined in the context of specified requirements. The use of a simulation identifies which errors should be tracked and quantified, and it also determines the credible level of accuracy, that is, the acceptable level of accuracy. For example, a simulation may be credible for one use but not for another, even though the simulation accuracy is the same.

In general, simulations are deemed to be satisfactory in terms of their intended purposes if 1) the significant, simulated, and derived (inferred) quantities or important fluid-dynamics features or both are accurate to the level required; 2) the level of modeling complexity is appropriate; and 3) the cost of generating simulations as measured by man-hours, calendar time, user skills, computer resources, simulation, and modeling complexity, etc., is affordable.

It may appear that item 2 is a part of item 1. These items can be independent, however, because different levels of complexity may give the same level of accuracy, because the increase in the level of complexity does not necessarily increase the level of accuracy, or because the intended use determines the level of complexity. The latter is illustrated by the fact that the modeling complexity increases as the design of a fluid-dynamics system progresses from the conceptual-design stage to the preliminary-design stage to the final-design stage. For each level of complexity there is an acceptable level of accuracy for the intended use of simulations. In item 3, the schedule is included as a part of the cost, because time is money.

Two examples of acceptable levels of accuracy for the intended uses of simulations are presented. First, the understanding of turbulence phenomena for developing turbulence models mandates the almost complete elimination of computational uncertainties, or that there be only a negligible contribution of computational errors relative to the effects resulting from the turbulence model, in simulating the reality. The latter requirement necessitates the separation of computational uncertainties from fluid-dynamics uncertainties. If computational errors are not distinguished from fluid-dynamics errors, it is impossible to evaluate and compare different turbulence models and to assess whether the developed model confirms the reality.

Second, the quantification of increments is the most common use of simulations in engineering. Tests and simulations are used to define incremental effects or correction factors to a well-defined baseline.[28] This approach provides increments that account for the various modeling shortcomings. For example, the difference between the design expectation and actual performance of a fluid-dynamics system, say an airplane, is a measure of the variation or error inherent within the design process. Once this error has been determined, the same design simulation tools are used in the same manner to estimate the actual performance of other similar systems operating in the same environment; this is done by adding this error to the simulated performance value.

Verification and validation require the quantification of simulation accuracy, and the only measure of accuracy is error. Except when exact analytical solutions of conceptual models are available, computational errors cannot be determined. Simulation errors can only be estimated. Uncertainty is defined as the estimate of an error. The principal tool for determining uncertainty is sensitivity–uncertainty analysis. Sensitivity analysis is generally defined as a procedure for determining the sensitivities of output quantities to input values. This analysis provides the relative significance of different errors. Uncertainty analysis is generally defined as the analysis of the effect of the uncertainties involved in all stages of a process on the final responses. Uncertainty analysis is conducted by identifying the use of simulations, the sources of errors in modeling inputs (structures and parameters), and the sensitivity of the simulation output to these inputs, by propagating input uncertainties through the simulation process to obtain the resultant uncertainty in the outputs, and by comparing simulations with observed or assumed reality.

Principles for Developing and Assessing Models

The following are principles (with some explanations enclosed between parentheses) for developing simulation models:

1) The purpose of simulations and the success metrics for achieving this goal are defined. (For example, the purpose may be the use of simulations in developing turbulence models for a specific class of applications and for a specified range of flow conditions, whereas the statement of criteria may require a specified level of uncertainty in the simulations in order to fulfill this purpose.)

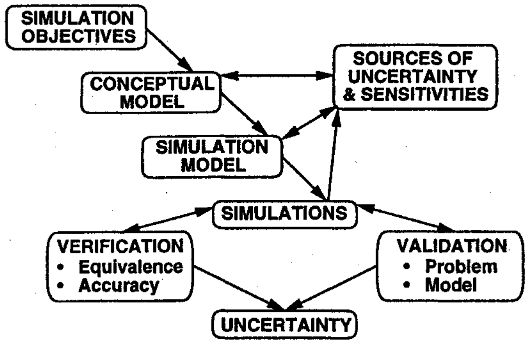

Fig. 4 Credibility assessment flowchart.

2) First, the conceptual model is properly formulated and then the simulation model is appropriately formulated. (The latter condition requires that the simulation model represents phenomena equivalent to those represented by the conceptual model. For example, computational models should not create spurious simulations.)

3) Computational models are selected such that they preserve relevant invariances.

4) The combination of explicit or built-in artificial–phenomenological models (e.g., artificial–viscosity models) and the discretization system are chosen such that there is a negligible effect of these models (e.g., on boundary-layer simulations and on simulations of significant waves traveling at different speeds). (What is considered as being negligible is defined by the success metrics.)

5) The various sources of relevant uncertainties are identified and their sensitivities are determined for choosing the appropriate simulation model. (The selection of this model is an iterative process, as shown in Fig. 4.)

The following are axioms for assessing the credibility of a simulation model:

1) The credibility of a simulation model is judged with respect to its intended use and to those measures of performance that will be used for decision making.

2) A simulation model is declared as being credible only for the conditions for which it is found to be credible.

3) The establishment of the credibility of submodels does not necessarily establish the credibility of the complete simulation model.

4) A credible simulation model does not guarantee credible simulations.

5) The outcome of a validation study is meaningless without some indication of the effects of the computational model.

6) A faulty model may appear to be correct when two or more errors cancel each other out or when the effect of the fault is insignificant.

7) A simulation result that is common to most simulation models is not necessarily the most reliable.

8) A comparison of the results of different, unverified simulation models solving the same conceptual model and the same fluid-dynamics problem does not establish confidence in any one of these models.

9) When derived quantities from one source are compared with the corresponding quantities from another source, preferably the same or essentially the same procedures should be used for determining both sets of derived quantities.

Principle 7 is based on the observation that models may use similar but possibly erroneous representations of the phenomena. Principle 8 is explained as follows.[17] All software may produce similar or different results, and similar results may all be erroneous. On the other hand, it is not at all obvious from such comparisons which one of these sets of results is the correct one. Without knowing the simulation uncertainties and their sources, it is not possible to identify the best among the sets of results.

Sensitivity–Uncertainty Analysis

Sensitivity–uncertainty methods are being extensively applied in various fields, such as experimental fluid dynamics, nuclear engineering, structural engineering, the environmental sciences, and in the design of aerospace systems. References 7–11 and 29–33 provide some examples. Sensitivity–uncertainty analysis is also appropriate for establishing the credibility of aerospace CFD simulation models. The credibility of the simulation model is established by conducting verification and validation of this model from the perspective of the intended uses of the simulations. Verification is conducted by using sensitivity analysis, and uncertainties in simulations are determined based on the results of this analysis. Uncertainties are also determined when verification is done with approximate analytical solutions and when validation is done using the real-world data. When virtual reality is simulated, validation is usually carried out by means of a sensitivity–uncertainty analysis (Figs. 1 and 5). Sensitivities and uncertainties are obtained either to investigate the final result and the simulation model or to investigate some intermediate result and submodel.

Sensitivity analysis is also known as what-if analysis and as perturbation analysis. Sensitivity analysis is a necessary step in the uncertainty analysis. The results of sensitivity analysis highlight which measurands (the measured quantities) and quantities derived from these measurands in tests and which simulated (raw and derived) quantities in simulations need to be determined accurately, and which quantities do not require such precision. This analysis also provides guidance with respect to identifying the important contributors to performance and the specification of fluid-dynamics systems. Sensitivity analysis is used to know how a model will behave if one or more of the model inputs are varied, and the information gained in this way can be used for further model development or for obtaining more accurate simulations.

Sensitivity analysis begins by identifying simulated (output) quantities. The sensitivity of each of these outputs to each of the modeling inputs is studied by varying each input (Fig. 2). Both structures and parameters related to computational models and global and local fluid-dynamics models may be changed. The objective is to seek modeling inputs that lead to simulations that are acceptable for their intended use. For example, the acceptability criteria are that simulations be essentially independent of discretization and of computational processes and that they essentially mimic the real world or virtual reality. Examples of modeling inputs (structures and parameters) that may be varied include the following: discretization methods used for discretizing the conceptual model; inherent or explicit artificial viscosity sources; discretization systems in terms of type, quality, and quantity; time-asymptotic state criterion; turbulence models; and transition models; and fluid-dynamics equations (thin-layer, slender-layer, or full Navier–Stokes equations). Sensitivity studies usually consider extreme values of the model parameters.

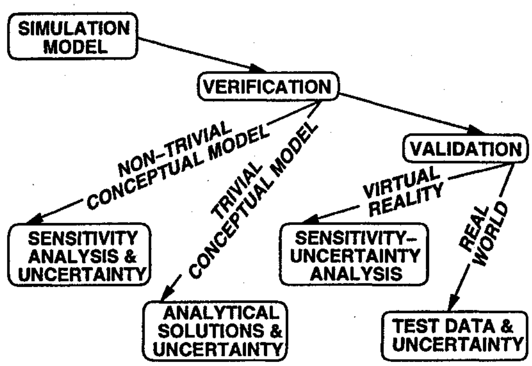

Fig. 5 Principal approaches to verifying and validating simulation models.

Reference 34 provides an illustration of a sensitivity study and of a procedure for determining uncertainty. Thin-layer, Navier–Stokes simulations are obtained for the hypersonic, laminar flow over a spherical nosetip. Simulation errors caused by artificial viscosity are evaluated by changing the coefficient of the explicit dissipation term. Simulations on three different grids are determined and Richardson extrapolation[35] is used to estimate the exact solution. Using this estimated solution, uncertainties in simulations with different grids are obtained. Surface pressure, surface heat flux, and density across the shock layer are the selected quantities of interest. Grid-refinement studies lead to the following conclusions. First, although a second-order spatial–discretization scheme is used, the simulations have second-order convergence behavior on the finest grid used, but this is not always true on the intermediate grid. Second, the heat-flux simulations require a finer grid than the surface-pressure simulations for the same level of uncertainty resulting from the explicit artificial viscosity. And third, simulations are not grid independent. The simulation model is not verified. The degree of veracity is established by obtaining uncertainties in quantities of interest during verification of the computational model.

One way of determining the sensitivity of an output to each of the input parameters is by computing the influence coefficient of each parameter, while neglecting the influence of the other inputs. These coefficients are obtained by perturbing the input parameters and obtaining the responses in the output quantities. For example, sensitivity derivatives may be obtained of the wing lift, drag, and pitching moment coefficients with respect to the second- and fourth-order artificial viscosity terms and to turbulence modeling parameters.[36]

Sensitivity information may be used in selecting the size of adaptive steps. An example is provided in Ref. 37. Stable and unstable freely propagating premixed laminar flames are studied with one-dimensional mixed initial-boundary-value formulation of the conceptual model with the *Le*, the nondimensional activation energy term, and the nondimensional heat-release term as input model parameters. Adaptive gridding and variable time-stepping are done, based on both the solution and first-order sensitivity coefficients. The effect of variations in these parameters on the temperature and species profiles and on the velocity of propagation are illustrated.

Sensitivity studies do not usually incorporate the error range or uncertainty of the input; this distinguishes sensitivity analysis from uncertainty analysis since in the latter, input uncertainties are incorporated. The effect of the uncertainties involved in all stages of a process are propagated to the final results. The process may be a wind-tunnel test or a computer simulation, with the responses being test data or simulated results, respectively.

Uncertainty can be evaluated subjectively (qualitatively or psychologically) or objectively (quantitatively or logically). The Delphi technique of sampling experts is a subjective evaluation of uncertainty. This evaluation determines a degree of belief that events or effects will occur. A qualitative evaluation of uncertainty may be meaningful only after there is an experience of quantitative evaluations under similar conditions. A quantitative assessment logically utilizes available evidence to quantify uncertainty.

Simulation modeling uncertainty is taken to refer to variability in a simulation arising from the choice of model or submodel structures or the choice of model or submodel parameters (Fig. 2). Typically, an assessment is made of the variability in a simulation resulting from variation in structures and parameters of a simulation model. At times, an assessment is done of the variability in simulations owing to the use of several simulation models. The method for assessing output uncertainty is much more developed for parameter uncertainty than for structural uncertainty.[38]

In simulations, identical values of the output are always produced when the same values of the modeling inputs are used; this is because of the deterministic nature of simulation. If inputs are random variables, then the output is a random variable. In this case the output can be studied with statistical techniques, just as experimental data are, for the purpose of determining the sensitivity of the output to the inputs, quantifying the uncertainty of the output, and gaining understanding of the simulation model. Reference 39 presents a procedure, based on the Latin hypercube sampling technique, for conducting the statistical uncertainty analysis. Inputs are treated as random variables with (classic or Bayesian) probability distributions, principally under the following circumstances. First, inputs are based on measurands and quantities derived from them, which have associated measurement uncertainties. Imprecise knowledge of the true values is taken into account through probability distributions. Second, most likely values of inputs are used, when their exact values are not known. Again, probability distributions can be used. For example, the values of constants used in two-equation, eddy–viscosity-type turbulence models are the most likely values.

After a simulation model has gone through verification, establishing a high level of veracity, routine simulations may be done with slightly different modeling inputs to reduce simulation cost. For example, instead of using N finite volumes, $0.9N$ finite volumes may be used. The uncertainty in simulation with the latter number of finite volumes is the difference between exact analytical solutions or estimated exact simulations or simulations with N finite volumes and $0.9N$ finite volumes.

If a conceptual model can be formulated in a few different ways by using different sets of dependent and independent variables, the choice among these different models for simulations may be made by conducting an uncertainty analysis and determining which model form introduces the least uncertainty in the simulations. An example of this is given in Ref. 40, wherein one out of five forms of the conceptual model, governing inviscid–transonic flows in convergent–divergent nozzles, is chosen using this analysis.

Verification

Assuming that there are no mistakes in transforming the conceptual model into the simulation model (including no mistakes in coding), verification, as defined previously, assesses whether the computational model solves the conceptual model correctly and determines the level of computational accuracy by estimating the uncertainty owing to a lack of equivalence and errors introduced by computational analysis (Fig. 5). The burden of evidence lies with the presenter of the simulations.

The following are recommended verification guidelines (with some explanations enclosed between parentheses) for simulation models exhibiting nonchaotic simulations:

1) Global features or characteristics should be independent of discretization and solution processes.

2) The contribution of artificial–phenomenological models is quantified and minimized. (The contribution of artificial–viscosity terms is assessed in boundary layers either by computing the ratio of these terms to those terms with laminar viscosity or by computing the ratio of the convective terms to viscous terms with laminar viscosity. Likewise, contributions of artificial conductivity terms and artificial species-diffusion terms need to be addressed, when appropriate.)

3) In one- and two-dimensional, steady or unsteady simulations, and in three-dimensional simulations, with one of the spatial directions being a marching direction, local features or characteristics of interest should be nearly independent of discretization and of solution processes. (This recommendation includes the requirement that in unsteady flows the phase errors are negligible.)

4) When simulations are conducted for developing phenomenological models, the contribution of the computational uncertainty should be preferably an order of magnitude smaller than the contribution of the phenomena being modeled.

5) When none of the space directions is a marching direction in three-dimensional problems and modeling of phenomena is not the purpose of the simulation, the sensitivity of the relevant simulated and derived results to discretization in each spatial direction is provided. (Localized simulations, that is, simulations in subdomains, may be shown to be nearly independent of discretization. This guideline is for addressing the limitation of computing power.)

6) When the sensitivity of simulations to discretization is determined, the actual order of discretization should be determined.

7) Global features or characteristics should be consistent with local features or characteristics, when multizonal simulation models are used.

8) The invariance uncertainty is determined (e.g., in global conservation of mass, momentum, energy, and, when appropriate, species).

9) The solution-adaptive discretization should recover proper known length and time scales.

10) Convergence and rate of convergence to steady state should be determined to demonstrate that the convergence uncertainty meets the success criteria.

11) Steady and time–asymptotic simulations should be essentially independent of the computational modeling of the conceptual initial conditions and of the conceptual boundary conditions.

12) Sensitivities of simulations to modeling inputs that are not addressed by the previous recommendations should be reported, if they are crucial for fulfilling the success metrics.

13) Verification of the simulation model is done for at least two values of each flow–input parameter, for its extreme values, and possibly for a third value, the nominal value, to establish the model's credibility over a range of flow conditions.

Guideline 8 is explained as follows. Computational models need to be inherently conservative for discretizing conservation laws. The imbalance in volume-integrated partial differential equations (PDEs) for primary or derived physical quantities of interest can be used as a measure of uncertainty. The simulated quantities may be mass, momentum, and energy. The derived quantities may be angular momentum and kinetic energy. Computational methods that are used for primary quantities must be used to determine whether the volume-integrated PDEs for derived quantities are in balance. The uncertainty caused by imbalance can be computed for finite difference, finite volume, or finite element methods over the full computational domain or over any subdomain. When this balance is computed, contributions of individual terms in the equation are quantified. This information may be used to improve the computational model or the conceptual model. Reference 41 provides an example.

The uncertainty in the simulated or derived–simulated result may be obtained by the use of the Richardson extrapolation.[35] Reference 42 presents a summary of how a generalization of this extrapolation to a pth-order computational model and r value of grid ratio can be used for estimating the exact values based on simulations done with two different size discretization systems. The estimated exact values should be determined only on the basis of the simulated–discretization order. If the simulated–discretization order is significantly different from the theoretical–discretization order, this extrapolation procedure should not be used. When this condition occurs, either the discretization is poor or the appropriateness of the conceptual model may be questionable or both. Reference 42 also discusses the limitations of this extrapolation procedure and its use, for example, in non-Cartesian, boundary-fitted, unstructured, or adaptive discretizations.

Validation

Validation, as defined previously, assesses whether the right simulation model is solved and the degree to which this model is an accurate representation of the real world or virtual reality, by estimating the uncertainties resulting from isolation of phenomena, extraneous phenomena, and the fluid-dynamics modeling.

Methods

The problem of validating a simulation model has been likened to the general problem of validating scientific theories. In the philosophy of science, the historical methods of validating theories are rationalism, empiricism, and positive economics.[43] Rationalism involves the logical development of the model based on indisputable axioms. For instance, most of CFD simulation models use some form or subform of the Navier–Stokes equations. Empiricism requires that every axiom, deduction, assumption, or outcome be empirically confirmed. For example, CFD simulation models are generally confirmed with test data. Positive economics is concerned with the model's predictive capability and not its structure, assumptions, or derivation. An example is the calibration of a model to predict certain features and quantities. When rationalism and empiricism are not feasible, the principal validation method for CFD simulation models is the sensitivity–uncertainty analysis (Fig. 6).

Simulations are checked against analytical results, test data, or other simulations that are believed to conform with reality. Simulations are inspected for consistency and for believability, and the range of applicability of the simulation model is demonstrated. Validation may lead to qualitative validity or validity of trends or to a degree of quantitative validity.

Empiricism

Since CFD simulates fluid-dynamics reality through modeling, the obvious uncertainty–analysis method consists of comparisons between simulated results and test data. The simulation-test approach by itself is of limited utility, primarily because of the following.

1) It is not always possible to measure all necessary quantities and measure them as often as required for a proper uncertainty analysis.

2) Sometimes it is not possible to carry out the relevant tests, introducing fluid-dynamics uncertainties.

3) This approach does not account for uncertainties in computation; these uncertainties need to be identified when computed results are compared with measurements. (Almost invariably, an excellent comparison between simulations and measurements is used to justify the validity of the simulation model and, in turn, of the computational model, without demonstrating, for example, the effect of grid refinement or of modeling parameters on the simulated results.)

4) This approach provides some, but not a sufficient, guidance for obtaining simulated results with the same uncertainties or accuracy at conditions other than those considered, but with the same fluid dynamics.

5) Unless experimental uncertainties are known, uncertainties of simulated results cannot be determined with test data.

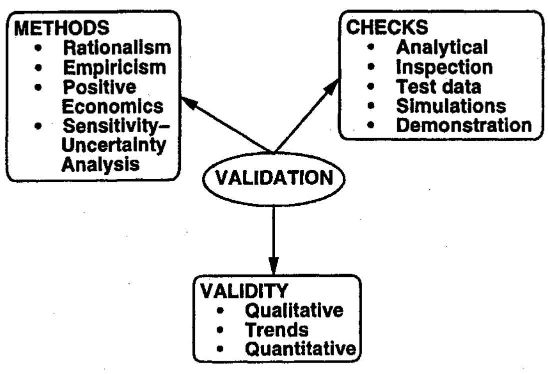

Fig. 6 Validation methods, checks, and types of validity.

Uncertainties are also inherent in experimental fluid dynamics (EFD). That is, both fluid dynamics and measurements contain uncertainties (Fig. 7). The fluid-dynamics uncertainties arise when testing is done under conditions other than the operating conditions of the fluid-dynamics system. Two sources of uncertainties related to fluid dynamics are phenomena of isolation and extraneous phenomena. For example, the ground-based facilities may manifest phenomena other than or in addition to those likely to occur in flight. In the case of measurements, ground-based or flight, there are interference uncertainties and data uncertainties (Fig. 8). Moreover, the insufficiency of data also introduces uncertainties. For example, the sources of uncertainties in aerodynamic reference condition in wind-tunnel tests are shown in Fig. 9. When this condition is used with other inputs to estimate the flight performance, additional sources of uncertainties arise.

When the test data approach is used, the uncertainties in the simulations are the differences between the measurements and the simulations. This definition assumes that the simulation model has gone through verification resulting in negligible computational uncertainties and that the test data are accurate.

Test Guidelines

The following are guidelines for tests that are conducted specifically to establish the level of validity of a simulation model[23]:

1) A statement of criteria for successful tests and for successful simulations is formulated.

2) Representative simulations of how the test article is going to perform to help design the test are performed, before the test article is fabricated.

3) The sensitivities of critical measurands and derived quantities to test parameters, test instruments, etc., are determined and various sources of experimental uncertainties are identified.

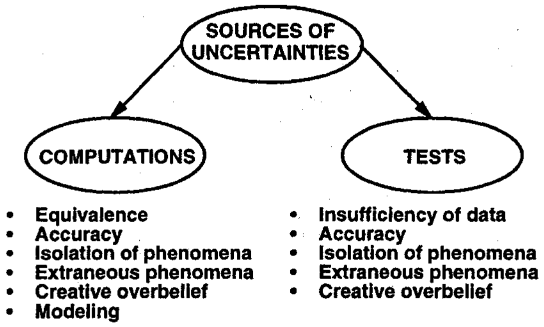

Fig. 7 CFD and experimental fluid dynamics have several sources of uncertainties in common.[17]

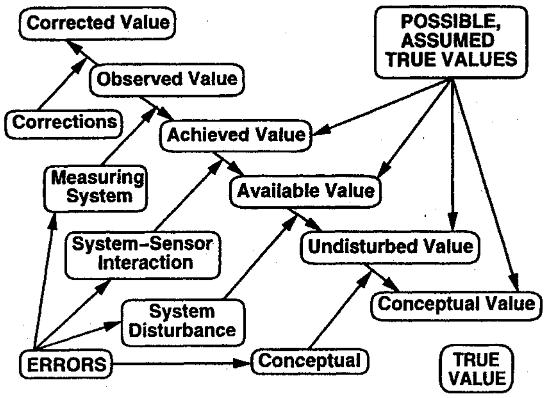

Fig. 8 Observed value and true value in tests. The bias component of measurement error is difficult to accurately determine because the true value of the measurement is not so easy to identify.[44]

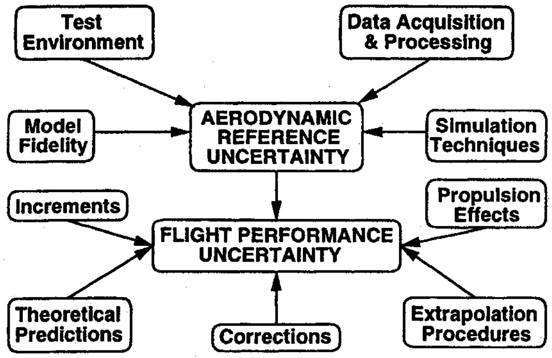

Fig. 9 Contributions to aerodynamic reference condition uncertainty and to flight performance uncertainty (adapted from Ref. 10).

4) A relevant and sufficient quantity of qualitative and quantitative data are taken.

5) A provision is made for having a redundancy of data to cross-check and to verify consistency.

6) Relevant quantities at boundaries are measured to facilitate simulations.

7) Performance quantities are obtained when design-like articles are tested.

8) The experimental uncertainties in measurands and derived quantities are determined, using the latest uncertainty assessment guide. (At present, one of the following guides is recommended, Refs. 9–11.)

9) An independent evaluation of the data is done.

10) Some tests are repeated in the same facility and in two other test facilities.

11) Documentation of all test-related activities is prepared.

Validation Guidelines

First, the computational uncertainties are determined with verification; then, the uncertainties or correction factors resulting from the simulation model are obtained with validation. The following are recommended validation guidelines:

1) Simulations are compared with measurements, whose experimental uncertainties are known and their levels are acceptable.

2) Credible simulations with known uncertainties are compared with the simulations to be assessed.

3) If neither measurements nor credible simulations are available for the flows of interest, conceptual model sensitivities and uncertainties are computed by changing this model and its parameters preferably while maintaining negligible computational uncertainties.

4) When the fluid-dynamics uncertainties are hard to determine, then the credibility is established subjectively by submitting the results to a team of independent experts for evaluation.

Note that simulations with established corrections factors in their domain of applicability are credible, provided these simulations are generated with the same simulation models and in the same manner as those simulations that were used for determining the correction factors.

An example of grid refinement and validation is discussed in Ref. 45. The computational uncertainty of simulations is first determined using the Richardson extrapolation, and then validation guideline 1 is used to determine the fluid-dynamics uncertainty.

Certification

Certification as defined herein requires that a software, in terms of its logic, conceptual and computational models, procedures, rules, documentation, and the simulations generated by it are in compliance with specified requirements. The verification and validation of the simulation model addresses the

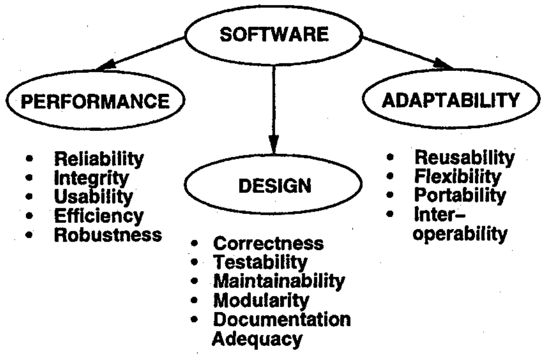

Fig. 10 Software-quality factors.

credibility of simulations, which in turn establishes the credibility of the conceptual and computational models. A determination is made as to whether the success criteria have been achieved or not for the intended use of simulations. If these criteria are met, then only further activities for certifying the software are carried out.

Software is developed for specific applications, whereas the computational and conceptual models are developed for possible wide applications. Software is developed according to the accepted conventions of software engineering, and the development team addresses the software-quality factors listed in Fig. 10. The assessment of these factors and the verification and validation software (as defined in software engineering) may be carried out following the recommendations made in Refs. 26, and 46–49.

The verification and validation of the simulation model cannot be done without conducting verification and validation of the software-quality factors related to the coding in the simulation code. Therefore, at the completion of the verification and validation of the simulation model, most of the requirements for certification of the software are addressed. These processes of establishing credibility also determine the reliability and the limits of applicability of the software. The remaining part of these requirements deals with the rules for use of the simulation model and of the simulation code and the documentation of all relevant aspects, including strengths and weaknesses, to assure or inform with certainty to whom it may concern that the software generates reliable simulations. A satisfactory certification guarantees that the software complies with its specified requirements and is acceptable for operational use.

The documentation is a very important quality factor in providing traceability and in helping qualify the user of the code. All requirements that a code must meet and does meet are identified and documented. These requirements pertain to performance, design, adaptability, utility, sophistication, attributes, credibility, and constraints. All verification and validation activities pertaining to the simulation model and software are also documented.

Concluding Remarks

Verification and validation of the simulation model are critical in establishing the credibility of simulated reality and in certifying simulation software. The only thing that matters in establishing the credibility of simulation is uncertainty, not veracity or validity. The sensitivity–uncertainty analysis is the key to the establishment of this credibility. The software certification is essential for establishing the reliability of software. Assessing the credibility of complex simulation study results and of the software poses a significant challenge. Terminology, concepts, framework, principles, and guidelines were presented for addressing this challenge.

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