ITTC Quality System Manual Recommended Procedures and Guidelines

Uncertainty Analysis in CFD Verification and Validation, Methodology and Procedures

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Abstract

The purpose of this guide is to provide a general overview of Verification, Validation, and Uncertainty Assessment (VVUA) as it relates to CFD for the ITTC. This guide seeks to provide a current set of definitions of the different aspects of the field of VVUA, and to provide references to several published methods that have shown to be practically useful for ITTC members to conduct VVUA analysis. Verification is the process that establishes the mathematical correctness of a computational model with respect to reference values that are used for comparison. Validation intends to identify modelling errors, the difference between the mathematical model and reality, which inevitably requires comparison with experimental data. Uncertainty assessment intends to quantify mathematically the uncertainties that arise from all sources present in calculation results, or collection of experimental data. This guide provides two approaches for VVUA along with step-by-step examples and discussions on practical issues such as the use of unstructured grids and wall functions.

Uncertainty Analysis in CFD, Verification and Validation Methodology and Procedures

1. PURPOSE OF PROCEDURE

The purpose of this guide is to provide a general overview of Verification, Validation, and Uncertainty Assessment (VVUA) as it relates to CFD for the ITTC. Here CFD is defined as solutions to the Reynolds-averaged Navier-Stokes (RANS) equations.

A companion guide 7.5-03-01-02 Quality Assurance in Ship CFD Application provides a Best Practice Guideline (BPG), quality assessment of the BPG methodology, and demonstration of quality, which can support the use of the present guide in practical ship CFD applications.

2. VERIFICATION AND VALIDATION METHODOLOGY

It is important to conduct uncertainty analysis to assess the accuracy of CFD predictions. There are several decades of research into different theories and methodologies for performing VVUA, and the historical developments of VVUA closely follow the development of the field of CFD itself. This guide does not cover the entire history of VVUA, nor does it summarize a single procedure that is suitable for the full range of calculations that are conducted by ITTC members. What this guide seeks to provide is a current set of definitions of the different aspects of the field of VVUA, and to provide references to several published methods that have shown to be practically useful for ITTC members to conduct VVUA analysis.

2.1 Definitions

In the ITTC context the goal of VVUA in CFD is to quantify numerical and modelling errors for practical calculations of complex turbulent flows. There has been a continual evolution of terminology as the field has advanced over the last several decades, and currently the process of VVUA can be described by three different activities.

1. Verification
2. Validation
3. Uncertainty Assessment

The following definitions of these activities are based directly on the International Standard of the American Society of Mechanical Engineers: VVUQ 1 – 2022.

2.1.1 Verification

Verification is the process that establishes the mathematical correctness of a computational model with respect to reference values that are used for comparison. Verification can be categorized as either code verification or solution verification.

Code Verification intends to verify that a given code correctly solves the equations of the model (RANS) that it contains. Thus, it compares the computational model to the mathematical model. Few exact (closed-form or analytical) solutions are available for assessing the accuracy of the computational results, so the method of manufactured solutions is commonly

used to provide a reference solution. Code verification is regarded as the responsibility of the code developer and is not a typical activity for ITTC members.

Solution Verification intends to estimate the error (which is usually impossible to determine for lack of the truth) or uncertainty (which is an estimate of the error) of a given calculation for which in general the exact solution is not known. The same computational model can produce different solutions due to the error sources of mesh discretization, number of iterations of the nonlinear or linear equations, and computer precision. Solution verification may need to be performed for each use of a computational model as the solution verification results may vary with changes to initial conditions, boundary conditions, gradients of the dependent variables, and modeling options.

2.1.2 Validation

Validation intends to identify modelling errors, the difference between the mathematical model (solution from simulation) and reality (physical truth), which inevitably requires comparisons with experimental data. It requires the estimation of experimental, numerical, and input uncertainties.

2.1.3 Uncertainty Assessment

Uncertainty Assessment (UA) intends to quantify mathematically the uncertainties that arise from all sources present in calculation results, or collection of experimental data. It is the process of generating and applying mathematical models to provide a measure of uncertainty in the empirical data or simulation results. There are two fundamental parts of UA, the error, and the uncertainty.

Error is the difference between a measured or a calculated value and the true value. Since the true value is rarely known, it is usually not possible to quantify error directly.

Uncertainty is the recognition of the imperfect knowledge about a system or quantity of interest. The recognition of uncertainty leads to the need to estimate the error, which is a primary goal of performing VV and UA.

3. VERIFICATION PROCEDURES

In steady CFD computations solution verification is performed by estimating the numerical uncertainty from solutions obtained on systematically refined grids. The error is estimated with power series expansions as a function of the typical cell size (Richardson extrapolation or RE). The error estimate from RE is converted to an uncertainty by multiplying it with a factor of safety to account for any complexities that are neglected in the conceptualization of Richardson extrapolation.

The literature on uncertainty analysis is vast, and it is recommended to consider the following two procedures that have shown to be useful to perform uncertainty analysis for ship CFD computations. These will be referred to as

1. The method of Stern et al. (Xing and Stern, 2010)

2. The method of Eça and Hoekstra. (Eça and Hoekstra, 2014)

Both methods use an asymptotic expansion of the simulation result that depends on the step size h as

$$S = S_0 + \alpha h^p + o(h^p) \quad (1)$$

where, S is simulation result, S_0 is the exact solution, and the coefficient α and the exponent p

are determined by using a set of different grids solving the same problem of interest. Then, the numerical discretization error is estimated as

$$\delta = S - S_0 \tag{2}$$

The method of Stern et al. determines the numerical uncertainty from solutions on three grids when only the first leading term of Eq. (1) is considered.

The method of Eça and Hoekstra determines the numerical uncertainty from solutions on at least four grids. Regardless of the number of grids, there is scatter in the numerical data due to a number of sources. To minimize the influence of the scatter the method Eça and Hoekstra uses a least-square fit through the data. Another advantage of using a fit to four or more grids is that the quality of the fit can be measured and used as an indicator of the accuracy of the error model.

Careful considerations on convergence conditions should be given while using the above methods. For a set of three solutions S_i, where i = 1, 2, and 3 representing the fine, medium, and coarse grid, respectively, the changes between the medium-fine $\varepsilon_{21} = S_2 - S_1$ solutions and the coarse-medium $\varepsilon_{32} = S_3 - S_2$ solutions are used to define a convergence ratio as

$$R = \varepsilon_{21}/\varepsilon_{32} \tag{3}$$

Depending on the sign and magnitude of R, the solutions exhibit one of the following four behaviours with the grid refinement:

i. Monotonic convergence for $0 < R < 1$
ii. Monotonic divergence for $R > 1$
iii. Oscillatory convergence for $-1 < R < 0$
iv. Oscillatory divergence for $R < -1$

For the monotonic convergence condition, both the method of Stern et al. and the method of Eca and Hoekstra work equally well. However, each method deals the other convergence conditions quite differently. The method of Stern et al. states that errors and uncertainties cannot be estimated for the monotonic and oscillatory divergence conditions but uses a certain error treatment method for the oscillatory convergence condition. Herein, only the monotonic convergence case of the method of Stern et al. is introduced and the readers are referred to Stern et al. (2006) for the other convergence cases. On the other hand, the method of Eca and Hoekstra states that for "practical problems" of complex geometries and complex equations data can be noisy with scatters in them and uses error estimators for the convergence conditions (ii) – (iv).

3.1 The method of Stern et al.

For monotonic convergence condition, generalized Richardson Extrapolation (RE) is used to estimate the error δ in Eq. (2). The error is expanded in a power series expansion of grid spacing Δx corresponding to the step size h in Eq. (1). The accuracy of the estimate depends on how many terms are retained in the expansion, the magnitude (importance) of the higher-order terms, and the validity of the assumptions made in RE theory.

With solutions on three different grids, only the leading term can be estimated, which provides direct estimates for order of accuracy and error as

$$p = \frac{\ln(\varepsilon_{32}/\varepsilon_{21})}{\ln(r)} \tag{4}$$

$$\delta_{RE} = \frac{\varepsilon_{21}}{r^p - 1} \tag{5}$$

A factor of safety approach (Roache, 1998) can be used to define the uncertainty U where an error estimate from RE is multiplied by a factor of safety FS to bound simulation error as

$$U_{FS} = FS \cdot |\delta_{RE}| \quad (6)$$

Xing and Stern (2010) define a distance metric P as the ratio of the estimated order of accuracy, p_{RE} to the theoretical order of accuracy, p_{th} as

$$P = p_{RE}/p_{th} \quad (7)$$

and derived FS as functions of P as

$$FS(P) = \begin{cases} 2.45 - 0.85P, & 0 < P \leq 1 \\ 16.4P - 14.8, & P > 1 \end{cases} \quad (8)$$

determined using a statistical analysis for a large number of samples based on analytical or numerical benchmarks.

3.2 The method of Eça and Hoekstra

To account for scatter in the numerical solutions, common in complex flows with relatively coarse grids, or where the use of unstructured grids leads to variability in the grids, the error can be estimated using a Least Squares Root method (LSR) by Eça and Hoekstra (2014).

This requires solutions on at least four different grids to perform a curve fit of

$$\phi_i = \phi_0 + \alpha {h_i}^p \quad (9)$$

in the least-squares sense to determine the estimate of the exact solution ϕ_0, the coefficient α, and the observed order of accuracy p. Then, an error estimate can be written as follows.

$$\delta_{RE} = \phi_i - \phi_0 = \alpha {h_i}^p \quad (10)$$

Since p is strongly influenced by the amount of scatter in the solutions, such that it may be larger than the theoretical order of accuracy, leading to an underestimate of the error, three alternative error estimates are provided, also found by curve fitting.

$$\delta_1 = \alpha h_i \quad (11)$$

$$\delta_2 = \alpha {h_i}^2 \quad (12)$$

$$\delta_{12} = \alpha_1 h_i + \alpha_2 {h_i}^2 \quad (13)$$

in Eqns. (11) and (12), the subscript i is the grid number from 1 to the number of grids, and $h_i$is the grid (or the time-step) size.

Appendices A and B in Eça and Hoekstra (2014) provide the Least-Squares solutions and the standard deviation σ of the curve-fits using Eqns. (11) – (13), both with and without using weights.

The uncertainty estimation is determined by first by defining a data range parameter to judge the quality of the data fit as

$$\Delta_\phi = \frac{(\phi_i)_{\max} - (\phi_i)_{\min}}{(n_g) - 1} \quad (14)$$

For $\sigma < \Delta_\phi$,

$$U(\phi_i) = F_S \epsilon_\phi + \sigma + |\phi_i - \phi_{\text{fit}}| \quad (15)$$

For $\sigma \geq \Delta_\phi$,

$$U(\phi_i) = 3\frac{\sigma}{\Delta_\phi}\left(\epsilon_\phi + \sigma + |\phi_i - \phi_{\text{fit}}|\right) \quad (16)$$

The error estimate ϵ_ϕ in Eqns. (15) and (16) is chosen based on the observed order of accuracy, p. For $0.5 \leq p \leq 2$, $\epsilon_\phi \cong \delta_{RE}$ from Eq. (10) is used. For $p > 2$, between δ_1 and δ_2, the one with the smaller σ is used as ϵ_ϕ, and for $p < 0.5$, the one with the smallest σ is chosen among δ_1, δ_2, and δ_{12}.

The factor of safety F_S in Eq. (15) is chosen based on both the observed order of accuracy p and the data range parameter Δ_ϕ. For $0.5 \leq p < 2.1$ and if $\sigma < \Delta_\phi$, $F_S = 1.25$ is used, whereas $F_S = 3$ is used otherwise.

3.3 Practical issues

The practical issues of iterative convergence, unstructured grids, and wall functions are considered in this section.

Iterative and parameter convergence studies are to be conducted using multiple solutions (at least 3) with systematic parameter refinement by varying the i^{th} input parameter Δx_i (or h_i), while holding all other parameters constant. Richardson Extrapolation assumes that input parameters are selected such that the finest resolution corresponds to range where the leading-order error term in the Taylor series dominates all other terms, and this is also called the *asymptotic range*. In practice this it is rarely possible to build a sufficiently fine grid such that one can prove that the solution is in the asymptotic range. This means additional ad hoc measures are required to adapt RE for application to ship CFD, hence the different methods of Xing and Stern (2010) and Eça and Hoekstra (2014), among others.

Another important consideration is that nearly all ship CFD grids have stretching in the spatial discretization, and many grids are unstructured. RE is most clearly applied for uniform structured grids, which are employed in only the rarest cases for ship CFD. In order to account for the stretching and unstructured nature of most CFD grids in application, it is important to generate the set of grids that are refined with a systematic relationship between the different grids. This means the local ratio of the grid size between any two grids is nearly constant throughout space. If this is done, then a single grid metric can be calculated to represent the grid spacing for each grid. For example, the grid spacing for a grid with three spatial dimensions can be calculated as the cube root of the ratio of the volume of the entire grid divided by the number of cells in the grid.

Additionally, a uniform parameter refinement ratio

$$r = \frac{\Delta x_{i,2}}{\Delta x_{i,1}} = \frac{\Delta x_{i,3}}{\Delta x_{i,2}} = \frac{\Delta x_{i,m}}{\Delta x_{i,m-1}} \tag{17}$$

between solutions is assumed for presentation purposes, but not required. Iterative errors must be accurately estimated or negligible in comparison to errors due to input parameters before accurate convergence studies can be conducted.

Careful consideration should be given to selection of uniform parameter refinement ratio. The most appropriate values for industrial CFD are not yet fully established. Small values (i.e., very close to one) are undesirable since solution changes will be small and sensitivity to input parameter may be difficult to identify compared to iterative errors. Large values alleviate this problem; however, they also may be undesirable since the finest step size may be prohibitively small (i.e., require many steps) if the coarsest step size is designed for sufficient resolution such that similar physics are resolved for all m solutions. Also, solution changes for the finest step size may be difficult to identify compared to iterative errors since iterative convergence is more difficult for small step size. Another issue is that for parameter refinement ratio other than $r = 2$, interpolation to a common location is required to compute solution changes, which introduces interpolation errors. Roache (1998) discusses methods for evaluating interpolation errors. However, for industrial CFD, $r = 2$ is too large in most cases. A good alternative may be $r = \sqrt{2}$, as it provides fairly large parameter refinement ratio and at least enables prolongation of the coarse-parameter solution as an initial guess for the fine-parameter solution.

A final practical issue that requires attention is the challenge of refining the grid in the near-wall region. If a wall-resolved grid is used for the finest grid, then systematic refinement can

be pursued without any further consideration. On the other hand, wall-functions are often used, especially for full-scale Reynolds number simulations. In this case, as the near-wall mesh is refined, the wall-function introduces an error that is fundamentally different than the discretization error, and often its role is significant and can confound the uncertainty assessment activity. It is encouraged to in the least ensure that the multiple sets of grids used in the UA activity are in logarithmic regime.

To summarize the practical issues.

1. Iterative convergence should be monitored and users should ensure that it is negligibly small.
2. A refinement ratio should be chosen as large as possible that allows for a meaningful solution on the coarse grid and a fine solution that is computationally affordable.
3. On unstructured grids care should be taken to keep the local refinement ratio constant throughout the domain.
4. When wall functions are used it is best to keep the near wall spacing constant for the set of grids used in the VVUA study.

3.4 Verification Examples

Steady-state simulations performed for the JBC and KCS cargo/container ship (Starke et al., 2024) are used to demonstrate the use of the two different verification approaches introduced in Sections 3.1 and 3.2.

The JBC simulations were done by the Shipbuilding Research Centre of Japan (SRCJ). Simulation conditions for the calculations are Froude number Fr = 0.14 and Reynolds number Re = 7.4×10^6.

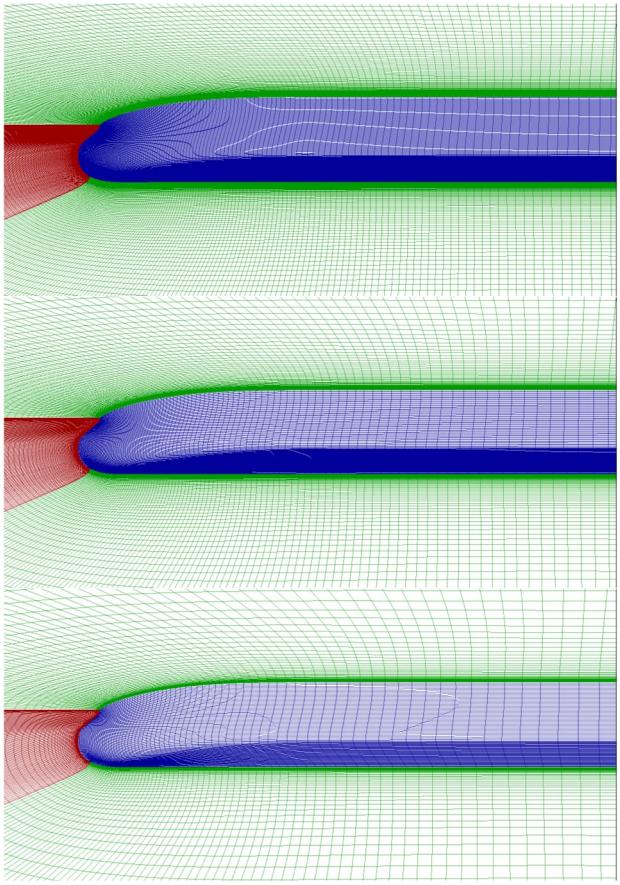

Figure 1. Grid meshes used for JBC simulations (Grid 1, Grid 3, and Grid 5 from the top).

Figure 1 shows a few of example plots of the grid mesh. The grid topology is an OO-type structured mesh. The outer boundary shape is a hemispherical ellipsoid with upper-lower symmetric boundary conditions applied by the assumption of a double-model flow. Grid studies were conducted using a total of five grids (n_g = 5), with the grid refinement ratio $r = \sqrt[4]{2}$.

Table 1. Grid data and the outcomes of the JBC simulations.

Grid, i	Total number of points, N_i	r_i	C_{FM} (e-3)	C_{TM} (e-3)
1	25,088,000	1.000	3.2148	4.0957
2	15,482,880	1.175	3.2116	4.0991
3	9,216,000	1.396	3.2075	4.1015
4	5,483,520	1.660	3.2021	4.1060
5	3,354,624	1.956	3.1945	4.1099

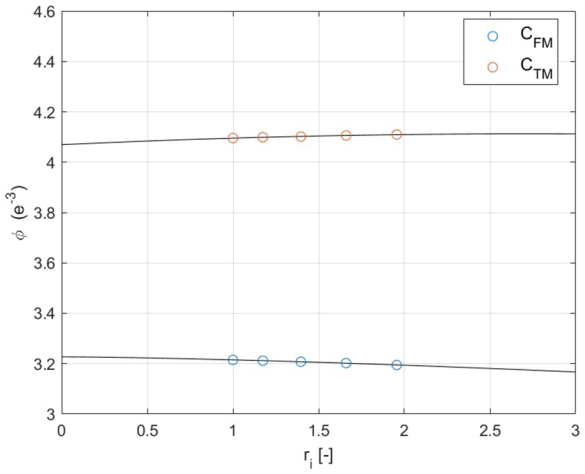

Figure 2. JBC simulation results.

Table 1 presents the grid data and the simulation results. The variable selected for the present verification are the friction resistance coefficient C_{FM} and the total resistance coefficient C_{TM}. Figure 2 shows the simulation outcomes as functions of the grid refinement ratio r_i. Here, r_i is the relative grid spacing with respect to the spacing of the finest grid (i.e., the Grid 1) and is defined as

$$r_i = \sqrt[3]{N_1/N_i} \tag{18}$$

Note that this r_i is different from the uniform refinement ratio $r = \sqrt[4]{2}$ mentioned above (see Eq. (17) for its definition).

First, the method of Stern et al. is used for a set of three grids, Grids 1, 3, and 5. The grid refinement ratio is $r = \left(\sqrt[4]{2}\right)^2 = \sqrt{2}$ for this grid-triplet. To check the convergence condition of this data set, the convergence ratio is calculated per Eq. (3) as

$$R = \frac{3.2075 - 3.2148}{3.1945 - 3.2075} = 0.567$$

Since $0 < R < 1$, the data converges monotonically. The observed order of accuracy p and the error δ_{RE} are calculated using Eq. (4) and Eq. (5), respectively as

$$p = \frac{\ln(-0.0130/-0.0074)}{\ln\sqrt{2}} = 1.69$$

$$\delta_{RE} = \frac{-0.0074}{\left(\sqrt{2}\right)^{1.69} - 1} = -0.00964$$

Next, the distance metric P in Eq. (7) and a factor of safety FS in Eq. (8) are calculated as

$$P = 1.69/2 = 0.845$$

$$FS = 2.45 - 0.85 \times 0.845 = 1.73$$

where, the theoretical order of accuracy $p_{th} = 2$ is used for the P calculation. Lastly, the uncertainty is estimated by using Eq. (6) as

$$U_{FS} = 1.73 \times |-0.00964| = 0.0167$$

corresponding to 0.52% of C_{FM} of Grid 1. The uncertainty for C_{TM} can be estimated in a similar way.

Next, the method of Eça and Hoekstra is used. Since this method requires a set of four or more grids (without an upper limit), all the 5 grids are used. Table 3 presents a summary of the assessment results.

For $\phi = C_{FM}$, first Eq. (9) is solved for ϕ_0, α, and p using the least-squares method. Here, Eq. (9) is rewritten as

$$\phi_i = \phi_0 + \alpha^* r_i^p \tag{19}$$

where, $\alpha^* = \alpha \cdot h_1^p$ and $r_i = h_i/h_1$ is equivalent to Eq. (18). The solution gives $p = 1.717$ that satisfies $0.5 \le p \le 2$, thus δ_{RE} in Eq. (10) is selected as the error estimator ϵ_ϕ, with α and h_i replaced with α^* and r_1, respectively,

$$\epsilon_\phi(\phi_1) = |-0.0093 \times (1)^{1.717}| = 0.0093$$

Table 2. Uncertainty assessment results by using the method of Stern et al. for JBC.

Variable	C_{FM}	C_{TM}
R	0.567	0.688
ε_{21}	-0.0074	0.0058
ε_{32}	-0.0130	0.0084
p	1.69	1.12
δ_{RE}	-0.00964	0.01274
p_{th}	2	2
P	0.845	0.558
FS	1.73	1.98
U_{FS}	0.0167	0.0252
$U_{FS}(\%S_1)$	0.52	0.61

Table 3. Uncertainty assessment results by using the method of Eça and Hoekstra for JBC.

Variable	C_{FM}	C_{TM}
ϕ_0	3.2240	4.0748
α^*	-0.0093	0.0225
p	1.717	0.7216
σ	0.0001	0.0002
Δ_ϕ	0.0051	0.0036
$\epsilon_\phi(\phi_1)$	-0.0093	0.0225
F_S	1.25	1.25
$U_\phi(\phi_1)$	0.0118	0.0286
$U_\phi(\%\phi_1)$	0.37	0.70

The data range parameter is calculated as

$$\Delta_\phi = \frac{3.2148 - 3.1945}{5 - 1} = 0.0051$$

The safety factor is chosen as $F_S = 1.25$ since $0.5 \leq p < 2.1$ and $\sigma < \Delta_\phi$. Lastly, the uncertainty is calculated using Eq. (15), again since $\sigma < \Delta_\phi$,

$$U(\phi_1) = 1.25 \times 0.0093 + 0.0001 + |3.2148 - 3.2147| = 0.0118$$

corresponding to 0.37% of ϕ_1. Here, $\phi_{\text{fit}} = 3.2147$ is obtained from the least-squares curve-fit. Similar calculations can be made for $\phi = C_{TM}$, resulting in $U_\phi(\phi_1) = 0.70\%$. It is noted that the U_ϕ values are comparable with the U_{FS} values in Table 2 by using the method of Stern et al. for both variables.

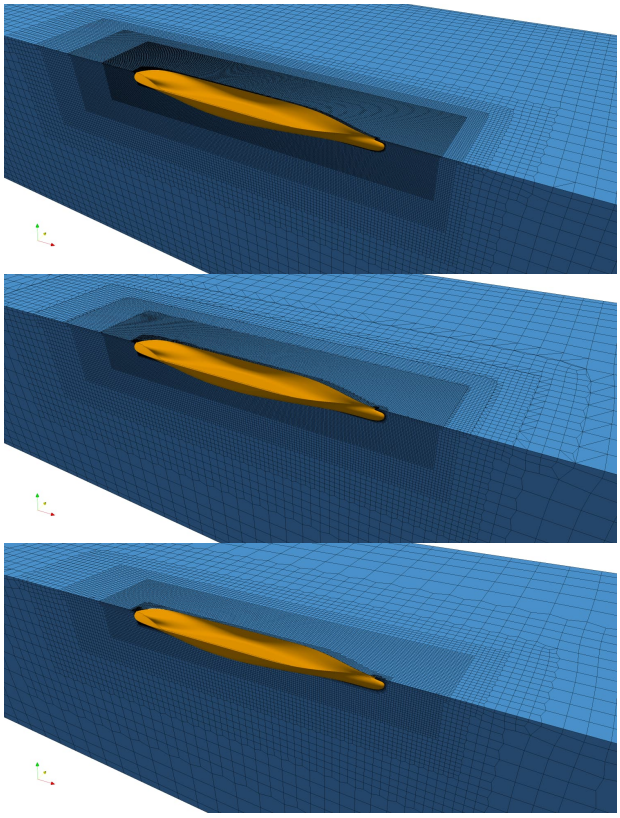

Figure 3. Grids used for KCS simulations (Grid 1, Grid 3, and Grid 5 from the top).

The next example is the KCS simulations done by the University of Genova (UniGe), Italy. Simulation conditions are Froude number Fr = 0.26 and Reynolds number Re = 1.4×10^7. Grid studies were conducted for a total of six grids ($n_g = 6$). The grid topology is an unstructured hex-dominant cartesian mesh on a parallel-piped domain. Figure 3 shows example mesh plots for three grids.

Table 4. Grid data and the outcomes of the KCS simulations.

Grid	Total number of points	r_i	C_{FM} (e-3)	C_{TM} (e-3)
1	12,444,794	1.000	2.8074	3.0632
2	7,368,997	1.191	2.8091	3.0708
3	3,432,556	1.536	2.8476	3.1253
4	1,902,446	1.870	2.8402	3.1482
5	1,084,560	2.256	2.8504	3.1710
6	642,810	2.685	2.8571	3.1901

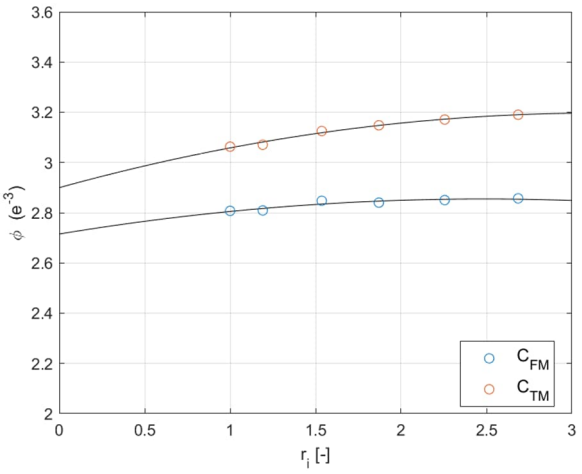

Figure 4. KCS simulation results.

Table 5. Uncertainty assessment results by using the method of Eça and Hoekstra for KCS.

Variable	C_{FM}	C_{TM}
ϕ_0	2.8804	4.7707
α^*	-0.0761	-1.7126
p	-1.209	-0.08351
σ	0.0041	0.0037
Δ_ϕ	0.0099	0.02538
$\epsilon_\phi(\phi_1)$	0.0898	0.1584
F_S	1.25	1.25
$U_\phi(\phi_1)$	0.1186	0.2067
$U_\phi(\%\phi_1)$	4.23	6.75

Table 4 and Figure 4 present the grid data and the outcomes of the KCS simulations for C_{FM} and C_{TM}. This example shows how it is often not possible to have the refinement ratio be constant throughout the domain, yet the user has attempted to keep it constant in the grid generation process. Thus, the present grid-set does not have a uniform grid refinement ratio and this fact precludes the use of the method of Stern et al.

Table 5 presents a summary of the uncertainty assessment results by using the method of Eça and Hoekstra. The overall calculation procedures are the same for the JBC case, i.e., determination of the observed order-of-accuracy p, selection of a proper error estimator δ, and the assessment of the uncertainty U_ϕ by using the least-squares fit along with the choice for a safety factor F_S. One difference compared to the JBC case is the selection for δ. From Table 5, both C_{FM} and C_{TM} data show $p < 0.5$ and δ is to be selected among δ_1, δ_2, or δ_{12} in Eq. (11) – (13). The choice is the one that gives the smallest standard deviation σ value from the data curve-fits. Both the C_{FM} and C_{TM} data show the smallest σ when δ_{12} is used, which is used to calculate ϵ_ϕ in Table 5. The resulting $U_\phi(\phi_1)$ values are larger than the JBC case, 4.23% and 6.75% for C_{FM} and C_{TM}, respectively.

4. VALIDATIOAN PROCEDURES

4.1 Validation Methodology

Validation is defined as a process for assessing simulation modelling uncertainty U_{SM} by using benchmark experimental data and, when conditions permit, estimating the sign and magnitude of the modelling error δ_{SM} itself.

The simulation error δ_S is defined as the difference between a simulation result S and the truth T and is composed of additive modelling δ_{SM} and numerical δ_{SN} errors (i.e., $\delta_S = S - T = \delta_{SM} + \delta_{SN}$). The error in data δ_D is the difference between the data and the truth (i.e., $\delta_D = D - T$). The comparison error E is given by the difference in the data $D$and simulation S values.

$$E = D - S = \delta_D - (\delta_{SM} + \delta_{SN}) \tag{20}$$

Numerical error δ_{SN} is decomposed into contributions from iteration number δ_I, grid size δ_G, time step δ_T, and other parameters δ_P, which gives the following expressions.

$$\delta_{SN} = \delta_I + \delta_G + \delta_T + \delta_P \tag{21}$$

$$U_{SN}^2 = U_I^2 + U_G^2 + U_T^2 + U_P^2 \tag{22}$$

Iteration number error/uncertainty is often considered negligible (usually reduced to machine accuracy). Without taking into consideration of other parameters, the simulation error is the sum of grid size and time step errors, $\delta_{SN} = \delta_G + \delta_T$, and similarly the simulation uncertainty is the root-sum-square of grid size and time step uncertainties, $U_{SN}^2 = U_G^2 + U_T^2$. Here, U_G corresponds to U_{FS} or U_ϕ discussed in Sections 3.1 and 3.2, and U_T can be found by using similar approaches as for U_G.

Modelling errors δ_{SM} can be decomposed into modelling assumptions and use of previous data. To determine if validation has been achieved, E is compared to the validation uncertainty U_V given by

$$U_V^2 = U_D^2 + U_{SN}^2 \tag{23}$$

If $|E| < U_V$, the combination of all the errors in $D$and S is smaller than U_V and validation is achieved at the U_V level. If $U_V << |E|$, the sign and magnitude of $E \approx \delta_{SM}$ can be used to make modelling improvements.

4.2 Interpretation of the Results of a Validation Effort

First, consider the approach in which the simulation numerical error is taken to be stochastic and thus the uncertainty U is estimated. From a general perspective, if we consider the three variables U_V, $|E|$, and programmatic requirements/tolerances U_{reqd}, there are six combinations (assuming none of the three variables are equal):

1) $|E| < U_V < U_{reqd}$

2) $|E| < U_{reqd} < U_V$

3) $U_{reqd} < |E| < U_V$

4) $U_V < |E| < U_{reqd}$ (24)

5) $U_V < U_{reqd} < |E|$

6) $U_{reqd} < U_V < |E|$

In cases 1, 2 and 3, $|E| < U_V$; validation is achieved at the U_V level; and the comparison error is below the noise level, so attempting to estimate δ_{SMA} is not feasible from an uncertainty standpoint. In case 1, validation has been achieved at a level below U_{reqd}, so validation is successful from a programmatic standpoint.

In cases 4, 5 and 6, $U_V < |E|$, so the comparison error is above the noise level and using the sign and magnitude of E to estimate δ_{SMA} is feasible from an uncertainty standpoint. If $U_V << |E|$, then E corresponds to δ_{SMA} and the error from the modelling assumptions can be determined unambiguously. In case 4, validation is successful at the $|E|$ level from a programmatic standpoint.

5. REVISION HISTORY

Revision 01 was a revision of QM Procedures 4.9-04-01-01 "Uncertainty Analysis in CFD, Uncertainty Assessment Methodology" and 4.9-04-01-02 "Uncertainty Analysis in CFD, Guidelines for RANS Codes," which were prepared and recommended by 22nd Resistance Committee and adopted as interim procedures. The QM Procedures were largely based on the methodology and procedures of Stern et al. (1999) [most recently Stern et al. (2001) and Wilson et al. (2001)] and Coleman and Stern (1997). Valuable experience was also gained at Gothenburg 2000 A Workshop on Numerical Ship Hydrodynamics (Larsson et al., 2000) where present QM Procedures were recommended and used.

Revision 01 of the present guide (or procedure) QM Procedure 7.5-03-01-01 "Uncertainty Analysis in CFD, Verification and Validation Methodology and Procedures" was updated for clarity of presentation and expanded discussion of verification procedures and implementation based on three years of experience, as discussed in Section 7 of 23rd ITTC RC Report. In particular, verification procedures were expanded to include user options of either correction factors or factor of safety approaches for estimating numerical errors and uncertainties and discussion was provided on fundamental and practical issues to aid in implementation of verification procedures.

Revision 02 of this procedure is a minor update of Revision 01, in which the latest revisions to the correction factor approach have been incorporated.

Revision 03 of this procedure is a minor update of Revision 02, in which the references to the ISO document have been updated to the latest issue of the JCGM GUM, and further details of the Least Squares Root method for estimating error have been added.

Revision 04 of this procedure is a minor update of Revision 03, in which the procedure was checked against the list of symbols in Annex J on the JCGM GUM and the use of upper-case letters was retained for the uncertainty symbols but with minor modifications in using the subscripts of the symbols. Also, subscripts of subscripts were replaced with the use of a comma separating the items.

6. PARAMETERS; SYMBOLS

Symbol	Description
h	Grid spacing or step size of numerical discretization
p	Observed order of accuracy
p_{th}	Theoretical order of accuracy of the simulation numerical scheme
r	Grid refinement ratio (or uniform parameter refinement ratio)
r_i	Grid refinement ratio of the i-th grid with respect to the finest grid
R	Convergence ratio
S	Simulation result
S_0	Exact solution of a simulation
U_{FS}	Simulation uncertainty by using the method of Stern at al.
U_ϕ	Simulation uncertainty by using the method of Eça and Hoekstra
δ	Numerical discretization error
ϕ	Simulation result (equivalent to S)
ϕ_0	Exact solution of a simulation (equivalent to S_0)

7. REFERENCES

Coleman, H. W. and Stern, F., 1997, "Uncertainties in CFD Code Validation", ASME J. Fluids Eng., Vol. 119, pp. 795-803.

Coleman, H, Stern, F., Di Mascio, A., Campagna, E. "Technical Note: The Problem with Oscillatory Behavior in Grid Convergence Studies", ASME J. Fluids Eng., Vol. 123, Issue 2, June 2001, pp. 438-439.

Eça, L., and Hoekstra, M., 1999, "On the numerical verification of ship stern flow calculations", 1st MARNET workshop, Barcelona, Spain.

Eça, L., and Hoekstra, M., 2000, "On the Application of Verification Procedures in Computational Fluid Dynamics", 2nd MARNET workshop, Copenhagen, 2000.

Eça, L., Vaz, G., and Hoekstra, M., "Code verification, solution verification and validation in RANS solvers, Proceedings of ASME 29th

International Conference, OMAE2010, Shanghai, China.

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, vol 262, pp 104-130.

Eça, L., Klaij, C.M., Vaz, G., Hoekstra, M., and Pereira, F.S., 2016, "On code verification of RANS solver", Journal of Computational Physics, 310:418-439.

Eça, L., Vaz, G., Toxopeus, S.L., and Hoekstra, M., "Numerical Errors in Unsteady Flow Simulations", Journal of Verification, Validation and Uncertainty Quantification, 4(2):021001-1-10, June 2019.

Eça, L., Lopes, R., Pereira, F.S., and Vaz, G., "Numerical and parameter uncertainties: are they independent?", ASME Verification and Validation Symposium (V&V), VVS2019-5125, Las Vegas, NV, May 2019.

Eça, L., Dowding, K., and Roache, P.J., "One the interpretation and Scope of the V&V Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer", ASME Verification and Validation Symposium (V&V), VVS2020-8826, Baltimore, MD, May 2020.

Eça, L., Pereira, F.S., Vas, G., Lopes, R., and Toxopeus, S.L., "On the Role of Discretization Errors in the Quantification of Parameter Uncertainties", ASME Verification and Validation Symposium (V&V), VVS2020-8825, Baltimore, MD, May 2020.

Eça, L., Silva, C., Muralha, J., Klaij, C.M., Toxopeus, S.L., and Hoekstra, M., "Discretization Error Estimation in Subsonic, Transonic and Supersonic Flows of an Inviscid Fluid over a Bump", ASME Verification and Validation Symposium (V&V), VVS2021-65290, May 2021.

Hoekstra, M., Eça, L., Windt, J., and Raven, H., 2000 "Viscous Flow Calculations for KVLCC2 AND KCS Models Using the PARNASSOS Code", Proceedings Gothenburg 2000 A Workshop on Numerical Ship Hydrodynamics, Gothenburg, Sweden.

JCGM, 2008, "Evaluation of measurement data – Guide to the expression of uncertainty in measurement," JCGM 100:2008 GUM 1995 with minor corrections, Joint Committee for Guides in Metrology, Bureau International des Poids Mesures (BIPM), Sèvres, France.

Larsson, L., Stern, F., Bertram, V., 2000 "Gothenburg 2000 A Workshop on Numerical Ship Hydrodynamics", Chalmers University of Technology, Gothenburg Sweden, Sept.

Larsson, L., Stern, F., and Visonneau, M., "Numerical Ship Hydrodynamics: An assessment of the Gothenburg 2010 Workshop", Springer, 2014.

Roache, P.J., 1998, Verification and Validation in Computational Science and Engineering, Hermosa publishers, Albuquerque, New Mexico.

Roache, P.J., 2003, "Criticism of the Correction Factor Verification Method", ASME J. Fluids Eng., Vol. 125, July 2003.

Roache, P.J., 2029, *Fundamentals of Verification and Validation*, Hermosa Publishers.

Stern, F., Wilson, R.V., Coleman, H., and Paterson, E., 2001, "Comprehensive Approach to

Verification and Validation of CFD Simulations-Part 1: Methodology and Procedures", ASME J. Fluids Eng., Vol. 123, Dec. 2001.

Stern, F., Wilson, R. V., Shao, J., "Quantitative V&V of CFD simulations and certification of CFD codes," Int. J. Numer. Meth. Fluids 2006; 50:1335-1355.

Verification, Validation, and Uncertainty Quantification Terminology in Computational Modeling and Simulation. VVUQ 1 - 2022. American Society of Mechanical Engineers. https://www.asme.org/codes-standards/find-codes-standards/vvuq-1-verification-validation-uncertainty-quantification-terminology-computational-modeling-simulation

Wackers, J., Deng, G.B., Guilmineau, E., Leroyer, A., Queutey, P., Visonneau, M., Palmieri, A. and Liverani, A., "Can adaptive grid refinement produce grid-independent solutions for incompressible flows?". Journal of Computational Physics, Vol. 344, pp 364--380., 2017.

Wilson, R., Stern, F., Coleman, H., and Paterson, E., 2001, "Comprehensive Approach to Verification and Validation of CFD Simulations-Part2: Application for RANS Simulation of A Cargo/Container Ship", ASME J. Fluids Eng., Vol. 123, Dec. 2001.

Wilson, R. and Stern, F., 2002, "Verification and Validation for RANS Simulation of a Naval Surface Combatant", Standards for CFD in the Aerospace Industry, 2002 AIAA Aerospace Sciences Meeting, Reno, Nevada, 14-17 January 2002.

Wilson, R., Shao, J. and Stern, F., 2004, "Discussion: Criticism of the Correction Factor Verification Method", ASME J. Fluids Eng., Vol. 126, July 2004.

Xing , T. and Stern, F., 2010, "Factors of Safety for Richardson Extrapolation," ASME J. Fluids Eng., Vol. 132, June 2010.

8. KEYWORDS

CFD, Verification and Validation, Uncertainty Assessment