Quantitative V&V of CFD Solutions and Certification of CFD Codes

Frederick Stern
IIHR-Hydroscience & Engineering
The University of Iowa
Iowa City, IA USA 52242
frederick-stern@uiowa.edu

ABSTRACT
Concepts, definitions, equations and procedures are provided for quantitative assessment of numerical (verification) and modeling (validation) errors and uncertainties for CFD simulations and of intervals of certification for CFD codes at 95% level of confidence. Examples are provided for ship hydrodynamics. Comparisons are made with alternative approaches.

1.0 INTRODUCTION
The purpose of the author’s and colleagues’ research on verification and validation (V&V) of computational fluid dynamics (CFD) simulations [1,2,3] and certification of CFD codes [4] is to provide methodology and procedures for estimating quantitative metrics, i.e., intervals of uncertainty at a specified level of confidence for solution V&V and code certification for industrial applications. The focus is on multi-user-purpose industrial CFD codes for practical applications. It is assumed that code verification and software quality assurance and model validation for simple benchmarks were properly dealt with during previous code development phases.

The approach uses experimental fluid dynamics (EFD) uncertainty analysis concepts and definitions for errors/uncertainties, systematic/random categorizations, and large sample size/normal distribution 95% level of confidence assumptions [5]. [5] is equivalent to the AIAA [6], AGARD [7], and ANSI/ASME [8] standards. These references adopt the same mathematical procedures but differ conceptually from the ISO and US Guides [9,10], as discussed in [5]. ISO and US Guides focus on uncertainties and consider concepts of error/true value as ideals since unknowable and categorize uncertainties as type A (evaluated by statistical analysis of a series of observations) and type B (evaluated by other means), which are combined as standard (estimated standard deviations) and expanded (at specified level of confidence) uncertainties. For engineering experiments and CFD (as shown below) the concepts of error/true value and systematic/random categorizations are useful and retained. It is disconcerting for users of EFD uncertainty analysis and does not bode well for CFD uncertainty analysis that after more than 50 years of publication on EFD uncertainty analysis large conceptual differences exist between professional society standards and international/national guides.

V&V of CFD simulations are conducted at the individual user, code, model, grid-type, etc. level (simulation level) for specified applications with available benchmark EFD validation data and uncertainties: solution V&V. The error estimates are based on fixed values with the same reasoning for 95% level of confidence as used for single-realizations and 0-order–replication level bias limit (systematic uncertainty) estimation in EFD. This is the smallest uncertainty interval that could be achieved with the CFD code for the specified application. The V&V methodology and resulting definitions are based on equations derived for simulation numerical and modeling errors and uncertainties, which provide the
overall mathematical framework. Simulation modelling and numerical errors are assumed additive such that simulation uncertainties root sum square (RSS). For solutions in the asymptotic range, the estimated numerical error and its estimated error are used to obtain a corrected solution (numerical benchmark) and its uncertainty. Verification procedures identify the most important numerical error sources (such as iterative, grid size, and time step errors) and provide error and uncertainty estimates. Validation methodology and procedures use benchmark experimental data and properly take into account both numerical and experimental uncertainties in estimating modelling errors and validation uncertainty, including the option of using corrected solutions. Simulation based design requires verification of all simulations, but hopefully validation only for the final or unusual designs.

Certification of CFD codes is done at the multiple codes or users, models, grid types, etc. level (code level) using standard and expanded uncertainties, which has been referred to as N-version testing [11]. Multiple users are appropriate for many user codes, whereas multiple codes are appropriate for various few user codes (often case for industrial applications). Differences between versions and implementations are due to myriad possibilities for modeling, numerical methods, and their implementation as CFD codes and simulations. As with estimating EFD precision limits (random uncertainty) using multiple realizations and 1-order-replication level testing, such estimates only include those factors turned on, which can be used to isolate differences, e.g., by using same models or grid types. The approach extends concept of N-version testing for consideration bias uncertainties (solution V&V) and use of reference values (experimental data and uncertainties) for estimating interval of certification. Presumably codes would be certified for range of applications using interpolation/extrapolation methods.

The present approaches for solution V&V and certification of CFD codes differ substantially from alternative approaches such as Roache [12,13], AIAA [14], ASME [15], and Hemsch [11]; and has been criticized by Roache [16,17] and Oberkampf [18], which were rebutted by [19,20,21,22]. As discussed in [4] and below the differences are largely conceptual since the detailed V&V and certification procedures used are similar.

### 2.0 V&V OF CFD SIMULATIONS

#### 2.1 Simulation Errors and Uncertainties

The simulation error $\delta_s$ is defined as the difference between a simulation result $S$ and the truth $T$ (objective reality) and is assumed composed of additive modelling $\delta_{SM}$ and numerical $\delta_{SN}$ errors

$$\delta_s = S - T = \delta_{SM} + \delta_{SN} \quad (1)$$

Modeling errors are due to the mathematical physics problem formulation in terms of a continuous initial boundary value problem (IBVP) and numerical errors are due to numerical solution of the discrete IBVP. The simulation uncertainty equation follows directly by considering (1) as a data reduction equation

$$U_s^2 = U_{SM}^2 + U_{SN}^2 \quad (2)$$

Equations (1) and (2) neglect correlated errors such as correlated modeling/numerical errors, which is justified as a reasonable first approximation in consideration of the development and execution of RANS CFD codes; however, correlations between modeling and numerical errors are also possible especially for LES simulations and should be incorporated into the methodology and procedures in future work. Again as a reasonable first approximation it would be assumed that correlated errors and uncertainties are additive and RSS, respectively.

For simulations (unlike experiments except for calibrations), it is possible under certain conditions to
estimate the numerical error both in sign and magnitude $\delta_{SN}^*$ such that

$$\delta_{SN} = \delta_{SN}^* + \varepsilon_{SN}$$  \hfill (3)$$

where $\varepsilon_{SN}$ is the error in the estimate. In this case, the simulation value is corrected to provide a numerical benchmark $S_C$, which is defined as

$$S_C = S - \delta_{SN}$$  \hfill (4)$$

with corrected simulation error $\delta_{SC}$ and uncertainty $U_{SC}$, equations

$$\delta_{SC} = S_C - T = \delta_{SM} + \varepsilon_{SN}$$  \hfill (5)$$

$$U_{SC}^2 = U_{SM}^2 + U_{SN}^2$$  \hfill (6)$$

where $U_{SC,N}$ is the uncertainty estimate for $\varepsilon_{SN}$.

### 2.2 Verification and Validation Methodology

Verification is defined as a process for assessing simulation numerical uncertainty $U_{SN}$ and, when conditions permit, estimating the sign and magnitude $\delta_{SN}^*$ of the simulation numerical error itself and the uncertainty in that error estimate $U_{SN}$.

The numerical error is decomposed into contributions from iteration number $\delta_I$, grid size $\delta_G$, time step $\delta_T$, and other input parameters $\delta_P$,

$$\delta_{SN} = \delta_I + \delta_G + \delta_T + \delta_P = \delta_I + \sum_{j=1}^{J} \delta_j$$  \hfill (7)$$

which again as a first approximation errors are assumed additive with simulation numerical uncertainty

$$U_{SN}^2 = U_I^2 + U_G^2 + U_T^2 + U_P^2$$  \hfill (8)$$

Similarly, for the corrected simulation

$$\delta_{SN}^* = \delta_I^* + \delta_G^* + \delta_T^* + \delta_P^*$$  \hfill (9)$$

$$U_{SN}^2 = U_I^2 + U_G^2 + U_T^2 + U_P^2$$  \hfill (10)$$

Substituting (9) into (4) yields

$$S = S_C + (\delta_I^* + \sum_{j=1}^{J} \delta_j^*)$$  \hfill (11)$$

Verification procedures are based on (11).

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 $\delta_{SM}^*$ itself.

The comparison error $E$ is defined by the difference between the data $D$ and simulation $S$ values

$$E = D - S = \delta_D - (\delta_{SM} + \delta_{SN}^*)$$  \hfill (12)$$

where $\delta_D$ is the experimental error. Equation (12) follows directly from (1) with $T$ estimated by $D - \delta_D$. It is assumed that $D$ is based on an appropriate averaging of individual measurements and $\delta_D$ is estimated using standard EFD uncertainty analysis procedures as $U_D$. Modeling errors $\delta_{SM}$ can be decomposed into
modeling assumptions $\delta_{\text{SMA}}$ and estimated, e.g., use of previous data $\delta_{\text{SME}}$. To determine if validation has been achieved, $E$ is compared to the validation uncertainty $U_V$ given by

$$U_V^2 = U_D^2 + U_{\text{SMA}}^2 + U_{\text{SME}}^2 + U_{SN}^2$$

(13)

If $|E| < U_V$, the combination of all the errors in $D$ and $S$ that can be estimated is smaller than $U_V$ and validation is achieved at the $U_V$ interval, which is a more stringent requirement than $|E| < U_E$. If $U_V << |E|$, the sign and magnitude of $E \approx \delta_{\text{SM}}$ can be used to make modeling improvements. For the corrected simulation,

$$E_C = D - S_C = \delta_D - (\delta_{\text{SM}} + \delta_{\text{SN}})$$

(14)

$$U_{V_C}^2 = U_D^2 + U_{\text{SMA}}^2 + U_{\text{SME}}^2 + U_{SN}^2$$

(15)

Validation procedures are based on (12)-(15).

### 2.3 Verification Procedures

Solution verification procedures provide error and uncertainty estimates for all possible numerical error sources; however, in view of root-sum-square (RSS) representation of total uncertainty estimate only those most significant need be considered, which for many CFD solutions are iterative, grid size, and time step errors. Other error sources that may also be significant include: artificial compressibility or other similar input parameters; domain size or other similar errors; and round-off errors. For some error sources (e.g., domain size and turbulence model parameters), estimates can be based on sensitivity studies. Current solution verification procedures for iterative and grid/time convergence are based on graphical methods and generalized Richardson extrapolation (RE), respectively. Future work requires improved procedures for iterative convergence for unsteady simulations and single grid size and time step convergence.

#### 2.3.1 Convergence Studies

Iterative and grid/time convergence studies are conducted using multiple solutions and systematic parameter refinement by varying the numerical input parameter ($\Delta x$ and $\Delta t$) while holding all other parameters constant. A uniform parameter refinement ratio $r_k$ between solutions is not required, but used to simplify the analysis. $r_k$ cannot be too large or small. Too small values are undesirable since solution changes will be small and sensitivity to input parameter may be difficult to identify compared to iterative errors. Ideally, $r_k$ should be as large as possible. However, $r_k$ may not be too large since the finest step size may be prohibitively small if the coarsest step size is designed for sufficient resolution such that similar physics are resolved for all solutions. For very fine grid spacing or time-step, simulations require expensive resources and it may be difficult to identify the solution changes compared to the iterative errors as they are at the same levels. For industrial CFD, the finest grid size is based on available resources and $r_k = 2$ is often too large in consideration of the physics and/or errors on the coarsest grid. $r_k$ other than 2 requires interpolation to a common location to compute solution changes, which introduces interpolation errors.

Convergence studies require a minimum of three solutions to evaluate convergence with respect to input parameter. The convergence ratio $R_k = \varepsilon_{k_1} / \varepsilon_{k_2}$ is defined as the ratio of solution changes for medium-fine $\varepsilon_{k_2} = S_{k_2} - S_{k_1}$ and coarse-medium $\varepsilon_{k_3} = S_{k_3} - S_{k_2}$ solutions, which defines four convergence
conditions: (i) monotonic convergence \(0 < R_k < 1\), (ii) oscillatory convergence \(R_k < 0; |R_k| < 1\), (iii) monotonic divergence \(R_k > 1\), and (iv) oscillatory divergence \(0 < R_k < 0; |R_k| > 1\). Errors and uncertainties cannot be evaluated for divergence conditions (iii) and (iv). For oscillatory convergence (ii), uncertainty can be evaluated based on the determination of the upper \(S_U\) and lower \(S_L\) bounds of solution oscillation \(E^2 = (S_U - S_L)/2\). Errors and uncertainties for monotonic convergence are evaluated using generalized RE. For point variables, a global convergence ratio based on the \(L_2\) norm of the solution changes is used to avoid ill conditions when solution changes for medium-fine and coarse-medium solutions both go to zero.

2.3.2 Iterative Convergence

Iterative errors \(U_i\) must be evaluated before grid/time-step studies can be conducted. Iterative error is defined as the difference between the current iterative solution to the discretized equations and the exact solution to the discretized equations. Iterative convergence to machine zero is desirable, but is often not possible for complex geometry and conditions for most industrial applications, especially for finer grids on which iterative methods converge much slower. Thus iterative convergence requires the establishment of a stopping criteria and a procedure for estimating the iterative errors and uncertainties for both integral and point variables, where for the latter an \(L_2\) norm over all grid points is often used as a global metric.

The stopping criteria for iterative convergence can be assessed by the solution residual (absolute or relative difference between successive iterates), which could be misleading when convergence is slow. A better approach is to evaluate the number of order magnitude drop of the solution residual ranging from at least three orders of magnitude drop [2,15] and final magnitude of the solution residual to be \(\leq 10^{-4}\) [2] to five or six orders of magnitude drop [14].

Methods for estimating iterative errors for steady problems can be either theoretical [23,24] or graphical [2] and are dependent on the type of iterative convergence: (a) oscillatory, (b) convergence, or (c) mixed oscillatory/convergent. Theoretical approaches require estimation of the principal eigenvalue of the iteration matrix. The approach is relatively straightforward when the eigenvalue is real and the solution is convergent. However, for cases in which the eigenvalue is complex and the solution is oscillatory or mixed, the estimation is not as straightforward and additional assumptions are required. Graphical approach is to examine the iterative history of a dependent variable and use the deviation of the dependent variable for oscillatory \(E^2 = (S_U - S_L)/2\), a curve fit of an exponential function for convergence, or the solution envelope for mixed oscillatory/convergent.

For unsteady simulations using implicit methods, iterative convergence of the solution needs to be checked at each time step, which requires the solution is independent of the inner iterations for implicit coupling of, e.g., free-surface, velocity–pressure, and ship motions. Iterative error and uncertainties can be estimated for the zeroth harmonics or statistical averaging (running mean) of a specific variable (e.g., force coefficients, moments) using the same procedures for steady flow simulations.

It should be noted that the requirement of \(U_i << U_G\) (i.e., \(U_i\) is at least one or two orders of magnitude smaller than \(U_G\)) could be difficult to be satisfied for very fine grids due to very small \(U_G\). More iterations or implementation of more efficient iterative methods to speed up the convergence (e.g., multi-grid) will be necessary.
2.3.3 Grid/Time Convergence

Grid/time-step convergence studies are conducted with multiple solutions (at least 3) using systematically refined grid sizes or time steps. For monotonic convergence, procedures for estimating grid size errors are based on generalized RE, which is developed on the assumption that the error terms are in the form of power series expansion, which for the \( k \)th parameter and \( m \)th solution is:

\[
\delta^*_{k_m} = \sum_{i=1}^{s} (\Delta x_k)^i g_k^{(i)}
\]  

(16)

Substituting equation (16) to equation (11) results in:

\[
S_{k_m} = S_C + \sum_{i=1}^{s} (\Delta x_k)^i g_k^{(i)} + \sum_{j=1,j\neq k}^{f} \delta^*_{j_m}
\]

(17)

The accuracy of the estimates depends on how many terms \( n \) are retained in the expansion, the magnitude (importance) of the higher-order terms, and the validity of the assumptions made in RE theory.

Since each term \( (i) \) contains 2 unknowns, \( m=2n+1 \) solutions are required to estimate the numerical benchmark \( S_C \) and the first \( n \) terms in the expansion in equation (17). For three solutions \( (m=3, n=1) \), only the leading-order term can be evaluated. The error and order of accuracy are:

\[
\delta^*_{RE_i} = \frac{\epsilon_{k_{i1}}}{r_k^{p_k} - 1}
\]

(18)

\[
p_k = \frac{\ln(\epsilon_{k_{i1}} / \epsilon_{k_{i2}})}{\ln(r_k)}
\]

(19)

Solving for the higher-order terms (i.e., second order term) is more difficult since evaluation of the \( m=5 \) solutions for \( S_C, P_k^{(i=1,2)} \) and \( g_k^{(i=1,2)} \) additionally requires that the solutions are relative close to the asymptotic range.

Convergence studies for analytical benchmarks (1D wave and 2D Laplace equations) show that equation (18) has the correct form, but the order of accuracy is poorly estimated by equation (19) except in the asymptotic range. The error estimate can be improved using correction factors, which provide a quantitative metric for defining distance of solutions from the asymptotic range and approximately account for the effects of higher-order terms. The numerical error is defined as:

\[
\delta^*_{i} = C_k \delta^*_{RE_i} = C_k \left( \frac{\epsilon_{k_{i1}}}{r_k^{p_k} - 1} \right)
\]

(20)

Where correction factor \( C_k \) is based on solution of (20) for \( C_k \) with \( \delta^*_{RE_i} \) based on (18) but replacing observed \( p_k \) with the improved estimate \( p_{kw} \) with:

\[
C_k = \frac{r_k^{p_k} - 1}{r_k^{p_{kw}} - 1}
\]

(21)

where \( p_{kw} \) 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 \( C_k \rightarrow 1 \). Usually \( p_{kw} = p_{th} \) where \( p_{th} \) is the theoretical order of accuracy; however, in some cases better estimates may be available, e.g., including the effects of non-uniform grids. Substitution of (21) into (20) results in:

\[
\delta^*_{i} = C_k \left( \frac{\epsilon_{k_{i1}}}{r_k^{p_{th}} - 1} \right)
\]

(22)
For $C_k$ sufficiently less than or greater than 1 and lacking confidence, uncertainties caused by grid/time-step is estimated:

$$U_k = \begin{cases} 9.6(1-C_k)^2 + 1.1 |\delta_{RE_k}| & |1 - C_k| < 0.125 \\ 2|1 - C_k| + 1 |\delta_{RE_k}| & |1 - C_k| \geq 0.125 \end{cases}$$

(23)

For uncorrected solutions, $U_k$ (23) is based on the absolute value of the corrected error estimate plus the amount of the correction. For corrected solutions (i.e. corrected error estimate is used both in sign and magnitude to define numerical benchmark $S_{kE} = S - C_k \delta_{RE_k}$), $U_{kC}$ is based on the absolute value of the amount of the correction

$$U_{kC} = \begin{cases} 2.4(1-C_k)^2 + 0.1 |\delta_{RE_k}| & |1 - C_k| < 0.25 \\ |1 - C_k| |\delta_{RE_k}| & |1 - C_k| \geq 0.25 \end{cases}$$

(24)

It should be noted that the use of corrected solution is only useful when solutions are sufficiently close to the asymptotic range, within which the lack of conservation properties (e.g., mass and momentum) for $S_{kC}$ can be neglected. Additionally, there are situations that might prevent correction of the solution including variability in the observed order of accuracy, lack of complete iterative convergence, and solutions further from the asymptotic range.

The correction factor approach has similarities to that proposed in [25]

$$U_{C&K} = C_k |\delta_{RE_k}|$$

(25)

An alternative approach is the GCI [26] as recommended by AIAA [14], ASME [15], and [27]. The uncertainty is defined using the error estimate from RE multiplied by a factor of safety ($F_S$)

$$U_k = F_S |\delta_{RE_k}|$$

(26)

Where $\delta_{RE_k}$ is based on a single-term estimate as given by (18) with either assumed (e.g. based on theoretical values) or estimated (observed) order of accuracy, where for the former only two solutions are required. $F_S$ is based on empirical data and $F_S = 1.25$ is recommended [12] for careful grid convergence studies using three or more grid solutions and $F_S = 3$ for cases in which only two grids are used and order of accuracy is assumed from the theoretical value $p_{th}$. In [28], the GCI approach was extended for situations where the solution is corrected with an error estimate from RE as:

$$U_{kC} = (F_S - 1) |\delta_{RE_k}|$$

(27)

[12] suggested:

$$U_{kC} = \left( \frac{1}{r_k p_k - 1} \right) |\delta_{RE_k}|$$

(28)

$\delta_{RE_k}$ is estimated using equation (18) but with $\epsilon_{k1} = S_{k2} - S_{k1}$ replaced by $\epsilon_{kC} = S_{k1} - S_{kC}$. This form shows that the amount of conservatism is a function of $r_k$ and $p_k$. Thus for $r_k < \sqrt{2}$, the multiplication factor is greater than 1 giving unacceptable result that the uncertainty in the corrected solution is larger than the error in the uncorrected solution.

[22] shows that the correction factor approach is equivalent to the GCI, but with a variable factor $F_S$. 

---

For $kC$ sufficiently less than or greater than 1 and lacking confidence, uncertainties caused by grid/time-step is estimated:
which increases with distance of solutions from the asymptotic range. \( C_k \) provides a metric for estimating distance of solutions from the asymptotic range: \( = 1 \) when solutions are in asymptotic range; \(< 1 \) when \( p_k < p_{k\text{ asymptotic}} \); and \( > 1 \) when \( p_k > p_{k\text{ asymptotic}} \). For GCI approach, \( F_S \) is constant for all \( C_k \): 1.25 for careful grid studies otherwise 3. For \( C_k \) approach, \( F_S \) varies linearly with \( C_k \) with slope 2 (uncorrected solution) and 1 (corrected solution) and symmetric about \( C_k = 1 \). The intersection points between \( C_k \) and GCI approaches depends on value \( F_S \) used in GCI: for \( F_S = 1.25 \) \( C_k = (0.875, 1.125) \) and for \( F_S = 3 \) \( C_k = (0, 2) \) for uncorrected solutions. When \( F_S = 1.25 \) and solutions are between the intersections points (closer to the asymptotic range), GCI approach is more conservative than \( C_k \) approach. When \( F_S = 1.25 \) and solutions are outside the intersection points (further from the asymptotic range), GCI approach is less conservative than \( C_k \) approach. When \( F_S = 3 \), GCI is always more conservative than \( C_k \) approach except for solutions very far from the asymptotic range. The previously mentioned analytical benchmarks confirmed the \( F_S \) slope predicted by \( C_k \) approach for \( C_k < 1 \), which admittedly may not be best for all cases and needs future research especially for \( C_k > 1 \). \( U_{C&K} \) is similar to correction factors for \( C_k > 1 \) in providing variable \( F_S \) which increases with distance from the asymptotic range; however, less conservative than correction factors which includes the amount of the correction. Also, for \( C_k = 0 \) \( U_{C&K} \) predicts 50% uncertainty and for \( C_k < 1 \) gives an unacceptable result of \( F_S < 1 \). Figure 1 compares \( F_S \) predicted by correction factors, GCI, and \( U_{C&K} \).

Results in total suggest that the variable factor of safety predicted by the correction factor approach, which increases with distance from the asymptotic range, is a “common-sense” advantage compared to GCI as it provides a quantitative metric to determine proximity of the solutions to the asymptotic range and approximately accounts for the effects of higher-order terms.

Figure 1: Factors of safety for correction factor, GCI, and Celik & Karatekin verification methods

2.3.4 Status of Ship Hydrodynamics Verification Studies at IIHR

The verification procedures have been used for quantitative verification of integral (forces, moments, motions) and point (wave profiles and elevations, velocity and turbulence profiles) variables for ship
hydrodynamics over the past 10 years at IIHR for many ship geometries and flow conditions in support of code development of a general-purpose RANS/DES code CFDSHIP-IOWA versions 3 [29] and 4 [30,31]. Geometries and flow conditions include surface-piercing flat plate, surface-piercing NACA0024 hydrofoil using RANS and DES, Wigley hull pitch and heave motions in head seas, Series 60 (S60) cargo/container and surface combatant 5415 in straight ahead calm water, Esso Osaka tanker with rudder in static manoeuvring conditions using overset grids, tanker KVLCC, TEB ducted rotor using overset grids, Athena barehull with skeg free to pitch and heave using overset grids, and DTMB 5512 in regular head waves.

For the simpler geometries (S60, Wigley hull, and NACA 0024) about 1 M and for the practical geometries about 7 M grid points were used. For steady flows \( \sqrt{2} \) grid refinement ratio and for unsteady flow \( \sqrt{2} \) grid refinement ratio and \( \sqrt{2} \) time refinement ratio were used. Use of finer grid is not always possible due to available resources, speed of the code and difficulties in separating iterative and grid errors. Typically \( U_I (0.01\% S_I \leq U_I \leq 0.4\% S_I) \) is at least an order of magnitude smaller than \( U_G \), such that \( U_{SN} \approx U_G \). For monotonically converged cases, \( 0.14 \leq R_G \leq 0.71 \). In many cases the observed order of accuracy is fairly close to \( p_{est} = p_t = 2.0 \) for 2\(^{nd}\) order numerical scheme (or 3.0 for 3\(^{rd}\) order scheme), but in many cases it is not ranging from \( 1.1 \leq p_G \leq 7.5 \). Correction factors range from \( 0.29 \leq C_G \leq 6.72 \), but in most cases are between \( 0.5 \leq C_G \leq 2.0 \). Intervals of verification for resistance and thrust and torque are \( U_G \approx 3\% S_I \). For point variables grid uncertainties range from \( 0.2\% S_I \leq U_G \leq 29\% S_I \) where largest values are for most complicated flow. Verification results for time-step studies are similar to those for grid size studies. The large deviation of \( p_G \) from the estimated order of accuracy and the large deviation of \( C_G \) from 1 suggest that the existence and behavior of the asymptotic range for ship hydrodynamics has not yet been demonstrated.

Achieving the asymptotic range for practical applications, at least for ships, has not yet been demonstrated. [32] investigated the issue of achieving the asymptotic range by continuously refining the grid to 8.1 million (M) grid points for the Athena bare hull with skeg with 2 degrees of freedom (pitch and heave) at Froude number (Fr) 0.48. Due to the symmetry of the geometry, only half domain is simulated. Table 1 summarizes all the grids used for this study, with \( y^+ \) for the first grid point away from the wall. Grids 1 to 7 are designed with a systematic grid refinement ratio \( r_k = 2^{1/4} \), which allows 9 sets of grids for V&V with 5 sets with \( r_k = 2^{1/4} \) (1, 2, 3; 2, 3, 4; 3, 4, 5; 4, 5, 6; and 5, 6, 7), 3 sets with \( r_k = 2^{1/2} \) (1, 3, 5; 2, 4, 6; and 3, 5, 7), and 1 set with \( r_k = 2^{3/4} \) (1, 4, 7). \( U_I (0.1\% S_I \leq U_I \leq 0.3\% S_I) \) is of the same order of magnitude for all the grids. As shown in Table 2, \( C_{TX} \) monotonically converges for grids (2,4,6), (3,5,7), (3,4,5), (4,5,6), and (5,6,7), of which grids (3,5,7) have the smallest grid uncertainty and grids (4,5,6) are closest to the asymptotic range based on 1-\( C_G \) closest to zero. \( C_{TX} \) monotonically diverges on grids (1,2,3), (1,3,5), and (2,3,4), which is likely due to the insufficient resolution of the coarsest grids 1 and 2. As shown in Figure 2(a), \( C_{TX} \) for grid 1 does not follow the trend as shown for grids 2 to 7. Figure 2(a) also shows frictional resistance coefficient \( C_{FX} \) and \( C_{PX} \) on all the grids. Figure 2(b) shows the magnitudes of the relative changes of solutions \( \varepsilon_N \) between two successive grids with respect to the solutions on the finest grid 7. When grids are refined from 3 to 8, \( \varepsilon_N \) systematically decreases for \( C_{TX} \) and \( C_{FX} \) while oscillatory decreases for \( C_{PX} \). Compared to resistance coefficients, sinkage and trim are more difficult to achieve converged solutions. Monotonically converged solutions are achieved for both sinkage and trim on grids (3,5,7) and (4,5,6) with additional converged solution for trim on grids (5,6,7) (Table 3 and figure 2(c)). Sinkage has smaller grid uncertainties even though trim seems to be closer to the asymptotic range based on 1-\( C_G \). Figure 2(d) shows \( \varepsilon_N \) of motions with respect to the solution on grid 7. For grids coarser than grid 5, \( \varepsilon_N \) shows linear increase and oscillatory increase for sinkage and trim, respectively. For grids finer than grid 5, \( \varepsilon_N \) shows oscillatory decrease and linear decrease for sinkage and trim, respectively. Tables 2 and 3
show that separating iterative errors from grid uncertainties is problematic for the finer grids since iterative and grid uncertainties are of the same order of magnitude. However, $\varepsilon_N$ of the current study does show systematic decreasing for $\text{CTX}$ and $\text{CFX}$ and oscillatory decreasing for $\text{CPX}$. $\text{CTX}$, $\text{CFX}$, and $\text{CPX}$ show different rates of approaching the asymptotic range and $1-C_G$ shows a large range of values, which suggests that the finest grid is still out of the asymptotic range. Further refinement with $y^+$ of the first grid point away from the wall less than 1 may help but requires a minimum of 38M grid points. This number will be doubled if a whole domain simulation is conducted. Solutions on such fine grids are not trivial and raise issues of code efficiency and available computer resources. It should be noted that although further grid refinement is required to achieve the asymptotic range it does not reduce the interval of validation since $U_G<<U_D$.

The wave field using grid 3 is shown in Figure 3.

<table>
<thead>
<tr>
<th>Grids</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ship</td>
<td>$111\times29\times56$</td>
<td>$132\times34\times66$</td>
<td>$157\times41\times79$</td>
<td>$187\times49\times94$</td>
<td>$222\times58\times112$</td>
<td>$264\times69\times133$</td>
<td>$314\times82\times158$</td>
</tr>
<tr>
<td></td>
<td>$=180,264$</td>
<td>$=296,208$</td>
<td>$=508,523$</td>
<td>$=861,322$</td>
<td>$=1,442,112$</td>
<td>$=2,422,728$</td>
<td>$=4,068,184$</td>
</tr>
<tr>
<td>Background</td>
<td>$111\times29\times56$</td>
<td>$132\times34\times66$</td>
<td>$157\times41\times79$</td>
<td>$187\times49\times94$</td>
<td>$222\times58\times112$</td>
<td>$264\times69\times133$</td>
<td>$314\times82\times158$</td>
</tr>
<tr>
<td></td>
<td>$=180,264$</td>
<td>$=296,208$</td>
<td>$=508,523$</td>
<td>$=861,322$</td>
<td>$=1,442,112$</td>
<td>$=2,422,728$</td>
<td>$=4,068,184$</td>
</tr>
<tr>
<td>Total</td>
<td>360,528</td>
<td>592,416</td>
<td>1,017,046</td>
<td>1,722,644</td>
<td>2,884,224</td>
<td>4,845,456</td>
<td>8,136,368</td>
</tr>
<tr>
<td>$y^+$</td>
<td>4.26</td>
<td>3.58</td>
<td>3.06</td>
<td>2.56</td>
<td>2.15</td>
<td>1.80</td>
<td>1.52</td>
</tr>
</tbody>
</table>

### Table 1: Grids used for verification for Athena bare hull with skeg ($Fr=0.48$).

### Table 2: V&V study for integral force coefficient $C_{TX}$

<table>
<thead>
<tr>
<th>Grids</th>
<th>Refinement ratio</th>
<th>$R_G$</th>
<th>$P_G$</th>
<th>1-$C_G$</th>
<th>$U_G$ (%)</th>
<th>$E$ (%)</th>
<th>$U_Y$ (%)</th>
<th>$U_D$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2, 4, 6</td>
<td>$\sqrt{2}$</td>
<td>0.63</td>
<td>1.32</td>
<td>0.42</td>
<td>4.90</td>
<td>1.83</td>
<td>5.12</td>
<td>1.5</td>
</tr>
<tr>
<td>3, 5, 7</td>
<td>$\sqrt{2}$</td>
<td>0.40</td>
<td>2.66</td>
<td>-0.51</td>
<td>0.01</td>
<td>2.10</td>
<td>1.50</td>
<td>1.5</td>
</tr>
<tr>
<td>3, 4, 5</td>
<td>$\sqrt{2}$</td>
<td>0.80</td>
<td>1.27</td>
<td>0.64</td>
<td>9.08</td>
<td>1.23</td>
<td>9.20</td>
<td>1.5</td>
</tr>
<tr>
<td>4, 5, 6</td>
<td>$\sqrt{2}$</td>
<td>0.60</td>
<td>2.98</td>
<td>0.01</td>
<td>0.94</td>
<td>1.83</td>
<td>1.77</td>
<td>1.5</td>
</tr>
<tr>
<td>5, 6, 7</td>
<td>$\sqrt{2}$</td>
<td>0.50</td>
<td>4.00</td>
<td>-0.47</td>
<td>0.56</td>
<td>2.10</td>
<td>1.60</td>
<td>1.5</td>
</tr>
</tbody>
</table>

%$S_5$, $S_6$, $S_7$ or $\%$EFD; * $C_{TX}$ is based on the static wetted area (EFD data $C_{TX}=0.00575$).

### Table 3: Verification study for motions of Athena bare hull with skeg ($Fr=0.48$)

<table>
<thead>
<tr>
<th>Grids</th>
<th>Refinement ratio</th>
<th>$R_G$</th>
<th>$P_G$</th>
<th>1-$C_G$</th>
<th>$U_G$ (%)</th>
<th>$E$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sinkage</td>
<td>3, 5, 7</td>
<td>$\sqrt{2}$</td>
<td>0.31</td>
<td>3.4</td>
<td>-1.25</td>
<td>0.77</td>
</tr>
<tr>
<td>Sinkage</td>
<td>4, 5, 6</td>
<td>$\sqrt{2}$</td>
<td>0.13</td>
<td>12</td>
<td>-9.28</td>
<td>0.81</td>
</tr>
<tr>
<td>Trim</td>
<td>3, 5, 7</td>
<td>$\sqrt{2}$</td>
<td>0.48</td>
<td>2.13</td>
<td>-0.09</td>
<td>3.88</td>
</tr>
<tr>
<td>Trim</td>
<td>4, 5, 6</td>
<td>$\sqrt{2}$</td>
<td>0.53</td>
<td>3.69</td>
<td>-0.31</td>
<td>4.37</td>
</tr>
<tr>
<td>Trim</td>
<td>5, 6, 7</td>
<td>$\sqrt{2}$</td>
<td>0.53</td>
<td>3.71</td>
<td>-0.32</td>
<td>2.28</td>
</tr>
</tbody>
</table>

%$S_6$, $S_7$ or $\%$EFD
Figure 2: Verification for resistance and motions for Athena bare hull with skeg ($Fr=0.48$): (a) resistance coefficients, (b) relative change $\epsilon_N = \left| \frac{S_N - S_{N-1}}{S_1} \right| \times 100$ for resistance coefficients, (c) sinkage and trim, (d) relative change $\epsilon_N$ for sinkage and trim.

Figure 3: Free surface wave fields for Athena bare hull with skeg at $Fr=0.48$. 
3.0 CERTIFICATION OF CFD CODES

At the code level uncertainties are further decomposed into systematic (bias) and random (precision) components

\[ U_S^2 = B_S^2 + P_S^2 = (B_{SM}^2 + B_{SN}^2) + P_S^2 \]  

(29)

where bias uncertainties are estimated at the simulation (single realization) level and precision uncertainties at the code (N-version, multiple realization) level. Equation (29) can be written both for an individual code \( S_i \) and the average of N-version codes (mean code)

\[ \bar{S} = \frac{1}{N} \sum_{i=1}^{N} S_i \]  

(30)

as

\[ U_{\bar{S}}^2 = B_{\bar{S}}^2 + P_{\bar{S}}^2 \]  

(31)

and

\[ U_S^2 = B_S^2 + P_S^2 \]  

(32)

V&V studies (simulation level) provide \( B_{S_i}^2 = B_{SMi}^2 + B_{SNi}^2 \). Modeling uncertainties are decomposed into known and estimated \( B_{SMi}^2 = B_{SMEi}^2 + B_{SMAi}^2 \) and numerical uncertainties are decomposed into estimates for iterative, grid, time, and other input parameters \( B_{SNi}^2 = B_{SNIi}^2 + B_{SNGi}^2 + B_{SNTi}^2 + B_{SNPi}^2 \). The mean code bias error is based on the average RSS for the individual codes

\[ B_{\bar{S}}^2 = \frac{1}{N} \sum_{i=1}^{N} B_{S_i}^2 \]  

(33)

N-version testing (code level) provides

\[ P_{S_i} = 2\sigma_{S_i} \]  

(34)

where

\[ \sigma_{S_i} = \frac{1}{N-1} \sum_{i=1}^{N} (S_i - \bar{S})^2 \]  

(35)

and

\[ P_{\bar{S}} = \frac{2\sigma_{\bar{S}}}{\sqrt{N}} \]  

(36)

For \( N \geq 10 \) and normal \( S_i \) distributions, the estimated truth \( \overline{S}_{ET} \) lies within the confidence intervals

\[ S_i - U_{S_i} \leq \overline{S}_{ET} \leq S_i + U_{S_i} \]  

(37)

and

\[ \bar{S} - U_{\bar{S}} \leq \overline{S}_{ET} \leq \bar{S} + U_{\bar{S}} \]  

(38)

The individual code and mean code levels correspond to 1st-order and N-order replication level analysis in EFD, respectively. The mean code is a fictitious code, which uses an average of the modelling and numerical methods used by the individual codes. The mean code seems more fictitious than the mean measurement systems and data acquisition and reduction processes envisioned in going from 1st to Nth-order EFD replication level. Nonetheless the differences between the solutions from the individual codes are assumed to result from many small errors of equal magnitude and equally likely to be positive or negative such that for \( N \to \infty \) \( S_i \) distribution is normal, which is valid even if error sources have non-normal distributions according to the central limit theorem.
The mean comparison error is defined as the difference between the mean code and experimental values

\[ E = D - \bar{S} \]  

(39)

Following the same reasoning and approach used for validation, certification uncertainty \( U_C \) is defined as

\[ U_C^2 = U_E^2 - \frac{B_{\text{SMA}}^2}{S^2} = U_D^2 + B_{\text{SNR}}^2 + B_{\text{SNR}}^2 + P_S^2 \]  

(40)

If \( |E| \leq U_C \), mean code is certified at interval \( U_C \), whereas for \( |E| > U_C \) mean code is not certified due to modeling assumptions. \( E \) can be used for modeling assumptions improvements, i.e., for \( |E| >> U_C \), \( E \approx \delta_{\text{SMA}} \). Similar analysis can be done for the individual code

\[ E_i = D - S_i \]  

(41)

\[ U_{C_i}^2 = U_{E_i}^2 - U_{\text{SMA}}^2 = U_{D_i}^2 + B_{\text{SNR}}^2 + B_{\text{SNR}}^2 + P_S^2 \]  

(42)

and for \( |E_i| \leq U_{C_i} \) individual code is certified at interval \( U_{C_i} \), whereas for \( |E_i| > U_{C_i} \) individual code is not certified due to modeling assumptions. \( E_i \) can be used for modeling assumptions improvements, i.e., \( |E_i| >> U_{C_i} \), \( E_i \approx \delta_{\text{SMA}} \).

Certification provides additional confidence compared to validation; since, additionally based on statistics of normal distribution of \( N \)-versions. Certification uncertainty also an improvement over simply identifying outliers [11] based on \( P_S \) alone; since additionally includes considerations of bias uncertainties. As with EFD uncertainty analysis, maximum confidence is achieved if both bias and precision uncertainties are considered. Ref. [33] provides subgroup analysis procedures for isolating and assessing differences due to use of different models and/or numerical methods, including comparisons with the method of analysis of the means [11].

### 4.0 CERTIFICATION OF SHIP HYDRODYNAMICS CODES

The purpose of the CFD Workshop Tokyo 2005 [34] was to assess viscous flow CFD simulations for ship hydrodynamics and accelerate research and development. Previous workshops were held in 1980, 1990, 1994, and 2000.

The 1980 workshop had 2 test cases for tanker and cargo hull forms with 17 submissions. 16 boundary-layer and 1 RANS code were used. The boundary layer simulations were considered satisfactory for the fore and mid body, but failed completely near the stern.

The 1990 workshop had 1 open and 1 blind test cases for two tanker hull forms with 19 submissions. 17 RANS, 1 boundary-layer, and 1 LES code were used. The average number of grid points was 80K. The results were a milestone in prediction capability for ship boundary layers and wakes; however, none of the methods accurately predicted the stern bilge vortices and hooked shaped axial velocity contours.

The 1994 workshop had 3 test cases for cargo and two tanker hull forms. The test cases included resistance, boundary layer and wave pattern at low (10 RANS submissions) and medium (11 RANS and 8 potential flow submissions) Froude number for cargo and boundary layer for tanker (8/5 submissions) hull...
forms. Turbulence models included 0, 1, 2 and Reynolds Stress (RS). Free surface models were surface tracking. The average number of grid points was 190K. The RS simulations showed marked improvement in the prediction of the stern bilge vortices and hooked shaped axial velocity contours. The wave pattern results were a milestone in prediction capability for ship hydrodynamics; however, for y/L>0.2 the waves suffered considerable damping. It was apparent that the better CFD codes were useful for design.

The 2000 workshop [35] had 20 organizations from 11 countries for 3 test cases for modern tanker (13 submissions), container (7 submissions), and combatant (7 submissions) hull forms, including self-propulsion for the container and full-scale for the tanker. 16 different RANS codes were used. Most of the codes were industrialized or commercial for multiple users and applications. Turbulence models included 0, 1, 2 and RS. Free surface models included surface tracking and level set (LS) or volume of fraction (VOF) surface capturing. Numerical methods included finite volume (FV), 2nd order, multi-block structured, pressure equation or artificial compressibility, and fast iterative solvers. The average number of grid points was 700K. [1,2] V&V procedures were recommended and mostly used; however, implementation difficulties were apparent due to lack of familiarity with the procedures especially for practical applications and fact that solutions were far from the asymptotic range. 10 organizations provided quantitative verification. Iterative convergence was usually not well documented. 8 simulations showed monotonic and 2 simulations showed oscillatory grid convergence. The resistance coefficient C_T results for five simulations were validated for container and combatant hull forms with intervals ranging from 3-15%C_T(TEFD). The average comparison error E for C_T is 4.8%, which is larger than the average validation uncertainty U_V at 3.6%. The average experimental uncertainty U_E is 1.6% and average U_S is 3.2%. Efforts to reduce intervals of validation will require reduction in both numerical and experimental uncertainties since both are of similar order of magnitude. Quantitative validation for point variables was not possible because U_S was seldom assessed. The RS models performed best, but improvements needed for accurate prediction of the Reynolds stresses. Free surface predictions showed increased resolution near the hull and reduced damping away from the hull, but improvements still needed. In general, more codes performed satisfactory for more test cases and conditions than the previous workshop. [4] used the resistance coefficient predictions from the 2000 workshop for the tanker hull form as an example for certification of ship hydrodynamics codes.

The 2005 workshop had 24 organizations participated from 12 countries using 19 different RANS codes for 5 test cases for the same 3 hull forms used at the 2000 workshop. Several codes had multiple submissions from different organizations or from the same organization with different turbulence models. Test cases include: bare hull fixed (1.1, 1.2, 1.4) and free (1.3); appended hull with and without propeller fixed (2); bare hull fixed static drift angle β = 0 (3.1), 3 (3.2), 6 (3.3), 9 (3.4, and 12 (3.5) deg; bare hull fixed in regular head waves (4); and bare hull fixed finest (5.1), fine (5.2), medium (5.3), coarse (5.4) and coarsest (5.5) grid study. Turbulence models included RS (4), two-equation (17), one-equation (5), algebraic (3), and vortex element (1). Near wall models (16) and wall functions (8) were used with y<+1 and 100-400 (mostly 100), respectively. Free surface modeling included tracking (5) and LS (7) or VOF (4) capturing methods. Body forces were used to model the propeller. Numerical methods included FD (3), FV (13), FA (1), FE (1), and I (1). Structured single (11) and multi block (13) with and without overset and unstructured (1) grid systems were used. The number of blocks varied from 1 to 48 with average 17. 75% used commercial grid generation software. Most codes were multi-block and parallel. The CPU time ranged from 4.2 to 8000 hours with average 715 hours, which is 10 times larger than at the previous workshop.

Tables 4 summarizes the test cases analyzed, including number of submissions, grid points, turbulence models, and resistance coefficient mean solution V&V and code certification variables (%mean solution), including results from the 2000 workshop for comparison. Test cases 1.3, 2, 4, 5.1, and 5.2 had relatively few submissions (1, 4, 3, 6) and were not included in the analysis. A similar summary table was made using median variables. The summary tables for mean and median variables are based on detailed tables, histograms and running records prepared for each of the test cases. The normality of the histograms was
assessed using Anderson-Darling, Shapiro-Wilk and probability plot correlation tests. 7 of the 11 distributions passed all three tests and if outliers were removed all cases tested normal. Correlations between submissions were apparent for same code and different turbulence models or different codes and the same turbulence models, although the differences were less than subgroup or ANOM analysis. Average (test cases 1.1, 1.2, and 1.4) number of grid points for half domain simulations was 2.3 million, which is more than twice as many as at the 2000 workshop. The average standard deviations of total, pressure, and frictional resistance coefficients are 5%, 13%, and 6%, respectively, which indicates that the largest source of variability is the pressure. The grid study test case 5 shows decreasing standard deviations for increasing grid resolution. The trends using median variables are similar, but with somewhat lower values for all variables, as is also the case for intervals of V&V and certification. The magnitudes and the trends for the resistance coefficient standard deviations and median variables are similar to those reported for aerodynamics applications drag prediction workshops [11,37,38].

[1,2] V&V procedures were recommended and mostly used. More organizations provided quantitative intervals of verification than at the 2000 workshop. The average intervals of verification, experimental uncertainty, validation uncertainty, and comparison error are 3.5%, 1.2%, 4%, and 4.2%, respectively. Thus, on average the simulations were (nearly) validated at an interval of about 4%. Including facility biases $U_D=2.2%$ [36] and $U_V=4.2%$. Reduction comparison error requires modelling improvements, whereas reduction interval validation primarily requires reduction in simulation numerical uncertainty since it is larger than EFD data uncertainty.

The average random component and certification uncertainties for the individual codes are 10.5% and 11.4%, respectively. Thus, the average individual code is certified at an interval of 11.4%. The largest contributor to the interval of certification is the random component of the simulation uncertainty, which is about 4 and 11 times larger than the systematic component and experimental uncertainties, respectively. Consideration of the mean code reduces the interval of certification to 4.9% since in this case the systematic and random components are comparable and about 3 times larger than the experimental uncertainty. Based on $P_5^C$ alone, the average number of outliers is 1.

The 2005 and 2000 workshop results are very similar, as also shown in table 4. The overall results indicate that the intervals of comparison error and validation and certification uncertainties are 4%, 4%, and 11.4%, respectively, for resistance simulations for tanker, container, and combatant hull forms with and without waves and small drift angles, as shown in table 5. The differences between turbulence and free surface models are statistically indistinguishable. The largest contributors to validation and certification uncertainties are the individual code systematic and random components, respectively. The largest contributor to the individual code systematic uncertainty is the grid uncertainty, which is consistent with the fact that at the current level of grid resolution for practical applications the solutions are far from the asymptotic range. It is estimated that an order of magnitude more grid points are required for the solutions to achieve the asymptotic range. The overall conclusion is to reduce the intervals of verification using substantially increased grid resolutions; since, this will reduce the intervals of validation and hopefully differences between the codes and thereby also the intervals of certification. More codes performed satisfactory for more tests cases and conditions than the 2000 workshop, which was also the case for the 2000 workshop with respect to its predecessor. Noteworthy was the satisfactory performance of several URANS codes for test case 4 (forward speed diffraction), which indicates promise for extending the codes for ship motions simulations, as has already taken place. The next workshop will be held in 2008 with focus on assessment of systems and CFD based manoeuvring prediction methods using captive and free model EFD test data [http://www.simman2008.dk/].
5.0 CONCLUSIONS AND FUTURE WORK

Many viewpoints exist on all aspects of CFD uncertainty analysis ranging from concepts and definitions to methodology to detailed procedures. As discussed in [4], the largest differences are with concepts, definitions, and methodology.


The actual procedures used for V&V of solutions and N-version testing of codes are similar to those described in Sections 2.3 and 3; thus, the largest differences are in how the results are used and interpreted. Only the present approach provides quantitative metrics for solution V&V and code certification using error/uncertainty equations, which add/RSS combine elemental error/uncertainty sources. Solution verification (all solutions) and validation and code certification activities all have specific technical completion points with quantitative metrics, i.e., intervals of uncertainty at a specified level of confidence documenting the results.

It is difficult to assess the penalty for such large conceptual differences between EFD and especially CFD uncertainty analysis approaches. Clearly from a user point of view this makes for difficulties in their practical application and interpretation of results and can be blamed for lack of their use. Since commonality of procedures seems to be the strongest link it would seem that greater emphasis should be placed on these and their use, including quantitative metrics so that inter- and multi-disciplinary comparisons can be made. The highest priority is for development of procedures for correlated modeling/numerical and single-grid errors and uncertainties. The most likely prognosis for reducing CFD solution and code errors and uncertainties is to use substantially larger grid resolutions of about 38M grid points, which hopefully will be sufficient for the solutions to achieve the asymptotic range, at least for calm water resistance and propulsion for ship hydrodynamics CFD codes.

Acknowledgements

The Office of Naval Research under Grants N00014-01-1-0073 and N00014-06-1-0420, administered by Dr. Patrick Purtell, sponsored this research. The considerable help of Dr Tao Xing and Mr Matthew Marquardt and Stuart Breczinski is very much appreciated.


Table 4: CFD Gothenburg 2000 and CFD Tokyo 2005 ship hydrodynamics mean resistance coefficient solutions, verification and validation parameters, and code certification intervals.

<table>
<thead>
<tr>
<th>CFD Workshop Gothenburg 2000</th>
<th>Turbulence Model Use (%)</th>
<th>Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>0-eq</td>
<td>1-eq</td>
</tr>
<tr>
<td>KVLCC2</td>
<td>13</td>
<td>10</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>CFD Workshop Tokyo 2005</th>
<th>Turbulence Model Use (%)</th>
<th>Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case</td>
<td>0-eq</td>
<td>1-eq</td>
</tr>
<tr>
<td>1.1 KCS</td>
<td>11</td>
<td>9</td>
</tr>
<tr>
<td>1.4 KVLCC2M</td>
<td>13</td>
<td>9</td>
</tr>
</tbody>
</table>

Table 5: Summary of Case 1.1, 1.2, and 1.4, towed condition case, ship hydrodynamic code certification for CFD Tokyo 2005.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>D</th>
<th>C1 (%)</th>
<th>C2 (%)</th>
<th>C3 (%)</th>
<th>E (%)</th>
<th>Uc (%)</th>
<th>Uo (%)</th>
<th>Bn (%)</th>
<th>Vs (%)</th>
<th>Uc (%)</th>
<th>Ps (%)</th>
<th>Outliers (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cases 1.1, 1.2, 1.4</td>
<td>1.002</td>
<td>5.24</td>
<td>12.69</td>
<td>6.22</td>
<td>4.16</td>
<td>3.99</td>
<td>1.23</td>
<td>3.54</td>
<td>11.43</td>
<td>10.49</td>
<td>4.90</td>
<td>3.06</td>
</tr>
</tbody>
</table>
Quantitative V&V of CFD Solutions and Certification of CFD Codes

Paper No. 21

Discusser’s Name: W. Oberkampf

Question: In your method the uncertainties are summed using an RMS technique. The basic assumptions to use the RMS are that all of the contributors are random variables, and they are independent. However, neither of the assumptions applies. How can this approach be defended?

Author’s Reply: My perspective is that uncertainties in simulations arise from modeling and numerical errors and their correlations. As a first approximation, the assumption is made that these errors are additive such that their uncertainties root sum square. The errors/uncertainties are further decomposed into simulation level and code level. At the simulation level (individual user, code, model, grid-type, etc. level), error/uncertainty estimates are based on fixed values with the same reasoning for 95% level of confidence as used for single-realizations and 0-order–replication level bias limit (systematic uncertainty) estimation in EFD. This is the smallest uncertainty interval that could be achieved with the CFD code for the specified application. At the code level (multiple codes or users, models, grid types, etc.), standard and expanded uncertainties (random uncertainty) are estimated using N-version testing extended to include bias uncertainties (solution V&V) and use of reference values (experimental data and uncertainties) for estimating interval of certification. Differences between versions and implementations are due to myriad possibilities for modeling, numerical methods, and their implementation as CFD codes and simulations. As with estimating EFD precision limits using multiple realizations and 1-order-replication level testing, such estimates only include those factors turned on, which can be used to isolate differences, e.g., by using same models or grid types.

Discusser’s Name: L. Eca

Question: Iterative errors are reported to be between 0.4 and 3%. For the proposed grid refinement to attain the “asymptotic range” the iterative errors will have to be smaller. Will this be a problem for the demonstration of the existence of the “asymptotic range?”

Author’s Reply: Yes. Iterative errors must be at least an order of magnitude smaller than grid/time errors in order to make accurate grid/time error estimates. This presents an additional challenge for practical applications since solution changes in the asymptotic range are small (tenths of a percent or smaller) requiring iterative errors to be even smaller (hundredths of a percent or smaller), which raises issues of iterative solver accuracy, efficiency and computer resources.

Discusser’s Name: I. Celik

Question: In view of a lot of uncertainty with regards to the assumptions in your procedure, how can one trust the estimates calculated without validation of the procedure itself?

Answer: The verification procedures have been validated using simple analytical and numerical benchmarks. However, your point is well taken that more advanced numerical benchmarks are available such as the backward facing step that can and should be used to validate not only the verification but also the validation procedures. I hope to pursue such a study in the near future.

Discusser’s Name: Charles Hirsch

Question: Your approach is largely based on linear assumptions, while CFD is about nonlinearities. The interaction between grids and turbulence models is nonlinear, and there is no asymptotic range for RANS
when one refines the grid, as this leads to modeling smaller and smaller scales, which leads to unsteady flow features.

**Answer:** I agree that fluid mechanics of interest to CFD and EFD for industrial applications is largely nonlinear; however, as with EFD uncertainty analysis my perspective is that errors are additive and therefore uncertainties root sum square. For CFD errors arise from modeling and numerical errors and their correlations. For RANS codes I argue that correlated errors are relatively small, whereas correlations between modeling and numerical errors are likely significant for LES simulations and should be incorporated into the methodology and procedures in future work. The concept of asymptotic range does not require linearity or steady flow, as has been demonstrated for advanced numerical benchmarks such as backward facing step flow, but rather requires that solutions achieve independence of further iterative, grid/time step and other numerical parameter refinement such that the numerical benchmark has been obtained for specified application, models, and conditions: numerical and correlated numerical errors/uncertainties are zero and the only errors/uncertainties are due to modelling. Different models will have different numerical benchmarks at least for RANS models, whereas for LES numerical benchmark should be same as fully resolved DNS.