CONTENTS

INTERIM RECOMMENDED PROCEDURE

PREPARED BY RESISTANCE COMMITTEE OF 22nd ITTC

Uncertainty Analysis in CFD, Uncertainty Assessment Methodology

1. PURPOSE OF PROCEDURE

To provide a methodology for estimating the uncertainty in a simulation result.

2. INTRODUCTION

Discussion and methodology for estimating errors and uncertainties in CFD simulations has reached a certain level of maturity with increased attention and recent progress on common concepts and terminology (AIAA, 1998), advocacy and detailed methodology (Roache, 1998), and numerous case studies (e.g., Mehta, 1998). Progress has been accelerated in response to the urgent need for achieving consensus on concepts and terminology and useful methodology, 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 and off-design conditions). In spite of the progress and urgency, the various viewpoints have not converged and current methodology falls short of providing practical procedures and methodology for estimating errors and uncertainties in CFD simulations.

The approach reported by the 21st RC (ITTC, 1996) was more pragmatic in providing verification procedures for making quantitative estimates for simulation numerical errors and uncertainties. Some RC members have continued their work in CFD uncertainty analysis methodology development. In particular, a new approach to CFD validation has been developed (Coleman and Stern, 1998) and was recently combined with extensions and more rigorous foundation for verification to provide the framework for overall procedures and methodology for verification and validation of CFD simulations (Stern et al., 1999a, b). These are the overall procedures and methodology along with an example for resistance and flow recommended for interim adoption.

3. VERIFICATION AND VALIDATION METHODOLOGY

Verification (Section 3.2) and validation (Section 3.3) methodology is presented for CFD simulation results from an already developed CFD code applied for specified objectives, geometry, conditions, and available benchmark information. Section 3.1 discusses concepts and definitions for errors and uncertainties and verification and validation, which provide the mathematical framework for the verification and validation methodologies.

3.1 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, which is 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 non-continuity, 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

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

A derivation of the simulation error equation (1) is provided in Appendix A of Stern et al. (1999b). The uncertainty equation corresponding to error equation (1) is

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

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

$$d_{SN} = d_{SN}^* + e_{SN} \quad (3)$$

where d_{SN}^* is an estimate of the sign and magnitude of δ_{SN} and e_{SN} is the error in that estimate (and will be 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

$$S_C = S - d_{SN}^* \quad (4)$$

with error equation

$$d_{S_C} = S_C - T = d_{SM} + e_{SN} \quad (5)$$

The uncertainty equation corresponding to error equation (5) is

$$U_{S_C}^2 = U_{SM}^2 + U_{S_C N}^2 \quad (6)$$

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

Debate on verification and validation has included discussion on whether errors such as δ_{SN} are deterministic vs. stochastic and thus how they should be treated in uncertainty analysis was unclear. In the approach given by equations. (3)-(6), a deterministic estimate d_{SN}^* of δ_{SN} and consideration of the error e_{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, 1999). In the "uncorrected" approach given by equations (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 $U_{S_C N}^2$).

Verification is defined as a process for assessing numerical uncertainty U_{SN} and, when conditions permit, estimating the sign and magnitude of the numerical error d_{SN}^* itself and the uncertainty in its error $U_{S_C N}$. Iterative and parameter convergence studies are conducted using multiple solutions with systematic parameter refinement. Verification methodology is described in Section 3.2. Analytical benchmarks can be defined as the truth and are useful in development and confirmation of verification procedures and methodology and in code development, but can not be used for validation and are restricted to simple equations. Results from the use of analytical benchmarks are provided in Appendix C of Stern et al. (1999b).

Validation is defined as a process for assessing 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. The comparison error E (difference between data D and simulation S values) and the validation uncertainty U_V (combination of uncertainties in data and portion of simulation uncertainties that can be estimated) are used in this process. Validation methodology is described in Section 3.3.

3.2 Verification

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

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

$$U_{SN}^2 = U_I^2 + U_G^2 + U_T^2 + U_P^2 = U_I^2 + \sum_{j=1}^{J} U_j^2 \quad (8)$$

Similarly, error estimates δ* can be decomposed as

$$d_{SN}^* = d_I^* + \sum_{j=1}^{J} d_j^* \quad (9)$$

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

$$S_C = S - (d_I^* + \sum_{j=1}^{J} d_j^*) = T + d_{SM} + e_{SN} \quad (10)$$

$$U_{S_C N}^2 = U_{I_C}^2 + \sum_{j=1}^{J} U_{j_C}^2 \quad (11)$$

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

$$S = S_C + (d_I^* + \sum_{j=1}^{J} d_j^*) \quad (12)$$

Equation (12) expresses S as the corrected simulation value S_C plus errors. S_C is also referred to as a numerical benchmark since it is equal, as shown by equation (10), to the truth plus simulation modeling and presumable small error ε_{SN} in the estimate of the numerical error d_{SN}^*. Power-series expansions about S_C for each input parameter using multiple solutions are used to obtain estimates for the d_j^*'s in equation (12). d_I^* must be accurately estimated or be negligible for each solution.

3.2.1 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 $r_k = \Delta x_{k2}/\Delta x_{k1} = \Delta x_{k3}/\Delta x_{k2} = \Delta x_{km}/\Delta x_{km-1}$ between solutions is assumed/required.

Parameter refinement ratio $r_k = 2$ is ideal as it provides large parameter refinement and enables use of the coarser-parameter solutions as initial guesses for the finer-parameter solutions without interpolation; however, parameter doubling is often impractical. Alternatively, $r_k = \sqrt{2}$ is suggested which also provides fairly large parameter refinement and at least enables prolongation of the coarse-parameter solution as an initial guess for the fine-parameter solution. Selection of grid refinement ratio is dependent on the level of iterative convergence. As grid refinement ratio r_G approaches unity (i.e., as the three grids become nearly identical), solution changes *e* due to grid refinement go to zero such that iterative errors can become

dominant. For this reason, it is recommended that grid refinement ratio be sufficiently large. However, for relatively large grid refinement ratio, the finest grid size may be prohibitively large if the coarsest grid is designed with sufficiently small step size. Also, in general, as the step size is reduced the errors also reduce. However, typical iterative methods require more iterations on finer step sizes to reach the same level of iterative uncertainty. Therefore, it becomes more difficult/resourceful to reduce the iterative error to at least one order of magnitude less than the parameter error as the parameter is refined.

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

$$S_{k_m} = S_C + d^*_{I_{k_m}} + d^*_{k_m} + \sum_{j=1,\, j\neq k}^{J} d^*_{j_m} \qquad (13)$$

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. Methods for estimating U_I or d^*_I and U_{I_C} are described in Section 3.2.2. With $d^*_{I_{k_m}}$ evaluated, S_{k_m} is corrected for iterative errors as

$$\hat{S}_{k_m} = S_{k_m} - d^*_{I_{k_m}} = S_C + d^*_{k_m} + \sum_{j=1,\, j\neq k}^{J} d^*_{j_m} \qquad (14)$$

Equation (13) shows that iterative errors $d^*_{I_{k_m}}$ must be accurately estimated or negligible in comparison to $d^*_{k_m}$ for accurate convergence studies and that they should be considered within the context of convergence studies for each input parameter.

$\hat{S}_{k_m}$ can be calculated for both integral (e.g., resistance coefficients) and point (e.g., surface pressure, wall-shear stress, and velocity) variables. If point variables are not at the same location (e.g., when grid doubling is not used) or time, interpolation to a common location and time is required. Roache (1998) discusses methods for evaluating interpolation errors. $\hat{S}_{k_m}$ 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 and to estimate errors and uncertainties. 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 *k*th input parameter. Solution changes ε for medium-fine and coarse-medium solutions and their ratio R_k are defined by

$$\begin{aligned} e_{21_k} &= \hat{S}_{k_2} - \hat{S}_{k_1} \\ e_{32_k} &= \hat{S}_{k_3} - \hat{S}_{k_2} \\ R_k &= \varepsilon_{21_k} / \varepsilon_{32_k} \end{aligned} \qquad (15)$$

Three convergence conditions are possible:

(i) Converging condition: $0 < R_k < 1$

(ii) Oscillatory condition: $R_k < 0$ (16)
(iii) Diverging condition: $R_k > 1$

For the converging condition (i), the solutions exhibit monotonic convergence and generalized RE is used to estimate U_k or d_k^* and U_{k_C}. Methods for estimating errors and uncertainties for the converging condition (i) are described in Section 3.2.3.

For the oscillatory condition (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., 1999). Depending on where the three points fall on the curve, the condition could be incorrectly diagnosed as either converging or diverging. Methods for estimating uncertainties U_k for the oscillatory condition (ii) require more than m=3 solutions and are described in Section 3.2.4.

For the diverging condition (iii), the solutions exhibit divergence and errors and uncertainties can not be estimated. Additional remarks are given in Section 3.2.5.

Determination of the convergence ratio R_k for point variables can be problematic since solution changes e_{21_k} and e_{32_k} 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., $R_k = \|e_{21_k}\|_2 / \|e_{32_k}\|_2$.

3.2.2 Iterative Convergence

Iterative convergence must be assessed and simulation results 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. Methods for estimating U_I or d_I^* and U_{I_C} are described in this section. The methods are applicable to both integral and point variables. For point variables, an L2 norm over all grid points is often used as a global metric. There are many integral and point variables that can be monitored to establish iterative stopping criteria; however, present discussion is specifically within the context of evaluating U_I or d_I^* and U_{I_C} for use in the parameter convergence study for S_{k_m}. Further work is needed on assessing iterative errors and their role in parameter convergence studies and for assessing iterative errors and uncertainties for unsteady flows.

Typical CFD solution techniques for obtaining steady state solutions involve beginning with an initial guess and performing time marching or iteration until a steady state solution is achieved. For time-accurate

calculations using implicit methods, convergence of the solution is required at each time step. Care must be exercised in evaluating iterative convergence based solely on solution residuals, i.e., change in solution from iteration to iteration. Small time steps and/or relaxation parameters can result in small solution residuals while iterative error can be large (Ferziger and Peric, 1997). If S_{k_m} is a primary dependent variable, an alternative approach that removes this problem is to use the residual imbalance of the discretized equations (i.e., the difference in the left- and right-hand sides) as a measure of convergence; since, the iterative error satisfies the same equation as this residual imbalance.

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

$$U_I = \left| \frac{1}{2}(S_U - S_L) \right| \tag{17}$$

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

$$\begin{aligned} U_I &= \left| S - CF_\infty \right| \\ d_{I_{k_m}}^* &= S - CF_\infty, U_{I_C} = 0 \end{aligned} \tag{18}$$

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 d_I^* and U_{I_C}

$$\begin{aligned} U_I &= \left| \frac{1}{2}(S_U - S_L) \right| \\ d_{I_{k_m}}^* &= S - \frac{1}{2}(S_U - S_L), U_{I_C} = 0 \end{aligned} \tag{19}$$

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 (1997) 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.

3.2.3 Convergent Condition: Generalized Richardson Extrapolation

For the converging condition (i) in equation (16), generalized RE is used to estimate U_k or d_k^* and U_{k_C}. RE is generalized for J input parameters and accounting for the effects of higher-order terms, as summarized in the following. Appendix B of Stern et al. (1999b) provides a detailed description.

Generalized RE begins with equation (14). The error terms on the right-hand-side of equation (14) are of known form (i.e., power series expansion in Δx_k) based on analysis of the modified (A.6) and numerical error (A.9) equations, as shown in Appendix A of Stern et al. (1999b) equation (A.12), which is written below as a finite sum (i.e., error estimate) and for the kth parameter and mth solution

$$d_{k_m}^* = \sum_{i=1}^{n} (\Delta x_{k_m})^{p_k^{(i)}} g_k^{(i)} \qquad (20)$$

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. Substituting equation (20) into equation (14) results in

$$\hat{S}_{k_m} = S_C + \sum_{i=1}^{n} (\Delta x_{k_m})^{p_k^{(i)}} g_k^{(i)} + \sum_{j=1,\, j\neq k}^{J} d_{j_m}^* \qquad (21)$$

Subtraction of multiple solutions eliminates the $d_{j_m}^*$ terms in equation (21) and provides equations for S_C, $p_k^{(i)}$, and $g_k^{(i)}$. Since each term (i) contains 2 unknowns, m=2n+1, 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 equation (20) and the magnitude (importance) of the higher-order terms. For sufficiently small Δx_k, the solutions are in the asymptotic range such that higher–order terms are negligible. 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. Usually d_k^* is estimated for the finest value of the input parameter, i.e., $d_k^* = d_{k_1}^*$ corresponding to the finest solution S_{k_1}.

For *m=3*, only the leading-order term can be evaluated. Equations are obtained for $d_{k_1}^*$ and order-of-accuracy p_k

$$d_{k_1}^* = d_{RE_{k_1}}^* = \frac{e_{21_k}}{r_k^{p_k} - 1} \qquad (22)$$

$$p_k = \frac{ln(\varepsilon_{32_k} / \varepsilon_{21_k})}{ln(r_k)} \qquad (23)$$

Appendix B of Stern et al. (1999b) includes results for m=5.

Appendix C of Stern et al. (1999b) provides verification for two analytical benchmarks (one-dimensional wave and two-

dimensional Laplace equations). Multiple solutions were used to evaluate the RE error estimates, including the effects of higher-order terms. Solving for the first-order term is relatively easy since evaluation of equations (22) and (23) only requires that the m=3 solutions are monotonically convergent, even if the solutions are far from the asymptotic range and equations (22) and (23) are inaccurate. 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 relatively close to the asymptotic range, i.e., within about 6% of the theoretical order of accuracy based on the modified equation $p_{k_{th}}$ and $q_{k_{th}}$.

The solutions show that equation (22) has the correct form, but the order of accuracy is poorly estimated by equation (23) except in the asymptotic range. Therefore, one approach is to correct equation (22) by a multiplication correction factor accounting for the effects of higher-order terms. Two correction factors were investigated

$$C_k = \frac{r_k^{p_k} - 1}{r_k^{p_{k_{est}}} - 1} \tag{24a}$$

$$C_k = \frac{(e_{23_k}/e_{12_k} - r_k^{q_{k_{est}}})(r_k^{p_k} - 1)}{\left(r_k^{p_{k_{est}}} - r_k^{q_{k_{est}}}\right)(r_k^{p_{k_{est}}} - 1)} + \frac{(e_{23_k}/e_{12_k} - r_k^{p_{k_{est}}})(r_k^{p_k} - 1)}{(r_k^{p_{k_{est}}} - r_k^{q_{k_{est}}})(r_k^{q_{k_{est}}} - 1)} \tag{24b}$$

$p_{k_{est}}$ and $q_{k_{est}}$ are estimates for the 1st and 2nd term order of accuracy p_k^1 and p_k^2. The estimated value can be based either on $p_{k_{th}}$ and $q_{k_{th}}$ or solutions for simplified geometry and conditions. In either case, preferably including the effects of grid stretching. Equation (24a) 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 (24b) more rigorously accounts for higher-order terms since it is derived from the two-term estimate with 1st and 2nd term order of accuracy p_k^1 and p_k^2 replaced by $p_{k_{est}}$ and $q_{k_{est}}$. Equation (24b) simplifies to equation (24a) in the limit of the asymptotic range. Both correction factors only require solutions for three parameter values. $C_k < 1$ 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. C_k given by equation (24) may be fairly universal in that it only implicitly depends on geometry and conditions.

Combining equation (22) and (24) provides an estimate for $d_{k_1}^*$ accounting for the effects of higher-order terms

$$d_{k_1}^* = C_k \, d_{RE_{k_1}}^* = C_k \left(\frac{e_{21_k}}{r_k^{p_k} - 1} \right) \tag{25}$$

The estimate includes both sign and magnitude. Equation (25) is used to estimate U_k or d_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 equation (25). There are many reasons for lack of confidence, especially for complex three-dimensional flows. Point variables

invariably are not uniformly convergent, which is particularly evident near inflection points and zero crossings.

Equations (24) and (25) need further testing both for additional analytical benchmarks and practical applications. Also alternative strategies for including effects of higher-order terms may be just as viable. Note that equation (25) differs significantly from the GCI proposed by Roache (1998). Herein $C_k = C_k\left(e, r_k, p_k, p_{k\,est}, q_{k\,est}\right)$, whereas in the GCI, C_k is a constant referred to as a factor of safety F_S which equals 1.25 for careful grid studies and 3 for cases for which only two grids are used.

For C_k sufficiently less than or greater than 1 and lacking confidence, U_k is estimated, but not d_k^* and U_{k_C}. Based on the analytical benchmark studies [Appendix C of Stern et al. (1999b)], it appears that equation (25) can be used to estimate the uncertainty by bounding the error by the sum of the absolute value of the corrected estimate from RE and the absolute value of the amount of the correction

$$U_k = \left| C_k\, d^*_{RE_{k_1}} \right| + \left| (1 - C_k)\, d^*_{RE_{k_1}} \right| \tag{26}$$

For C_k sufficiently close to 1 and having confidence, d_k^* and U_{k_C} are estimated. Equation (25) is used to estimate the error d_k^*, which can then also be used in the calculation of S_C [in equation (10)]. The uncertainty in the error estimate is based on the amount of the correction

$$U_{k_C} = \left| (1 - C_k)\, d^*_{RE_{k_1}} \right| \tag{27}$$

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

3.2.4 Oscillatory Condition

For the oscillatory condition (ii) in equation (16), 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

$$U_k = \frac{1}{2}(S_U - S_L) \tag{28}$$

3.2.5 Diverging Condition

For the diverging condition (iii) in equation (16), 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.

3.3 Validation

Validation is defined as a process for assessing 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 3.2. Approaches to estimating experimental uncertainties are presented and discussed by Coleman and Steele (1999).

The validation methodology of Coleman and Stern (1997) which properly takes into account the uncertainties in both the simulation and the experimental data is described in this section. The methodology is also demonstrated using an estimated numerical error and corrected simulation and validation uncertainty values.

3.3.1 Methodology

The validation comparison for a simulated and measured result r that is a function of the variable X is shown in figure 1. The experimentally determined *r*-value of the $(\boldsymbol{X}_i, r_i)$ **d**ata point is *D* and, as before, the simulated r-value is *S*. Recall from equation (1) that the simulation error d_S is the difference between *S* and the truth *T*. Similarly, the error d_D in the data is the difference between *D* and the truth *T*, so setting the simulation and experimental truths equal

$$D - d_D = S - d_S \tag{29}$$

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

$$\begin{aligned} E &= D - S = d_D - d_S \\ &= d_D - (d_{SMA} + d_{SPD} + d_{SN}) \end{aligned} \tag{30}$$

with δ_{SM} decomposed into the sum of δ_{SPD}, error from the use of previous data such as fluid properties, and δ_{SMA}, error from modeling assumptions. 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 d_{SN}^* of the sign and magnitude of δ_{SN} is made, all of these errors are estimated with uncertainties. (As will be shown, during the validation process an estimate of the sign and magnitude of δ_{SMA} can be made under certain conditions.)

If $\boldsymbol{X}_i, r_i$, and *S* share no common error sources, then the uncertainty U_E in the comparison error can be expressed as

$$U_E^2 = \left(\frac{\partial E}{\partial D}\right)^2 U_D^2 + \left(\frac{\partial E}{\partial S}\right)^2 U_S^2 = U_D^2 + U_S^2 \tag{31}$$

or

$$U_E^2 = U_D^2 + U_{SMA}^2 + U_{SPD}^2 + U_{SN}^2 \tag{32}$$

where subscripts are used in the same manner as for the δ's .

Ideally, we would like to 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, the authors know of no 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

$$U_V^2 = U_E^2 - U_{SMA}^2 = U_D^2 + U_{SPD}^2 + U_{SN}^2 \quad (33)$$

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."

If the corrected approach of equations (3)-(6) is used, then the equations equivalent to equations (30) and (33) are

$$E_C = D - S_C = \delta_D - (\delta_{SMA} + \delta_{SPD} + \varepsilon_{SN}) \quad (34)$$

for the corrected comparison error and

$$\begin{aligned} U_{V_C}^2 &= U_{E_C}^2 - U_{SMA}^2 \\ &= U_D^2 + U_{SPD}^2 + U_{S_CN}^2 \end{aligned} \quad (35)$$

for the corrected validation uncertainty. 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_CN} should be smaller than U_{SN}.

For the data point $(\boldsymbol{X}_i, r_i)$, U_D should include both the experimental uncertainty in r_i and the additional uncertainties in r_i arising from experimental uncertainties in the measurements of the *n* independent variables $(X_j)_i$ in $\boldsymbol{X}_i$. The expression for U_D that should be used in the U_V (U_{V_C}) calculation is then

$$U_D^2 = U_{r_i}^2 + \sum_{j=1}^{n} \left(\frac{\partial r}{\partial X_j} \right)_i^2 (U_{X_j})_i^2 \quad (36)$$

In some cases, the terms in the summation in equation (36) may be shown to be very small, using an order-of-magnitude analysis, and then neglected. This would occur in situations in which the U_{X_j} values are of "reasonable" magnitude and gradients in r are small. In regions with high gradients (e.g., near a surface in a turbulent flow), these terms may be very significant and the partial derivatives would be estimated using whatever $(\boldsymbol{X}_i, r_i)$ data is available.

There is also a very real possibility that measurements of different variables might share identical bias errors. This is easy to imagine for measurements of *x*, *y*, and *z*. Another possibility is *D* and *S* sharing an identical error source, for example if the same density table (curve fit) is used both in data reduction in the experiment and in the simulation. In such cases, additional correlated bias terms must be included in equation (31), (32), (33), and (35).

To estimate U_{SPD} for a case in which the simulation uses previous data D_i in m instances, one would need to evaluate

$$U_{SPD}^2 = \sum_{i=1}^{m} \left(\frac{\partial S}{\partial D_i} \right)^2 \left(U_{D_i} \right)^2 \qquad (37)$$

where the U_{D_i} are the uncertainties associated with the data.

3.3.2 Single CFD Code

Consideration of equation (32) shows that (1) the more uncertain the data, and/or (2) the more inaccurate the code (greater U_{SN} and U_{SPD}), the easier it is to validate a code, since the greater the uncertainties in the data and the code predictions, the greater the noise level U_V. 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 there is a programmatic validation requirement, denote it as U_{reqd} since validation is required at that uncertainty level or below. 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):

$$\begin{aligned} &1. \quad |E| < U_V < U_{reqd} \\ &2. \quad |E| < U_{reqd} < U_V \\ &3. \quad U_{reqd} < |E| < U_V \\ &4. \quad U_V < |E| < U_{reqd} \\ &5. \quad U_V < U_{reqd} < |E| \\ &6. \quad U_{reqd} < U_V < |E| \end{aligned} \qquad (38)$$

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 decrease the error δ_{SMA} due to the modeling assumptions in the simulation is not feasible from an uncertainty standpoint. In case 1, validation has been achieved at a level below U_{reqd}, so validation is successful from a programmatic standpoint.

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

A similar comparison table 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. However, the band $E_C \pm U_{E_C}$ should always give a smaller (therefore better) range within which the true value of E lies than the band $E \pm U_E$, assuming that one's confidence in using the estimate d^*_{SN} is not misplaced. Furthermore, for cases 4, 5, and 6, one can argue that E_C more likely corresponds to δ_{SMA}.

In general, validation of a code's predictions of a number (N) of different variables is desired, and this means that in a particular validation effort there could be N different E, E_C, U_V, U_{V_C}, and U_{reqd} values and (perhaps) some successful and some unsuccessful validations. For each variable, a plot of the simulation prediction versus X compared with the $(\boldsymbol{X}_i, r_i)$ data points gives a traditional overview of the validation status, but the interpretation of the comparison is greatly affected by choice of the scale and the size of the symbols. A plot of $\pm U_V$ ($\pm U_{V_C}$) and E (E_C), and U_{reqd} (if known) versus X for each variable is particularly useful in drawing conclusions, and the interpretation of the comparison is more insensitive to scale and symbol size choices.

3.3.3 Comparison of Multiple Codes and/or Models

When a validation effort involves multiple codes and/or models, the procedure discussed above -- comparison of values of E and U_V (and U_{reqd} if known) for the N variables -- should be performed for each code/model.

Since each code/model may have a different U_V, some method to compare the different codes'/models' performance for each variable in the validation is useful. The range within which (95 times out of 100) the true value of E lies is $E \pm U_E$. From equation (32), when U_{SMA} is zero then $U_V = U_E$, so for that ideal condition the maximum absolute magnitude of the 95% confidence interval is given by $|E| + U_V$. Comparison of the ($|E| + U_V$)'s for the different codes/models then shows which has the smallest range of likely error assuming all U_{SMA}'s are zero. This allows appropriate comparisons of (low E)/(high U_V) with (high E/low U_V) codes/models.

A similar discussion holds if the corrected values are used.

3.3.4 Predictions of Trends

In some instances, the ability of a code or model to predict the trend of a variable may be the subject of a validation effort. An example would be the difference in drag for two ship configurations tested at the same Froude number. The procedure discussed above -- comparison of $|E|$ and U_V for the drag -- should be performed for each

configuration. The difference Δ in drag for the two configurations should then be considered as the variable that is the subject of the validation. As discussed in Coleman and Steele (1999), because of correlated bias uncertainty effects in the experimental data the magnitude of the uncertainty in Δ may be significantly less than the uncertainty in either of the two experimentally determined drag values. This means that the value of U_V for Δ may be significantly less than the U_V's for the drag values, allowing for a more stringent validation criterion for the difference than for the absolute magnitudes of the variables. Choice of the corrected or uncorrected approach should be made on a specific case-by-case basis.

3.3.5 Corrected vs. Uncorrected Simulation Results

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. 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.)

As discussed in Section 3.3.2, however, the band $E_C \pm U_{E_C}$ should always give a smaller (therefore better) range within which the true value of E lies than the band $E \pm U_E$, assuming that one's confidence in using the estimate d^*_{SN} is not misplaced.

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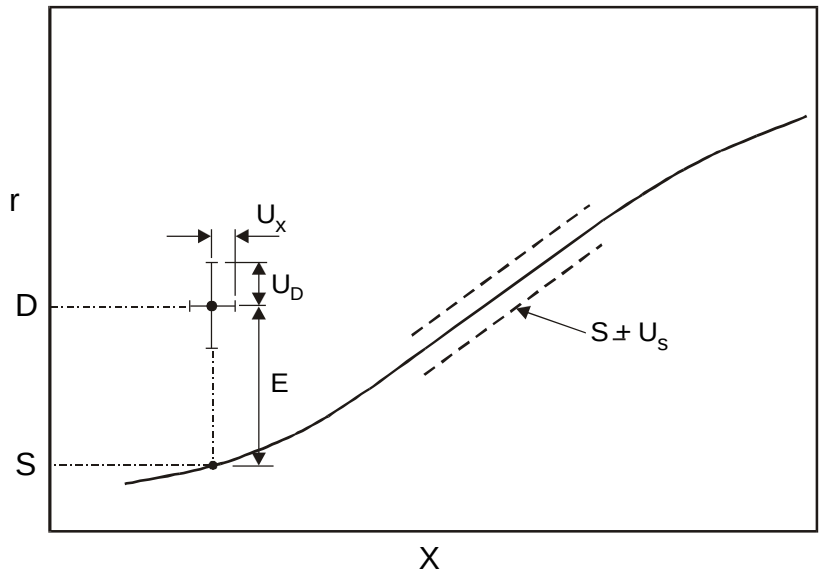

Figure 1 Definition of comparison error.