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QUANTITATIVE V&V OF CFD SIMULATIONS AND CERTIFICATION OF CFD CODES WITH EXAMPLES

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ABSTRACT Definitions and equations are provided for quantitative assessment of numerical (verification) and modeling (validation) errors and uncertainties for CFD simulations and of intervals of certification for CFD codes. Verification, validation, and certification methodology and procedures are described. Examples are presented of quantitative V&V for RANS and DES simulations and certification of RANS codes for ship hydrodynamics applications. Opportunities and challenges for achieving consensus and standard V&V and certification methodology and procedures are discussed.

INTRODUCTION

In spite of the ever-increasing need and importance for standards for computational fluid dynamics (CFD) uncertainty analysis/accuracy estimation, there are currently many viewpoints covering all aspects from basic concepts and definitions to detailed methodology and procedures. A similar situation existed for experimental fluid dynamics (EFD) uncertainty analysis ca. 1960 for which currently standards are widely accepted and available, although widespread use is still lacking.

Pioneering work was done by Roache [1] who proposed the grid convergence index (GCI) for estimating uncertainty due to grid and time step errors based on Richardson extrapolation (RE) using multiple solutions on systematically refined grids; thereby, providing a quantitative metric for verification. Ref. [2] expanded on this work through overall discussion of verification and validation (V&V), including: use of EFD definitions for errors and uncertainties; phrases (e.g., verification deals with equations solved correctly and validation with correct equations and verification deals with mathematics and validation with physics) and activities (e.g., method of manufactured solutions and benchmark solutions for verification and use of experimental data for validation) defining V&V; discussion for V&V of both codes and solutions; many case studies demonstrating use of GCI; single grid error estimation methods; and broader issues such as code quality assurance and certification. Such definitions for V&V, however, in the authors' viewpoint are inadequate. Quantitative metrics are needed for both verification and validation, and methodology is needed for combining errors and uncertainties.

The AIAA Committee on Standards for CFD [3] and Guide for V&V of CFD Simulations [4] uses definitions from information theory for errors and uncertainties with emphasis on measurement of accuracy as opposed to estimation of errors and uncertainties; follows Roache's phrases and expands considerably on his activities along with broad statements in defining V&V; discusses mostly code, but also solution V&V; and additionally discusses policy statements on experimental and numerical accuracy. Code verification activities measure accuracy in relation to benchmark analytical and ordinary and partial differential equation solutions for simplified problems along with software quality assurance: identify, quantify, and reduce errors in the computational model and its numerical solution. Model validation activities measure accuracy in relation to experimental data with emphasis on validation tiers based on unit problems, benchmark cases, subsystem cases, and complete systems: identify and quantify error and uncertainty in the conceptual and computational models, quantify the numerical error in the computational solution, estimate the experimental uncertainty, and compare the computational and experimental results. Solution verification largely follows Roache in using GCI along with consistency and iterative convergence checks. Rigorous implementation is impressive [5, 6]; nonetheless, these definitions are subject to same criticisms mentioned earlier. Another problem with such definitions is lack of an overall mathematical framework for V&V, which is considered essential in the author's viewpoint similarly as it is an essential and integral part of EFD uncertainty analysis.

The literature also includes editorial policy statements [7], additional guidelines [8], and numerous case studies, which mostly focus on verification procedures for 2D problems (e.g., volume 36 of the AIAA Journal and volume 124 of the ASME Journal of Fluids Engineering). In general this literature follows approaches similar to that described above.

The authors and colleagues [9] developed an alternative quantitative approach to solution V&V specifically for already developed CFD codes for industrial applications (geometry and domain; models; initial, boundary and other conditions; fluid properties) and input parameters (such as iteration numbers and grid and time step sizes), which differs considerably from previous approaches. It is assumed that code verification and quality assurance issues have already been dealt with during code development. Similarly, if appropriate, it is assumed that model validation for simplified problems has also already been dealt with during model development. The philosophy is strongly influenced by EFD uncertainty analysis [10], including use of EFD definitions for errors and uncertainties. The methodology is based on concepts, definitions, and equations derived for simulation errors and uncertainties, which provide the overall mathematical framework. Verification procedures for estimating numerical errors and uncertainties include (1) the options of estimating the numerical uncertainty or the numerical error itself, which is used to obtain a corrected solution, and its uncertainty; and (2) the concept of correction factors based on analytical benchmarks. Previously developed validation methodology and procedures for estimating modeling errors and uncertainties [11] were extended to include the option of use of corrected solutions.

The V&V approach [9] has been shown successful in establishing intervals of V&V for RANS simulations for ship hydrodynamics by present authors and colleagues [12-18] and international colleagues through its use at recent Gothenburg 2000 Workshop on CFD in Ship Hydrodynamics [19].

A shortcoming of this and other V&V approaches is that the justification for uncertainty estimates at 95% confidence level is based on reasoning similar to that used for EFD bias uncertainties at the 0-order-replication level without additional statistical 1-order-replication level precision uncertainties, which in combination provides N-order-replication level and increased confidence for EFD uncertainty analysis. Recently, present authors addressed this issue through development of a statistical approach for CFD code certification [20]. As with V&V there are many viewpoints on certification [2]. Certification is defined as a process for assessing probabilistic confidence intervals for CFD codes for specific benchmark applications and certification variables. Presumably, range of applications requires interpolation and extrapolation methods. The approach combines previous V&V approach with extensions of concept of N-version testing [21] for consideration bias uncertainties and use of reference values (experimental data and uncertainties) for estimating interval of certification.

The V&V approach [9] has also undergone criticism; most notably, [22] believes there is a conceptual flaw in the proposed approach to validation based on three criticisms and [23] presents seven criticisms of the correction factor verification method. We disagree with [22], as discussed in [24]. We agree with the first criticism of [23] and as a result have made revisions to the correction factor uncertainty estimates; however, we disagree with the other criticisms, as discussed in [25].

The present paper summarizes and combines the V&V of CFD simulation and certification of CFD code approaches into a single presentation with examples, including presentation and use of the revised correction factor uncertainty estimates. Clarification is provided of some important aspects. Opportunities and challenges for achieving consensus and standard V&V and certification methodology and procedures are discussed.

SIMULATION AND CODE LEVEL ERRORS AND UNCERTAINTIES

The simulation error δ_S is defined as the difference between a simulation result S and the truth T (objective reality) and is assumed composed of additive modeling δ_{SM} and numerical δ_{SN} errors

$$\delta_S = S - T = \delta_{SM} + \delta_{SN} \tag{1}$$

Modeling errors are due to the mathematical physics problem formulation in terms of a continuous initial boundary value problem (IBVP), whereas numerical errors are due to numerical solution of the discrete IBVP. Equation (1) is considered a reasonable first approximation in consideration of the development and execution of CFD codes; however, correlations between modelling and numerical errors are also possible and should be considered in the future. Appendix A of [26] provides a derivation of (1) based on linear operator theory, which clarifies the source and role of modelling and numerical errors and provides additional justification for their being additive. The simulation uncertainty equation follows directly by considering (1) as a data reduction equation, as per EFD uncertainty analysis

$$U_S^2 = U_{SM}^2 + U_{SN}^2 \tag{2}$$

For simulations (unlike experiments except for calibrations), it is possible under certain conditions to estimate the numerical error both in sign and magnitude δ_{SN}^* such that

$$\delta_{SN} = \delta_{SN}^* + \varepsilon_{SN} \tag{3}$$

where ε_{SN} is the error in the estimate. In this case, the simulation value is corrected to provide a numerical benchmark S_C, which is defined as

$$S_C = S - \delta_{SN}^* \tag{4}$$

with corrected simulation error δ_{S_C} and uncertainty U_{S_C} equations

$$\delta_{S_C} = S_C - T = \delta_{SM} + \varepsilon_{SN} \tag{5}$$

$$U_{S_C}^2 = U_{SM}^2 + U_{S_CN}^2 \tag{6}$$

where U_{S_CN} is the uncertainty estimate for ε_{SN}. The concept of deterministic error estimate for simulations seems appropriate and has been advocated by others. Equations (1)-(6) are fundamental to the present V&V of CFD simulation and certification of CFD code approaches and form the basis of the definitions, methodology, and procedures that follow.