

## THE ISSUE OF NUMERICAL UNCERTAINTY

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### ABSTRACT

Computational Fluid Dynamics (CFD) computer codes have become an integral part of the analysis and scientific investigation of complex, engineering flow systems. Unfortunately, inherent in the solutions from simulations performed with these computer codes is error or uncertainty in the results. The issue of numerical uncertainty is to address the development of methods to define the magnitude of error or to bound the error in a given simulation. This paper reviews the status of methods for evaluation of numerical uncertainty, and provides a direction for the effective use of some techniques in estimating uncertainty in a simulation.

### NOMENCLATURE

$d$  diffusion coefficient  
 $h$  grid size  
 $u$  characteristic velocity  
  
 $\rho$  density  
 $\mu$  dynamic viscosity

### INTRODUCTION

Albert Einstein succinctly stated the essence of the issue of numerical uncertainty when he stated that: "As far as the laws of mathematics refer to reality, they are not certain, and as far as they are certain, they do not refer to reality." Our ability to accurately simulate complex fluid flows is limited by our mathematical or numerical approximations to the differential governing equations, our limited computer capacity, and our essential lack of full understanding of the laws of physics. Certainly we can demonstrate the ability of a numerical simulation or technique to accurately resolve a model problem (with essentially no error). However, as suggested by Einstein, those problems have little to do with reality. To be effective in design and analysis of engineering systems, users of CFD tools need to know the level of accuracy of a given simulation of realistic flows. Unfortunately, it is not common practice to estimate error in numerical simulations. The perception is that error estimation is difficult and time consuming, and that the trends are the important result rather than the magnitude of the results. Yet, the consequences of the implementation of a large scale engineering design based on inaccurate simulation results can be far more costly than that associated with the additional analysis effort.

From a fundamental viewpoint, the only effective method to advancing the state of the art in CFD is to be able to differentiate between inherent numerical errors of a simulation and those errors associated with a model. As

we all know, fluid flows of engineering and scientific interest are very difficult to accurately simulate. Nonlinear effects in these flows, historically, forced the development of robust, first-order methods that were successful because they introduced spurious damping that artificially smoothed solutions. For years, these first-order methods were used to evaluate the accuracy of turbulence models. Clearly, the ability to differentiate between the artificial viscosity introduced by these first-order numerical discretizations and the augmented viscosity due to turbulence calculated by time-averaged models was lacking. In general, complex flow physics are nearly always represented by approximate mathematical models whose accuracy needs to be assessed. A valid model assessment can only be completed when other sources of error are quantified. Improvements to these models are then only possible when numerical errors are significantly smaller than the acceptable model error.

So, how does one effectively determine the magnitude of numerical error or bound the uncertainty in a calculation. Unfortunately, methods for performing this type of analysis are an active area of research, and no consensus of the computational community has yet to be reached. Which is somewhat surprising since the most highly cited paper on this subject was written nearly 90 years ago, i.e., Richardson's paper on  $h^2$  extrapolation (1910). The intent of this paper, then, is to attempt to encapsulate the current status of the philosophy of assessing numerical error and approaches to providing an estimate of numerical uncertainty bounds.

### A BRIEF HISTORY

Evaluation of and concern for numerical accuracy has been of interest to analysts since the time of L. F. Richardson. However, the impetus for significant advancements in the understanding of numerical methods and error was the development of modern computers in 1946. The first community activity to address in some sense numerical uncertainty was the Stanford Olympics of 1968 (Kline et al., 1968). The primary objective of this meeting was to identify the fundamental predictive capabilities of early CFD codes and turbulence models, as they related to turbulent boundary layer flows. The first editorial policy statement promulgated by a journal on the control of numerical accuracy was in 1986 in the *ASME Journal of Fluids Engineering* (Roache et al., 1986). The policy statement simply stated that the journal would *not accept for publication any paper reporting the numerical solution of a fluids engineering problem that fails to address the task of systematic truncation error testing and accuracy estimation*. It did not, however, define procedures for performing such testing or estimation.

The author became involved with formulation of procedures and techniques for estimation of numerical uncertainty in the summer of 1988, when the *Fluids Engineering Division of ASME* formed the Coordinating Group on CFD. The focus of this group was to be the driving force behind a community discussion of the quantification of numerical uncertainty and to develop guidelines, procedures, and methods for verification, validation, and uncertainty estimation. Over the next 10 years, this group organized a series of ASME Forums and Symposia to discuss these topics. These sessions are documented in Celik and Freitas (1990), Celik et al. (1993), Freitas (1993a, 1995a), and Freitas and Kodama (1999). A significant outcome of these technical discussions was a new policy statement on the reporting of numerical uncertainty for archival publications in the *Journal of Fluids Engineering* (Freitas, 1993b). The essential elements of this policy statement are discussed later in this paper. Unfortunately, this policy statement led to nearly two years of intense discussions as to its appropriateness in nonacademic analysis (Freitas 1994, 1995b). Eventually, other journals adopted various forms of a policy statement to address numerical uncertainty; i.e., *AIAA Journal* and *International Journal of Numerical Methods in Fluids*, both in 1994. Finally, in 1998 the AIAA CFD Committee on Standards released the *Guide for Verification and Validation of Computational Fluid Dynamics Simulations* (AIAA G-077-1998). The purpose of this guide was to formalize definitions and basic methodology for verification and validation in CFD. It does not present techniques for estimating uncertainty.

This brief history is not intended to be comprehensive of all activities addressing numerical uncertainty. Only those that the author has been involved with directly. For a truly comprehensive review of the history of numerical uncertainty the reader is directed to Roache (1998).

## DEFINITIONS

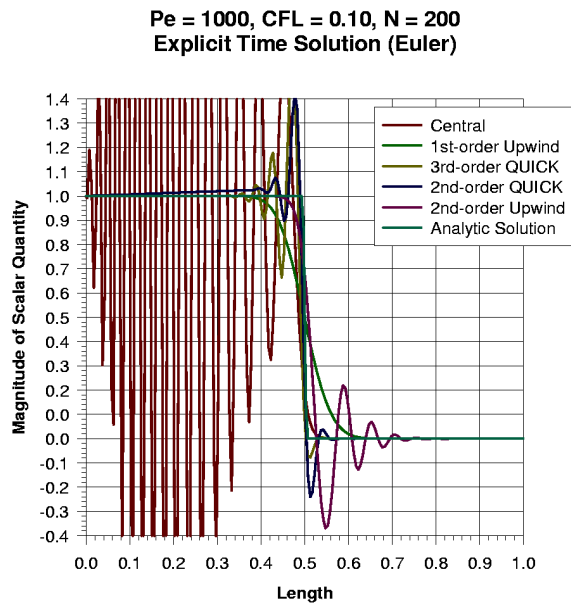
There are inherent inaccuracies in any numerical simulation of any continuum problem. These inherent inaccuracies are due solely to the fact that we are approximating a continuous system by a finite length, discrete approximation. The inherent assumption in this process is that as  $h$  (the grid size)  $\rightarrow 0$ , we recover the continuum differential equation and the exact solution. This assumption is qualified by the conditions of *consistency* and *convergence*. It is the objective of verification and validation procedures to demonstrate that the above assumption is true for each specific realization.

The reader should recognize that verification and validation are processes. Verification is defined to be the process to determine whether the mathematical model is solved correctly. Roache (1998) simplifies the definition of verification to – *solving the equations right*. Validation is defined to be the process of assessing the accuracy of the simulation model for its domain of application. Again, Roache (1998) simplifies the definition of validation to – *solving the right equations*. This succinct phrase masks an important issue, however, that the *right equations* in this context must be the sum of the effects of the mathematical model and the discretization scheme. A more informative approach is to segregate the *right equations* into the *right model equations* and the *right numerical technique*. By

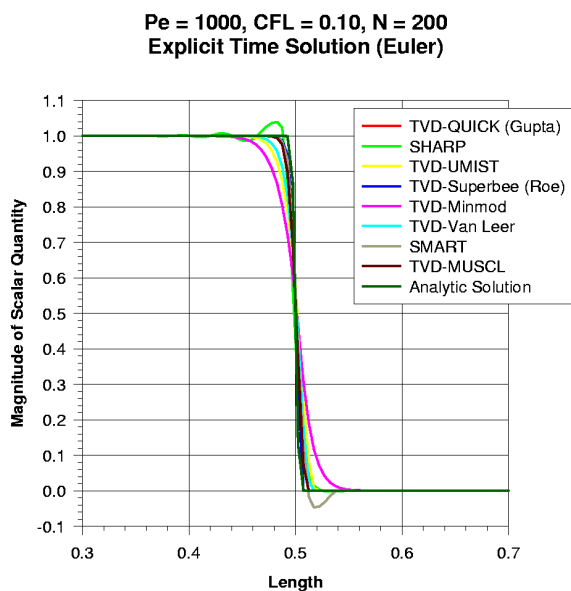
making this distinction, one can then associate error with each component and allow for identification of model shortcomings from numerical uncertainty introduced by discretization truncation. Thus, a more complete specification for validation perhaps should be – *solving the right model equations with the right methods*. For example, one could have two fully verified algorithms – we are solving the equations correctly with the specified methods. However, when we simulate a specific problem with both codes, one code successfully meets our criteria for validation, while the other code does not. The model equations are the same between the two codes, but one code solves the equations with a bounded scheme, for example, and the other solves them with an unbounded scheme. So, for certain values of the input parameters, both codes will generate the same results, but for another set of input values they generate widely different results. By allowing the distinction between the *right model equations* and the *right methods* one can then determine, in this example, that the method is generating the error and not the model equations.

Figure 1 illustrates this point by displaying the results for a boundary value problem of the time-dependent, one-dimensional, convection-diffusion equation. Figure 1a displays results from an instant in the simulation in which a series of unbounded schemes for the convective term of the partial differential equation were used. The input parameters are the Peclet number ( $Pe = \rho u h / d$ ) and the Courant number ( $CFL = u \Delta t / h$ ). Figure 1b displays similar results, for the same input parameters and the same instant in the time dependent simulation, but for a series of bounded, TVD schemes, applied to the convective term. Clearly, the unbounded schemes for this set of input parameters are not the “right method” when compared to the analytic solution, plus (without the analytic solution) we can make no judgement on the veracity of the model equation due to the characteristics (e.g. overshoots) of these convective schemes. Figure 1b, however, clearly indicates that both the model equations and the convective schemes are correct.

This example highlights two essential elements of the verification and validation processes. First, one verifies a code. Second, one validates a simulation or potentially a group of simulations. In the validation process one must be certain that the range of input parameters used are relevant to the criteria of success that the user has defined for their application. In the context of Figure 1a, if a smaller value of the Peclet number had been selected, the overshoot characteristic of some of these schemes would not have been manifested, and the validation process may have been erroneously identified as successfully completed. Finally, the objective of verification and validation is twofold. The first objective is to minimize error in the code and model equations. The second objective is to establish uncertainty bounds for a simulation.



**(a) Unbounded convective schemes**



**(b) Bounded convective schemes**

**Figure 1:** Illustration of the use of “right methods” in the validation process.

Error is defined as the difference between an observed or calculated value and a true value; e.g., variation in measurements, calculations, or observations of a quantity due to mistakes or to uncontrollable factors. Generally, error may be associated with consistent or repeatable sources, called systematic or bias errors, or they may be associated with random fluctuations which tend to have a Gaussian distribution if truly random. In the context of numerical simulations on today’s computers, systematic or bias errors are the only type of error that will occur. The only source of random error that may be introduced in a simulation is through the user, and for a single user even this error would have a bias (i.e., consistently setting a parameter to an incorrect value, for example). Systematic errors can be studied through inter-comparisons based on parameter variations, such as variation in grid resolution, variation in numerical schemes, and variation in models

and model inputs. As already discussed, error in numerical simulations does not necessarily imply a mistake or blunder. If you know about a mistake or blunder, then you can at least (in principle) fix the problem and eliminate it. However, because of the fact that we are representing a continuous system by a finite length, discrete approximation, error becomes intrinsic to the process and we can only hope at this time to minimize it. Fortunately, we do understand that this error is created by those terms truncated in the Taylor series representation of derivatives, or introduced by the iterative solution process, if appropriate. These discretization errors have a definite magnitude and an assignable cause, and can all be cast, eventually, in terms of two parameters – the grid size and the time step size.

Uncertainty is defined as the estimated amount or percentage by which an observed or calculated value may differ from the true value. Uncertainty may have three origins in a simulation: (1) input uncertainty, (2) model uncertainty, and (3) numerical uncertainty. Input uncertainty results from the fact that some input parameters are not well defined. For example, the magnitude of equation of state parameters for different materials, or the thermal conductivity of different materials. This uncertainty exists independently of the model or computer code. Model uncertainty results from alternative model formulations, structure, or implementation. Figure 2 demonstrates this type of uncertainty. Here we have a suite of computer codes that are using the same stated formulations of different time-averaged turbulence models with similar discretization schemes. However, each code implements these models differently and was written by different teams. The problem studied in Figure 2 is that of turbulent flow past a cylinder of square cross-section imbedded in a two-dimensional channel (Freitas, 1995). Displayed in Figure 2 are experimental and computed mean, axial velocity profiles along the centerline of the cylinder (blue square). Although the reported models are the same in formulation, implementation leads to significant differences between code results. Granted, not all the differences displayed in Figure 2 are due solely to implementation variations of a given turbulence model - grid resolutions were not the same across these calculations. However, one reason for differences in simulated results between commercial codes using the same formulation of a turbulence model is implementation. It should be recognized then that some error and uncertainty is introduced by this code to code variation.

Numerical uncertainty, the one of primary interest here, results from the influence of discretization and iterative convergence errors. This is the only uncertainty that can not be eliminated, but only minimized or bounded in a simulation. Input uncertainty for example, has the potential to be eliminated or made a second order effect through improved definition of the input parameter (i.e., a better-measured value) or through the use of probabilistic methods which define the uncertainty bounds for the parameter on the simulation results. Model uncertainty can be minimized, or eliminated by the use of a different model or even code. But, numerical uncertainty is a first-order effect that for the foreseeable future (until we can routinely perform simulations with spatial and temporal resolutions defined by the smallest scales) we are stuck

with. The challenge then is to develop effective error estimators that quantify this numerical uncertainty. The vision is that on-the-fly or single-grid error estimators would be imbedded directly in the solution process and, with no additional effort expended by the user, provide an error bound on the solution. The simulation result plus the error bound would then allow the user or code developer to determine when the mathematical model is incorrect. Further, such an approach would allow code users the flexibility to perform lower fidelity simulations and then state the accuracy of the simulation. So, if a 50% accurate answer is acceptable then the user could expend that level of effort in the analysis. The reader should recognize that the error bound provided by this approach is approximate, just like the value determined in experimental uncertainty analysis, but provides an essential element to fully understanding the value of the data.

To summarize, code mistakes can be eliminated through the process of verification. Model mistakes can be eliminated by the process of validation. What remains are the uncontrollable factors, those introduced by using finite length, discrete methods to represent a continuum system. The goal then is to minimize and bound these uncontrollable factors. If successful, with a verified code and a validated model, one can then state that a given predicted quantity  $f(x,y,z,t)$  is true, plus and minus an uncertainty magnitude.

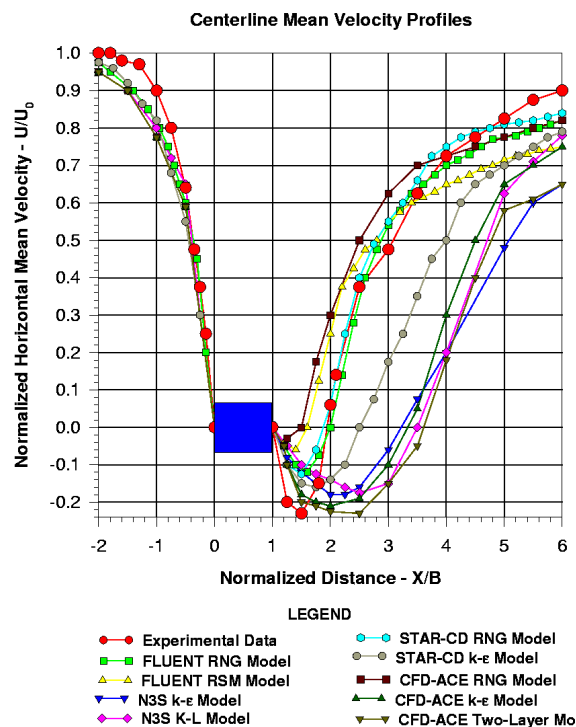


Figure 2: Uncertainty introduced by model variations.

## STANDARDS

In September of 1993, the *Journal of Fluids Engineering* defined a ten element policy statement for the control of numerical accuracy. After six years, this policy statement is still the most comprehensive set of requirements for archival publication of papers dealing with computational simulations. The ten elements of the policy statement cover documentation, verification and validation. As

stated in the policy it is *recognized that the effort to perform a thorough study of numerical accuracy may be great and that many practical engineering calculations will continue to be performed by first-order methods, on a single fixed grid. However, such analyses would not be appropriate for presentation in this archival journal. With the gains in performance of low-end workstations, it is now reasonable to require papers on solutions by CFD to meet these fundamental criteria...*

The ten elements of the policy are:

1. the basic features of the method must be described,
2. methods must be at least second-order in space,
3. inherent or explicit artificial viscosity must be assessed and minimized,
4. grid independence or convergence must be established,
5. iterative convergence must be addressed, where appropriate,
6. in transient calculations, phase error must be assessed and minimized,
7. the accuracy and implementation of boundary and initial conditions must be fully explained,
8. an existing code must be fully cited,
9. benchmark solutions may be used for validation for specific classes of problems,
10. reliable experimental results may be used to validate a solution.

Elements 1 and 8 deal with documentation issues; elements 2, 3, 6, and 7 deal with the process of verification; and, elements 4, 5, 9, and 10 deal with the process of validation. Again, as stated in the introduction to this policy statement, it was not the *intent of this ...policy statement to eliminate a class of simulations which some have referred to as "practical engineering project simulations"*. The justification by these individuals for performing a single grid simulation has been that budget constraints, schedule constraints, or computer resource constraints prevent a systematic analysis of accuracy from being performed. It is assumed that in performing CFD analyses for "practical engineering projects", for which experimental data is usually not available, that one must perform, in the natural course of the project, an evaluation of the accuracy of the simulation results in order to determine the validity of these particular calculations. Without such an effort there is no clear justification for presenting a simulation as representative of the physical phenomena. Therefore, it would seem only natural, even in the solution of practical engineering problems, that the items addressed here, be used to validate a simulation. The flexibility in this policy statement is that the techniques to be used in satisfying these elements is not specified and left to the ingenuity of the paper's authors to establish and demonstrate.

As indicated earlier in this paper, the AIAA has also recently released a guide for verification and validation. This report is presented as a first level of standards document, and is to be viewed as a guide to recommended practices. The purpose of the guide is to formalize definitions and basic methods for verification and validation in CFD. In addition to these two approaches to reporting of numerical uncertainty, there have been standards on code certification promulgated by

government agencies such as the U. S. Nuclear Regulatory Commission. These certification standards define verification, validation, and quality assurance procedures to ensure that software is error-free and that it is applicable to the application areas for which it has been designed. These procedures are designed to deal with those issues that could prevent an estimation of uncertainty. These assurances must be attained before uncertainties associated with production-level software can be determined by calculations. Quality assurance procedures or protocols (QAP) such as the NRC/SwRI TOP-018 define a set of requirements that must be met for release of computer software for production use. These requirements generally address or define documentation procedures both for code development and modification, verification procedures, validation procedures with validating data or solutions, and archival characteristics for providing a controlled version of the computer code.

It is clear that the infrastructure or framework for performing verification and validation exists. What is left is to develop and acquire a consensus among the CFD code developers and users as to the techniques to be used in reporting results of verification, validation, and uncertainty.

## STATUS

Systematic grid refinement studies are the most common approach used in assessing numerical accuracy of a simulation, when performed. Two methods of grid refinement are used, classical Richardson Extrapolation and Roache's Grid Convergence Index (GCI). GCI is in fact Richardson Extrapolation defined as a range with a safety factor of 3. Richardson Extrapolation is based on the assumption that discrete solutions  $f$  have a series representation in the grid spacing  $h$ . If the formal order of accuracy of an algorithm is known, then the method provides an estimate of the error when using solutions from two different (halved or doubled) grids. If the formal order of accuracy is not known, then three different (twice halved or doubled) grids and solutions are required to determine the order of the method and the error. Although grid doubling (or halving) is used with Richardson Extrapolation, it is not required (Roache, 1998). Assuming a 2<sup>nd</sup> order method, Richardson Extrapolation gives that

$$f_{\text{exact}} = f_r + (f_r - f_c) / (r^2 - 1) = 1.33 f_r - 0.33 f_c$$

where subscript  $f$  refers to the fine grid solution,  $c$  refers to the course grid solution, and  $r$  is the ratio of grid spacing on the two grids. Once again, Roache (1998) provides complete details on the implementation of these two methods.

Currently, methods such as Richardson Extrapolation are applied as *a posteriori* methods, or post-processor style operations. By their very nature they are applied to fully developed flow fields or steady state problems. Application of these methods in a post-processor style to time-dependent flows does require snap-shots of the flow fields, at the same instant in time on each grid system. For users of commercial codes, assessment of numerical uncertainty is only achievable through the use of a

*a posteriori* methods such as GCI or Richardson Extrapolation.

There are no successfully applied *a priori* methods for estimating numerical uncertainty. And, it is unlikely, that such methods will ever be successful, since we need to have a solution first in order to predict an error estimate, based on current methods. There are currently a few suggested methods for on-the-fly error estimation. Some adaptive grid error estimators may be a precursor to appropriate on-the-fly error estimators. However, in their current form the error predicted by adaptive methods is inappropriate for estimating levels of uncertainty. Other suggested methods use the residual or imbalance on a per zone basis of quantities which are not conserved inherently in the calculation method. The magnitude of the imbalance is then used as an error estimator (see Haworth et al., 1993).

It is the author's opinion, that Richardson Extrapolation or GCI be used to estimate numerical uncertainty in all current, worthwhile computations performed by analysts. However, for code developers, these methods do not discriminate between numerical uncertainty and model inadequacies. Further, it should be our ultimate objective to develop "dynamic" measurement techniques of numerical uncertainty. These techniques would then be imbedded directly into an algorithm and provide on-the-fly, self-diagnostics of the simulation. The challenge then is to derive and formulate measures of local and global error that can be used dynamically in calculations. If successful, these measures could become a standard library package, such as LINPACK or NSPCG that can be easily integrated into any algorithm.

## CONCLUSION

Computational Fluid Dynamics (CFD) computer codes have become an integral part of the analysis and scientific investigation of complex, engineering flow systems. Unfortunately, inherent in the solutions from simulations performed with these computer codes is error or uncertainty in the results. These inherent inaccuracies are due solely to the fact that we are approximating a continuous system by a finite length, discrete approximation. The issue of numerical uncertainty is to address the development of methods to define the magnitude of error or to bound the error in a given simulation. The objective of this paper has been to attempt to encapsulate the current status of the philosophy of assessing numerical error and approaches to providing an estimate of numerical uncertainty bounds. It is suggested that for users of commercial codes, assessment of numerical uncertainty be performed through the use of *a posteriori* methods such as Grid Convergence Index or Richardson Extrapolation. It is further recommended that the challenge be for the CFD community to derive and formulate measures of local and global error that can be used dynamically in calculations and thus provide on-the-fly diagnostics of a given simulation.

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