NISTIR 8298

A Summary of Industrial Verification, Validation, and Uncertainty Quantification Procedures in Computational Fluid Dynamics

DongHun Yeo

This publication is available free of charge from:
https://doi.org/10.6028/NIST.IR.8298

National Institute of
Standards and Technology
U.S. Department of Commerce

NISTIR 8298

A Summary of Industrial Verification, Validation, and Uncertainty Quantification Procedures in Computational Fluid Dynamics

DongHun Yeo
Materials and Structural Systems Division
Engineering Laboratory

This publication is available free of charge from:
https://doi.org/10.6028/NIST.IR.8298

March 2020

U.S. Department of Commerce
Wilbur L. Ross Jr., Secretary

National Institute of Standards and Technology
Walter Copan, Director and Under Secretary of Commerce for Standards and Technology

National Institute of Standards and Technology Interagency or Internal Report 8298
Natl. Inst. Stand. Technol. Interag. Intern. Rep. 8298, 33 pages (March 2020)

This publication is available free of charge from:
https:/doi.org/10.6028/NIST.IR.8298

ABSTRACT

Within a variety of Computational Fluid Dynamics (CFD) applications, maturity levels can vary significantly depending upon modeling approach and the user's knowledge and skills. Recently, application of CFD techniques for Computational Wind Engineering (CWE) has generated strong interest among wind and structural engineers as a possible substitute for or supplement to wind tunnel experimentation, even though CWE is still in a developmental stage. A necessary step toward advancing CWE simulations in wind and structural engineering applications credible is the development of reliable verification and validation (V&V) procedures.

Fundamental factors that determine the degree to which CWE simulations are the credible include: (i) the quality of the mathematical modeling of the physics of interest; (ii) the depth of understanding by the users/analysts of the details of the model and the simulation results; (iii) the quality of the verification and validation (V&V) procedures applied to the simulation results, and (iv) the quality of the uncertainty quantification procedure applied to those results.

This report deals in detail with the sources of inaccuracy in CFD simulations, and concepts and procedures used in V&V and uncertainty quantification.

ACKNOWLEDGEMENTS

Critical comments by Dr. Emil Simiu and Dr. Tarak N. Nandi of the National Institute of Standards and Technology and Dr. Anikesh Pal of Oak Ridge National Laboratory are acknowledged with thanks.

NOTE.

NIST definitions and terminology in the Verification, Validation, and Uncertainty Quantification fields differ from their counterparts used in current applications to Computational Fluid Dynamics (CFD). Applications of those fields to CFD consistent with NIST practice are currently being developed.

CONTENTS

LIST OF FIGURES

1. INTRODUCTION

The US National Research Council identified five phases of the CFD (Computational Fluid Dynamics) development cycle with a view to evaluating its maturity and potential impact in scientific computing (NRC 1986)

Phase I. Developing and enabling technology: scientific papers, know-how.

Phase II. Demonstration and confidence building: limited pioneering applications, subject to surprise.

Phase III. Putting it all together: major commitment made, graduate evolution of capacity.

Phase IV. Learning to use effectively: changes the engineering process, value exceeds expectations, user groups acquire new skills.

Phase V. Mature capabilities: reliable and cost-effective design applications, most analysis done without supporting experimental comparison

The maturity levels of CFD applications can vary significantly, depending upon the modeling approach and the user's knowledge and skills. In recent years, the application of CFD to wind engineering problems, referred to as Computational Wind Engineering (CWE), has been considered as a potential substitute for or supplement to wind tunnel testing. However, CWE is still in a developmental stage, and its credibility remains to be established. The fundamental elements for achieving the credibility are: (i) quality of physical modeling, (ii) quality of users/analysts performing the simulations and using the results, (iii) verification and validation (V&V) activities, and (iv) uncertainty quantification of the simulation results (Oberkampf and Roy 2010). The quality of computational simulations is highly dependent upon the degree to which the mathematical model for representing the physics of interest is appropriate, and upon the CFD users' depth of understanding of the details in the model and the associated simulation results. Verification and validation are independent procedures that work together as the primary processes for assessing the accuracy of simulation results. Uncertainty quantification is the process that identifies, characterizes, and estimates quantitatively the factors in the analysis affecting the accuracy of simulation results. These are necessary conditions but not sufficient for achieving the credibility of simulations other than those for which verification and validation have been performed.

The following sections deal in some detail with CFD concepts regarding sources of inaccuracy (Section 2), V&V procedures (Section 3), uncertainty quantification (Section 4), and the use of the validation level concept (Section 5).

2. SOURCES OF INACCURACY IN CFD SIMULATIONS

A computational model calculated in a computing machine cannot avoid errors or uncertainties in the simulation results due to a wide range of sources of inaccuracy. At this stage, the difference between the notions of error and uncertainty will be ignored (but revisited in Section 4) and the term error will be used to identify the sources leading to inaccuracy of the CFD results.

The errors in CFD simulation results can be classified into four types (Oberkampf and Roy 2010; Zikanov 2010):

1) Physical modeling errors

2) Errors of discretization

3) Errors of iterative convergence/round off

4) Programming/user errors.

Physical modeling errors

A CFD simulation provides results based on physical modeling that approximates the behavior of the actual physics. The difference between the behavior of the model and real behavior can be defined as:

$$\delta_{\text{model}} = p_{\text{model}} - p_{\text{real}} \tag{1}$$

where δ_{model} is the physical modeling error, and p_{model} and p_{real} are the property of interest (e.g., velocity or pressure) in the model and the real physics, respectively.

The numerical modeling errors could arise from the approximation of complex behavior in the governing equations (e.g., turbulence modeling), effects of computational domain size and boundary conditions, and assumptions on the fluid properties (e.g., constant air density and temperature).

Discretization errors

A CFD simulation does not solve the equations of the physical model analytically, but rather the equations discretized in space and time. This fact introduces the discretization error, δ_{h}, that is, the difference between the exact analytical solution p_{model} of the model PDE (Partial Differential Equation) and the exact solution p_{h} of the discretized equations:

$$\delta_{\text{h}} = p_{\text{h}} - p_{\text{model}}. \tag{2}$$

The discretization error depends on not only the numerical schemes in space and time and the resolution and quality of the grids used in simulations, but also on the behavior of the solution. The error should be estimated whenever a new grid type, a new scheme, or a new application is employed in a simulation. Among the sources associated with numerical errors, the discretization errors are usually the largest and their estimation is the most challenging (Oberkampf and Roy 2010).

Iterative errors

The difference between the exact solution and the computed iterative solution of the discretized equations is called iterative error, δ_{it}:

$$\delta_{\text{it}} = p_{\text{comp}} - p_{\text{h}} \tag{3}$$

where p_{comp} is the computed solution from a computing machine, which may entail round-off errors and iterative convergence errors inherent in iterative methods. The round-off error results from low precision in computer calculations and can be reduced by increasing the number of digits associated with the precision of the numerical solution. In simulations with a stable scheme and no round-off error accumulation, the round-off error is usually very small in comparison to other type errors (e.g., several orders lower than δ_h) (Zikanov 2010).

The iterative convergence error exists in CFD solutions because in iterative methods a linear or a linearized system of discretized equations is typically solved. The iterative errors commonly accepted are at least one order or two of magnitude lower than the discretization errors (Oberkampf and Roy 2010; Zikanov 2010). However, when a flow solver uses an implicit time integration method for unsteady simulations, a loose iterative convergence criterion at each time step may significantly influence the accuracy of the numerical solution (Eça et al. 2017).

Programming/user errors

Programming errors, caused by mistakes or bugs in the software, can be classified into two types (Oberkampf and Roy 2010). The former is a critical error by which the software cannot execute a simulation or generate reasonable results. The latter is related to a less critical, or dormant fault which may not be easily identified by code verification. This hidden error could generate non-negligible, incorrect results., especially if a simulation is beyond the coverage of the code verification process.

Another error is related to blunders or mistakes from users in input preparation for simulation and in post-processing analysis of output data. The human errors cannot be easily detected, especially when simulations of complex systems of large scale are performed.

3. VERIFICATION AND VALIDATION

The objective of verification and validation (V&V) is to establish the credibility of a computational model by assessing the degree of accuracy of the simulation results (Oberkampf and Roy 2010). Since Department of Defense (DoD) developed the first definition of V&V for numerical modeling and simulations (DoD 1994), practicing communities, such as American Institute of Aeronautics and Astronautics (AIAA 1998), American Society of Mechanical Engineers (ASME 2006; 2009) and U.S. Department of Energy (Pilch et al. 2001), have developed their V&V philosophies, definitions, and procedures. The general definitions can be introduced as follows:

Verification: the process of determining that a computational model accurately represents the underlying mathematical model and its solution (ASME 2006)

Validation: 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. (AIAA 1998).

Figure 1 illustrates a comprehensive diagram of the verification and validation (V&V) activities and outcomes, based on a conceptual model of real physics, its mathematical modeling for simulation, its physical modeling for experimentation, and their interaction (ASME 2006). V&V processes start with determining the intended uses of the computational model. The relevant physics should be included in the model and the experiment for validating the model. Once the responses of interest and the associated accuracy requirements for the intended application are determined, the corresponding modeling activities and experimental activities should be planned. In the modeling activities, errors in the code are addressed (*code verification*) and numerical errors associated with solutions of discretized equations of the mathematical model are estimated (*solution verification*). The verified simulation results and relevant experiment data are used for quantifying their uncertainties, and the predictive capacity of the model in the physics of interest is assessed (*model validation*). If the agreement between model predictions and experimental outcomes satisfies the accuracy requirement, the V&V processes end. The success of V&V

can claim that the accuracy of the computational model is adequate for the intended use of the model. Otherwise, the V&V processes are repeated until the agreement is acceptable by updating the model and carrying out additional experiments if necessary. Note that the documentation of the results and the rationale in all the V&V activities is important not only for tracing the justification of the current intended use, but also for providing information/experience for potential future uses.

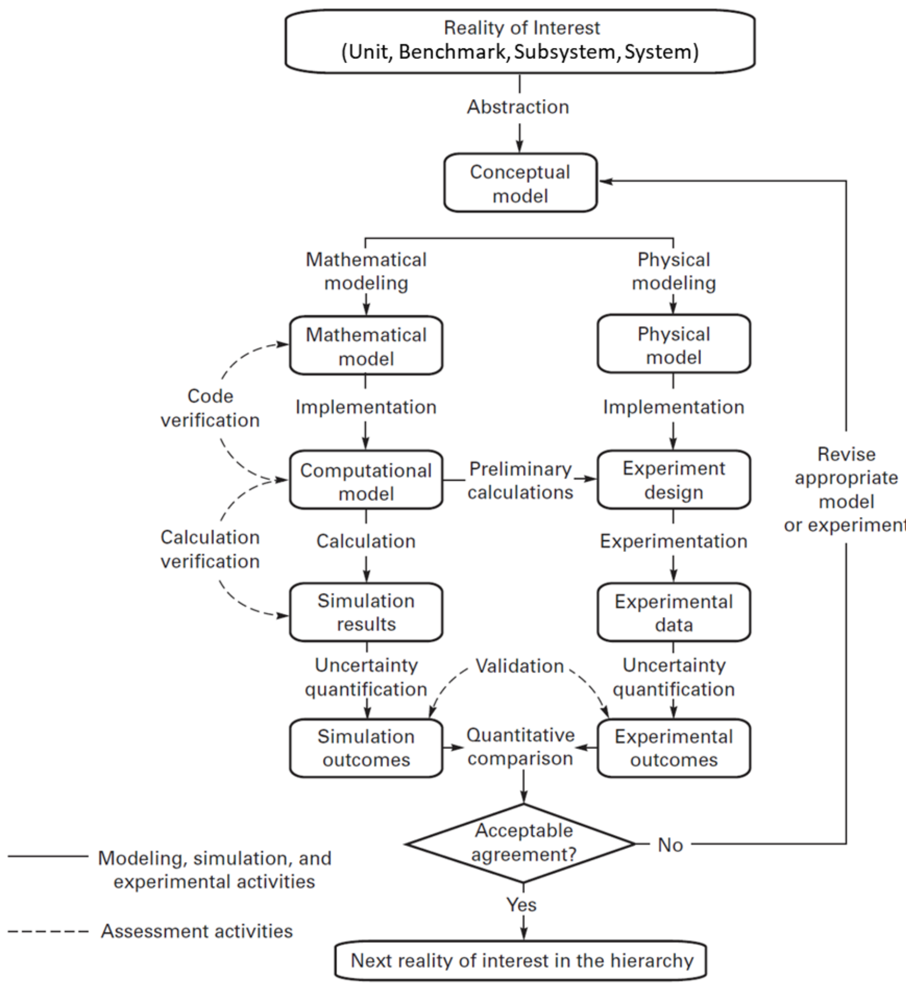

Figure 1 Verification and Validation activities and outcomes (ASME 2006)

The objective of verification is to estimate the numerical errors in simulation results and is not associated with any accuracy of physical modeling. The verification process can be divided into code verification and solution verification, as shown in Fig. 1.

Code verification

The code verification addresses the correct implementation of the numerical algorithm in the computer code specifically by evaluating the error for a known solution with high accuracy, referred as verification benchmark. Code verification in grid-based simulations can be performed by a systematic discretization convergence test (e.g., Roache 1994) and its convergence to a benchmark solution. For example, the code verification process would demonstrate that a code can produce the expected convergence rate as the discretization is refined.

The best approach to code verification employs exact analytical solutions that can represent problems of interest. However, it is impossible to find them in complex problems, such as wind engineering applications. Practical approaches have been developed, e.g., the method of manufactured solutions (Roache 2002), to generate exact analytical solutions required for code verification.

The code verification is usually performed by code developers/vendors. However, it is also recommended that the users of commercial/open source code independently perform the code verification process because the documentation might not be appropriate for the users' specific applications (ASME 2009).

Solution verification

The solution (or calculation) verification deals with i) correctness of the input and output data for a particular solution of a problem of interest and ii) numerical accuracy (error/uncertainty estimation) for the simulated solution (Oberkampf and Roy 2010). The code verification is a prerequisite for the solution verification. The code and solution verification processes concern mathematical and numerical issues. They do not account for the relationship between the simulation results from a mathematical model and the physical data from the real world, which is the subject of validation. However, the solution and its error estimation from the solution verification process are employed in the validation process.

The sources in numerical solution errors include discretization in space and time, iteration-convergence, and round-off calculations. For nontrivial CFD problems based on nonlinear PDEs, numerical errors can be quantitatively estimated in a posteriori technique only, using e.g., multiple simulations with different grid resolutions (Roache 1997).

Solution verification should be performed by CFD users and be required by analysts and decision-makers who use CFD simulation results.

Model validation

Once the code and solution verification processes are completed, the validation process can be performed. While verification deals with mathematical issues, validation concerns physical reality issues. The ultimate interest of CFD users in V&V lies in the validation results for the intended use. The validation relates the computational model to the real physical world and quantifies the degree of accuracy of the model, as indicated in Fig. 1.

Figure 2 shows the three aspects to validation (Oberkampf and Roy 2010; Oberkampf and Trucano 2008). Aspect 1 (model validation) deals with the quantification of the accuracy of the computational model by comparing the computational results of interest and the corresponding experimental counterparts (i.e., using the validation metric operation in the figure). Aspect 2 (model prediction) deals with estimation of predictive uncertainty in the results of interest due to interpolation or extrapolation of the model to the intended use. Aspect 3 (model adequacy assessment) deals with decision-making in the adequacy of the model for the intended use by checking whether the simulation results comply with the accuracy requirement for the intended use.

As described above, code verification, solution verification and validation are interactive in the process of estimating the accuracy of the computational model in simulated results of the application of interest.

The comprehensive and in-depth knowledge on V&V is provided in Oberkampf and Roy (2010) and Roache (2009).

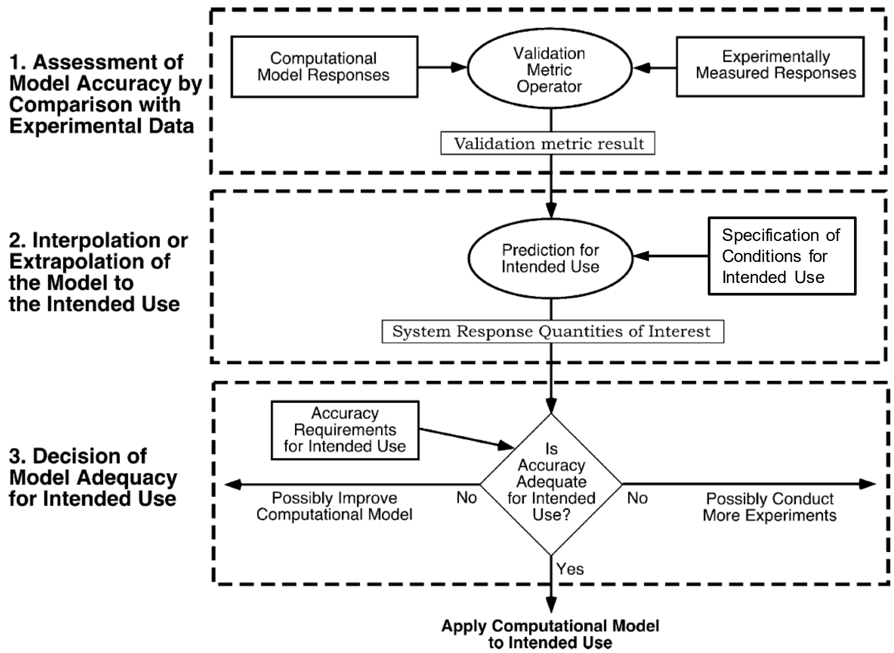

Figure 2 Three aspects of model validation (Oberkampf and Trucano 2008)

Modeling Complex Systems and its V&V approach

Typical real-world physical systems in CFD applications are inherently complex. To address the complexity efficiently, the concept of hierarchy in the systems has been adopted (AIAA 1998; ASME 2006). In the AIAA guide (Fig. 3), a complete system of interest is divided into subsystem cases which commonly show reduced coupling between flow phenomena of the complete system. Each subsystem consists of two or more benchmark cases which exhibit more restricted geometric or flow features. In this benchmark case phase, experimental data covering a wide range of flow features are usually well documented. A benchmark case is composed of multiple unit problems representing a flow feature.

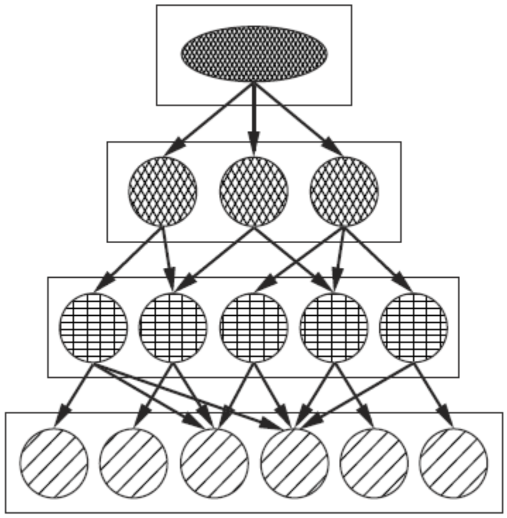

Figure 3. Hierarchical structure of physical systems (AIAA 1998)

Such unit problems identified from a top-down decomposition of a real-world physical system play a critical role in developing a model of the system. In the V&V procedure, once the hierarchical structures of a physical system of interest are established by identifying physical phenomena at each hierarchical level as stated above, the V&V procedure of Fig. 1 should be performed at each hierarchical level using a bottom-up approach. For the unit problems, all numerical issues (e.g., grid sensitivity and iterative convergence) are extensively investigated. For benchmark cases, the physical model for a specified flow feature is typically assessed. For the subsystems, coupling effects of multiple geometric and flow features are studied. For the complete system, the results for predicting real system of interest are simulated by employing the most appropriate physical models and grids obtained from the lower-level V&V procedures. Based on uncertainty of numerical and experimental results and the difference between the simulation and the associated experiment, the accuracy of the computational model is accessed for predictive capacity of the physical system of interest, which are defined first at the V&V procedure, as shown in Fig. 1.

4. PROCEDURES FOR ERROR AND UNCERTAINTY QUANTIFICATION

Error and uncertainty are often used interchangeably in estimating accuracies of CFD results. The AIAA V&V guide for CFD (1998) defines the two terms as follows:

Error: A recognizable deficiency in any phase or activity of modeling and simulation that is not due to lack of knowledge.

Uncertainty: A potential deficiency in any phase or activity of the modeling process that is due to the lack of knowledge.

The errors can be classified as acknowledged errors and unacknowledged errors. The acknowledged errors can be identified and eliminated (e.g., round-off errors, discretization errors, iterative errors). The unacknowledged errors cannot be found or removed (e.g., programming errors, improper use of the CFD code). The uncertainties can be classified as aleatory and epistemic. The aleatory uncertainty (irreducible uncertainty) is connected to inherent randomness (e.g., input parameters of a model). The epistemic uncertainty (reducible uncertainty) is related to a lack of knowledge of (or information on) a physical model. For details, see Oberkampf and Roy (2010).

The ASME V&V approach (2009) provides quantitative evaluation of uncertainties in simulation results by their comparison with their counterpart in experiments, and employs concepts and the definitions of error and uncertainty from metrology, as follows (JCGM 2012):

Errors (of measurement), δ: Measured quantity value minus a reference ('true') quantity value

Uncertainty (of measurement), u: Non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurand, based on the information used.

These concepts were extended to V&V in CFD simulations, aiming at evaluating quantitatively the errors and uncertainty in simulation results to be validated by comparing those results with their experimental counterparts.

The procedures for the error and uncertainty quantification included in the ASME Standard V&V 20-2009 (2009) are summarized below.

An error, δ, is a quantity that has a particular +/- sign and magnitude. Each error whose sign and magnitude is known can be eliminated by correction. A specific error δ_i is defined as the difference caused by error source i between the measured or simulated quantity and its true value. For an unknown error, its signs and magnitude cannot be removed, thus its uncertainty u is estimated by an interval $\pm u$ containing δ. A standard uncertainty is an estimate of standard deviation of the parent distribution of δ.

In the validation process, a simulation result is assessed by comparison with an experimental result for specified variables under restricted conditions (*validation point*). Figure 4 is a schematic showing the nomenclature for a validation process of, as an example, a simulation for the flow past a building in the atmospheric boundary layer. The variable of interest is assumed to be the aerodynamic pressure on the building. The predicted pressure value from the simulation is denoted by S, the value determined from experimental data by D, and the true (but unknown) value by T. Note that the order of the variables shown in Fig. 4 can be varied.

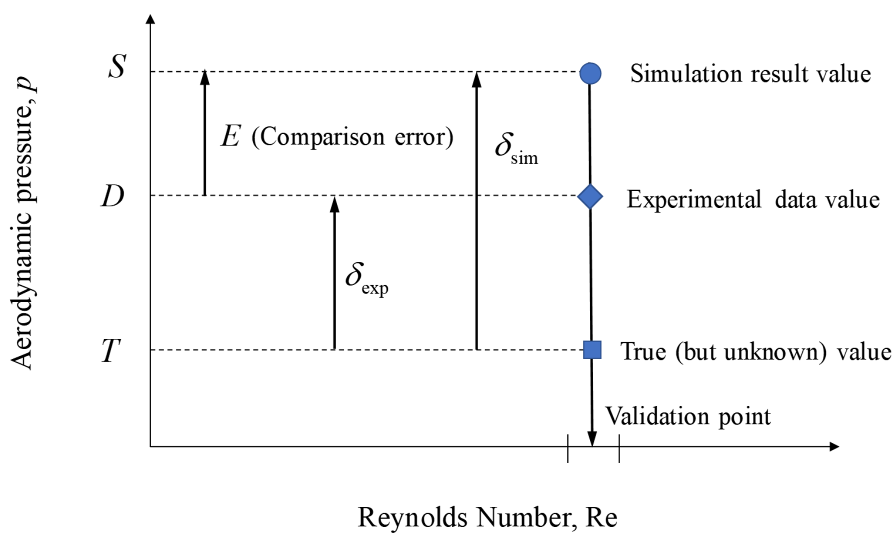

Figure 4. Schematic showing nomenclature for validation approach (ASME 2009).

The validation comparison error, E, is defined as

$$\begin{aligned} E &\equiv S - D \\ &= \delta_{\text{sim}} - \delta_{\text{exp}} \end{aligned} \tag{4}$$

where the error in the simulation value, δ_{sim}, is the difference between the simulated value and the true value:

$$\delta_{\text{sim}} = S - T \tag{5}$$

and similarly, the error in the experimental value is

$$\delta_{\text{exp}} = D - T \tag{6}$$

Thus, the validation comparison error combines all the errors in the simulation result and the experimental data.

Figure 5 illustrates the validation process with sources of error. The experimental "as run" is the reality of interest (truth) given the condition called *validation point* (shown in Fig. 4). The error in simulation value, δ_{sim}, consists of three errors associated with numerical calculations:

$$\delta_{\text{sim}} = \delta_{\text{model}} + \delta_{\text{num}} + \delta_{\text{input}} \tag{7}$$

where δ_{model} is the error due to modeling assumptions and approximations, δ_{num} is the error due to the numerical solution of the discretized equations, and δ_{input} is the error in the simulation result due to errors in the simulation input parameters.

As shown in Fig. 5, the validation comparison error, E, can be determined from Eqs. (4) and (7) as

$$E = \delta_{\text{model}} + \delta_{\text{num}} + \delta_{\text{input}} - \delta_{\text{exp}}. \tag{8}$$

To estimate δ_{model} in this validation process example, Eq. (8) needs to be rearranged as

$$\delta_{\text{model}} = E - \left(\delta_{\text{num}} + \delta_{\text{input}} - \delta_{\text{exp}}\right). \tag{9}$$

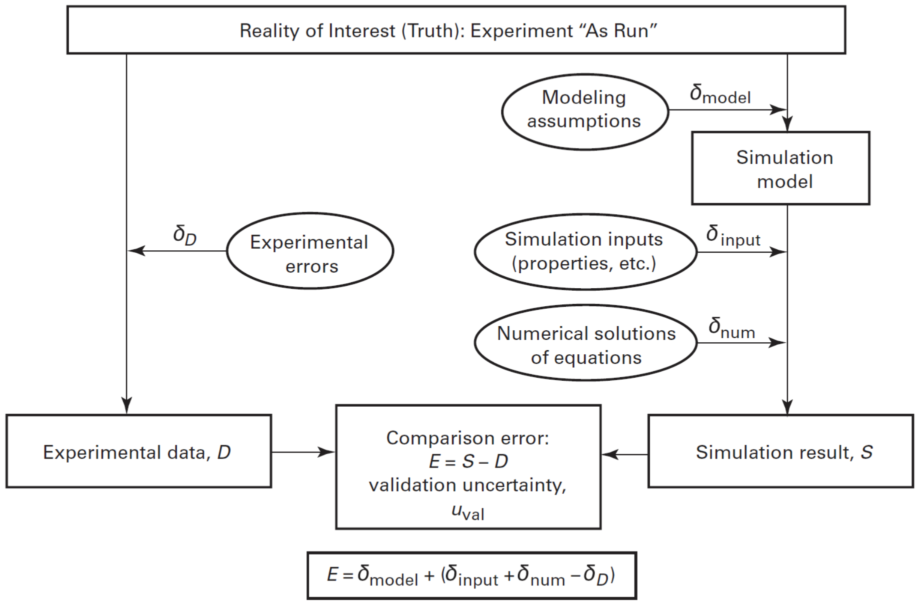

Figure 5. Overview of the Validation Process with Sources of Error in Ovals (ASME 2009).

As explained above, once the simulation value (S) and the experimental data (D) are determined, the comparison error (E) can be calculated from Eq. (4) (i.e., the sign and magnitude of E can be known). However, because the signs and the magnitudes of δ_{num}, δ_{input}, and δ_{exp} are unknown, the standard uncertainties corresponding to those errors can be estimated by u_{num}, u_{input}, and u_{exp}, respectively.

The validation standard uncertainty due to combination of the errors, u_{val}, is defined as

$$u_{val} = \sqrt{u_{num}^2 + u_{input}^2 + u_{exp}^2}. \tag{10}$$

This relationship is valid when the three errors are independent of each other and their uncertainty sources are aleatory (i.e., random).

The validation results can be interpreted in two ways: i) with no assumptions on error distributions associated with ($\delta_{num} + \delta_{input} - \delta_{exp}$) and ii) with assumption on the error distributions. In the method with no assumption on error distribution, δ_{model} is inferred approximately by comparing the magnitudes of E with

u_{val}. When the magnitude of E is much larger than u_{val}, E may be viewed as approximately equal to δ_{model}. When the magnitude of E is not larger than u_{val}, δ_{model} can be considered to be of the same order as the error contribution ($\delta_{\mathrm{num}} + \delta_{\mathrm{input}} - \delta_{\mathrm{exp}}$). That is:

$$\begin{aligned} &\text{If } \left|E\right| \gg u_{\mathrm{val}}, \qquad \delta_{\mathrm{model}} \approx E \\ &\text{If } \left|E\right| \leq u_{\mathrm{val}}, \qquad \delta_{\mathrm{model}} \approx (\delta_{\mathrm{num}} + \delta_{\mathrm{input}} - \delta_{\mathrm{exp}}). \end{aligned} \tag{11}$$

In the method that assumes the probability distribution of $\delta_{\mathrm{num}} + \delta_{\mathrm{input}} - \delta_{\mathrm{exp}}$ (e.g., uniform or Gaussian distribution) (ISO 1993), an interval can be estimated within which δ_{model} is positioned at a given degree of confidence:

$$U_{\%} = k_{\%} u_{\mathrm{val}} \tag{12}$$

where $U_{\%}$ is the overall or expanded validation uncertainty at a specified percentage level of confidence, and $k_{\%}$ is the coverage factor which depends on the assumed parent distribution of error and the desired confidence level. For example, $k_{\%} = 2$ is for the 95% confidence interval of a Gaussian distribution. Typically, $k_{\%}$ is in the range between 2 and 3 (ASME 2009). A coverage interval can be directly calculated by Monte Carlo methods. Thus, the true value of the validation variable will be located within a $\pm\ U_{\%}$ band around E with a given confidence interval:

$$\delta_{\mathrm{model}} \in \left[E - U_{\%}, \quad E + U_{\%}\right]. \tag{13}$$

This is the estimated accuracy of the simulation result. The adequacy of the simulation result depends on the accuracy required for the application of interest.

For estimating u_{val} and, ultimately, δ_{model}, the standard uncertainties (u_{num}, u_{input}, and u_{exp}) in the RHS term of Eq. (10) should be estimated through the solution verification and model validation processes. Their quantitative evaluations are briefly explained in the following.

4.1 Estimation of numerical error uncertainty (u_{num})

The uncertainty due to numerical errors, u_{num}, can consist of the discretization error uncertainty (u_{h}), the iterative error uncertainty (u_{it}), and the round-off error uncertainty (u_{ro}), associated with the corresponding errors described in Section 2, as:

$$u_{\mathrm{num}} = u_{\mathrm{h}} + u_{\mathrm{it}} + u_{ro}. \tag{14}$$

The combined error is recommended to be conservatively estimated by simple addition, instead of RMS addition (Eq. 10) because the uncertainties cannot be assumed to be uncorrelated (Eça and Hoekstra 2009). Thus, the resulting numerical error uncertainty is treated as epistemic. Note that all uncertainty values in Eq. (14) are positive.

The round-off errors can be assessed by comparing CFD/CWE results based on different levels of precision in a computing machine and the associated uncertainty can be assumed to be considerably smaller than u_{it} (i.e., $u_{\mathrm{ro}} \approx 0$ in Eq. 14)

Prior to estimation of any discretization error, the iterative error should be estimated first to avoid amplifying the uncertainty induced by the incomplete iterative convergence error. The uncertainty due to iterative error can be estimated by, e.g., the method of manufactured solutions (Eça and Hoekstra 2009). For unsteady flow simulations, iterative convergence at every time step should be monitored to make sure that the iterative error is considerably smaller by, e.g., 2 to 3 orders of magnitude than the errors of discretization. When the estimated iterative error is assumed to be significantly smaller than the discretization error for the contribution to the numerical error uncertainty, the uncertainty in the numerical errors, u_{num}, can be

$$u_{\mathrm{num}} = u_{\mathrm{h}}. \tag{15}$$

and in the case the iterative error uncertainty (u_{it}) needs to be considered,

$$u_{\mathrm{num}} = u_{\mathrm{h}} + u_{\mathrm{it}}. \tag{16}$$

For the estimation of discretization error, the classical Richardson Extrapolation (RE) (Richardson 1911; Richardson 1927) has been most widely used and its various versions have been developed (e.g., a Least Squares version (Eça and Hoekstra 2014)). Roache's Grid Convergence Index (GCI) (Roache 1994; Roache 1997) can estimate the uncertainty of numerical errors by multiplying the absolute value of the RE error estimate by a safety factor, F_s. At least three successive levels of grid refinement are recommended to be used for ensuring an acceptable level of accuracy. The CGI method is summarized below:

Let three grids be h_1 (finest) < h_2 < h_3 (coarsest) where h_i (i = 1, 2, 3) is the characteristic grid size of grid i for estimating u_{num} using the GCI method. The CGI for grids 2 and 1 is calculated from

$$\mathrm{GCI}^{21} = \frac{F_s\, e_a^{21}}{(r_{21})^p - 1} \tag{17}$$

where the grid spacing ratio $r_{21} = h_2/h_1$, p is the observed order in convergence of the simulated value of the solution variable (S) with respect to mesh size from the three simulations, e_a^{21} is the absolute change of S over grids 1 and 2, and F_{s} is the safety factor recommended to be 1.25 for structured grids and 3 for unstructured grids (Roache 1994). The GCI for grids 2 and 3 is determined in a similar manner. The standard uncertainty u_h corresponding to each grid refinement level can be estimated using the GCI value. Because the GCI is estimated at 95 % of confidence from empiricism (i.e., GCI = $U_{95\%}$) , the standard uncertainty u_h required for Eq. (10) is determined by

$$u_h = \frac{\mathrm{GCI}}{k_{\%}} \tag{18}$$

where $k_{\%}$ is the coverage (or expansion) factor, as explained in Eq. (12). The value of $k_{\%}$ is recommended to be 2 for Gaussian error distribution about the fine grid solution and 1.1 to 1.15 for roughly shifted Gaussian error distribution. The non-dimensional standard uncertainty of u_h (Eq. (18)) can be converted to dimensional form by multiplying it by the representative simulated value of the solution variable S. For the detail of the GCI method, see the ASME Standard (2009).

The systematic grid refinement study should use sufficiently fine grids to predict the flow physics of interest. Appropriate boundary conditions (e.g., inflow/outflow boundaries far enough from the structures of interest in the computational domain) should be employed to guarantee zero discretization error when the grid sizes approach infinitesimally small values. Such errors, categorized as modeling errors, can be addressed by sensitivity tests (Oberkampf and Roy 2010).

4.2 Estimation of input parameter uncertainty (u_{input})

One part of uncertainty in simulation results comes from the uncertainty of simulation input parameters, u_{input} in Eq. (10). Since experiments typically use the input parameters that have their own uncertainties, so do the numerical simulations based on the values of input parameters determined by the experiments. For example, in the case of simulations for pressures on a structure, the input parameters for their uncertainty estimation could include air density, wind speed, and terrain exposure condition. The contribution of each input parameter X_i to u_{input} is estimated by using a local or a global approach. As a local method, the sensitivity coefficient method[1] describes the input uncertainty propagation equation for a simulation result S caused by n uncorrelated random input parameters, as described below (Coleman and Steele 2009):

$$u_{\text{input}} = \sqrt{\sum_{i=1}^{n}\left(\frac{\partial S}{\partial X_i}u_{X_i}\right)^2} = \sqrt{\sum_{i=1}^{n}\left(\bar{X}_i\frac{\partial S}{\partial X_i}\frac{u_{X_i}}{\bar{X}_i}\right)^2} \tag{19}$$

where the partial derivative $\partial S/\partial X_i$ is the sensitivity coefficient of the validation variable S with respect to input X_i, $\bar{X}_i$ is the nominal (e.g., mean) value of X_i, and the $u_{X_i}/\bar{X}_i$ is the relative standard uncertainty (i.e., coefficient of variation). The input parameter uncertainty u_{X_i} can be determined from measurements of parameters in experiments, database, or expert's opinion. The sensitivity coefficients can be computed by local techniques, such as finite difference method. The detail of the computing techniques is provided

[1] The sensitivity coefficient method was used for estimating the uncertainty in the wind load in Ellingwood et al. (1980).

in ASME (2009). This local method evaluates the input uncertainty propagation equation (Eq. (19)) within a small (local) neighborhood around the nominal values of the input parameters. When the result S has a high non-linear behavior in the parameter space, the local method cannot estimate properly the uncertainty inherent in input parameters.

A more reliable approach to estimating u_{input} is to employ global samples in the parameter space by e.g., Monte Carlo methods. The samples are randomly collected from the distribution functions of input parameters. If the input parameters are not independent, the correlation should be addressed in an appropriate method. Since the full Monte Carlo method is known to be computationally expensive, a less computer-intensive method (e.g., Latin hypercube sampling method (McKay et al. 1979)) is preferred for practical applications.

4.3 Estimation of experimental result uncertainty (u_{exp})

In the experimental uncertainty analysis, the uncertainties are estimated for individual variables. Among many error sources of a measured variable X_i, known errors should be eliminated by a calibration process. The unknown errors are represented by standard uncertainty u_i.

As shown in Fig. 6, the total error in an experimental result, defined as the difference between the measured value and the true value (δ_{exp} in Fig. 4), consists of random error (precision) and systematic error (bias). The random error varies randomly in repeated measurements during the test, mainly caused by uncontrolled or non-repeatable test conditions. The systematic error remains constant in repeated measurements during the test, largely caused by imperfect calibration corrections and measurement methods. The "total" uncertainty in an experimental measurement can be described as the combination of uncertainties contributed by the random and systematic errors (ASME 2013).

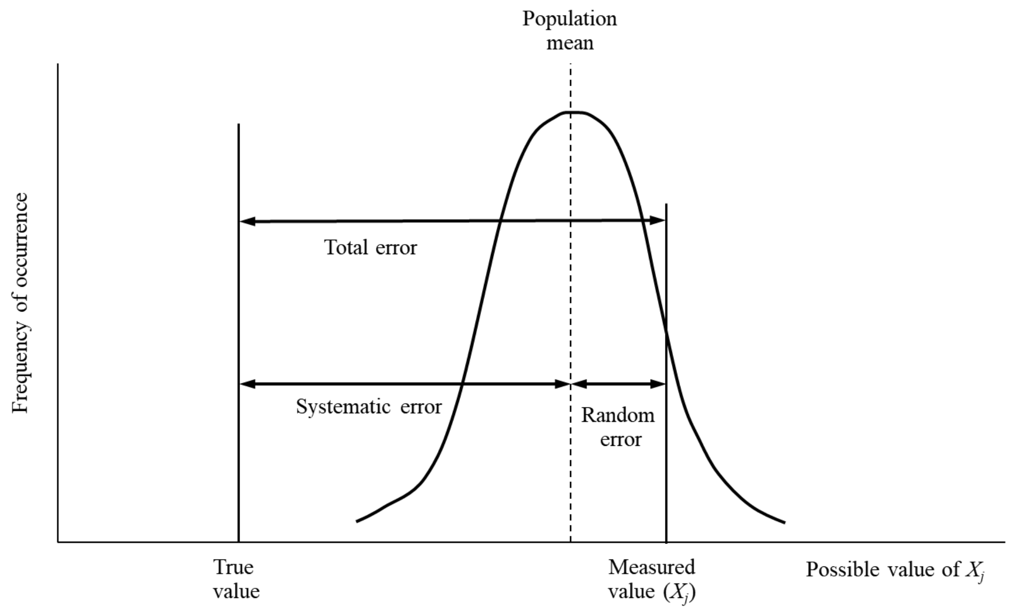

Figure 6. Measurement errors (ASME 2013).

The standard uncertainty of an experimental result r determined from j measured variables ($X_1, X_2, \ldots, X_j$), denoted by $u_{\exp}$, is defined in ASME (2009) as

$$u_{\exp} = \sqrt{b_r^2 + s_r^2} \tag{20}$$

where b_r is the systematic standard uncertainty of the experimental result r:

$$b_r^2 = \sum_{i=1}^{j} \left(\frac{\partial r}{\partial X_i} b_i \right)^2 + 2 \sum_{i=1}^{j-1} \sum_{k=i+1}^{j} \left(\frac{\partial r}{\partial X_i} \frac{\partial r}{\partial X_k} b_{ik} \right), \tag{21}$$

and s_r is the random standard uncertainty of the experimental result r:

$$s_r^2 = \sum_{i=1}^{j} \left(\frac{\partial r}{\partial X_i} s_i \right)^2 + 2 \sum_{i=1}^{j-1} \sum_{k=i+1}^{j} \left(\frac{\partial r}{\partial X_i} \frac{\partial r}{\partial X_k} s_{ik} \right). \tag{22}$$

In Eqs. (21-22), b_i and s_i are the elemental systematic and random standard uncertainties, respectively; b_{ik} and s_{ik} are the covariance of the systematic and random standard uncertainties, respectively. The random contribution to the measurement uncertainty (s_D) can also be estimated as the standard deviation in the measurements of r from multiple (say, 10) experiments. As explained for the u_{input} estimation, alternative methods of the u_{exp} estimation to the local sensitivity coefficient propagation approach (Eqs. 21-22) are global sampling (Monte Carlo) methods.

For validation purposes, the uncertainty of experimental result is fixed as a systematic standard uncertainty and the experimental result has a single value with a fixed (but unknown) error (ASME 2009). Thus, the experimental uncertainty u_{exp} in Eq. (20) becomes

$$u_{\text{exp}} = u_{\text{exp}}\big|_{b_r=0} = s_r . \tag{23}$$

5. USAGE OF VALIDATION LEVEL

The word "validation" has been used at various levels of interpretation as an indicator of acceptable tolerance for agreement between simulation and experiment results (ASME 2009). In a loose usage, a model is deemed "validated" once the simulation results are compared with experimental counterparts, regardless of the agreement level. The validation in this case refers to the process and is not related to the quality of the model and its simulated results. As a moderate usage, the model is considered validated when the validation uncertainty of $E \pm u_{\mathrm{val}}$ is quantified through the procedure described in Sect. 4. This level of validation provides a quantitative assessment without judgement of pass or fail validation. In a strict usage, the validation can be used as pass or fail evaluation to check whether or not the accuracy level of results is within the error tolerance specified in standards for a particular application. In CWE applications, most studies to date have employed the loose usage of validation. There is no clear consensus on validation usage and acceptance level in CWE results for structural design.

6. SUMMARY

Recently, applications of CFD techniques for CWE has generated strong interest among wind and structural engineers as a possible substitute for or supplement to wind tunnel experimentation. However, at present CWE is still in a developmental stage. A necessary step toward advancing CWE simulations in wind and structural engineering applications credible is the development of reliable verification and validation (V&V) procedures. The fundamental elements for building the credibility of CWE simulations are (i) quality of physical modeling, (ii) quality of users/analysts conducting the simulations, (iii) verification and validation (V&V) activities, and (iv) uncertainty quantification of the simulation results. This report summarizes (i) the sources of inaccuracy in CFD simulations and (ii) concepts and procedures of verification and validation (V&V) and uncertainty quantification, and (iii) the usage of validation levels.

The sources leading to the inaccuracy of CFD results can be classified into four types: (i) physical modeling, (ii) discretization, (iii) iteration, and (iv) programming/user. The physical modeling errors could arise from the approximation of complex behavior in the governing equations, effects of computational domain size and boundary conditions, and assumptions on fluid properties. The discretization error depends on the numerical schemes in space and time, the resolution and quality of the grids used in simulations, and solution behaviors. Among the sources associated with numerical inaccuracy, the discretization errors are usually the largest and their estimation is the most challenging. The iterative errors could result from round-off errors and iterative convergence errors inherent in iterative methods. The latter should be carefully monitored for unsteady flow simulations. The programming/user errors are associated with mistakes in coding and in pre-/post-processing of data, respectively.

The verification process can consist of code verification and solution verification. The former addresses the correct implementation of the numerical algorithm in the computer code and is usually performed by code developers/vendors. The latter deals with (i) correctness of the input and output data for a particular solution of a problem of interest and (ii) numerical accuracy (error/uncertainty estimation) for the simulated solution. Solution verification should be performed by CFD users and be required by analysts and decision-makers who use CFD simulation results structural engineers. Once the code and solution verification processes are completed, the validation process can be performed. The ultimate interest of CFD users in V&V lies in the validation results for the intended use. The validation relates the computational model to the real physical world and quantifies the degree of accuracy of the model.

The procedures for the error and uncertainty quantification based on the ASME V&V 20 Standards provide quantitative evaluation of uncertainties in simulation results by their comparison with their counterparts in experiments, and employs concepts and definitions of error and uncertainty taken from metrology. To estimate the validation uncertainty and, ultimately, the modeling error in the simulation results, the standard uncertainties of numerical errors, input parameters, experimental results should be estimated.

The word "validation" has been used at various levels of interpretation (e.g., loose, moderate, and strict usages) as an indicator of acceptable tolerance for agreement between simulation and experiment results. In CWE applications, most of studies to date have employed the loose usage of validation. There is no clear consensus on validation usage and acceptance level in CWE results for structural design. Such research should be performed for assuring appropriate safety margins in structural design for wind when CWE-based wind loads are used in practical applications.

REFERENCES

AIAA (1998). *Guide for the verification and validation of computational fluid dynamics simulations*. AIAA-G-077-1998, American Institute of Aeronautics and Astronautics, Reston, Virginia.

ASME (2006). *Guide for verification and validation in computational solid mechanics*, ASME V&V 10-2006, American Society of Mechanical Engineers, New York, NY.

ASME (2009). *Standards for verification and validation in computational fluid dynamics and heat transfer*, ASME V&V 20-2009, American Society of Mechanical Engineers, New York, NY.

ASME (2013). *Test uncertainty: Performance test codes*, ASME PTC 19.1-2013, American Society of Mechanical Engineers, New York, NY.

Coleman, H. W. and Steele, W. G. (2009). *Experimentation, validation, and uncertainty analysis for engineers*, 3rd ed., John Wiley & Son, Hoboken, NJ.

DoD (1994). *Modeling and Simulation (M&S) Management*. DoD Directive No. 5000.59, Department of Defense.

Eça, L. and Hoekstra, M. (2009). "Evaluation of numerical error estimation based on grid refinement studies with the method of the manufactured solutions." *Computers & Fluids*, 38(8), 1580-1591.

Eça, L. and Hoekstra, M. (2014). "A procedure for the estimation of the numerical uncertainty of CFD calculations based on grid refinement studies." *Journal of Computational Physics*, 262(Supplement C), 104-130.

Eça, L., Vaz, G., and Hoekstra, M. (2017). "Iterative errors in unsteady flow simulations: Are they really negligible?" *20th Numerical Towing Tank Symposium (NuTTS 2017)*, Wageningen, The Netherlands, Oct. 1-3, 2017.

Ellingwood, B., Galambos, T. V., MacGregor, J. G., and Cornell, C. A. (1980). *Development of a probability-based load criterion for American National Standard A58*. NBS Special Publication 577, National Bureau of Standards, Washington, DC.

ISO (1993). *Guide to the expression of uncertainty in measurement*, International Organization for Standardization, Geneva.

JCGM (2012). *International vocabulary of metrology – basic and general concepts and associated terms* JCGM 200:2012 (JCGM 200:2008 with minor corrections), Joint Committee for Guides on Metrology.

McKay, M. D., Beckman, R. J., and Conover, W. J. (1979). "A Comparison of Three Methods for Selecting Values of Input Variables in the Analysis of Output from a Computer Code." *Technometrics*, 21(2), 239-245.

NRC (1986). *Current capabilities and future directions in Computational Fluid Dynamics*. National Research Council, Washington, DC.

Oberkampf, W. L. and Roy, C. J. (2010). *Verification and validation in scientific computing*, 1st ed., Cambridge University Press, Cambridge, UK.

Oberkampf, W. L. and Trucano, T. G. (2008). "Verification and validation benchmarks." *Nuclear Engineering and Design*, 238(3), 716-743.

Pilch, M., Trucano, T., Moya, J., Froehlich, G., Hodges, A., and Peercy, D. (2001). *Guidelines for Sandia ASCI verification and validation plans - Content and Format Version 2.0*. SAND2000-3101, Sandia National Laboratory, Albuquerque, NM.

Richardson, L. F. (1911). "The approximate arithmetical solution by finite differences of physical problems involving differential equations, with an application to the stresses in a masonry dam." *Philosophical Transactions of the Royal Society of London. Series A*, 210(459-470), 307-357.

Richardson, L. F. (1927). "The deferred approach to the limit." *Philosophical Transactions of the Royal Society of London. Series A*, 226(636-646), 299-361.

Roache, P. J. (1994). "Perspective: A Method for Uniform Reporting of Grid Refinement Studies." *Journal of Fluids Engineering*, 116(3), 405-413.

Roache, P. J. (1997). "Quantification of uncertainty in computational fluid dynamics." *Annual Review of Fluid Mechanics*, 29(1), 123-160.
Roache, P. J. (2002). "Code Verification by the Method of Manufactured Solutions." *Journal of Fluids Engineering*, 124(1), 4-10.
Roache, P. J. (2009). *Fundamentals of verification and validation*, 2nd ed., Hermosa publishers, Socorro, New Mexico.
Zikanov, O. (2010). *Essential computational fluid dynamics*, 1st Ed. ed., John Wiley & Sons, Hoboken, New Jersey.