Recent Progresses in Verification, Validation and Uncertainly Analysis in Computational Fluid Dynamic

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Abstract. Verification and validation (V&V) are indispensable tools to evaluate the accuracy and reliability in computational simulations. This paper highlights guidelines, related works, as well as recent progress for evaluating the credibility of model and simulation in computational fluid dynamics (CFD). Herein, detailed definitions of V&V that aims to help researchers to distinguish between the term verification and the term validation, define the conceptual sources of error and uncertainty as well as understanding the difference between them. Then, we discuss related works to V&V for CFD simulations, the most useful methodologies and algorithms have been introduced, problems have been faced as well as solutions has been proposed. Finally, an outlook and perspectives for future challenges in V&V for CFD Simulation have been proposed. For verification assessment, in order to assure the accuracy, the computational solution is compared with an analytical solution or a highly accurate solution. The main strategy of validation is to reflect the accuracy between the computational results and the experimental data, as well as the quantification and estimation of both error and uncertainty. It is hoped from this review to help in research, development as well as the use of CFD simulations by establishing robust methodologies and terminologies for V&V.

Keywords. Verification; validation; errors; uncertainty; computational fluid dynamic.

1. Introduction

1.1. Overview of Computational Fluid Dynamic Verification and Validation

Since the second middle of the nineteenth century, engineers and scientists start to involve computer simulations to study several physical phenomena, as well as analyzing and design engineered systems [1]. Computational fluid dynamic (CFD) known as a branch of fluid mechanic, it is a complex technology that strongly involve nonlinear partial differential equations (PDE). It attempts to compute theoretical and experimental models in discrete domain of a given geometry shape [2-5]. It is well known that the equations used in CFD simulations are mainly PDE, which means that a numerical method with specific algorithms
is required to find an approximate solution. In order to facilitate the CFD simulations for the users, many companies have developed different platforms with integrated geometries, models, numerical methods and algorithms. These software are solving the models using some numerical methods such as finite elements, finite volumes, and finite differences [6-8]. However, the solution of CFD equations mainly has an approximate value. This approximate value could affect the accuracy of simulated output which raises the question: How should evaluate the confidence in model and simulation? To answer this question the term verification and validation (V&V) has been created.

V&V of a given computational simulation is known as primary methods to build, evaluate, and quantify this confidence. The term verification can be defined as an assessment accuracy of mathematical model solution compared to the analytical solution. It can determine if the computer code and the computational implementation of the mathematical model is correct. On the other hand, the term validation can be defined as an assessment of the accuracy of a given numerical simulation compared to the experimental outputs. The verification does not focus to link the numerical simulation to the real world as the validation does, i.e., verification and validation are primarily mathematical and physical issues respectively [9]. There are extensive researches focus on V&V including books, papers, and policy statements [10, 11]. Researches dealing with V&V of CFD problems are related to many fields such as aerospace [12], aeronautics [13], microfluidic [14], ship hydrodynamic [15], and electrohydro dynamic systems [16], etc. The credibility of CFD simulation is obtained when the uncertainty and errors show an acceptable value, in the next section the term uncertainty and errors will be discussed in detail. Detailed evaluation of errors and uncertainties has to be carried out by putting into consideration the three roots of CFD: experiment, theory, and computation.

1.2. Errors and Uncertainties in CFD Simulations
The term error can be defined as the recognizable insufficiency in any phase or activity during the model or the simulation processes which caused not due to the lack of knowledge. On the other hand, the term uncertainty can be defined as the potential insufficiency in any phase or activity during the model process which caused due to the lack of knowledge of the physical process [9]. The CFD distinguishes four types of errors known as physical errors, Numerical errors, coding errors, and human errors [17]. The physical errors are mainly caused due to the physical model or geometry model. Numerical errors can be divided into three types: round-off error, iterative convergence errors or discretization errors. The coding errors are bugs in the code, and human errors are the errors made by users while writing codes.

The uncertainties mainly regroup input uncertainties and physical model uncertainties. The input uncertainties can be caused due to the mismatch between the real design and CFD geometry, weak information on the boundary conditions, or lacking information on the fluid proprieties. The physical model uncertainty can be caused due to mismatch between the experimental flow and CFD flow. This mismatch can occur due to the negligence of turbulence, chemical reaction, incompressibility, unsteadiness, etc. [9].

By defining the notion errors and uncertainty, the aim of verification is to quantify the errors of the numerical method which include: mesh and time step dependency tests. The aim of validation is to quantify uncertainty which include evaluation of input uncertainty and comparison to experiment outputs.

2. Verification Assessment Process
In 1992, the American Institute of Aeronautics and Astronautics (AIAA), CFD committee has made legislation to standardize and formulate the basic methodology and terminology in verification and validation of CFD. These efforts have culminated by the publication of the guide for V&V of CFD, also known as the AIAA guide [11]. This guide highlights the fundamental concepts and discussing the main
procedures to perform V&V in CFD. The AIAA has defined the verification as the process that determines if the implemented model accurate with its conceptual description and its solution.

The verification test includes many examinations such as: (1) Examines the implementation of the computational model with the conceptual model (2) if the proposed algorithm can be properly used for analysis, the next step is to define and quantify the errors in the implemented model and its solution. Verification also includes the right solving of the equations, it is intended to focus on the mathematical aspect rather than the engineering aspect.

In CFD, verification assessment can be divided into two general branches: Code verification emphasis and Calculation verification emphasis.

2.1. Computer Programming & Code Examination (Code Verification)

Reviewing the computer programming is one of the most basic tasks during the verification testes, it aims to identify and check the computer programming errors/bugs. This can be done by manually checking the code. If the code is quite large it is better to use test code to run subprograms. This step is quite important in the detection of computer programming errors. Since the last decades, several methods for performing code examination has been developed and they are mainly classified into static, and dynamic testing. In this section, we do not give a detailed description of testing methods due to their association with software implementation. However, some definitions and reasons for applying testing in verification assessment has been introduced.

2.1.1. Why Code Examination? Code examination is an essential item of verification assessment in CFD. A critical study has been presented by Hatton [18] when he measured the consistency of many software over seven years written in C and FORTRAN and containing millions of lines. He has performed both static and dynamic testing (defined as T1 and T2 experiments). He has found that for 1000 executable lines written in C there are about 8 serious static mistakes, and about 12 serious static mistakes when using FORTRAN. In the dynamic test, Hatton analyzed the differences between different implementations of the same algorithm using the same language and input. The testing experiments presented by Hatton has open the way to process the results of scientific calculations in the same way and measure of disbelief that engineers have traditionally attached to results of untrusted physical experiments. A recent literature has summarized that code errors might occur due to one of the following contexts [19]:

(a) Lack of comprehension or providing poor protection against the numerical accuracy as well as precision restrictions in numerical algorithms.
(b) The numerical type conversion is not considered by some developers which may affect the accuracy of the results. Noting that many software development environments do not detect such types of errors during the compilation.
(c) Many software accepts inputs of data values or constants which may be not really accurate.
(d) Some smallest positive values are known as "platform epsilon" are represented in every computing environment and any computations of values smaller than this may affect the accuracy of the results.

2.1.2. Static and Dynamic Testing. The static testing or static analysis has been defined by fairly as analyzing the code without executing the software or considering a specific inputs [20]. This method is mainly used to check if the code fulfills its specification, it may also look for violations of logical or recommended programming practice. Static analysis finds wide applications in software testing and software engineering. Briefly, a recent study published by Sing et al. [21] have evaluated how static analysis can reduce the code review effort by detecting common mistakes. By performing a study on Programming Mistake Detector (PMD) tool, it was found that PMD could prove to reduce the workload of code reviewers. Unlike static
analysis, dynamic analysis, or dynamic testing describes the dynamic behavior of the code, compute, as well as evaluates the results by detecting bugs in design that can cause coding errors [20].

2.2. Calculation Verification Emphasis
The calculation verification can be classified into three categories: Iterative convergence examination, spatial convergence examination, and temporal convergence examination.

2.2.1. Iterative Convergence Examination. The iterative convergence is required for any CFD simulation. The term iterative convergence associate to the number of iteration required in order to get residual errors that have sufficiently low value, either for a steady-state problem or for each time step in an unsteady problem [22]. A research has discussed the CFD 2030 vision noted to inconsistent/incomplete convergence behavior as an obstacle in current CFD technology [23]. Noting that, in the recent years some progress has been made to develop some solving methods with high convergence capabilities.

An efficient code or program must decrease rapidly the residual error in the early stages of convergence. The defect correction method is affected by the linear change of the convergence rate. This lead to a large number of iterations to get residual error close to zero [24]. The large computational cost of decreasing the residual error into value close to zero often leads CFD programmers to an early stop of the simulation and accepting partially converged results with the risk of large values of remaining iterative error. Another alternative method to the defect correction method known as Newton’s method. Newton’s method has the advantage to converge quadratically instead of linearly, which makes it a good alternative method [25]. However, in order to obtain a quadratic convergence Newton’s method requires an accurate Jacobians. Calculating an accurate Jacobians may still be challenging. Many research has been performed to estimate an accurate Jacobian [26-29]. An estimated Jacobian is easier for implementation and requires less memory to store. An inaccurate formula of Newton’s Method known as the Jacobian-Free Newton-Krylov (JFNK) method [30]. The JFNK method applies a Krylov subspace method as the linear solver, it only requires the product of the Jacobian matrix and the solution update vector. However, for turbulent aerodynamic flows, JFNK is not a perfect method in the solution of the compressible Navier-Stokes equations. This can be related to some unclear aspects of JFNK methods if the method is poorly handled. To solve this problem Chisholm and Zingg [31] have proposed some strategies, leading to an efficient JFNK algorithm for the efficient solution of subsonic, which is shown a better performance than the approximate factorization method.

2.2.2. Spatial Convergence Examination. The examination of grids convergence of CFD simulation is indispensable for determining the discretization error in a CFD simulation. The term grid convergence study can also be defined in other references as the grid refinement study. Several methods and algorithms examining the temporal and spatial convergence have been presented by others. Many of these methods are based on Richardson’s extrapolation [32-34].

Sosnowski [35] shows that the discretization of the computational domain could affect the CFD simulation solution. He found that the mesh size and geometry directly influence on the simulation results with noticeable advantages of polyhedral mesh over the tetrahedral mesh. Li et al. [36] has proved that the flow field variables selected for verification will affect the mesh convergence of the numerical simulation. In addition, the inlet and outlet configurations used in CFD simulations have shown a significant impact on mesh convergence. Almohammadi et al. [37] have investigated the fitting method, namely mesh refinement, Grid convergence index, and general Richardson extrapolation methods in order to obtain a mesh independent solution by simulating a wind turbine using CFD. Eca et al. [38], have offered a procedure to estimate the numerical uncertainty of CFD simulation based on grid refinement studies.
2.2.3. Temporal Convergence Examination. An efficient CFD simulation requires discrete-time steps to examine the accuracy of simulation results to the magnitude of the time step. In order to assure the accuracy of unsteady CFD simulation, it is necessary to ascertain that the temporal discretization error is small as well as the convergence is achieved. The temporal convergence error is known as a function of time step. This error increase proportionally with increasing of time step. Ideally, in order to understand the effect of time step on the results, it is better to perform several independent simulations using different time steps. However, there is a lack of studies that investigate the effect of time step on the temporal convergence because these kind of simulations are computationally expensive. Another intrinsic parameter influences the temporal convergence known as Newton sub-iterations. Mittal et al. [39], have studied the effect of temporal convergence on the simulation of a wind turbine. They found that Newton sub-iterations may be more important than the time step to reach a temporal convergence.

3. Validation Assessment Process
Validation is the step that determines the accuracy of the representation of the real world according to the perspective of the intended uses of the model. The identification and quantification of errors and uncertainty between the computational and conceptual models are the main strategies of the validation process. Since one of the fundamental roles of CFD in engineering is to present high-accuracy results, it is necessary to develop an efficient, robust, and systematic code validation process that could be applied to a wide variety of engineering research. It was noted that comparing CFD simulations with experimental data is the method of measuring the accuracy of a representation of the real world. However, this does not mean that all experimental data has a high accuracy. All experimental data contain some errors known as random and bias errors. The estimation of these errors must be calculated while comparing with the computational solution. Nothing that several practical issues must be considered:

1. The number of validation tests and the accuracy levels required for each test case is varied according to each application. There are no global criteria for all applications.
2. It is desirable but not necessary to have very high accuracy in engineering. Although the error and uncertainty can be estimated, it is acceptable that the accuracy of the CFD simulation is not perfect.
3. The validation process has to be realistic as well as achievable within engineering environment.

In addition, the validation process requires the flexibility, varied levels of accuracy as well as the tolerance of incremental improvements.

3.1. Estimation of Validation Errors and Uncertainty
Previously, the validation technique was defined as the process that quantifies errors and uncertainties between the computational model and the real world. Many CFD validation methodologies have been developed to quantify errors and uncertainties in different applications. Using the Line Comparison and Validation Error Quantification (LCVEQ) approach, the error has been quantified by calculating the difference between the computational and the experimental models.

Raschi et al. [42] have analyzed the blood flow field using PIV and CFD. The errors were quantified by calculating the magnitude similarity index (MSI). The MSI is based on the absolute difference between normalized outputs (Computational output and experimental outputs). The perfect accuracy is obtained when MSI is equal to 1. However, the previous approaches do not quantify the error in the simulation results due to the CFD solver’s model assumptions which may have a potential effect on the validation accuracy. To solve this problem, an accurate validation methodology for cardiovascular CFD simulation has been proposed by Paliwal et al. [41]. Paliwal strategy was based on the quantification of the errors due to the model assumption. As shown in figure 1, this methodology quantifies errors from three independent sources: model assumption errors, input errors, and numerical discretization errors. Moreover, Paliwal has demonstrated the advantage of his approach by comparing it with other validation techniques in literature.
such as Qualitative comparison [43], Line comparison and validation error quantification [40], as well as Angular and magnitude similarity approach [40].

![Diagram of validation process with error sources]

**Figure 1.** Overview of validation process with error sources according to Paliwal et al. [41].

### 3.2. Validation Hierarchy for Complex Systems

Scientists have developed several validations techniques for complicated designs. However, most of them have not been developed these tentative in depth. A common validation method is known as validation hierarchy which has been recommended by the AIAA guide [9]. The Hierarchy divides the whole system into subsystem cases, the subsystem cases are divided into benchmark cases, the benchmark cases are divided into unit problems as well. As an example, a hierarchical validation of an air-launched, air-breathing, hypersonic cruise missile was presented by Oberkampf et al. [44]. As shown in figure 2a, the missile was considered as a complete system. This complete system contains propulsion, airframe, GNC, and warhead as individual systems. These individual systems would normally be present or absent as well as other systems that can be added in other engineering designs such as ships, vehicles, etc. Each individual system contains at least one subsystem, for the cruise missile there is aero/thermal protection subsystem, a structural subsystem, as well as an electrodynamics subsystem. Each subsystem element contains at least one benchmark, the identified benchmarks are laminar and turbulent hypersonic flow with ablation, ablation of thermal protective coating, boundary-layer transition with ablation, and heat transfer to the metal substructure. The benchmark level is also divided into unit problems level. Each benchmark element contains at least one unit problem. Eight unit elements were identified: turbulent hypersonic flow, turbulent hypersonic flow with wall blowing, turbulent boundary layer interaction, boundary layer transition, low-temperature sublimation, and non-isotropic heat conduction.
Figure 2. Validation hierarchy of composed system: (a) A hypersonic cruise missile [44], (b) solid sorbent-based carbon capture [45].
Another hierarchy validation was proposed by Lai et al by studying CFD models for solid sorbent-based carbon capture [45]. Lai has validated a sequence of increasingly complex “unit problems” using statistical calibration substructures. As shown in figure 2b, the complete system has been minimized into a pilot-scale system. The pilot-scale system has been divided into two laboratories subsystems with coupled benchmark cases. The subsystem elements contain bubbling bed adsorber and moving bed regenerator. The coupled benchmark cases elements are divided into decoupled benchmark cases. The benchmark cases contain unit problems. This hierarchical validation and calibration methodology have demonstrated the significance of parallel data exchange and knowledge low in multi-physics simulations.

3.3. Calibration Process
Calibration is known as the process of enhancing the physical or numerical model parameters in computational models in order to improve the match with the experimental data. Unlike the validation, the calibration is not the process to determine the accuracy of the CFD model but it is the adjustment of the input parameters to get matched with existing experiments. The calibration process has mainly arisen when there is no enough experiment data due to some circumstances such as experiment cost, the lack of equipment, etc. [11]. Hajdukiewicz et al. [46] have presented a calibration methodology for CFD models of naturally ventilated indoor environments. This methodology describes how to perform a qualitative and quantitative V&V for a CFD model as well as performing parametric analysis by using the response surface technique to support a robust calibration process. Chen et al. [47] have studied the air quality and thermal analysis of kitchen environment. The CFD model was calibrated by testing the data obtained experimentally by measuring the fume concentration during cooking in the kitchen.

4. V&V Horizons and Perspectives
CFD is maturing. However, the professional disagreement on the procedure extraction for V&V shows that it still emerging technology. The fundamental terminology and transactions required to formalize V&V are properly established. However, effective and robust methodologies for V&V in CFD are still in the early stages of development. Intensive work is required to improve the accurate experimental and computational procedures for quantifiable and effective V&V. Although the estimation of errors is possible for simplified problems, we believe that a high accuracy solution is very limited for complex CDF simulations. As an alternative, it is recommended to perform intensive mathematical researches in order to pursue the estimation of errors. We advise researchers to perform derivations of complex solutions of the nonlinear PDEs in CFD. These solutions can be considered as benchmark solutions for complicated physics such as two and multi-phase flow, turbulence, combustion, etc.

Regarding the validation assessment, the application of the validation hierarchy for complex engineered systems still an emerging technology. However, it may have a wide application in the future as it was highly recommended by the AIAA. Consequently, it is hoped that companies and organizations that use CFD model in certification, production, or design of engineered systems to start the construction and application of validation hierarchical structure. It is well known that an effective validation hierarchy is the one that emphasizes only one single physic phenomenon at the lower level. On the other hand, it emphasizes the engineered system level at the highest levels.

5. Conclusion
V&V are the primary tools to evaluate the accuracy and reliability in computational simulations. In this paper, a detailed definition of V&V with literature review have been presented.

For the verification assessment, we have discussed the following technique: Computer programming code examination and general good programming practice. Defining the iterative, spatial, and temporal examinations with a detailed discussion of the most useful algorithms and methodologies. Moreover, the
difficulties have been faced and the solutions proposed for each examination. For validation assessment, we presented relevant methodologies for error estimation, presented the validation hierarchy as a promised technique for validation of complicated systems with some examples, as well as discussed the calibration’s methodology for CFD validations. To date, further research indeed for developing analytic and semi-analytic solutions for complex CFD, as well as developing effective methodologies for analysing convergence will have a great potential in verification assessment. Moreover, we strongly suggest further research on the validation hierarchy for complicated CFD, as it still an immerging technology, and very few works have been reported. However, it is predicted to have wide applications in validation assessments.

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