Validation Procedure for 3rd Workshop on CFD Uncertainty Analysis

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Introduction

The required validation procedure is adapted from the following ASME/ANSI Standard document, cited herein as V&V 20.

ASME V&V 20-2008: Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer, ASME Committee PTC 61, (expected) 2008

This document uses internationally accepted concepts of uncertainty defined in the following document on experimental procedures, also an ASME/ANSI Standard document.

ANSI/ASME PTC 19.1-2005. 2006. Test Uncertainty. ASME, New York, NY.

The validation process is preceded by Code Verification and Calculation (Solution) Verification. Code Verification (required only for those code options involved in the validation problem) shall be achieved using the Method of Manufactured Solutions. Calculation (Solution) Verification shall be achieved using the GCI or Least Squares GCI, or any other method for uncertainty estimation. If non-GCI methods are used, note that (1) any methods for error estimation (e.g. single-grid error estimation methods) must provide error estimates for the validation quantities of engineering interest, and (2) these error estimates must be used to obtain uncertainty estimates, e.g. by being multiplied by a Factor of Safety F_s (as in the GCI procedure).

The Workshop Validation Procedure

The validation procedure for the Workshop, to be applied to the ERCOFTAC C-30 test case, is a simple version of the more general and elaborate V&V 20 procedure. It assumes independence of error sources and fixed parameters ("strong model" concept), and uses a target uncertainty level of 95% confidence¹, consistent with the GCI. The objective is to evaluate the validation comparison error E and the validation uncertainty U_{val} and to interpret the result, according to the following prescriptions.

The validation comparison error E is defined as the difference between the Simulation value and the experimental Data value.

$$E = S - D \tag{1}$$

The validation uncertainty U_{val} at 95% confidence level is estimated as

$$U_{val} = \sqrt{U_{num}^2 + U_{input}^2 + U_D^2} . {2}$$

 U_{num} is the 95% confidence level estimate of numerical uncertainty; if the GCI or Least Squares GCI is used, $U_{num} = \text{GCI}$. U_D is the experimental \underline{D} ata uncertainty, also at the 95% confidence level. U_{input} is due to parameter uncertainty, = 0 for the strong model concept (but see "Parameter Uncertainty" below).

Interpretation of Validation Results Using E and U_{val}

The validation comparison error E = S - D can also be written in terms of component errors δ as

$$E = \delta_{\text{mod }el} + \delta_{\text{num}} + \delta_{\text{input}} - \delta_{D}$$
 (3)

The term δ_{model} is the modeling error which we intend to assess. It is composed of the errors in the governing *continuum* equations of the model (e.g. the RANS model used) and errors due to any other non-ordered approximations such as inflow and outflow boundary conditions; these

¹ The more general V&V20 procedure (a) covers in detail the important cases wherein error sources are not independent, (b) treats input parameter uncertainties, and (c) uses standard uncertainties in all derivations so that any confidence level can be chosen by the user.

errors do $not \to 0$ as $\Delta \to 0$ (where Δ is a representative measure for the grid cell size). The error δ_{num} is composed of the ordered numerical errors; these errors $do \to 0$ as $\Delta \to 0$. The error δ_{input} is composed of the (non-ordered) errors arising from the use of incorrect parameter values in the model equations. Here we use a strong model concept so that $\delta_{input} = 0$. The error δ_D is composed of the total experimental errors.

A validation *standard* uncertainty u_{val} (referred to in the V&V 20 procedure) is defined as an estimate of the standard deviation of the parent population of the combination of all errors $(\delta_{num} + \delta_{input} - \delta_D)$ except the modeling error. Once a validation exercise has determined values S and D of a validation variable, then the sign and magnitude of the validation comparison error E = S - D are known. $(E \pm u_{val})$ then defines an interval within which δ_{model} falls (with some as-yet unspecified degree of confidence). Thus E is an estimate of δ_{model} and u_{val} is the standard uncertainty of that estimate and can properly be designated as u of δ_{model} or u_{val} . For the simple validation procedure of the Workshop, we use the more specific and common engineering target U_{val} with 95% confidence, rather than standard uncertainty u_{val} .

Thus, $(E \pm U_{val})$ defines an interval within which δ_{model} falls, with ~95% confidence, or

$$\delta_{\text{mod }el} \in [E - U_{VAL}, E + U_{VAL}], Confidence \sim 95\%$$
 . (4)

Application

(1) If
$$|E| \gg U_{\text{val}} \tag{5}$$

then probably $\delta_{\text{model}} \approx E$.

(2) If
$$|E| \le U_{\text{val}} \tag{6}$$

then probably δ_{model} is of the same order as, or less than, $(\delta_{num} + \delta_{input} - \delta_d)$.

In the first case one has information that can possibly be used to improve the model (i.e., reduce the modeling error). In the second case, however, the modeling error is within the "noise level" imposed by the numerical, input, and experimental uncertainties, and formulating model improvements is more problematic.

Parameter Uncertainty

Although evaluation of parameter uncertainty U_{input} (or, as in V&V 20, u_{input}) is highly recommended for thorough validation exercises, it is not strictly necessary, since the decision of which parameter values to include in U_{input} and which to consider hard-wired is somewhat arbitrary. The limit situation of all parameter values fixed has been termed the strong model concept, in which $U_{input} = 0$ by definition. Regardless of which parameters (if any) are included in U_{input} , nothing is ignored in the validation procedure. The errors and uncertainties are still present and produce error and uncertainty in the final model validation; E = S - D is not changed.

To obtain an estimate of U_{input} , the sensitivity of the simulation results (in the quantities of interest) to parameter variation must be determined numerically, and an estimate of the distribution of these input parameters must be made. The two methods described in V&V 20 are based on an uncertainty propagation method (local) and a sampling (Monte Carlo) Note that in situations (not uncommon) in which the same parameter uncertainty affects both the simulation and the experimental uncertainty (via experimental data reduction dependencies) it is not possible to separate the three contributions to uncertainty as in Eq. 2. Instead, U_{val} must be estimated in a tightly coupled and complicated procedure to avoid problems. (One particular problem is the case where the effects of a parameter uncertainty should approximately cancel between U_{input} and U_D if treated correctly, but will contribute two terms if Eq. 2 is used.) The estimation of U_{val} (or u_{val}) in such coupled cases is at the core of the methodology presented in V&V 20. For the Workshop exercises, we will assume that U_{input} and U_D may be determined independently, and use Eq. 2.

It is not required to investigate parameter sensitivity for the Workshop participation, but such results would be of great interest. At this stage in the development of RANS turbulence models, it is probably not of interest to further investigate numerical parameters of these models. The most significant candidates for parameter uncertainty are the inflow boundary

conditions, and to a lesser extent the outflow conditions. (The latter can in principle be made negligible by using a long enough computational domain L and possibly by extrapolation to $L = \infty$.)

Summary of Workshop Activities

Required:

- 1. Code Verification by MMS
- 2. Calculation (Solution) Verification for the ERCOFTAC C-30 test case (Local and Integral flow quantities identical to the previous editions of the Workshop)
- 3. Validation exercise for the ERCOFTAC C-30 test case:
 - a) Estimation of $U_{num} = GCI$ or Least Squares GCI or other 95% uncertainty estimator (not merely an error estimator).
 - b) Evaluation of:
 - the validation comparison error E from Eq. (1)
 - the validation 95% uncertainty U_{val} from Eq. (2)
 - c) Interpretation of the validation results using Eqs. (4,5,6)

Optional:

Evaluation of parameter sensitivity and/or uncertainty [using U_{input} in Eq. (2)], preferably to assess the significance of the inflow boundary conditions.