Fred Stern
Professor Mechanical Engineering and
Research Engineer
Fellow ASME

Robert V. Wilson
Assistant Research Engineer
Mem. ASME

Iowa Institute Hydraulic Research,
The University of Iowa,
Iowa City, IA 52242

Hugh W. Coleman
Eminent Scholar in Propulsion,
Professor of Mechanical Engineering,
Propulsion Research Center,
Mechanical and Aerospace Engineering
Department,
University of Alabama in Huntsville,
Huntsville, AL 35899
Fellow ASME

Eric G. Paterson
Associate Research Engineer,
Iowa Institute Hydraulic Research,
The University of Iowa,
Iowa City, IA 52242
Mem. ASME

Comprehensive Approach to Verification and Validation of CFD Simulations—Part 1: Methodology and Procedures

Part 1 of this two-part paper presents a comprehensive approach to verification and validation methodology and procedures for CFD simulations from an already developed CFD code applied without requiring availability of the source code for specified objectives, geometry, conditions, and available benchmark information. Concepts, definitions, and equations derived for simulation errors and uncertainties provide the overall mathematical framework. Verification is defined as a process for assessing simulation numerical uncertainty and, when conditions permit, estimating the sign and magnitude of the numerical error itself and the uncertainty in that error estimate. The approach for estimating errors and uncertainties includes (1) the option of treating the numerical error as deterministic or stochastic, (2) the use of generalized Richardson extrapolation for J input parameters, and (3) the concept of correction factors based on analytical benchmarks, which provides a quantitative metric to determine proximity of the solutions to the asymptotic range, accounts for the effects of higher-order terms, and are used for defining and estimating errors and uncertainties. Validation is defined as a process for assessing simulation modeling uncertainty by using benchmark experimental data and, when conditions permit, estimating the sign and magnitude of the modeling error itself. The approach properly takes into account the uncertainties in both the simulation and experimental data in assessing the level of validation. Interpretation of results of validation efforts both where the numerical error is treated as deterministic and stochastic are discussed. Part 2 provides an example for RANS simulations for a cargo/container ship where issues with regard to practical application of the methodology and procedures and interpretation of verification and validation results are discussed.
[DOI: 10.1115/1.1412235]

1 Introduction

Discussion and methodology for estimating errors and uncertainties in computational fluid dynamics (CFD) simulations have reached a certain level of maturity with recognition of importance through editorial policies (Freitas [1]), increased attention and recent progress on common terminology (AIAA, [2]), advocacy and detailed methodology (Roache [3]), and numerous case studies (e.g. [4]). Progress has been accelerated in response to the urgent need for achieving consensus on concepts, definitions, and useful methodology and procedures, as CFD is applied to increasingly complex geometry and physics and integrated into the engineering design process. Such consensus is required to realize the goals of simulation-based design and other uses of CFD such as simulating flows for which experiments are difficult (e.g., full-scale Reynolds numbers, hypersonic flows, off-design conditions). In spite of the progress and urgency, the various viewpoints have not converged and current approaches fall short of providing practical methodology and procedures for estimating errors and uncertainties in CFD simulations.

The present work provides a pragmatic approach for estimating errors and uncertainties in CFD simulations. Previous work on verification (Stern et al. [5]) is extended and put on a more rigorous foundation and combined with subsequent work on validation (Coleman and Stern [6]) thereby providing a comprehensive framework for overall procedures and methodology. The philosophy is strongly influenced by experimental fluid dynamics (EFD) uncertainty analysis (Coleman and Steele [7]), which has been standardized. Hopefully, CFD verification and validation procedures and methodology can reach a similar level of maturity and user variability can reach similar low levels, as for EFD. The work is part of a larger program (Rood [8]) for developing and implementing a strategy for verification and validation of Reynolds-averaged Navier-Stokes (RANS) ship hydrodynamics CFD codes. The program includes complementary CFD and EFD towing-tank investigations and considers errors and uncertainties in both the simulations and the data in assessing the success of the verification and validation efforts. The work also benefited from collaboration with the 21st and 22nd International Towing Tank Resistance Committees (ITTC [9,10]). The procedures proposed in this paper were adopted on an interim basis by the 22nd ITTC and also were recommended and used at the recent Gothenburg 2000 Workshop on CFD in Ship Hydrodynamics (Larsson et al. [11]).

The focus is on verification and validation methodology and procedures for CFD simulations with an already developed CFD code applied without requiring availability of the source code for specified objectives, geometry, conditions, and available benchmark information. The methodology and procedures were developed considering RANS CFD codes, but should be applicable to a fairly broad range of codes such as boundary-element methods and certain aspects of large-eddy and direct numerical simulations. The present work differs in many respects from recent literature. The presentation is relatively succinct with intention for use for practical applications (i.e., industrial CFD) for which numerical errors and uncertainties cannot be considered negligible or overlooked.

Contributed by the Fluids Engineering Division for publication in the JOURNAL OF FLUIDS ENGINEERING. Manuscript received by the Fluids Engineering Division November 4, 1999; revised manuscript received July 10, 2001. Associate Editor: P. E. Raad.

The definitions of errors and uncertainties and verification and validation that are used in any approach need to be clearly stated. The present and Roache [3] definitions for errors and uncertainties are consistent with those used for EFD. The AIAA [2] definitions are from an information theory perspective and differ from those used in EFD, but are not contradictory to the present definitions. The present concepts and definitions for verification and validation are closely tied to the present definitions of errors and uncertainties and equations derived for simulation errors and uncertainties thereby providing the overall mathematical framework. The Roache [3] and AIAA [2] definitions are broader, but not contradictory to the present definitions. The present approach includes both the situations (1) of estimating errors and the uncertainty of those estimates and (2) of estimating uncertainties only. Richardson extrapolation (RE) is used for verification, which is not new; however, the present generalizations for J input parameters and concept of correction factors based on analytical benchmarks, which provides a quantitative metric to determine proximity of the solutions to the asymptotic range, accounts for the effects of higher-order terms, and are used for defining and estimating errors and uncertainties constitute a new approach. The use of quantitative estimates for errors and the use of uncertainties for those estimates also constitute a new approach in verification and validation.

Part 1 of this two-part paper presents the verification and validation methodology and procedures. In Section 2, the overall verification and validation methodology is presented by providing concepts, definitions, and equations for the simulation numerical and modeling errors and uncertainties. In Section 3, detailed verification procedures for estimation of various sub-components of the simulation numerical error and uncertainty are given. In Section 4, validation procedures are given including a discussion of the interpretation of validation results and use of corrected simulation results. Finally, conclusions are provided in Section 5. Part 2 provides an example for RANS simulations for a cargo/container ship where issues with regard to practical application of the methodology and procedures and interpretation of verification and validation results are discussed (Wilson et al. [12]). Present papers are based on Stern et al. [13], which is sometimes referenced for additional details. However, presentation and expanded discussions of verification procedures and implementation were improved based on nearly two years experience with present approach, especially through ITTC community and Gothenburg 2000 Workshop on CFD in Ship Hydrodynamics.

2 Overall Verification and Validation Methodology

In Section 2.1, the overall verification and validation methodology is presented by providing key concepts, definitions, and derivation of equations for the simulation error and uncertainty, as sum and root-sum-square (RSS) of simulation numerical and modeling errors and uncertainties, respectively. The verification and validation equations are derived in Sections 2.2 and 2.3, respectively, where subcomponents of the simulation numerical error are identified and an approach for assessing the simulation modeling uncertainty is presented.

2.1 Concepts and Definitions. Accuracy indicates the closeness of agreement between a simulation/experimental value of a quantity and its true value. Error δ is the difference between a simulation value or an experimental value and the truth. Accuracy increases as error approaches zero. The true values of simulation/experimental quantities are rarely known. Thus, errors must be estimated. An uncertainty U is an estimate of an error such that the interval $\pm U$ contains the true value of δ 95 times out of 100. An uncertainty interval thus indicates the range of likely magnitudes of δ but no information about its sign.

For simulations, under certain conditions, errors can be estimated including both sign and magnitude (referred to as an error estimate δ^*). Then, the uncertainty considered is that corresponding to the error in δ^*. When δ^* is estimated, it can be used to obtain a corrected value of the variable of interest.

Sources of errors and uncertainties in results from simulations can be divided into two distinct sources: modeling and numerical. Modeling errors and uncertainties are due to assumptions and approximations in the mathematical representation of the physical problem (such as geometry, mathematical equation, coordinate transformation, boundary conditions, turbulence models, etc.) and incorporation of previous data (such as fluid properties) into the model. Numerical errors and uncertainties are due to numerical solution of the mathematical equations (such as discretization, artificial dissipation, incomplete iterative and grid convergence, lack of conservation of mass, momentum, and energy, internal and external boundary noncontinuity, computer round-off, etc.). The present work assumes that all correlations among errors are zero, which is doubtless not true in all cases, but the effects are assumed negligible for the present analyses.

The simulation error δ_S is defined as the difference between a simulation result S and the truth T. In considering the development and execution of a CFD code, it can be postulated that δ_S is comprised of the addition of modeling and numerical errors

$$\delta_S = S - T = \delta_{SM} + \delta_{SN} \tag{1}$$

Support for this postulation is provided by using the model value M in definitions for modeling and numerical errors. The simulation modeling error $\delta_{SM} = M - T$ is defined as the difference between the true T and model M values while the simulation numerical error $\delta_{SN} = S - M$ is defined as the difference between the simulation S and model M values. The simulation S and model M values are obtained by numerical and exact solutions of the continuous equations used to model the truth, respectively. Since exact solution of nonlinear equations is seldom possible, approximations are used to replace the continuous modeled equations with discrete ones that are solved algebraically with a CFD code to yield the simulation value S.

The uncertainty equation corresponding to error equation (1) is

$$U_S^2 = U_{SM}^2 + U_{SN}^2 \tag{2}$$

where U_S is the uncertainty in the simulation and U_{SM} and U_{SN} are the simulation modeling and numerical uncertainties.

For certain conditions, the numerical error δ_{SN} can be considered as

$$\delta_{SN} = \delta_{SN}^* + \varepsilon_{SN} \tag{3}$$

where δ_{SN}^* is an estimate of the sign and magnitude of δ_{SN} and ε_{SN} is the error in that estimate (and is estimated as an uncertainty since only a range bounding its magnitude and not its sign can be estimated). The corrected simulation value S_C is defined by

$$S_C = S - \delta_{SN}^* \tag{4}$$

with error equation

$$\delta_{S_C} = S_C - T = \delta_{SM} + \varepsilon_{SN} \tag{5}$$

The uncertainty equation corresponding to error equation (5) is

$$U_{S_C}^2 = U_{SM}^2 + U_{S_C N}^2 \tag{6}$$

where U_{S_C} is the uncertainty in the corrected simulation and $U_{S_C N}$ is the uncertainty estimate for ε_{SN}.

Debate on verification and validation has included discussion on whether errors such as δ_{SN} are deterministic or stochastic, and thus how they should be treated in uncertainty analysis was unclear. In the ''corrected'' approach given by Eqs. (3)–(6), a deterministic estimate δ_{SN}^* of δ_{SN} and consideration of the error ε_{SN} in that estimate are used. The approach is analogous to that in EFD when an asymmetric systematic uncertainty is ''zero-centered'' by inclusion of a model for the systematic error in the data reduction equation and then the uncertainty considered is that associated with the model (Coleman and Steele [7]). In the ''uncorrected''

approach given by Eqs. (1)–(2), any particular δ_{SN} is considered as a single realization from some parent population of δ_{SN}'s and the uncertainty U_{SN} is interpreted accordingly in analogy to the estimation of uncertainties in EFD (with a similar argument for ε_{SN} and U_{S_CN}). Oberkamp and Trucano [14] have criticized Coleman and Stern [6] for treating U_{SN} statistically; however, the present approach is well justified both conceptually and mathematically for reasons just given.

The overall CFD verification and validation procedures can be conveniently grouped in four consecutive steps. The first step is preparation, which involves selection of the CFD code and specification of objectives, geometry, conditions, and available benchmark information. The objectives might be prediction of certain variables at certain levels of validation (e.g., programmatic validation requirements U_{reqd}). The variables can either be integral (e.g., resistance) or point (e.g., mean velocities and turbulent Reynolds stresses) values and the programmatic validation requirements may be different for each variable. The second and third steps are verification and validation, which are described in Sections 2.2 and 2.3. The fourth step is documentation, which is detailed presentation of the CFD code (equations, initial and boundary conditions, modeling, and numerical methods), objectives, geometry, conditions, verification, validation, and analysis.

2.2 Verification. Verification is defined as a process for assessing *s*imulation *n*umerical 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. For many CFD codes, the most important numerical errors and uncertainties are due to use of iterative solution methods and specification of various input parameters such as spatial and time step sizes and other parameters (e.g., artificial dissipation). The errors and uncertainties are highly dependent on the specific application (geometry and conditions).

The errors due to specification of input parameters are decomposed into error contributions from iteration number δ_I, grid size δ_G, time step δ_T, and other parameters δ_P, which gives the following expressions for the simulation numerical error and uncertainty

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

$$U^2_{SN}=U^2_I+U^2_G+U^2_T+U^2_P=U^2_I+\sum_{j=1}^{J}U^2_j \tag{8}$$

Similarly, error estimates δ^* can be decomposed as

$$\delta^*_{SN}=\delta^*_I+\sum_{j=1}^{J}\delta^*_j \tag{9}$$

which gives the following expressions for the corrected simulation and corrected simulation numerical uncertainty

$$S_C=S-\left(\delta^*_I+\sum_{j=1}^{J}\delta^*_j\right)=T+\delta_{SM}+\varepsilon_{SN} \tag{10}$$

$$U^2_{S_CN}=U^2_{I_C}+\sum_{j=1}^{J}U^2_{j_C} \tag{11}$$

Verification is based on equation (10), which is put in the form

$$S=S_C+\left(\delta^*_I+\sum_{j=1}^{J}\delta^*_j\right) \tag{12}$$

Equation (12) expresses S as the corrected simulation value S_C plus numerical errors. S_C is also referred to as a numerical benchmark since it is equal, as shown by Eq. (10), to the truth plus simulation modeling error and presumable small error ε_{SN} in the estimate of the numerical error δ^*_{SN}.

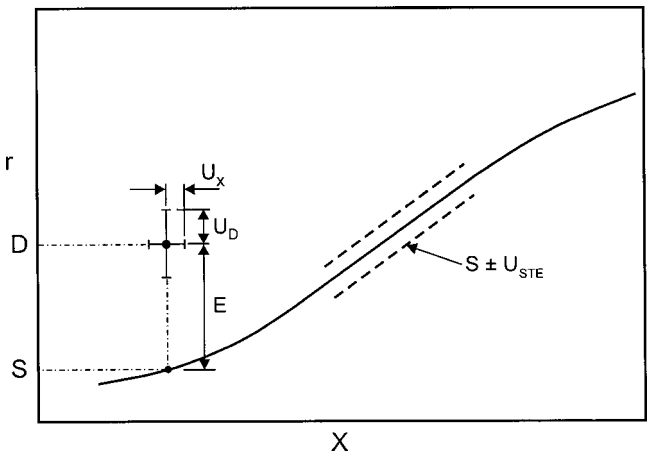

Fig. 1 Definition of comparison error.

2.3 Validation. Validation is defined as a process for assessing simulation modeling uncertainty U_{SM} by using benchmark experimental data and, when conditions permit, estimating the sign and magnitude of the modeling error δ_{SM} itself. Thus, the errors and uncertainties in the experimental data must be considered in addition to the numerical errors and uncertainties discussed in Section 3. Approaches to estimating experimental uncertainties are presented and discussed by Coleman and Steele [7].

The validation methodology of Coleman and Stern [6] which properly takes into account the uncertainties in both the simulation and the experimental data is discussed in this section for both approaches of treating the numerical error as stochastic and as deterministic.

The validation comparison is shown in Fig. 1. The experimentally determined r-value of the (X_i, r_i) data point is D and simulated r-value is S. Recall from Eq. (1) that the simulation error δ_S is the difference between S and the truth T. Similarly, the error δ_D in the data is the difference between D and the truth T, so setting the simulation and experimental truths equal results in

$$D-\delta_D=S-\delta_S \tag{13}$$

The comparison error E is defined as the difference of D and S

$$E=D-S=\delta_D-\delta_S=\delta_D-(\delta_{SMA}+\delta_{SPD}+\delta_{SN}) \tag{14}$$

with δ_{SM} decomposed into the sum of δ_{SPD}, error from the use of *p*revious *d*ata such as fluid properties, and δ_{SMA}, error from *m*odeling *a*ssumptions. Thus E is the resultant of *all* the errors associated both with the experimental data and with the simulation. For the approach in which no estimate δ^*_{SN} of the sign and magnitude of δ_{SN} is made, all of these errors are estimated with uncertainties.

If (X_i, r_i), and S share no common error sources, then the uncertainty U_E in the comparison error can be expressed as

$$U^2_E=\left(\frac{\partial E}{\partial D}\right)^2U^2_D+\left(\frac{\partial E}{\partial S}\right)^2+U^2_S=U^2_D+U^2_S \tag{15}$$

or

$$U^2_E=U^2_D+U^2_{SMA}+U^2_{SPD}+U^2_{SN} \tag{16}$$

Ideally, one would postulate that if the absolute value of E is less than its uncertainty U_E, then validation is achieved (i.e., E is "zero" considering the resolution imposed by the "noise level" U_E). In reality, there is no known approach that gives an estimate of U_{SMA}, so U_E cannot be estimated. That leaves a more stringent

validation test as the practical alternative. If the validation uncertainty U_V is defined as the combination of all uncertainties that we know how to estimate (i.e., all but U_{SMA}), then

$$U_V^2 = U_E^2 - U_{SMA}^2 = U_D^2 + U_{STE}^2 \tag{17}$$

where $U_{STE}^2 = U_{SPD}^2 + U_{SN}^2$ is the total estimated simulation uncertainty, as shown in Fig. 1.

If $|E|$ is less than the validation uncertainty U_V, the combination of all the errors in D and S is smaller than the estimated validation uncertainty and validation has been achieved at the U_V level. U_V is the key metric in the validation process. U_V is the validation ''noise level'' imposed by the uncertainties inherent in the data, the numerical solution, and the previous experimental data used in the simulation model. It can be argued that one cannot discriminate once $|E|$ is less than this; that is, as long as $|E|$ is less than this, one cannot evaluate the effectiveness of proposed model ''improvements.'' On the other hand, if $|E| \gg U_V$ one could argue that probably $E \approx \delta_{SMA}$.

Oberkamp and Trucano [14] have criticized Coleman and Stern [6] for fact that U_V excludes U_{SMA}. As already acknowledged, there is no known way for directly estimating U_{SMA}. However, the present approach does provide a more stringent validation metric U_V which sets the level that validation can be achieved as the root sum square of the experimental U_D and the total estimated simulation U_{STE} uncertainties. Additionally, under certain conditions, the simulation modeling error δ_{SMA} itself can be estimated, as further discussed in Section 4. Consideration of Eq. (17) shows that (1) the more uncertain the data (greater U_D) and/or (2) the more inaccurate the code (greater U_{STE}), the easier it is to validate a code, since the greater the uncertainties in the data and code predictions, the greater the noise level U_V. Both Roache [3] and Oberkamp and Trucano [14] have criticized Coleman and Stern [6] for this fact. However, if the value of U_V is greater than that designated as necessary in a research/design/development program, the required *level of validation* could not be achieved without improvement in the quality of the data, the code, or both. Also, if U_{SN} and U_{SPD} are not estimated, but $|E|$ is less than U_D, then a type of validation can be argued to have been achieved, but clearly as shown by the present methodology, at an unknown level.

If the ''corrected'' approach of Eqs. (3)–(6) is used, then the equations, equivalent to Eqs. (14) and (17) are

$$E_C = D - S_C = \delta_D - (\delta_{SMA} + \delta_{SPD} + \varepsilon_{SN}) \tag{18}$$

for the corrected comparison error and

$$U_{V_C}^2 = U_{E_C}^2 - U_{SMA}^2 = U_D^2 = U_D^2 + U_{S_C TE}^2 \tag{19}$$

for the corrected validation uncertainty where $U_{S_C TE}^2 = U_{SPD}^2 + U_{S_C N}^2$ is the total estimated corrected simulation uncertainty, also shown in Fig. 1. Note that S_C and E_C can be either larger or smaller than their counterparts S and E, but U_{E_C} and U_{V_C} should be smaller than U_E and U_V, respectively, since $U_{S_C N}$ should be smaller than U_{SN}.

If there is a programmatic validation requirement, there is another uncertainty U_{reqd} that must be considered since validation is required at that uncertainty level or below. Interpretation of the meaning of the relative magnitudes of E (or E_C), U_{reqd} and U_V (or U_{V_C}) and of the implications on the possibility of estimating δ_{SMA} are discussed in Section 4. Additional discussion is provided in Coleman and Stern [6] on: estimating U_{SPD}; estimating U_D for the data point (X_i, r_i), including both the experimental uncertainty in r_i and the additional uncertainties in r_i arising from the experimental uncertainties in the measurements of the n independent variables $(X_j)_i$ in X_i; and for validation of a CFD code, multiple codes and/or models, and prediction of trends.

3 Verification Procedures

In Section 2, the simulation numerical error and uncertainty were decomposed into contributions from iteration number, grid size, time step, and other parameters in Eqs. (7) and (8). In this section, detailed verification procedures are given for estimation of these contributions through convergence studies (Section 3.1). Iterative (Section 3.2) and parameter (Sections 3.3–3.5) convergence studies are conducted using multiple solutions with systematic parameter refinement to estimate numerical errors and uncertainties. Three convergence conditions are possible: (*i*) monotonic convergence; (*ii*) oscillatory convergence; and (*iii*) divergence and are described in Sections 3.3, 3.4, and 3.5, respectively. For condition (*i*), as already mentioned, errors and uncertainties are estimated using generalized RE. For condition (*ii*), uncertainties are estimated simply by attempting to bound error based on oscillation maximums and minimums. For condition (*iii*), errors and uncertainties cannot be estimated. As discussed below and later in Section 5, there are many issues in estimating errors and uncertainties for practical applications.

3.1 Convergence Studies. Iterative and parameter convergence studies are conducted using multiple (m) solutions and systematic parameter refinement by varying the kth input parameter Δx_k 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 $r_k = \Delta x_{k_2}/\Delta x_{k_1} = \Delta x_{k_3}/\Delta x_{k_2} = \Delta x_{k_m}/\Delta x_{k_{m-1}}$ between solutions is assumed for presentation purposes, but not required as discussed later.

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 $r_k = 2$, interpolation to a common location is required to compute solution changes, which introduces interpolation errors. Roache [3] discusses methods for evaluating interpolation errors. However, for industrial CFD, $r_k = 2$ may often be too large. A good alternative may be $r_k = \sqrt{2}$, 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.

Equation (12) is written for the *kth* parameter and *mth* solution as

$$S_{k_m} = S_C + \delta^*_{I_{k_m}} + \delta^*_{k_m} + \sum_{j=1, j\neq k}^{f} \delta^*_{j_m} \tag{20}$$

Iterative convergence must be assessed and S_{k_m} corrected for iterative errors prior to evaluation of parameter convergence since the level of iterative convergence may not be the same for all m solutions used in the parameter convergence studies. Equation (20) shows that iterative errors $\delta^*_{I_{k_m}}$ must be accurately estimated or negligible in comparison to $\delta^*_{k_m}$ for accurate convergence studies and that they should be considered within the context of convergence studies for each input parameter. Methods for estimating U_I or δ^*_I and U_{I_C} are described in Section 3.2.2.

With $\delta^*_{I_{k_m}}$ evaluated, S_{k_m} is corrected for iterative errors as

$$\hat{S}_{k_m} = S_{k_m} - \delta^*_{I_{k_m}} = S_C + \delta^*_{k_m} + \sum_{j=1, j\neq k}^{J} \delta^*_{j_m} \tag{21}$$

$\hat{S}_{k_m}$ can be calculated for both integral (e.g., resistance coefficients) and point (e.g., surface pressure, wall-shear stress, and velocity) variables. $\hat{S}_{k_m}$ can be presented as an absolute quantity (i.e., non-normalized) or normalized with the solution as a percentage change; however, if the solution value is small, a more appropriate normalization may be the range of the 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. Consider the situation for 3 solutions corresponding to fine $\hat{S}_{k_1}$, medium $\hat{S}_{k_2}$, and coarse $\hat{S}_{k_3}$ values for the *kth* input parameter. Solution changes ε for medium-fine and coarse-medium solutions and their ratio R_k are defined by

$$\begin{aligned} \varepsilon_{k_{21}} &= \hat{S}_{k_2} - \hat{S}_{k_1} \\ \varepsilon_{k_{32}} &= \hat{S}_{k_3} - \hat{S}_{k_2} \\ R_k &= \varepsilon_{k_{21}} / \varepsilon_{k_{32}} \end{aligned} \tag{22}$$

Three convergence conditions are possible:

$$\begin{aligned} &(i)\ \text{Monotonic convergence:} \quad 0<R_k<1 \\ &(ii)\ \text{Oscillatory convergence:} \quad R_k<0^1 \\ &(iii)\ \text{Divergence:} \quad R_k>1 \end{aligned} \tag{23}$$

For monotonic convergence (*i*), generalized RE is used to estimate U_k or δ^*_k and U_{k_C}. Methods for estimating errors and uncertainties for condition (*i*) are described in Section 3.3.

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. [15]). Depending on where the three points fall on the curve, the condition could be incorrectly diagnosed as either monotonic convergence or divergence. Methods discussed here for estimating uncertainties U_k for condition (*ii*) require more than $m=3$ solutions and are described in Section 3.4.

For divergence (*iii*), the solutions diverge and errors and uncertainties cannot be estimated. Additional remarks are given in Section 3.5.

Determination of the convergence ratio R_k for point variables can be problematic since solution changes $\varepsilon_{k_{21}}$ and $\varepsilon_{k_{32}}$ 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_k, which overcomes ill conditioning, based on the L2 norm of the solution changes, i.e., $\langle R_k \rangle = \|\varepsilon_{k_{21}}\|_2 / \|\varepsilon_{k_{32}}\|_2$. $\langle\ \rangle$ is used to denote an averaged value and $\|\varepsilon\|_2 = [\Sigma_{i=1}^{N} \varepsilon_i^2]^{1/2}$ 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 ($R_k<1$) cannot be diagnosed since $\langle R_k \rangle$ will always be greater than zero. Local values of R_k at solution maximums or minimums should also be examined to confirm the convergence condition based on an L2 norm definition. An alternate approach suggested by Hoekstra et al. [16] 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_k.

3.2 Iterative Convergence. The number of order magnitude drop and final level of solution residual (or residual imbalance) can be used to determine stopping criteria for iterative solution techniques. Iterative convergence to machine zero is desirable, but for complex geometry and conditions it is often not possible. Three or four orders of magnitude drop in solution residual to a level of 10^{-4} is more likely for these cases. Methods for estimation of iterative errors and uncertainties can be based on graphical, as discussed below, or theoretical approaches and are dependent on the type of iterative convergence: (*a*) oscillatory; (*b*) convergent; or (*c*) mixed oscillatory/convergent.

For oscillatory iterative convergence (*a*), the deviation of the variable from its mean value provides estimates of the iterative uncertainty based on the range of the maximum S_U and minimum S_L values

$$U_I = \left| \frac{1}{2} (S_U - S_L) \right| \tag{24}$$

For convergent iterative convergence (*b*), a curve-fit of an exponential function can be used to estimate U_I or δ^*_I and U_{I_C} as the difference between the value and the exponential function from a curve fit for large iteration number CF_∞

$$\begin{aligned} U_I &= |S - CF_\infty| \\ \delta^*_{I_{k_m}} &= S - CF_\infty, U_{I_C} = 0 \end{aligned} \tag{25}$$

For mixed convergent/oscillatory iterative convergence (*c*), the amplitude of the solution envelope decreases as the iteration number increases, the solution envelope is used to define the maximum S_U and minimum S_L values in the Ith iteration, and to estimate U_I or δ^*_I and U_{I_C}

$$\begin{aligned} U_I &= \left| \frac{1}{2} (S_U - S_L) \right| \\ \delta^*_{I_{k_m}} &= S - \frac{1}{2} (S_U - S_L), U_{I_C} = 0 \end{aligned} \tag{26}$$

An increase in the amplitude of the solution envelope as the iteration number increases indicates that the solution is divergent.

Estimates of the iterative error based on theoretical approaches are presented in Ferziger and Peric [17] and involve estimation of the principal eigenvalue of the iteration matrix. The approach is relatively straightforward when the eigenvalue is real and the solution is convergent. For cases in which the principal eigenvalue is complex and the solution is oscillatory or mixed, the estimation is not as straightforward and additional assumptions are required.

3.3 Monotonic Convergence: Generalized Richardson Extrapolation. For monotonic convergence, i.e., condition (*i*) in Eq. (23), generalized RE is used to estimate U_k or δ^*_k and U_{k_C}. RE is generalized for J input parameters and concept of correction factors based on analytical benchmarks is introduced. More detailed derivations are provided by Stern et al. [13].

As already mentioned, since Stern et al. [13] there has been nearly two years experience with present approach, especially through ITTC community and Gothenburg 2000 Workshop on CFD in Ship Hydrodynamics. In particular, detailed verification procedures have been the focus of attention (Eca and Hoekstra [18]; Ebert and Gorski [19]). After some background for generalized RE is given, two approaches for estimating errors and uncertainties are presented and are based on (*i*) correction factors proposed in the current paper and (*ii*) factor of safety approach proposed by Roache (1998). Finally, a discussion of fundamental and practical issues for verification is provided.

[1] As discussed in the text that follows, $0<R_k<1$ and $R_k>1$ may also occur for the oscillatory condition.

Background for Generalized RE. Generalized RE begins with Eq. (21). The error terms on the right-hand side of Eq. (21) are of known form (i.e., power series expansion with integer powers of Δx_k) based on analysis of the modified and numerical error equations which is written below as a finite sum (i.e., error estimate) and for the kth parameter and mth solution

$$\delta^*_{k_m} = \sum_{i=1}^{n} (\Delta x_{k_m})^{p_k^{(i)}} g_k^{(i)} \tag{27}$$

n = number of terms retained in the power series, powers $p_k^{(i)}$ correspond to order of accuracy (for the ith term), and $g_k^{(i)}$ are referred to as "grid" functions which are a function of various orders and combinations of derivatives of S with respect to x_k. It is assumed that the power series in Eq. (27) is convergent (i.e., the finite sum convergence to the infinite series value as more terms are included). Substituting Eq. (27) into Eq. (21) results in

$$\hat{S}_{k_m} = S_C + \sum_{i=1}^{n} (\Delta x_{k_m})^{p_k^{(i)}} g_k^{(i)} + \sum_{j=1, j\neq k}^{J} \delta^*_{j_m} \tag{28}$$

Subtraction of multiple solutions where input parameter Δx_k is uniformly refined eliminates the $\delta^*_{j_m}$ terms in Eq. (28) since $\delta^*_{j_m}$ is independent of Δx_k and provides equations for S_C, $p_k^{(i)}$, and $g_k^{(i)}$. This assumes $p_k^{(i)}$ and $g_k^{(i)}$ are also independent of Δx_k. 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 Eq. (28) (i.e., for $n=1$, $m=3$ and for $n=2$, $m=5$, etc). The accuracy of the estimates depends on how many terms are retained in Eq. (27), the magnitude (importance) of the higher-order terms, and the validity of the assumption that $p_k^{(i)}$ and $g_k^{(i)}$ are independent of Δx_k. For sufficiently small Δx_k, the solutions are in the asymptotic range such that higher-order terms are negligible and the assumption that $p_k^{(i)}$ and $g_k^{(i)}$ are independent of Δx_k is valid. However, achieving the asymptotic range for practical geometry and conditions is usually not possible and $m>3$ is undesirable from a resources point of view; therefore, methods are needed to account for effects of higher-order terms for practical application of RE. Additionally, methods may be needed to account for possible dependence of $p_k^{(i)}$ and $g_k^{(i)}$ on Δx_k, although not addressed herein. Usually δ^*_k is estimated for the finest value of the input parameter, i.e., $\delta^*_k = \delta^*_{k_1}$ corresponding to the finest solution S_{k_1}.

With three solutions ($m=3$), only the leading-order term of Eq. (27) can be estimated. Solution of the three equations for S_C, $p_k^{(i)}$, and $g_k^{(i)}$ yields estimates for the error $\delta^*_{k_1}$ and order-of-accuracy p_k

$$\delta^*_{k_1} = \delta^*_{RE_{k_1}} = \frac{\varepsilon_{k_{21}}}{r_k^{p_k} - 1} \tag{29}$$

$$p_k = \frac{\ln(\varepsilon_{k_{32}}/\varepsilon_{k_{21}})}{\ln(r_k)} \tag{30}$$

Solving for the first-order term is relatively easy since evaluation of Eqs. (29) and (30) only requires that the $m=3$ solutions are monotonically convergent, even if the solutions are far from the asymptotic range and Eqs. (29) and (30) are inaccurate. With solutions from five systematically refined input parameters ($m=5$), more complicated expressions can be derived to estimate the first two terms of the power series expansion. However, their range of applicability is more restrictive since all five solutions must be both monotonically convergent *and* sufficiently close to the asymptotic range for the expressions to be used.

As previously mentioned, solutions from three values of input parameter where the refinement ratio between the medium and fine input parameters $r_{k_{21}}$ is not equal to that between coarse and medium input parameters $r_{k_{32}}$ can be used to estimate $\delta^*_{k_1}$ from Eq. (29), provided that Eq. (30) for estimating order of accuracy is modified as

$$p_k = \frac{\ln(\varepsilon_{k_{32}}/\varepsilon_{k_{21}})}{\ln(r_{k_{21}})} + \frac{1}{\ln(r_{k_{21}})}[\ln(r_{k_{32}}^{p_k} - 1) - \ln(r_{k_{21}}^{p_k} - 1)] \tag{31}$$

For situations when $r_{k_{21}} \neq r_{k_{32}}$, Eq. (31) is a transcendental equation implicitly defining p_k and must be solved iteratively. If $r_{k_{21}} = r_{k_{32}}$, Eq. (31) degenerates to Eq. (30).

Estimating Errors and Uncertainties Using Generalized RE With Correction Factors. Results from the numerical solution of the one-dimensional (1D) wave and two-dimensional (2D) Laplace equation analytical benchmarks show that Eq. (29) has the correct form, but the order of accuracy is poorly estimated by Eq. (30) except in the asymptotic range. Analysis of the results suggests the concept of correction factors, which provide a quantitative metric to determine proximity of the solutions to the asymptotic range, account for the effects of higher-order terms, and are used for defining and estimating errors and uncertainties. Details are provided in Appendix A.

Multiplication of Eq. (29) by a correction factor C_k provides an estimate for $\delta^*_{k_1}$ accounting for the effects of higher-order terms

$$\delta^*_{k_1} = C_k \delta^*_{RE_{k_1}} = C_k \left(\frac{\varepsilon_{k_{21}}}{r_k^{p_k} - 1} \right) \tag{32}$$

If solutions are in the asymptotic range, correction of Eq. (29) is not required [i.e., $C_k = 1$ so that Eqs. (29) and (32) are equivalent]. For solutions outside the asymptotic range, $C_k < 1$ or $C_k > 1$ indicates that the leading-order term over predicts (higher-order terms net negative) or under predicts (higher-order terms net positive) the error, respectively. The estimate given by Eq. (32) includes both sign and magnitude and is used to estimate U_k or δ^*_k and U_{k_C} depending on how close the solutions are to the asymptotic range (i.e., how close C_k is to 1) and one's confidence in Eq. (32). There are many reasons for lack of confidence, especially for complex three-dimensional flows.

For C_k sufficiently less than or greater than 1 and lacking confidence, U_k is estimated, but not δ^*_k and U_{k_c}. Equation (32) is used to estimate the uncertainty by bounding the error δ^*_k by the sum of the absolute value of the corrected estimate from RE and the absolute value of the amount of the correction

$$U_k = |C_k \delta^*_{RE_{k_1}}| + |(1 - C_k)\delta^*_{RE_{k_1}}| \tag{33}$$

For C_k sufficiently close to 1 and having confidence, δ^*_k and U_{k_c} are estimated. Equation (32) is used to estimate the error δ^*_k, which can then also be used in the calculation of S_c [in Eq. (10)]. The uncertainty in the error estimate is based on the amount of the correction

$$U_{k_C} = |(1 - C_k)\delta^*_{RE_{k_1}}| \tag{34}$$

Note that in the limit of the asymptotic range, $C_k = 1$, $\delta^*_k = \delta^*_{k_1} = \delta^*_{RE_{k_1}}$, and $U_{k_C} = 0$.

Two definitions for the correction factor were developed. The first is based on solution of Eq. (32) for C_k with $\delta^*_{RE_{k_1}}$ based on Eq. (29) but replacing p_k with the improved estimate $p_{k_{est}}$

$$C_k = \frac{r_k^{p_k} - 1}{r_k^{p_{k_{est}}} - 1} \tag{35}$$

Similarly, the second is based on a two-term estimate of the power series which is used to estimate $\delta^*_{RE_{k_1}}$ where p_k and q_k are replaced with $p_{k_{est}}$ and $q_{k_{est}}$

$$C_k = \frac{(\varepsilon_{k_{23}}/\varepsilon_{k_{12}} - r_k^{q_{k_{est}}})(r_k^{p_k}-1)}{(r_k^{p_{k_{est}}} - r_k^{q_{k_{est}}})(r_k^{p_{k_{est}}}-1)} + \frac{(\varepsilon_{k_{23}}/\varepsilon_{k_{12}} - r_k^{p_{k_{est}}})(r_k^{p_k}-1)}{(r_k^{p_{k_{est}}} - r_k^{q_{k_{est}}})(r_k^{q_{k_{est}}}-1)} \tag{36}$$

$p_{k_{est}}$ and $q_{k_{est}}$ are estimates for limiting orders of accuracy of the first and second terms of the error expansion equation (27) as spacing size goes to zero and the asymptotic range is reached. Equation (35) roughly accounts for the effects of higher-order terms by replacing p_k with $p_{k_{est}}$ thereby providing an improved single-term estimate. Equation (36) more rigorously accounts for higher-order terms since it is derived from the two-term estimate with first and second term order of accuracy $p_k^{(1)}$ and $p_k^{(2)}$ replaced by $p_{k_{est}}$ and $q_{k_{est}}$. Equation (36) simplifies to Eq. (35) in the limit of the asymptotic range. Both correction factors only require solutions for three parameter values. The estimated values $p_{k_{est}}$ and $q_{k_{est}}$ can be based either on the assumed theoretical order of accuracy $p_{k_{th}}$ and $q_{k_{th}}$ or solutions for simplified geometry and conditions. In either case, preferably including the effects of grid stretching.

In Appendix A, exact (A) and numerical (S) solutions are used to compare the true simulation error ($A-S$) to (*i*) an uncorrected three-grid error estimate using Eq. (29) and (*ii*) corrected estimates based on Eq. (32) with correction factor defined by Eq. (35) or (36). Correction of error estimates with both definitions of C_k results in improved error estimates. Also, uncertainty estimates using Eq. (33) with correction factor defined by Eq. (35) or (36) are shown to bound the true simulation error ($A-S$), while uncertainty estimates using Eq. (34) are shown to bound the difference between the corrected solution and the truth (S_c-T). Additional testing of expressions for C_k given by Eqs. (35) and (36) is needed and development of improved expressions within the proposed general framework is certainly possible.

Estimating Uncertainties Using Generalized RE With Factors of Safety. In Roache [3], a GCI approach is proposed where a standard three-grid error estimate from RE is multiplied by a factor of safety F_S to bound the simulation error

$$U_k = F_S \left| \delta^*_{RE_{k_1}} \right| \tag{37}$$

Note that Eq. (37) with factor of safety differs significantly from Eq. (34). Herein $C_k = C_k\,(\varepsilon, r_k, p_k, p_{k_{est}}, q_{k_{est}})$, in contrast to Eq. (37) where C_k is a constant referred to as a factor of safety F_S. The exact value for factor of safety is somewhat ambiguous and Roache [3] recommends 1.25 for careful grid studies and 3 for cases in which only two grids are used.

Although not proposed in Roache [3], the factor of safety approach can be used for situations where the solution is corrected with an error estimate from RE. Equation (29) is used to estimate δ^*_k and the uncertainty in that error estimate is given by

$$U_{k_C} = (F_S - 1) \left| \delta^*_{RE_{k_1}} \right| \tag{38}$$

With this approach, a fixed percentage of a three-grid error estimate (e.g., 25% $\delta^*_{RE_{k_1}}$ for $F_S = 1.25$) is used to define the uncertainty of the error estimate regardless of how close solutions are to the asymptotic range.

Discussion of Fundamental and Practical Issues. Fundamental and practical issues for verification are discussed in this section. Fundamental issues include convergence of power series equation (27), assumptions that $p_k^{(i)}$ and $g_k^{(i)}$ are independent of Δx_k, and estimating $p_{k_{est}}$. Solution of analytical benchmarks has been used to address some of these fundamental issues while others need further research. Although both correction factor and factor of safety approaches were presented, the authors advocate the use of former. Results from the numerical solution of analytic benchmarks show that the factor of safety approach is overly conservative, especially when the solutions approach the asymptotic range (Appendix A). This is in contrast to the variable correction factor approach proposed in Eqs. (33) and (34), where the uncertainty in the error estimate correctly goes to zero as the asymptotic range is approached because $C_k \rightarrow 1$. Admittedly, others have recommended the factor of safety approach, e.g., Eca and Hoekstra [18], although examination of their results as with our own analysis indicates that such estimates are overly conservative.

For practical applications, especially complex flows with relatively coarse grids, solutions may be far from asymptotic range such that some variables are convergent while others are oscillatory or even divergent. 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 [18] suggest a least-squares approach to estimate the error by computing the three unknown parameters from RE when more than three solutions are available. The behavior of the asymptotic range was successfully demonstrated for simpler analytical benchmarks in Appendix A. However, the existence and behavior of the asymptotic range for practical problems has not been demonstrated due to lack of sufficiently refined grids, number of solutions to assess variability, and available resources, among other issues. Another practical issue involves selecting and maintaining appropriate parameter refinement ratio and resources for obtaining solutions with sufficient parameter refinement as well as number of solutions. Lastly, interpretation of results is an issue since, as already mentioned, there is limited experience and no known solutions for practical applications in the asymptotic range for guidance.

The present verification procedures represent the most rational approach presently known. However, alternative strategies for including effects of higher-order terms may be just as viable, e.g., treatment of the power series exponents as known integers as proposed by Oberkampf and investigated by Eca and Hoekstra [18]. Once available, improved verification procedures can be easily incorporated into the present overall verification and validation methodology. These issues are discussed further in Section 5 Conclusions and Recommendations and in Part 2 (Wilson et al. [12]).

3.4 Oscillatory Convergence. For oscillatory convergence, i.e., condition (*ii*) in Eq. (23), uncertainties can be estimated, but not the signs and magnitudes of the errors. Uncertainties are estimated based on determination of the upper (S_U) and lower (S_L) bounds of solution oscillation, which requires more than $m=3$ solutions. The estimate of uncertainty is based on half the solution range

$$U_k = \frac{1}{2}(S_U - S_L) \tag{39}$$

3.5 Divergence. For divergence, i.e., condition (*iii*) in Eq. (23), errors and or uncertainties can not be estimated. The preparation and verification steps must be reconsidered. Improvements in iterative convergence, parameter specification (e.g., grid quality), and/or CFD code may be required to achieve converging or oscillatory conditions.

4 Validation Procedures

In Section 2, an approach for assessing the simulation modeling uncertainty was presented where for successful validation, the comparison error, E is less than the validation uncertainty, U_V given by Eqs. (17) and (19) for uncorrected and corrected solutions, respectively. In this section, validation procedures are presented through discussions in Section 4.1 on interpretation of

validation results and in Section 4.2 on use of corrected simulation results. As previously mentioned, Coleman and Stern [6] provide additional discussion on validation procedures.

4.1 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):

$$\begin{aligned}
&1.\quad |E|<U_V<U_{reqd}\\
&2.\quad |E|<U_{reqd}<U_V\\
&3.\quad U_{reqd}<|E|<U_V\\
&4.\quad U_V<|E|<U_{reqd}\\
&5.\quad U_V<U_{reqd}<|E|\\
&6.\quad U_{reqd}<U_V<|E|
\end{aligned} \tag{40}$$

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 $U_V \ll |E|$, then E corresponds to δ_{SMA} and the error from the modeling 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 Eq. (40) 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.

4.2. Use of Corrected Versus Uncorrected Simulation Results. As previously stated in Section 3.3, 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 neighboring 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.)

5 Conclusions

The present comprehensive approach to verification and validation methodology and procedures sets forth concepts, definitions, and equations derived for simulation errors and uncertainties, which provide a well-founded mathematical framework. The approach should have applicability to a fairly broad range of CFD codes, including RANS, Navier-Stokes, Euler, boundary-element methods, and others. However, clearly much more work is needed for other CFD codes (such as large-eddy simulations), additional error sources, and alternative error and uncertainty estimation methods, e.g., single-grid methods and both results for additional analytical benchmarks (especially for nonlinear equations and using stretched grids) for improved definitions of correction factors and estimates of orders of accuracy, and alternative strategies to account for the effects of higher-order terms in RE. Improved verification procedures once available can be easily incorporated into the present overall verification and validation methodology. Furthermore, more experience is needed through application for different codes and geometry and conditions, especially for practical applications.

As mentioned in the Introduction, present verification and validation methodology and procedures were recommended and used at the recent Gothenburg 2000 Workshop on CFD in Ship Hydrodynamics (Larsson et al. [11]). 22 participating research groups from 12 countries and 19 different RANS codes were used for simulations of 3 test cases representing tanker, container, and surface combatant hull forms. Most groups implemented the recommended procedures, but lack of familiarity with the procedures and use of coarse grids led to difficulties. Coarser grid solutions are far from the asymptotic range and show variability such that not all variables display monotonic convergence and oscillatory convergence and even divergence is evident. For monotonic convergence, variability in the estimated order of accuracy was observed for some cases. The current 1 million point grids are clearly insufficient for more complex hull forms such as the tanker and an order of magnitude increase in points may be required to remove variability and achieve monotonic convergence for most variables. In spite of difficulties, the effort was beneficial in enabling quantitative evaluation of levels of verification and validation, increasing familiarity with verification and validation procedures, interpretation of results, and identification of grid requirements for decreasing levels of errors and uncertainties. Careful examination of verification results even for relatively coarse grid solutions provides a road map towards achieving acceptable levels of verification.

Verification and validation methodology and procedures should be helpful in guiding future developments in CFD through documentation, verification, and validation studies and in transition of CFD codes to design through establishment of credibility. Presumably, with a sufficient number of documented, verified, and validated solutions along with selected verification studies, a CFD code can be accredited for a certain range of applications. The contribution of the present work is in providing methodology and procedures for the former, which hopefully will help lead to the latter.

Part 2 provides an example for RANS simulations for a cargo/container ship where issues with regard to practical application of the methodology and procedures and interpretation of verification and validation results are discussed (Wilson et al. [12]).

Acknowledgments

This research was sponsored by the Office of Naval Research under Grants N00014-96-1-0018, N00014-97-1-0014, and N00014-97-1-0151 under the administration of Dr. E. P. Rood. The authors gratefully acknowledge Dr. Rood and other colleagues, especially Prof. W. G. Steele and Dr. H. Raven, who made significant contributions through insightful discussions and comments on early drafts. The recent Masters and Ph.D. theses of

Dr. B. Chen, Mr. G. Dolphin and Dr. S. H. Rhee, all at The University of Iowa, Department of Mechanical Engineering, were helpful both in the development and testing of the present verification and validation methodology and procedures.

Nomenclature

C_k = correction factor
D = benchmark data
E, E_C = comparison error, corrected
p_k = order of accuracy
R_k = parameter refinement ratio
S, S_C = simulation result, corrected
T = truth
U = uncertainty estimate
U_D = data uncertainty
U_E, U_{E_C} = comparison error uncertainty, corrected
U_I = iteration uncertainty
U_P, U_{P_C} = parameter uncertainty (e.g., grid size G and time step T), corrected
U_{reqd} = programmatic validation requirement
U_S, U_{S_C} = simulation uncertainty, corrected
U_{SM} = simulation modeling uncertainty
U_{SMA} = simulation modeling assumption uncertainty
U_{SPD} = simulation uncertainty due to use of previous data
U_{STE}, U_{S_CTE} = simulation total estimated numerical uncertainty
U_{SN}, U_{S_CN} = simulation numerical uncertainty, corrected
U_V, U_{V_C} = validation uncertainty, corrected
Δx_k = increment in *kth* input parameter (e.g., grid size G and time step T)
δ = error
δ^* = error estimate with sign and magnitude
δ_I, δ_I^* = iteration error, estimate
δ_P, δ_P^* = parameter error, estimate
δ_S, δ_{S_C} = simulation error, corrected
δ_{SN} = simulation numerical error
δ_{SMA} = simulation modeling assumption error
ε = solution change
ε_{SN} = error in δ^*

Appendix A. Analytical Benchmarks

The use of analytical benchmarks for development of the concept of correction factors as discussed in Section 3.3 is presented in this Appendix. For analytical benchmarks, the modeling error is zero such that the simulation error is solely due to numerical error. Results are obtained for two analytical benchmarks one-dimensional (1D) wave and two-dimensional (2D) Laplace equations. The results for the 2D Laplace equation were qualitatively similar to those for the 1D wave equation, which are presented. Exact solutions from analytical benchmarks are used to determine the exact simulation numerical error which is compared to estimates from RE, including use of correction factors. More details are provided in Stern et al. [13], including single grid error estimates.

Verification of Analytical Benchmarks. For verification using an analytical benchmark, the simulation error and uncertainty are given by $\delta_S = S - A = \delta_{SN}$ and $U_S^2 = U_{SN}^2$, while the corrected simulation error and uncertainty are given by $\delta_{S_C} = S_C - A = \varepsilon_{SN}$ and $U_{S_C}^2 = U_{S_CN}^2$. Simulations are verified if $|E| = |A - S| < U_{SN}$ and corrected simulations are verified if $|E_C| = |A - S_C| < U_{S_CN}$.

The first-order, linear 1D wave equation models the behavior of a more complicated (nonlinear) partial differential equation. The initial condition is prescribed by a Gaussian function centered at $x = 0.0$. Two discretization techniques were studied: (*i*) first-order (Euler) explicit method with first-order upwind spatial discretization; and (*ii*) a second-order implicit method with second-order central spatial discretization. Since trends from both schemes are similar, only the results from the first-order scheme are presented.

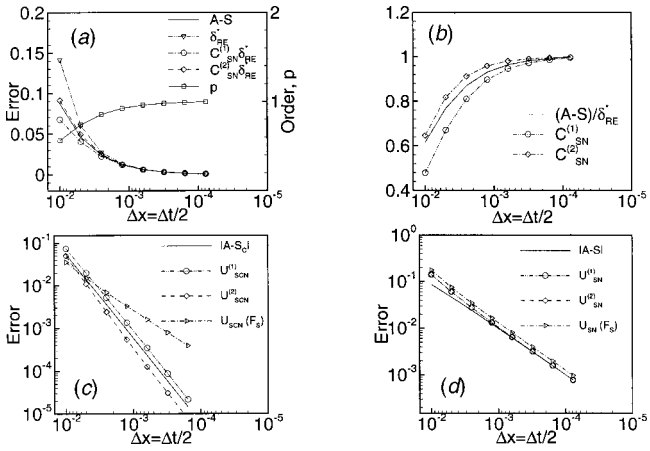

Fig. 2 Verification results for first-order numerical solution of 1D wave equation. (*a*) Comparison of true error $A-S$ to estimates from RE, (*b*) correction factor, and (*c*) comparison of $|A-S_C|$ and U_{SCN}, and (*d*) comparison of $|A-S|$ and U_{SN}.

A combined grid size and time step study was performed where ten solutions were obtained by successively doubling both the grid and time step such that $\Delta t/\Delta x = 0.5$ for all solutions. With this approach, solutions changes are used to estimate total (temporal and spatial) simulation errors and uncertainties. Accordingly, the generic subscript '*k*' appearing in expressions for errors and uncertainties in Section 3.3 is replaced with '*SN*' in this section where appropriate.

Errors, Uncertainties, and Correction Factors. The concept of a multiplication correction factor was introduced in Section 3.3. The correction factor C_k was used to define the numerical uncertainty in Eq. (33) or when conditions permit to improve error estimates in Eq. (32) and to define the uncertainty in that error estimate in Eq. (34). Error and uncertainty estimates given by Eqs. (32)–(34) are tested by numerical solution of analytical benchmarks as well as development of expressions for correction factor.

Figure 2(a) compares the true simulation error E to the three-grid error estimate $\delta^*_{RE_1}$ from Eq. (29) versus step size at one spatial location ($x = 1$ since maximums of numerical error occur there). The three-grid estimate accurately estimates the true error E for smaller step sizes, but over predicts E for larger step sizes. Closer examination reveals that Eq. (29) over estimates the error because Eq. (30) under estimates the order of accuracy, as also shown in Fig. 2(*a*).

Two definitions for C_k were investigated. The first is based on solving equation (32) for C_k with $\delta^*_{RE_{k_1}}$ defined in Eq. (29) but replacing p_k with the improved estimate $p_{k_{est}}$, which is provided by Eq. (35) where $p_{k_{est}}$ is an estimate of the limiting order of accuracy of the first term of the error expansion equation (27). Similarly, the second definition of correction factor is based on estimating $\delta^*_{RE_{k_1}}$ using the first two terms of the powers series and replacing p_k and q_k with improved estimates $p_{k_{est}}$ and $q_{k_{est}}$, which is provided by Eq. (36) where $p_{k_{est}}$ and $q_{k_{est}}$ are estimates for limiting orders of accuracy of the first and second terms of the error expansion equation (27) as spacing size goes to zero and the asymptotic range is reached. With this definition, correction factors approach one in the limit of zero spacing size. The estimated values $p_{k_{est}}$ and $q_{k_{est}}$ can be based either on the assumed theoret-

ical order of accuracy $p_{k_{th}}$ and $q_{k_{th}}$ or solutions for simplified geometry and conditions. In either case, preferably including the effects of grid stretching.

Figure 2(*a*) also compares the true error E to (*i*) an uncorrected three-grid error estimate using Eq. (29) and (*ii*) corrected estimates based on Eq. (32) with correction factor defined by Eq. (35) or (36). Both estimates are closer to E than the uncorrected three grid estimate $\delta^*_{RE_1}$, but for coarser grids $C_k^{(1)}$ is somewhat too small and $C_k^{(2)}$ is slightly too large. Figure 2(*b*) shows the same trends, but directly compares the exact correction factor E/δ^*_{RE} to Eqs. (35) and (36). In this case, $C_k<1$ indicates that the leading-order term over predicts (higher-order terms net negative) the error. However, for the general case, C_k is equally likely to be <1 or >1 depending whether the order of accuracy is approached from below or above, respectively. $C_k>1$ indicates that the leading-order term under predicts (higher-order terms net positive) the error. Thus, for the general case the correction to the leading-term error estimate is equally likely to be positive or negative and can be used to define the simulation numerical uncertainty.

For C_k sufficiently close to 1 and having confidence, δ^*_k and U_{k_C} are estimated. Correction factors $C_k^{(1)}$ and $C_k^{(2)}$ are used to estimate the error δ^*_k in Eq. (32) which can then also be used in the calculation of S_C [in Eq. (10)] and uncertainty U_{k_C} in Eq. (34). Figure 2(*c*) shows a comparison of $|A-S_C|$ and three uncertainty estimates: (*i*) $U^{(1)}_{S_CN}$ defined using $C_k^{(1)}$; (*ii*) $U^{(2)}_{S_CN}$ defined using $C_k^{(2)}$; and (*iii*) U_{S_CN} from a factor of safety approach given by Eq. (38) with $F_S=1.25$. The results show that the uncertainty estimate $U^{(1)}_{S_CN}$ successfully bounds $|A-S_C|$ over the entire range of step sizes and that $U^{(2)}_{S_CN}$ is not conservative enough since $U^{(2)}_{S_CN}<|A-S_C|$. The uncertainty estimate based on the factor of safety approach is not conservative enough for the coarsest two grids and is overly conservative by an order of magnitude for the four finest grids (i.e., when solutions are in the asymptotic range). For C_k sufficiently less than or greater than 1 and lacking confidence, U_k is estimated, but not δ^*_k and U_{k_C}. Correction factors $C_k^{(1)}$ and $C_k^{(2)}$ are used to estimate the uncertainty in Eq. (33) which is compared to factor of safety approach given by Eq. (37). Figure 2(*d*) shows that all three uncertainty estimates successfully bound the true error $|A-S|$ although the factor of safety approach is overly conservative for all grids.

Uncertainty estimates enable a quantitative measure of verification for analytical benchmarks. Figure 2(*c*, *d*) indicates that the present solutions are verified over the chosen range of grid size and time step. As expected, the largest levels of uncertainty are for the coarsest grid size and time step where levels are $(U_k, U_{k_C}) = (15\%, 7.5\%)$.

Eca and Hoekstra [18] also perform verification for the 2D Laplace equation analytical benchmark. Their results are consistent with our own in showing that uncertainty estimates using Eq. (33) always bounded the true error. Unlike our own results, their results indicate that the uncertainty estimate from Eq. (34) failed to bound the difference in the truth and numerical benchmark for some grid triplets when the apparent order of accuracy was estimated to be larger than the theoretical value.

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