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Discussion

Discussion: "Comprehensive Approach to Verification and Validation of CFD Simulations—Part 1: Methodology and Procedures" (Stern, F., Wilson, R. V., Coleman, H. W., and Paterson, E. G., 2001, ASME J. Fluids Eng., 123, pp. 793–802)

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The paper by Stern et al. proposes a comprehensive approach to verification and validation of computational fluid dynamics simulations. Although the authors present a new perspective for quantifying verification and validation, I believe there is a conceptual flaw in the proposed approach to validation. Three criticisms follow.

1 The authors define verification as "... a process for assessing simulation numerical uncertainty ..." I agree with the authors when they say that their definition of verification is not contradictory with the broader definitions developed by Roache [1] and the AIAA Guide [2]. However, as pointed out clearly by Roache and others, there are two other important facets of verification: code verification and software quality assurance. Code verification deals with assessing the correctness of the computer program in implementing the discrete form of the partial differential equations, as well as the numerical algorithms needed to solve the discrete equations. Software quality assurance deals with topics such as code robustness, version control, static and dynamic testing, and documentation. In this paper, the authors only address the issue of solution verification, neglecting to mention these two other topics of equal importance. For a paper claiming to present a comprehensive approach, this is misleading.

2 The authors state that their definition of verification is implemented in Eq. (10), which is

$$S_C = T + \delta_{SM} + \varepsilon_{SN}$$

where S_C is the result from the corrected simulation, T is the "truth," δ_{SM} is the simulation modeling error, and ε_{SN} is the estimated numerical error from the simulation. Although the authors do not clearly state what the "truth" is in this expression, the only interpretation that makes sense, based on their discussion starting with Eq. (1), is that T is the true value resulting from experimental measurement. Discussing verification in terms of experimental measurements and simulation modeling error causes a great deal of confusion when people are trying to understand the fundamental differences between verification and validation. As Roache [1] lucidly puts it, "Verification deals with mathematics, validation deals with physics."

When substituting the definition of δ_{SM} into Eq. (10), one obtains

$$S_C = M + \varepsilon_{SN}$$

where M is defined as the exact, or analytical, solution to the continuum partial differential equations. This equation appears to be consistent with accepted definitions of verification. However, in order to get to Eq. (10), the authors had to define the error in the corrected solution, δ_{S_C}, as

$$\delta_{S_C} = S_C - T$$

That is, the authors had to introduce the true value from experiment in order to get to their equation for verification. This is a confusing and circuitous route to verification.

3 The authors define validation as "... a process for assessing simulation modeling uncertainty ..." which is consistent with broader definitions of validation developed by Roache [1] and the AIAA Guide [2]. The authors claim to implement this definition using their Eq. (17) and the narrative that follows. Their result is

$$|E| < \sqrt{U_D^2 + U_{SPD}^2 + U_{SN}^2}$$

where E is the comparison error, U_D is the uncertainty in an individual experimental measurement, U_{SPD} is the uncertainty in the simulation model due to use of previous data, and U_{SN} is the uncertainty in the numerical error estimate. E is defined as $D - S$, where D is the result obtained from an individual experimental measurement, and S is the result from a numerical simulation.

The authors' implementation of validation does not embody their definition of validation because of the way they define the comparison error E. First, they define the comparison error using an individual experimental measurement D. This is in contrast to using the true experimental value T. As the number of experimental measurement samples increases, the statistical mean converges to the true value, ignoring systematic (bias) error. That is, as more experimental realizations are obtained, the key issue becomes: how does the simulation compare to the mean as opposed to any individual measurement?

Second, they define the comparison error using an individual numerical simulation result S. Since S can have an arbitrary magnitude of numerical error, it is not a reflection of the true value from the model, which is M. Validation should measure how well the true value from the model compares with the experiment, not how well a simulation value polluted by numerical error compares with the experiment.

Because of the way in which they define the comparison error E, the authors' implementation of validation is forced into the following situation. The simulation can be declared validated by increasing the right side of their validation equation. The right side can be increased by: (a) increasing the experimental uncertainty; (b) increasing the uncertainty in data used from previous analyses; or (c) increasing the numerical uncertainty in a given simulation. As pointed out by Roache [3] and Oberkampf and Trucano [4], this makes no sense.

The authors responded to Roache's criticism in a previous Author's Closure [3], as well as in the subject paper, by saying that what is really important is the magnitude of the validation measure required by the application of the code. In my opinion, this is sidestepping the criticism because the criticism is directed at the way the validation measure *itself* is defined, not how it might be used. Resorting to the use of application requirements in defining the validation measure is contrary to the fundamental meaning of validation. This misunderstanding, widespread in the community, presumes that validation means assessing whether the simulation has ''passed'' or ''failed'' an application requirement.

Validation, as defined by the AIAA Guide [2], and earlier by the Defense Modeling and Simulation Office of the Department of Defense [5], is: ''The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.'' Stated differently, validation is *only* a measure of the agreement between simulation and experiment. The magnitude of the measure is not an issue as far as validation is concerned. This may seem contradictory to people who are new to the terminology of verification and validation. Validation is defined in this way for two reasons. First, the required magnitude of the validation measure varies from one application to another. For example, the magnitude of a validation measure that is satisfactory for one application may be a factor of ten or more larger than what is needed for another application. Second, in multi-physics simulations one does not know before hand what level of validation is needed for each component of physics. There is actually an interaction of validation measure requirements, and trade-off between requirements, in order to achieve the accuracy required for the particular system response quantity of interest. That is why application requirements cannot be used to defend a particular implementation of a validation measure.

Acknowledgment

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References

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[4] Oberkampf, W. L., and Trucano, T. G., 2000, ''Validation Methodology in Computational Fluid Dynamics,'' American Institute of Aeronautics and Astronautics, AIAA 2000-2549, Fluids 2000 Conference, Denver, CO.
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Closure to ''Discussion of 'Comprehensive Approach to Verification and Validation of CFD Simulations—Part 1: Methodology and Procedures' '' (2002, ASME J. Fluids Eng., 124, p. 809)

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(1): I do not understand how the word ''simulation'' in the title can be misinterpreted as ''code'' or ''software.''

(2) and (3): I believe the confusion arises from his use of the definition of uncertainty as ''A potential deficiency in any phase of the modeling process that is due to lack of knowledge'' (which does not quantify a range within which truth lies with a specified degree of confidence) as opposed to the concepts and definitions used in current experimental uncertainty analysis [1] (which do quantify such a range).

The ranges $D \pm U_D$ and $S \pm U_S$ both contain (with 95% confidence) the truth T, which is independent of experiment or simulation. The assumption (also made in Oberkampf and Trucano, 2000) that *D* is ''an individual experimental measurement'' is inaccurate. The experimental result is *D*, and U_D *is the uncertainty considering any averaging, any correlated systematic uncertainties, and any correlated random uncertainties* [1].

M is the simulation result with the continuous equations solved exactly ($U_{SN}=0$) with no uncertainty in the inputs ($U_{\mathrm{SPD}}=0$), *but includes the errors due to modeling assumptions*. Thus, the assumption ''the true value from the model, which is *M*'' is inaccurate. Again, the true value T is independent of experiment or simulation.

After enlightening discussions over the last two years (particularly with Patrick Roache), my view has evolved to consider ''a validated simulation'' to mean that a simulation has undergone the validation process and that a level of validation (the larger of $|E|$ and $|U_V|$) has been established. I agree with Oberkampf that ''the magnitude of the measure''—in my words, the level of validation—''is not an issue as far as validation is concerned.'' However, it follows logically that the qualification ''from the perspective of the intended uses of the model'' should not be part of a definition of validation since the level of validation of a simulation variable is independent of the intended use of the model.

Reference

[1] Coleman, H. W., and Steele, W. G., 1999, *Experimentation and Uncertainty Analysis for Engineers*, 2nd Edition, Wiley, New York.

Closure to ''Discussion of 'Comprehensive Approach to Verification and Validation of CFD Simulations—Part 1: Methodology and Procedures' '' (2002, ASME J. Fluids Eng., 124, p. 809)

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In the discussion, the definitions of truth *T*, experimental result *D*, modeled solution *M*, and simulation solution *S* seem to differ from ours. These key variables were defined using a sequence of initial boundary value problems (IBVP) summarized in the paper and derived in [13].

The IBVP for T by definition contains no modeling or numerical errors. Approximate solutions for T are provided by experimental, analytical, and simulation methods. Experimental methods use measurement systems and data acquisition and reduction procedures to provide D with error $\delta_D = D - T$. Analytical and simulation methods reformulate the IBVP for T using approximate models for the partial differential equation operators, initial and/or boundary conditions. Analytical methods solve the IBVP for M and δ_{SM} exactly, and thus are limited to simple fluid mechanics problems. The continuous IBVP for M is reduced to a discreet IBVP for S, which is solved by the CFD computer code, introducing additional numerical errors. The $\delta_{SN} = S - M$ is defined by transforming the discreet IBVP back to a continuous IBVP. As this shows, we believe that D, M, and S inherently have errors, which are estimated using experimental uncertainty analysis and verification and validation (V&V) methodologies and procedures, respectively.

Response to criticism (1)

The focus of our paper is on V&V methodology and procedures for CFD simulations with an already developed CFD code. It is implicitly assumed that code verification and software quality assurance issues have already been addressed during code development.

Response to criticism (2)

T in Eq. (10) has been clearly defined as the truth, which differs from the simulation result S by simulation error δ_S and from the experimental result D by experimental error δ_D. Therefore, we in no way have introduced experimental measurements or simulation modeling error in discussing verification and deriving Eq. (10).

Response to criticism (3)

The experimental result D in Eqs. (13), (14), and (18) has been clearly defined as the experimental result with error δ_D and associated uncertainty U_D. D is not an individual measurement, but based on appropriate averaging. S is the simulation result with simulation error δ_S and associated uncertainty U_S, comprised of the addition and root-sum-square of numerical and modeling errors and uncertainties, as defined by Eqs. (1) and (2), respectively. S is based on iterative and input parameter convergence studies using multiple solutions and systematic parameter refinement. The value used is usually the finest value of input parameter. The numerical and modeling error and uncertainty estimates are not arbitrary. The V&V procedures described in our paper provide quantitative estimates for levels of numerical and modeling errors and uncertainties. We have not used application requirements in defining validation, but rather used our validation definition to assess application requirements. The level of validation is important in that it determines one's ability to discriminate among modeling assumptions/approaches, and to judge if a particular application requirement has been met. We have already addressed issues related to fact that validation uncertainty excludes modeling assumption uncertainty and ''noisy'' data and solutions are easier to validate in our paper and have no further comment.