ITTC Quality System Manual

Recommended Procedures and Guidelines

Procedure

Uncertainty Analysis in CFD Verification and Validation, Methodology and Procedures

7.5	Process Control
7.5-03	CFD
7.5-03-01	General
7.5-03-01-01	Uncertainty Analysis in CFD Verification and Validation, Methodology and Procedures

Disclaimer

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Uncertainty Analysis in CFD, Verification and Validation Methodology and Procedures

1. PURPOSE OF PROCEDURE

Provide methodology and procedures for estimating the uncertainty in a simulation result.

2. INTRODUCTION

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 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 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 QM Procedure 7.5-03-01-01 "Uncertainty Analysis in CFD, Verification and Validation Methodology and Procedures" is a minor update of Revision 01, in which the latest revisions to the correction factor approach have been incorporated. These modifications have been discussed in Section 4.3.

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.

The symbols used in the procedure have been checked against the list of symbols in Annex J of the JCGM document "Evaluation of measurement data – Guide to the expression of uncertainty in Measurement" or GUM (JCGM, 2008), proposed by the Quality Systems Group of the 28th ITTC to be used as a reference. The GUM is entirely and specifically intended for uncertainty estimation for measurements and therefore most of the symbols are not related to the recommended procedure at hand. The symbols most closely connected with this procedure are the ones for uncertainty. In the standards document the uppercase symbol (U) is used for expanded uncertainty of an estimate that defines an interval $y - U < Y < y + U$ having a high level of confidence and is equal to the coverage factor k times the standard combined uncertainty. Lower case symbol (u) is used for standard uncertainty of an estimate that is the positive square root of the estimated variance. Due to obvious similarities between the use of the coverage factor and the uncertainty estimation in this

procedure, the use of upper case symbols for uncertainty has been retained. Therefore, also in terms of symbols, only minor modifications have been. These are all related to the subscripts used. In the GUM the different input parameters are defined with subscript i. To be in line with the standards document the corresponding subscripts have been changed. Additionally, in order to improve legibility, the use of subscripts of subscripts has been minimized and most of these have been moved into subscripts with comma separating the items.

Present verification procedures are considered best presently available and further work is also recommended for improved procedures, which once available can be incorporated. Validation procedures were not changed. In the following an overview of the overall verification and validation approach is provided, including methodology and procedures. Stern et al. (2001) should be consulted for detailed presentation and discussions.

3. VERIFICATION AND VALIDATION METHODOLOGY

The definitions of errors and uncertainties directly follow those used in experimental uncertainty analysis. 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., $\delta_S = S - T = \delta_{SM} + \delta_{SN}$). For certain conditions, both the sign and magnitude of the numerical error can be estimated as $\delta_{SN} = \delta_{SN}^* + \varepsilon_{SN}$ where δ_{SN}^* is an estimate of the sign and magnitude of δ_{SN} and ε_{SN} is the error in that estimate. The simulation value is corrected to provide a numerical benchmark S_C, which is defined

$$S_C = S - \delta_{SN}^* \tag{1}$$

Verification is defined as a process for assessing simulation numerical uncertainty U_{SN} and, when conditions permit, estimating the sign and magnitude δ_{SN}^* of the simulation numerical error itself and the uncertainty in that error estimate U_{S_CN}. For the uncorrected simulation approach, numerical error 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 expression for simulation numerical uncertainty

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

For the corrected simulation approach, the solution is corrected to produce a numerical benchmark S_C and the estimated simulation numerical error δ_{SN}^* and corrected uncertainty U_{S_cN} are given by

$$\delta_{SN}^* = \delta_I^* + \delta_G^* + \delta_T^* + \delta_P^* \tag{3}$$

$$U_{S_cN}^2 = U_{I_C}^2 + U_{G_C}^2 + U_{T_C}^2 + U_{P_C}^2 \tag{4}$$

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 comparison error E is given by the difference in the data $D$and simulation S values

$$E = D - S = \delta_D - (\delta_{SM} + \delta_{SN}) \tag{5}$$

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

$$U_V^2 = U_D^2 + U_{SN}^2 \tag{6}$$

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. For the corrected simulation, equations equivalent to Eqs. (5) and (6) are

$$E = D - S_C = \delta_D - (\delta_{SM} + \varepsilon_{SN}) \quad (7)$$

$$U_{V_C}^2 = U_{E_C}^2 - U_{SM}^2 = U_D^2 + U_{S_CN}^2 \quad (8)$$

4. VERIFICATION PROCEDURES

4.1 Convergence Studies

Iterative and parameter convergence studies are conducted using multiple solutions (at least 3) with systematic parameter refinement by varying the i^{th} input parameter Δx_i while holding all other parameters constant. The present work assumes input parameters can be expressed such that the finest resolution corresponds to the limit of infinitely small parameter values. Many common input parameters are of this form, e.g., grid spacing, time step, and artificial dissipation. Additionally, a uniform parameter refinement ratio

$$r_i = \Delta x_{i,2}/\Delta x_{i,1} = \Delta x_{i,3}/\Delta x_{i,2} = \Delta x_{i,m}/\Delta x_{i,m-1}$$

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, similarly as for small values, 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 $r_i = 2$, 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, $r_i = 2$ may often be too large. A good alternative may be $r_i = \sqrt{2}$, 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.

Convergence studies require a minimum of $m = 3$ solutions to evaluate convergence with respect to input parameter. Note that $m = 2$ is inadequate, as it only indicates sensitivity and not convergence, and that $m > 3$ may be required. Changes between medium-fine $\varepsilon_{i,21} = \hat{S}_{i,2} - \hat{S}_{i,1}$ and coarse-medium $\varepsilon_{i,32} = \hat{S}_{i,3} - \hat{S}_{i,2}$ solutions are used to define the convergence ratio

$$R_i = \varepsilon_{i,21}/\varepsilon_{i,32} \quad (9)$$

and to determine convergence condition where $\hat{S}_{i,1}$, $\hat{S}_{i,2}$, $\hat{S}_{i,3}$ correspond to solutions with fine, medium, and coarse input parameter, respectively, corrected for iterative errors. Three convergence conditions are possible:

(i) Monotonic convergence: $0 < R_i < 1$

(ii) Oscillatory convergence: $R_i < 0$ (10)

(*iii*) Divergence: $R_i > 1$

For condition (*i*), generalized Richardson extrapolation (RE) is used to estimate $U_i$or δ_i^* and U_{i_C}. For condition (*ii*), uncertainties are estimated simply by attempting to bound the error based on oscillation maximums S_U and minimums S_L, i.e., $U_i = \frac{1}{2}(S_U - S_L)$. For oscillatory convergence (*ii*), the solutions exhibit oscillations, which may be erroneously identified as condition (*i*) or (*iii*). This is apparent if one considers evaluating convergence condition from three points on a sinusoidal curve (Coleman et al., 2001). Depending on where the three points fall on the curve, the condition could be incorrectly diagnosed as either mono-tonic convergence or divergence. Bounding the error based on oscillation maximum and minimum for condition (*ii*) requires more than $m = 3$ solutions. For condition (*iii*), errors and uncertainties cannot be estimated.

4.2 Generalized Richardson Extrapolation

For convergence condition (*i*), generalized RE is used to estimate the error δ_i^* due to selection of the i^{th} input parameter and order-of-accuracy p_i. The error is expanded in a power series expansion with integer powers of Δx_i as a finite sum. The accuracy of the estimates 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 three solutions, only the leading term can be estimated, which provides one-term estimates for error and order of accuracy

$$\delta_{RE_{i,1}}^{*(1)} = \frac{\varepsilon_{i,21}}{r_i^{p_i}-1} \tag{11}$$

$$p_i = \frac{\ln(\varepsilon_{i,32}/\varepsilon_{i,21})}{\ln(r_i)} \tag{12}$$

With five solutions, two terms can be estimated, which provides two-term estimates for error and orders of accuracy

$$\delta_{RE_{i,1}}^{*(2)} = \frac{r_i^{q_i}\varepsilon_{i,21}-\varepsilon_{i,32}}{\left(r_i^{q_i}-r_i^{p_i}\right)\left(r_i^{p_i}-1\right)} - \frac{r_i^{p_i}\varepsilon_{i,21}-\varepsilon_{i,32}}{\left(r_i^{q_i}-r_i^{p_i}\right)\left(r_i^{q_i}-1\right)} \tag{13}$$

$$p_i = \frac{\ln\left[\left(a_i+\sqrt{b_i}\right)/\left[2\left(\varepsilon_{i,21}\varepsilon_{i,43}-\varepsilon_{i,32}^2\right)\right]\right]}{\ln(r_i)}$$
$$q_i = \frac{\ln\left[\left(a_i-\sqrt{b_i}\right)/\left[2\left(\varepsilon_{i,21}\varepsilon_{i,43}-\varepsilon_{i,32}^2\right)\right]\right]}{\ln(r_i)} \tag{14}$$

where

$$a_i = \varepsilon_{i,21}\varepsilon_{i,54} - \varepsilon_{i,32}\varepsilon_{i,43}$$
$$b_i = -3\varepsilon_{i,32}^2\varepsilon_{i,43}^2 + 4\left(\varepsilon_{i,21}\varepsilon_{i,43}^3 + \varepsilon_{i,32}^3\varepsilon_{i,54}\right) - 6\varepsilon_{i,21}\varepsilon_{i,32}\varepsilon_{i,43}\varepsilon_{i,54} + \varepsilon_{i,21}^2\varepsilon_{i,54}^2$$

Solutions for analytical benchmarks show that the range of applicability for Eqs. (13) and (14) is more restrictive than that for Eqs. (11) and (12) since all five solutions must be both monotonically convergent and sufficiently close to the asymptotic range to evaluate p_i and q_i in Eq. (14). In general, $m = 2n + 1$ solutions are required to estimate the first n terms of the error expansion.

4.3 Estimating Errors and Uncertainties with Correction Factor

The concept of correction factors is based on verification studies for 1D wave equation, 2D Laplace equation, and Blasius boundary layer analytical benchmarks for which it is shown that a multiplicative correction factor is useful as a quantitative metric to determine proximity of the solutions to the asymptotic range, to account

for the effects of higher-order terms, and for estimating errors and uncertainties. The error is defined as

$$\delta_{i,1}^{*} = C_i \delta_{RE_{i,1}}^{*} = C_i \left(\frac{\varepsilon_{i,21}}{r_i^{p_i} - 1} \right) \tag{15}$$

where two expressions for the correction factor C_i were developed. The first is based on solution of Eq. (15) for $C_i$with $\delta_{RE_{i,1}}^{*}$ based on Eq. (11) but replacing $p_i$with the improved estimate $p_{i_{est}}$

$$C_i = \frac{r_i^{p_i} - 1}{r_i^{p_{iest}} - 1} \tag{16}$$

$p_{i_{est}}$ is an estimate for the limiting order of accuracy of the first term as spacing size goes to zero and the asymptotic range is reached so that $C_i \to 1$. Similarly, the second is based on a two-term estimate of the power series which is used to estimate $\delta_{RE_{i,1}}^{*}$ where p_i and q_i are replaced with $p_{i_{est}}$ and $q_{i_{est}}$

$$C_i = \frac{\left(\varepsilon_{i,32}/\varepsilon_{i,21} - r_i^{q_{iest}}\right)\left(r_i^{p_i} - 1\right)}{\left(r_i^{p_{iest}} - r_i^{q_{iest}}\right)\left(r_i^{p_{iest}} - 1\right)} + \frac{\left(\varepsilon_{i,32}/\varepsilon_{i,21} - r_i^{p_{iest}}\right)\left(r_i^{p_i} - 1\right)}{\left(r_i^{p_{iest}} - r_i^{q_{iest}}\right)\left(r_i^{q_{iest}} - 1\right)} \tag{17}$$

Eq. (16) roughly accounts for the effects of higher-order terms by replacing p_i with $p_{i_{est}}$ thereby improving the single-term estimate, while Eq. (17) more rigorously accounts for higher-order terms since it is derived from a two-term estimate. Both expressions for C_i only require three solutions to estimate errors using Eq. (15). Solutions for analytical benchmarks show that correction of error estimates with both expressions for C_i yields improved error estimates.

Expressions for uncertainties are developed from error estimates in Eq. (15). When solutions are far from the asymptotic range, C_i is sufficiently less than or greater than 1 and only the magnitude of the error is estimated through the uncertainty U_i. Eq. (15) is used to estimate U_i by bounding the error $\delta_{i,1}^{*}$ by the sum of the absolute value of the corrected estimate from RE and the absolute value of the amount of the correction

$$U_i = (|C_i| + |1 - C_i|)\left|\delta_{RE_{i,1}}^{*}\right| \tag{18}$$

It is shown by Wilson and Stern (2002) that Eq. (18) is not conservative enough for $C_i < 1$, which motivates development of an improved estimate

$$U_i = (2|1 - C_i| + 1)\left|\delta_{RE_{i,1}}^{*}\right| \tag{19}$$

When solutions are close to the asymptotic range, C_i is close to 1 so that δ_i^{*} is estimated using Eq. (15) and U_{i_C} is estimated by

$$U_{i_C} = |1 - C_i|\left|\delta_{RE_{i,1}}^{*}\right| \tag{20}$$

Eq. (20) has the correct form for both $C_i < 1$ and $C_i > 1$. It should be recognized that using the corrected simulation approach requires in addition to C_i close to 1 that one have confidence in Eq. (15). There are many reasons for lack of confidence, especially for complex three-dimensional flows.

As pointed out by Roache (2003) Eqs. (19) and (20) have the short-coming that as $C_k \to 1$ the method reverts to Richardson Extrapolation, which produces only ~50% uncertainty estimate. Based on this criticism a further revision of the uncertainty estimates have been presented by Wilson et al. (2004). The final uncertainty estimates for the uncorrected and corrected approaches respectively are given as

$$U_i = \begin{cases} [9.6(1-C_i)^2 + 1.1]\left|\delta^*_{RE_{i,1}}\right|, & |1-C_i| < 0.125 \\ [2|1-C_i| + 1]\left|\delta^*_{RE_{i,1}}\right|, & |1-C_i| \geq 0.125 \end{cases} \quad (21)$$

$$U_{i_C} = \begin{cases} [2.4(1-C_i)^2 + 0.1]\left|\delta^*_{RE_{i,1}}\right|, & |1-C_i| < 0.25 \\ [|1-C_i|]\left|\delta^*_{RE_{i,1}}\right|, & |1-C_i| \geq 0.25 \end{cases} \quad (22)$$

These uncertainty estimates merge smoothly with the previous uncertainty estimates and provide 10% factor of safety in the limit $C_i = 1$.

4.4 Estimating Uncertainties with Factors of Safety

Alternatively, a factor of safety approach (Roache, 1998) can be used to define the uncertainty U_i where an error estimate from RE is multiplied by a factor of safety $F_S$to bound simulation error

$$U_i = F_S\left|\delta^*_{RE_{i,1}}\right| \quad (23)$$

where $\delta^*_{RE_{i,1}}$ can be based on a single- or two-term estimate as given by Eq. (11) or (13), respectively with either assumed or estimated order of accuracy. If order of accuracy is assumed (e.g., based on theoretical values), only two or three solutions are required for evaluation of Eq. (11) or (13), respectively.

Although not proposed by Roache (1998), the factor of safety approach can be used for situations where the solution is corrected with an error estimate from RE as

$$U_{i_C} = (F_S - 1)\left|\delta^*_{RE_{i,1}}\right| \quad (24)$$

The exact value for factor of safety is somewhat ambiguous and $F_S = 1.25$ is recommended for careful grid studies and 3 for cases in which only two grids are used and order of accuracy is assumed from the theoretical value p_{th}.

4.5 Estimating Errors and Uncertainties using a Least Squares Root approach

Where there is 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) (Eça, 2010 and Larsson, 2014).

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

$$S_i = S_0 + \alpha {h_i}^p \quad (25)$$

where *i* is the grid number from 1 to the number of grids and $h_i$is the grid size ratio.

The convergence condition is determined based on the observed order of accuracy, *p*, such that $p > 0$ indicates monotonic convergence and $p < 0$ indicates monotonic divergence. Oscillatory convergence is defined as being when the solution is alternately above and below the exact solution.

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.

$$\delta_{RE} = S_i - S_0 = \alpha {h_i}^p \quad (26)$$

$$\delta^{02}_{RE} = S_i - S_0 = \alpha_{02} {h_i}^2 \quad (27)$$

$$\delta^{12}_{RE} = S_i - S_0 = \alpha_{11} h_i + \alpha_{12} {h_i}^2 \quad (28)$$

$$\delta_{\Delta_M} = \frac{(S_i)_{\max} - (S_i)_{\min}}{\left(h_{n_g}/h_1\right) - 1} \tag{29}$$

The error estimate is chosen based on the observed order of accuracy, p. For $0.5 \le p \le 2$, δ_{RE} from Eq. (26) is used. For $p > 2$, δ_{RE}^{02} from Eq. (27) is used, and for $p < 0.5$ the best fit of δ_{RE}^{02} or δ_{RE}^{12} is chosen.

The numerical uncertainty is calculated using a factor of safety approach, as in Eq. (23), but the error used and the factor of safety are based on p. For $0.5 \le p < 2.1$, assuming a theoretical order of accuracy equal to 2, the factor of safety of 1.25 is applied while for all other p a factor of safety equal to 3 is used.

For oscillatory or anomalous convergence the uncertainty is based on the data range parameter

$$U_i = 3\left|\delta_{\Delta_M}\right| \tag{30}$$

4.6 Estimating Errors and Uncertainties for Point Variables

Determination of the convergence ratio R_i for point variables can be problematic since solution changes $\varepsilon_{i,21}$ and $\varepsilon_{i,32}$ can both go to zero (e.g., in regions where the solution contains an inflection point). In this case, the ratio becomes ill conditioned. However, the convergence ratio can be used in regions where the solution changes are both non-zero (e.g., local solution maximums or minimums).

Another approach is to use a global convergence ratio R_i and order of accuracy p_i, which overcomes ill conditioning, based on the L2 norm of the solution changes, i.e.,

$$\langle R_i \rangle = \left\|\varepsilon_{i,21}\right\|_2 / \left\|\varepsilon_{i,32}\right\|_2 \tag{31}$$

$$\langle p_i \rangle = \frac{\ln\left(\left\|\varepsilon_{i,32}\right\|_2 / \left\|\varepsilon_{i,21}\right\|_2\right)}{\ln(r_i)} \tag{32}$$

where $\langle \quad \rangle$ denotes a profile-averaged quantity (with ratio of solution changes based on L2 norms) and $\|\varepsilon\|_2 = (\sum_{k=1}^{N} \varepsilon_k^2)^{1/2}$ denotes the L2 norm of solution change over the N points in the region of interest. Caution should be exercised when defining the convergence ratio from the ratio of the L2 norm of solution changes because the oscillatory condition ($R_i < 1$) cannot be diagnosed since $\langle R_i \rangle$ will always be greater than zero. Local values of R_i at solution maximums or minimums should also be examined to confirm the convergence condition based on an L2 norm definition.

For verification of the uncorrected solution Eqs. (21) or (23) are used to estimate distributions of U_i at each point from the local solution change $\varepsilon_{i,21}$, where p_i is estimated from Eq. (32). Similarly, for the corrected solution, $\langle p_i \rangle$ is used to estimate δ_i^* and U_{i_C} at each point using Eqs. (15) or (11) and (22) or (24), respectively. An L2 norm of point distributions of errors and uncertainties are then used to assess verification levels and to judge if validation has been achieved globally.

An alternate approach suggested by Hoekstra et al. (2000) is to transform the spatial profile to wave number space and to perform a convergence study on the amplitude distribution of the Fourier modes. In principle, this approach would remove the problem of ill-conditioning of the convergence ratio, R_i.

4.7 Discussion of Fundamental and Practical Issues

It should be recognized that implementation of verification procedures is not easy and re-

quire both experience and interpretation of results, especially for practical applications. However, their importance cannot be overemphasized to ensure fidelity and quality of CFD solutions.

Fundamental issues include from the outset selection of multiple vs. single grid approaches for estimating errors and uncertainties. However, as discussed in Section 7 of 23rd ITTC RC Report, the former approach can be used to establish convergence and is relatively inexpensive to implement and therefore recommended at this time. For multiple-grid approaches, important fundamental issues include appropriateness of power series representation [Eq. (27) of Stern et al. (2001)] and its convergence characteristics along with assumptions that $p_i^{(k)}$ and $q_i^{(k)}$ are independent of Δx_i. Also, issues concerning definitions and nature of solutions in asymptotic vs. non-asymptotic ranges.

These fundamental issues are exacerbated for practical applications along with additional is-sues, including selection of parameter refinement ratio, procedures for generation of multiple systematic grids and solutions, number of grids required and variability between grid studies, selection of appropriate verification procedures, and interpretation of results.

Selection of the parameter refinement ratio was discussed previously in Section 4.1 wherein the use of uniform value $r_i = \sqrt{2}$ was recommended; however, non-uniform and larger/smaller values may also be appropriate under certain circumstances. Wilson and Stern (2002) discuss procedures for generation of multiple systematic grids and solutions. Multiple systematic grids are generated using $r_i = \sqrt{2}$ and a post-processing tool in which the coarse grid is obtained by removing every other point from the fine grid and the medium grid is obtained by interpolation. Multiple solutions are obtained by first obtaining a solution for the coarse grid with a uniform flow initial condition, which is then used as an initial condition for obtaining a solution on the medium grid, which is then used as an initial condition for obtaining a solution on the fine grid. This procedure can be used to obtain solutions on all three grids in about 1/3 the time required to obtain only the fine grid solution without this procedure.

For complex flows with relatively coarse grids, solutions may be far from the asymptotic range such that some variables are convergent while others are oscillatory or even divergent. The order of accuracy and therefore correction factors and factors of safety may display large variability indicating the need for finer grids. Clearly, more than 3 grids are required to estimate errors and uncertainties for such cases. Eca and Hoekstra (1999, 2000) propose a least squares approach to estimate the error by computing the three unknown parameters from RE when more than three grids are used and there is variability between grid studies.

Both correction factor and factor of safety verification approaches have been presented with selection being a user option. Wilson and Stern (2002) have shown that the factor of safety approach is over conservative when solutions are close to the asymptotic range and under conservative when solutions are far from the asymptotic range. Nonetheless some users may prefer factors of safety over correction factors. An alternative is to select the more conservative uncertainty from the correction factor and factor of safety approaches. For the uncorrected simulation approach the more conservative uncertainty is given as the maximum of Eqs. (21) and (23).

For the corrected simulation approach, the more conservative uncertainty is given as the maximum of Eqs. (22) and (24).

For F_S = 1.25, uncorrected uncertainty estimates are based on the factor of safety approach when C_i is close to one (i.e., 0.875 < C_i < 1.125) and on the correction factor approach outside this range (i.e., $|1 - C_i| > 0.125$). For the corrected approach, uncertainties are based on the correction factor approach, when $|1 - C_i| > 0.25$. When using correction factors an important issue is selection of the best estimate for the limiting order of accuracy. Theoretical values can be used or values based on solutions for simplified geometry and conditions, in either case, preferably including the effects of stretched grids.

Lastly, analysis and interpretation of results is important in assessing variability for order of accuracy, levels of verification, and strategies for reducing numerical and modelling errors and uncertainties; since, as already mentioned, there is limited experience and no known solutions for practical applications in the asymptotic range for guidance.

4.8 The use of unstructured grids for V&V

As a preamble to this section it is reminded that the verification concerns code verification for correct coding of the model. The solution verification is aimed at estimating the numerical error/uncertainty of a given solution whereas the validation process is concerned by the numerical model meaning the modelling errors/uncertainties.

The CFD error related to the discretization error is the difference between the exact solution of the PDE and the exact (round-off-free) solution of the algebraic equations used. The possible sources of numerical error to consider for accurately control the precision of a physical model are, Roache (1998):

(i) Round-off errors: its influence is commonly neglected.

(ii) Iterative error (to solve the couplings/segregated equations and the non-linearities): its influence is often neglected assuming the condition of the residuals “low enough” for all the quantities. Eça et al. (2010) showed on manufactured solution that the iterative error - evaluated by comparing solutions obtained with less demanding convergence criteria - must be two orders of magnitude smaller than the discretization error to have a negligible influence.

(iii) Discretization error (or solution error due to incomplete grid convergence): it is computed from a series of systematically refined grids from which the exact solution is extrapolated and the uncertainty can be evaluated from the computed error.

For the estimation of the numerical uncertainty a set of geometrically similar grids is required where grid properties remain the same and the refinement ratio be constant in the computational domain. The task of generating a series of embedded grids by coarsening a fine grid or refining a coarse grid is easy with most of structured grid generators.

With an unstructured grid generation package it is more difficult to guarantee a perfect similarity between the grids where the ratios of the cell sizes are the same throughout the mesh. In practice, this limits the use of refinement studies with unstructured grids.

As an example Figure 1 illustrates hand drawing of a series of very simple full hexahedral meshes suited for grid convergence analysis. The location of the boundary between the

locally refined regions would not change between the grids. In this example the lower half of the domain will always be refined twice as the upper region and the cell size ratio from a coarse grid to its next fine grid remains the same throughout the computational domain: 2/3 for (a)/(b) , 3/4 for (b)/(c) and 4/5 for (c)/(d) . The detailed process to reach that requirement is of course generator-dependent and the information should be precisely documented by the software provider.

As an alternative and when available, adaptive grid refinement combined with finite-volume simulations can be used in a straightforward way to obtain grid-independent solutions by changing only the refinement threshold. The limitation is that the cells can only by divided in powers of two. This was shown by Wackers et al. (2017) for generating series of anisotropic refined meshes to study grid convergence and local flow analysis about the KVLCC2 tanker.

The grid convergence behaviour depends on the selected turbulence model. For wall-function approach the first cell in the fluid above the walls should be located at the same place in all grids, in the log-layer region with y+ higher than 15 for model ship. For full-scale ship and high Reynolds number it could be as high as 300.

In any case, the Richardson extrapolation and Least Squares Regression methods, described above, should be used to estimate the numerical uncertainty.

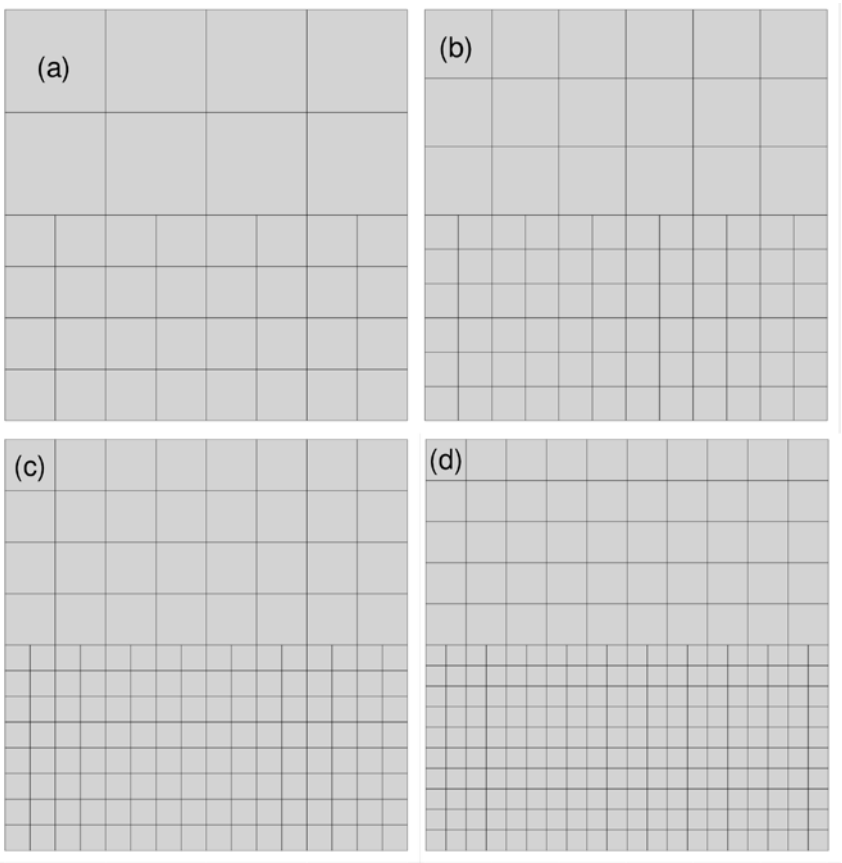

Figure 1: Example of a series of perfectly nested meshes. From coarse(a) to fine(d).

5. VALIDATION PROCEDURES

5.1 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_{SN} is estimated. From a general perspective, if we consider the three variables U_V, $|E|$, and U_{reqd} there are six combinations (assuming none of the three variables are equal):

$$\begin{aligned} &1)\ |E| < U_V < U_{reqd} \\ &2)\ |E| < U_{reqd} < U_V \\ &3)\ U_{reqd} < |E| < U_V \\ &4)\ U_V < |E| < U_{reqd} \\ &5)\ U_V < U_{reqd} < |E| \\ &6)\ U_{reqd} < U_V < |E| \end{aligned} \tag{33}$$

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.

Now consider the approach in which the simulation numerical error is taken to be deterministic and thus δ_{SN}^* and the uncertainty U_{V_C} are estimated. A similar set of comparisons as those in equation (33) can be constructed using $|E_C|$, U_{V_C}, and U_{reqd}. Since E_C can be larger or smaller than E, but U_{V_C} should always be less than U_V, the results for a given corrected case are not necessarily analogous to those for the corresponding uncorrected case. That is, a variable can be validated in the corrected but not in the uncorrected case, or vice versa. For cases 4, 5, and 6 in which $U_{V_C} < |E_C|$, one can argue that E_C is a better indicator of δ_{SMA} than is E, assuming that one's confidence in using the estimate δ_{SN}^* is not misplaced.

5.2 Use of Corrected vs. Uncorrected Simulation Results

The requirements for correcting the solution are that the correction factor be close to one and that confidence in solutions exist. Since the variability of the order of accuracy cannot be determined from solutions on three grids, confidence is difficult to establish in this case. As a result, caution should be exercised when correcting solutions using information from only three grids.

If a validation using the corrected approach is successful at a set condition, then if one chooses to associate that validation uncertainty level with the simulation's prediction at a neighbouring condition that prediction must also be corrected. That means enough runs are required at the new condition to allow estimation of the numerical errors and uncertainties. If this is not done, then the comparison error E and validation uncertainty U_V corresponding to the use of the uncorrected S and its associated (larger) U_{SN} should be the ones considered in the validation with which one wants to associate the prediction

at a new condition. (Whether to and how to associate an uncertainty level at a validated condition with a prediction at a neighboring condition is very much unresolved and is justifiably the subject of much debate at this time.)

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