Journal of Fluids Engineering Editorial Policy
Statement on the Control of Numerical Accuracy

Although no standard method for evaluating numerical uncertainty is currently accepted by the CFD community, there are numerous methods and techniques available to the user to accomplish this task. The following is a list of guidelines, enumerating the criteria to be considered for archival publication of computational results in the *Journal of Fluids Engineering.*

1. Authors must be precise in describing the numerical method used; this includes an assessment of the formal order of accuracy of the truncation error introduced by individual terms in the governing equations, such as diffusive terms, source terms, and most importantly, the convective terms. It is not enough to state, for example, that the method is based on a "conservative finite-volume formulation," giving then a reference to a general CFD textbook.
2. The numerical method used must be at least formally second-order accurate in space (based on a Taylor series expansion) for nodes in the interior of the computational grid. The computational expense of second, third, and higher order methods are more expensive (per grid point) than first order schemes, but the computational efficiency of these higher order methods (accuracy per overall cost) is much greater. And, it has been demonstrated many times that, for first order methods, the effect of numerical diffusion on the solution accuracy is devastating.
3. Methods using a blending or switching strategy between first and second order methods (in particular, the well-known "hybrid," "power-law," and related exponential schemes) will be viewed as first-order methods, unless it can be demonstrated that their inherent numerical diffusion does not swamp or replace important modeled physical diffusion terms. A similar policy applies to methods invoking significant amounts of explicitly added artificial viscosity or diffusivity.
4. Solutions over a range of significantly different grid resolutions should be presented to demonstrate grid-independent or grid-convergent results. This criterion specifically addresses the use of improved grid resolution to systematically evaluate truncation error and accuracy. The use of error estimates based on methods such as Richardson extrapolation or those techniques now used in adaptive grid methods, may also be used to demonstrate solution accuracy.
5. Stopping criteria for iterative calculations need to be precisely explained. Estimates must be given for the corresponding convergence error.
6. In time-dependent solutions, temporal accuracy must be demonstrated so that the spurious effects of phase error are shown to be limited. In particular, it should be demonstrated that unphysical oscillations due to numerical dispersion are significantly smaller in amplitude than captured short-wavelength (in time) features of the flow.
7. Clear statements defining the methods used to implement boundary and initial conditions must be presented. Typically, the overall accuracy of a simulation is strongly affected by the implementation and order of the boundary conditions. When appropriate, particular attention should be paid to the treatment of inflow and outflow boundary conditions.
8. In the presentation of an existing algorithm or code, all pertinent references or other publications must be cited in the paper, thus aiding the reader in evaluating the code and its method without the need to redefine details of the methods in the current paper. However, basic features of the code must be outlined according to Item 1, above.

9. Comparison to appropriate analytical or well-established numerical benchmark solutions may be used to demonstrate accuracy for another class of problems. However, in general this does not demonstrate accuracy for another class of problems, especially if any adjustable parameters are involved, as in turbulence modeling.
10. Comparison with reliable experimental results is appropriate, provided experimental uncertainty is established. However, "reasonable agreement" with experimental data alone will not be enough to justify a given single-grid calculation, especially if adjustable parameters are involved.

These ten items lay down a set of criteria by which the editors and reviewers of this Journal will judge the archival quality of publications dealing with computational studies for the *Journal of Fluids Engineering*. We recognize that the effort to perform a thorough study of numerical accuracy may be great and that many practical engineering calculations will continue to be performed by first order methods, on a single fixed grid. However, such analyses would not be appropriate for presentation in this archival journal. With the gains in performance of low-end workstations, it is now reasonable to require papers on solutions by CFD to meet these fundamental criteria for archiving of a publication.

With the details of these ten criteria now presented, a shortened statement will appear as follows:

The Journal of Fluids Engineering will not consider any paper reporting the numerical solution of a fluids engineering problem that fails to address the task of systematic truncation error testing and accuracy estimation. Authors should address the following criteria for assessing numerical uncertainty.

1. The basic features of the method including formal truncation error of individual terms in the governing numerical equations must be described.
2. Methods must be at least second order accurate in space.
3. Inherent or explicit artificial viscosity (or diffusivity) must be assessed and minimized.
4. Grid independence or convergence must be established.
5. When appropriate, iterative convergence must be addressed.
6. In transient calculations, phase error must be assessed and minimized.
7. The accuracy and implementation of boundary and initial conditions must be fully explained.
8. An existing code must be fully cited in easily available references.
9. Benchmark solutions may be used for validation for a specific class of problems.
10. Reliable experimental results may be used to validate a solution.

References

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Procedure for Estimation and Reporting of Uncertainty Due to Discretization in CFD Applications

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Since 1990, the Fluids Engineering Division of ASME has pursued activities concerning the detection, estimation and control of numerical uncertainty and/or error in computational fluid dynamics (CFD) studies. The first quality-control measures in this area were issued in 1986 (Roache et al., [1]), and revised in 1993 (Freitas [2]). Given the continued increase in CFD related publications, and the many significant advancements in computational techniques and computer technology, it has become necessary to revisit the issue and formulate a more detailed policy to further improve the quality of publications in this area. This brief note provides specific guidelines for prospective authors for calculation and reporting of discretization error estimates in CFD simulations where experimental data may or may not be available for comparison. The underlying perspective is that CFD-related studies will eventually aim to predict the outcome of a physical event for which experimental data is not available.

It should be emphasized that the requirements outlined in this note do not preclude those already published in the previous two policy statements [1, 2]. It is also important to keep in mind that the procedure recommended in this note cannot possibly encompass all possible scenarios or applications.

Preliminaries

The ***computer code*** used for an application must be fully referenced, and previous ***code verification studies*** must be briefly described or cited. The word "verification" is used in this note in its broadest sense, meaning that the computer code is capable of solving a system of coupled differential or integral equations with a properly posed set of initial and/or boundary

conditions correctly, and reproduces the exact solution to these equations when sufficiently fine grid resolution (both in time and space) is employed. The ***formal order of accuracy*** in time and space for each equation solved should be also stated clearly, with proper references where this information is accessible to the readers. Before any discretization error estimation is calculated, it must be shown that ***iterative convergence*** is achieved with at least three (preferably four) orders of magnitude decrease in the normalized residuals for each equation solved. (This commonly-used criterion does not always ensure adequate convergence; see Appendix A) For time-dependent problems, iterative convergence at every time step should be checked, and sample convergence trends should be documented for selected, critically important, variables. *A possible method for assessment of iteration errors is outlined in Appendix A.*

It should also be recognized that uncertainty in inlet flow boundary conditions could be a significant contributor to the overall uncertainty. Here we recommend that the degree of sensitivity of the presented solution to small perturbations in the inlet conditions be studied and reported.

The recommended method for discretization error estimation is the Richardson extrapolation (RE) method. Since its first elegant application by its originator (Richardson [3, 4]), this method has been studied by many authors. Its intricacies, shortcomings and generalization have been widely investigated. A short list of references given in the bibliography [2, 5-14] is selected for the direct relevance of these references to the subject, and for brevity. The limitations of the RE method are well known. The local RE values of the predicted variables may not exhibit a smooth, monotonic dependence on grid resolution, and in a time-dependent calculation, this non-smooth response will also be a function of time and space. Nonetheless, it is currently the most reliable method available for the prediction of numerical uncertainty. Prospective authors can find many examples in the above references. As new and more reliable methods emerge, the present policy statement will be re-assessed and modified as needed.

The GCI method (which is based on RE) described herein is an acceptable and recommended method that has been evaluated over several hundred CFD cases [1, 4, 8, 15, 16]. If authors choose to use it, the method per se will not be challenged in the paper review process.

If authors choose to use another method, the adequacy of their method will be judged in the review process. This policy is not meant to discourage further development of new methods; in fact, JFE encourages the development and statistically significant evaluation of alternative methods of estimation of error and uncertainty. Rather, this policy is meant to facilitate CFD publication by providing practitioners with a method that is straightforward to apply, is fairly well justified and accepted, and will avoid possible review bottlenecks, especially when the CFD paper is an applications paper rather than one concerned with new CFD methodology.

Recommended Procedure for estimation of discretization error

Step 1. Define a representative cell, mesh or grid size *h*. For example, for three-dimensional calculations

$$h = \left[\frac{1}{N} \sum_{i=1}^{N} (\Delta V_i) \right]^{1/3} . \qquad (1)$$

For two-dimensions,

$$h = \left[\frac{1}{N} \sum_{i=1}^{N} (\Delta A_i) \right]^{1/2} \qquad (2)$$

where ΔV_i is the volume, and ΔA_i is the area of the i^{th} cell, and N is the total number of cells used for the computations. Equations (1) and (2) are to be used when integral quantities, e.g., drag coefficient, are considered. For field variables, the local cell size can be used. Clearly, if an observed global variable is used, it is then appropriate to use also an average "global" cell size. *The area should be interpreted strictly according to the mesh being used, i.e. the mesh is either 2-D (consisting of areas) or 3-D (consisting of volumes) irrespective of the problem being solved.*

Step 2. Select three significantly different sets of grids, and run simulations to determine the values of key variables important to the objective of the simulation study, for example, a

variable ϕ critical to the conclusions being reported. It is desirable that the grid refinement factor, $r=h_{coarse}/h_{fine}$, be greater than 1.3. This value of 1.3 is based on experience, and not on formal derivation. The grid refinement should, however, be done systematically, that is, the refinement itself should be structured even if the grid is unstructured. Use of geometrically similar cells is preferable.

Step 3. Let $h_1 < h_2 < h_3$ and $r_{21}=h_2/h_1$, $r_{32}=h_3/h_2$, and calculate the apparent order, p, of the method using the expression

$$p = \frac{1}{\ln(r_{21})}\left|\ln\left|\varepsilon_{32}/\varepsilon_{21}\right| + q(p)\right| , \tag{3a}$$

$$q(p) = \ln\left(\frac{r_{21}^{p} - s}{r_{32}^{p} - s}\right) , \tag{3b}$$

$$s = 1 \cdot \mathrm{sign}(\varepsilon_{32}/\varepsilon_{21}) , \tag{3c}$$

where $\varepsilon_{32}=\phi_3-\phi_2$, $\varepsilon_{21}=\phi_2-\phi_1$, ϕ_k denoting the solution on the k^{th} grid. Note that $q(p)=0$ for $r=const.$ Equation (3) can be solved using fixed-point iteration, with the initial guess equal to the first term. The absolute value in Eq. (3a) is necessary to ensure extrapolation towards $h=0$ [6]. Negative values of $\varepsilon_{32}/\varepsilon_{21}<0$ are an indication of oscillatory convergence. If possible, the percentage occurrence of oscillatory convergence should also be reported. Agreement of the observed apparent order with the formal order of the scheme used can be taken as a good indication of the grids being in the asymptotic range; the converse should not necessarily be taken as a sign of unsatisfactory calculations. It should be noted that if either $\varepsilon_{32}=\phi_3-\phi_2$ or $\varepsilon_{21}=\phi_2-$

ϕ_1 is "very close" to zero, the above procedure does not work. This might be an indication of oscillatory convergence or, in rare situations, it may indicate that the "exact" solution has been attained. In such cases, if possible, calculations with additional grid refinement should be performed; if not, the results may be reported as such.

Step 4 Calculate the extrapolated values from

$$\phi_{ext}^{21} = (r_{21}^{p}\phi_1 - \phi_2)/(r_{21}^{p} - 1). \tag{4}$$

Similarly, calculate ϕ_{ext}^{32}.

Step 5 Calculate and report the following error estimates, along with the apparent order *p*:

Approximate relative error:

$$e_a^{21} = \left| \frac{\phi_1 - \phi_2}{\phi_1} \right|. \tag{5}$$

Extrapolated relative error:

$$e_{ext}^{21} = \left| \frac{\phi_{ext}^{12} - \phi_1}{\phi_{ext}^{12}} \right|. \tag{6}$$

The fine-grid convergence index:

$$\mathrm{GCI}_{\mathrm{fine}}^{21} = \frac{1.25 e_a^{21}}{r_{21}^{p} - 1}. \tag{7}$$

Table 1 illustrates this calculation procedure for three selected grids. The data used is taken from Celik & Karatekin [6]), where the turbulent two-dimensional flow over a backward

facing step was simulated on non-uniform structured grids with total number of cells N_1, N_2, and N_3. Hence, according to Table 1, the numerical uncertainty in the fine-grid solution for the reattachment length should be reported as 2.2%; note that this does not account for modeling errors.

Discretization Error Bars

When computed profiles of a certain variable are presented, it is recommended that numerical uncertainty be indicated by error bars on the profile, analogous to experimental uncertainty. It is further recommended that this be done using the GCI in conjunction with an average value of $p=p_{ave}$ as a measure of the global order of accuracy. This is illustrated in Figs. 1 and 2.

Figure 1 (data taken from Celik & Karatekin [6]) presents an axial velocity profile along y-axis at an axial location of x/H=8.0 for a *turbulent* two-dimensional backward-facing-step flow. The three sets of grids had 980, 4500, and 18000 cells, respectively. The local order of accuracy p calculated from Eq. (3) ranges from 0.012 to 8.47, with a global average p_{ave} of 1.49, which is a good indication of the hybrid method applied for that calculation. Oscillatory convergence occurs at 20% of the 22 points. This averaged apparent order of accuracy is used to assess the GCI indices values in Eq. (7) for individual grids, which is plotted in the form of error bars, as shown in Fig. 1(b). The maximum discretization uncertainty is 10%, which corresponds to ±0.35 m/s.

Table 1: Sample calculations of discretization error

	ϕ = dimensionless reattachment length (*with monotonic convergence*)	ϕ = axial velocity at x/H=8, y=0.0526 (p < 1)	ϕ = axial velocity at x/H=8, y=0.0526 (*with oscillatory convergence*)
N_1, N_2, N_3	18000, 8000, 4500	18000, 4500, 980	18000, 4500, 980
r_{21}	1.5	2.0	2.0
r_{32}	1.333	2.143	2.143
ϕ_1	6.063	10.7880	6.0042
ϕ_2	5.972	10.7250	5.9624
ϕ_3	5.863	10.6050	6.0909
p	1.53	0.75	1.51
ϕ_{ext}^{21}	6.1685	10.8801	6.0269
e_a^{21}	1.5%	0.6%	0.7%
e_{ext}^{21}	1.7%	0.9%	0.4%
GCI_{fine}^{21}	2.2%	1.1%	0.5%

Figure 2 (data taken from Celik & Badeau [17]) presents an axial velocity profile along the y-axis at the station x/H=8.0 for a *laminar* two-dimensional backward-facing-step flow. The Reynolds number based on step height is 230. The sets of grids used were 20x20, 40x40, and 80x80, respectively. The local order of accuracy p ranges from 0.1 to 3.7, with an average value of p_{ave} = 1.38. In this figure, 80% out of 22 points exhibited oscillatory convergence. Discretization error bars are shown in Fig. 2(b), along with the fine-grid solution. The maximum % discretization error was about 100%; this high value is relative to a velocity near zero, and corresponds to a maximum uncertainty in velocity of about ±0.012 m/s.

In the not unusual cases of noisy grid convergence, the least-squares version of GCI should be considered [15, 16].

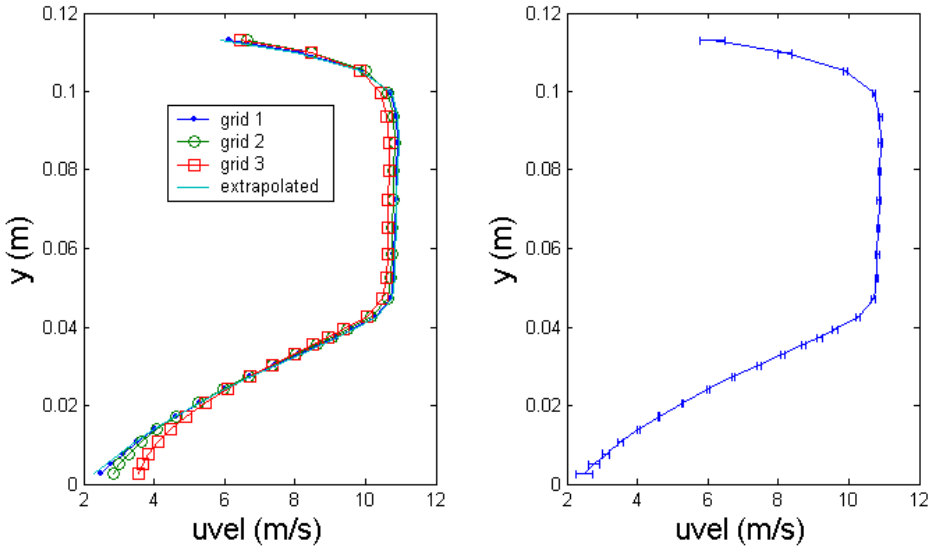

Figure 1(a): Axial velocity profiles for a two-dimensional turbulent backward-facing-step flow calculation, Ref: Celik & Karatekin [6];
(b): Fine-grid solution, with discretization error bars computed using Eq. (7).

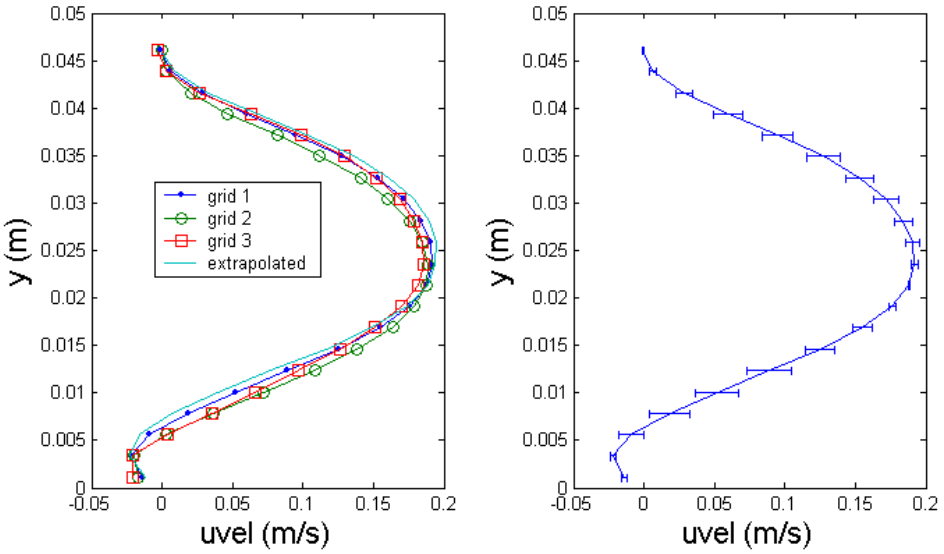

Figure 2(a): Axial velocity profiles for a two-dimensional laminar backward-facing-step flow calculation, Ref: Celik & Badeau [17];
(b): Fine-grid solution, with discretization error bars computed using Eq. (7).

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APPENDIX A : A Possible Method for Estimating Iteration Error

Following Ferziger [1, 2], the iteration error can be estimated by

$$\varepsilon_{iter,i}^{n} \cong \frac{\phi_i^{n+1} - \phi_i^{n}}{\lambda_i - 1} \tag{A.1}$$

where n is the iteration number, and λ_1 is the principal eigenvalue of the solution matrix of the linear system, which can be approximated from

$$\lambda_i \cong \frac{\left\| \phi_i^{n+1} - \phi_i^{n} \right\|}{\left\| \phi_i^{n} - \phi_i^{n-1} \right\|} \tag{A.2}$$

The uncertainty δ_{iter} in iteration convergence can then be estimated as

$$\delta_{iter} \cong \frac{\left\| \varepsilon_{iter,i}^{n} \right\|}{\lambda_{ave} - 1} \tag{A.3}$$

$\| \ \|$ is any appropriate norm, e.g., L_∞ norm. Here, λ_{ave} is the average value of λ_i over a reasonable number of iterations; if $\lambda_{ave} \approx 1.0$, the difference between two consecutive iterations would not be a good indicator of iteration error. In order to build conservatism into these estimates, it is recommended that a limiter of $|\lambda| < 2$ be applied in calculating λ_{ave}.

It is recommended that iteration convergence error calculated as suggested above (or in some other rational way) should be at least one order of magnitude smaller than the discretization error estimates for each calculation. For alternative methods see for example Eca and Hoekstra [3] or Stern et al.[4].

References to Appendix A

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