Richardson Extrapolation-based Discretization Uncertainty Estimation for Computational Fluid Dynamics

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ABSTRACT

This study investigates the accuracy of various Richardson extrapolation-based discretization error and uncertainty estimators for problems in computational fluid dynamics. Richardson extrapolation uses two solutions on systematically refined grids to estimate the exact solution to the partial differential equations and is accurate only in the asymptotic range (i.e., when the grids are sufficiently fine). The uncertainty estimators investigated are variations of the Grid Convergence Index and include a globally averaged observed order of accuracy, the Factor of Safety method, the Correction Factor method, and Least-Squares methods. Several 2D and 3D applications to the Euler, Navier-Stokes, and Reynolds-Averaged Navier-Stokes with exact solutions and a 2D turbulent flat plate with a numerical benchmark are used to evaluate the uncertainty estimators. Local solution quantities (e.g. density, velocity, and pressure) have much slower grid convergence on coarser meshes than global quantities resulting in non-asymptotic solutions and inaccurate Richardson extrapolation error estimates; however, an uncertainty estimate may still be required. The uncertainty estimators are applied to local solution quantities to evaluate accuracy for all possible types of convergence rates. Extensions were added where necessary for treatment of cases where the local convergence rate is oscillatory or divergent. The conservativeness and effectivity of the discretization uncertainty estimators are used to assess the relative merits of the different approaches.

1 Introduction

Computational Fluid Dynamics, or CFD, has enormous potential to impact the analysis, design, and optimization of engineering systems. The predictive capability of CFD depends not only on the validity of the sub-models employed (e.g., turbulence, chemistry, multi-phase flow) and the uncertainties present in the system and surroundings, but also on the ability to reliably estimate and reduce numerical errors. While there are several sources of numerical error in a CFD computation, the largest and most difficult to estimate is usually the error related to the resolution of the spatial grid, i.e., the spatial discretization error.

For a solution solved on a grid with spacing *h*, the discretization error, ε_h , is defined as the difference between the exact solution to the discrete equations, u_h , and the exact solution to the PDEs, \tilde{u} ,

$$\mathbf{\varepsilon}_h = u_h - \tilde{u}.\tag{1}$$

The exact solution to the discrete equations, u_h , assumes that round-off error, iterative error, and other sources of numerical error are zero (or negligible relative to discretization error). Richardson extrapolation uses a sequence of solutions to estimate discretization error and can be applied to almost any type of computational simulation as well as to both local and global quantities. The method is not code intrusive and is applied as a post processing step. For smooth solutions with no discontinuities, the exact solution can be written in terms of a power series expansion, $\tilde{u} = u_h - \sum_{p=p_f}^{\infty} \alpha_p h^p$, which can be used to rewrite Eq. 1 as

$$\varepsilon_h = \sum_{p=p_f}^{\infty} \alpha_p h^p = \alpha_{p_f} h^{p_f} + HOT.$$
⁽²⁾

For a fully verified code, the formal order of accuracy, p_f , is determined by the chosen discretization scheme and is the exponent of the first term in the series. If discontinuities are present, the formal order of the discretization scheme is reduced. A formal order of one is expected for a non-linear discontinuity and $p_s/(p_s + 1)$ for a linear discontinuity where p_s is the formal order for a smooth problem, see Banks et al. [1] for more discussion. To reasonably approximate the discretization error, the Higher Order Terms (HOT) are dropped reducing Eq. 2 to

$$\varepsilon_h \approx \bar{\varepsilon}_h = \alpha_{p_f} h^{p_f}. \tag{3}$$

The exclusion of the HOT introduces the assumption that numeric solutions are asymptotic (i.e., $HOT \ll \alpha_{p_f} h^{p_f}$) for the estimated discretization error, $\bar{\epsilon}_h$, to accurately approximate the true discretization error, ϵ_h . Richardson extrapolation is formulated to solve for the unknowns in Eq. 3, α_{p_f} and $\bar{\epsilon}_h$, using solutions on two systematically refined grids (see discussion in Section 2). This further extends the requirement of an asymptotic solution to not only the solution on which the discretization error is to be estimated but also to any additional solutions used in the extrapolation. In practice, for Eq. 3 to be accurate, all sources of numerical error must be negligible relative to discretization error, the solver should be verified to match the expected order of accuracy of the discretization scheme, and the two numerical solutions used to estimate the discretization error must be asymptotic. (While not accurate for a power series expansion, Richardson extrapolation can be applied to a solution with discontinuities but the expected order of accuracy is reduced from what would be found for smooth problems.) If any of the assumptions are not met, then the solution can exhibit a different order of convergence and a different type of convergence toward the exact solution. The observed order of accuracy requires three solutions on systematically refined grids to compute and is related to four different types of convergence: monotonic convergence, monotonic divergence, oscillatory convergence, and oscillatory divergence. Monotonic convergence and monotonic divergence occur when the difference between solutions computed on successively finer grids decreases and increases, respectively. Oscillatory convergence and oscillatory divergence occur when the difference between solutions on successively finer grids decreases and increases, respectively, and changes sign (i.e., the convergence is not monotone). The observed order of accuracy is typically used to determine the reliability of a Richardson extrapolation error estimate where an observed order of accuracy near the formal order of accuracy is indicative of a near asymptotic solution.

Multiple solutions in the asymptotic range are often difficult to achieve for practical engineering applications; in such cases, the discretization error estimates are often unreliable (i.e., there is uncertainty in the discretization error estimate). To account for this additional uncertainty, the estimated discretization error is modified using an absolute value to create a +/-band centered about the fine grid numerical solution. To improve the probability that the exact solution to the PDEs lies within this uncertainty band, the uncertainty is often multiplied by a factor of safety. The Grid Convergence Index (GCI) was initially developed by Roache [2] for uniform reporting of grid convergence studies and has evolved into a discretization uncertainty estimator recommended by ASME [3] and AIAA [4]. The GCI uncertainty estimate is computed by multiplying the absolute value of the Richardson extrapolation error estimate by a factor of safety where the factor of safety is determined based on knowledge of the nearness to the asymptotic range. For the GCI, Roache [5] does not give an explicit way to determine nearness to the asymptotic range but discusses expected asymptotic behavior and leaves the interpretation of nearness up to the implementer of the GCI. The other methods investigated in this study are based on Richardson extrapolation and follow similar formulations to the GCI with variations including factor of safety choice, proximity to the asymptotic range, et cetera.

The GCI and several variants have been evaluated over a wide range of applications. See for example, Roache [5], Logan and Nitta [6], Cadafalch et al. [7], and Xing and Stern [8]. Most studies focus on uncertainty estimation for global quantities and prescribe the reliability of the uncertainty estimate as the solutions achieve asymptotic convergence. The convergence of local solution quantities is much more "noisy" and it is much more difficult to reach asymptotic solutions because the discretization error at a given node or cell depends on every other node or cell in the domain to varying degrees depending on the application. This noisy convergence results in more frequent oscillatory convergence/divergence and monotone divergence. Most studies discard oscillatory convergence and divergence as these types of convergence do not fit within the theory of Richardson extrapolation. For engineering applications, it is difficult to achieve asymptotic convergence for local

solution quantities; however, an estimate of the discretization uncertainty may be desired. A few non-asymptotic points can cause order of accuracy problems in the entire domain due to the transport of error and can prevent the implementation of Richardson extrapolation as it is normally implemented for local quantities. This paper focuses on evaluating several existing uncertainty estimators for local solution quantities regardless of the type of convergence and relates the reliability of the uncertainty estimators to a distance metric (a metric which indicates how close to the asymptotic range the solution is). The error and uncertainty estimators are evaluated using a set of applications with exact solutions to the Euler, Navier-Stokes, and Reynolds-Averaged Navier-Stokes (RANS) equations and a numerical benchmark solution for the RANS equations.

2 Discretization Error and Uncertainty Estimation

Richardson extrapolation is derived from Eq. 3 by eliminating the coefficient α_{p_f} and estimating the discretization error in the fine grid solution using two systematically refined grids with spacing $h_1 = h$, and $h_2 = rh$

$$\bar{\varepsilon}_h = \frac{u_{rh} - u_h}{r^{p_f} - 1}.\tag{4}$$

For a grid to be systematically refined the grid spacing must be decreased by a constant factor in all coordinate directions and the grid quality must stay the same or improve. The constant factor is the grid refinement factor r which is the relative change is grid spacing from the coarse grid to the fine grid where r > 1. Roache [5] recommends that r > 1.1 to reduce the effects of other sources of numerical error. See Oberkampf and Roy [9] for more discussion regarding systematic grid refinement.

The reliability of the discretization error estimate depends on both solutions being asymptotic which can be determined by calculating the observed order of accuracy of the solution \hat{p} . If the solutions are asymptotic then $\hat{p} \approx p_f$. An additional coarser solution with grid spacing is required to calculate observed order of accuracy

$$\hat{p} = \frac{ln\left(\frac{u_{r^2h} - u_{rh}}{u_{rh} - u_h}\right)}{ln(r)}.$$
(5)

The coarser solution must also be asymptotic which further increases the grid requirements for an accurate estimate of discretization error. Equation 5 assumes that the refinement factor between the fine and medium grids are the same, $r = h_2/h_1 = h_3/h_2$.

A set of solutions can exhibit four different types of convergence. The convergence ratio [10] is defined as

$$R = \frac{u_{r^2h} - u_{rh}}{u_{rh} - u_h}.$$
(6)

The different types of convergence are

- (i) Monotonic convergence: 0 < R < 1
- (ii) Monotonic divergence: 1 < R
- (iii) Oscillatory convergence: -1 < R < 0
- (iv) Oscillatory divergence: R < -1

Some discretization error estimators use the formal order of accuracy and some use the observed order of accuracy. To easily clarify which error estimator is prescribed to use which order of accuracy, Eq. 4 is rewritten as a general function of the order of accuracy

$$\bar{\varepsilon}_h(p) = \frac{u_{rh} - u_h}{r^p - 1}.\tag{7}$$

The error estimate approaches infinity as $p \rightarrow 0$ and results in an unrealistically large error estimate. The observed order of accuracy should be limited to some small positive number, p_l . In our earlier work, we recommended limiting the minimum observed order of accuracy to 0.5 based on extensive testing with various exact solutions [11]. To also allow for error and uncertainty estimation for oscillatory converging solutions (where \hat{p} is undefined), we recommend setting $\hat{p} = 0.5$ unless prescribed otherwise for a given error or uncertainty estimator.

2.1 Grid Convergence Index

The Grid Convergence Index (GCI) was developed by Roache [2] as a method for uniform reporting of CFD results but has since evolved into an uncertainty estimator. Most current implementations of the GCI take the general form of a factor of safety multiplied by the absolute value of the discretization error estimate

$$U = FS|\bar{\mathbf{e}}_h(p)| \tag{8}$$

where FS is the factor of safety. Roache [5] gives two different implementations of the GCI depending on the number of available solutions and the observed order of accuracy

if solutions on only two grids are available

$$U_{GCI-2g} = 3.0 \left| \bar{\mathbf{e}}_h(p_f) \right| \tag{9}$$

if solutions on more than two grids are available and the observed order of accuracy is near the formal order of accuracy

$$U = 1.25 \left| \bar{\varepsilon}_h(\hat{p}) \right|. \tag{10}$$

The two grid error estimator is $E_{GCI-2g} = \bar{\epsilon}_h(p_f)$. Roache limited $\hat{p} \le p_f$ (Ref. [5]) and provided a discussion on a variety of considerations and studies evaluating and applying the GCI [12]. The use of a factor of safety of 1.25 for the GCI requires that the observed order of accuracy is near the formal order and requires the judgment of the user based on the results of the grid convergence study. Oberkampf and Roy [9] suggest an implementation of the GCI that defines which factor of safety to use depending on the observed order of accuracy for $p_f = 2$

$$U_{GCI-OR} = \begin{cases} 1.25 \left| \bar{\mathbf{\epsilon}}_h(p_f) \right|, & 1.8 \le \hat{p} \le 2.2\\ 3.0 \left| \bar{\mathbf{\epsilon}}_h(p_{OR}) \right|, & for all other values \end{cases}$$
(11)

where $p_{OR} = min(max(0.5, \hat{p}), p_f)$ and $p_{OR} = 0.5$ for oscillatory convergence. The error estimator is

$$E_{GCI-OR} = \begin{cases} \bar{\mathbf{e}}_h(p_f), & 1.8 \le \hat{p} \le 2.2\\ \bar{\mathbf{e}}_h(p_{OR}), \text{ for all other values.} \end{cases}$$
(12)

2.2 Global Averaging Method (GCI-glb)

Cadafalch et al. [7] used a global average of observed order of accuracy from the domain. First, the nodes are classified as Richardson nodes, oscillatory nodes, or converged nodes

Richardson Nodes: $(u_{r^2h} - u_{rh})(u_{rh} - u_h) > 0$ Oscillatory Nodes: $(u_{r^2h} - u_{rh})(u_{rh} - u_h) < 0.$

Converged nodes are nodes where the above product is below a specific tolerance and are treated the same as Richardson nodes. In their study, no converged nodes were found so the classification was omitted.

Cadafalch et al. [7] computed a global observed order of accuracy by averaging the observed orders of accuracy at the Richardson nodes. They also placed no restriction on the local observed orders of accuracy to prevent either an average above the formal order of accuracy or below zero. The averaging method is modified for our study to prevent global orders of accuracy outside an acceptable range, the local orders of accuracy were limited between 0.05 and p_f , thus allowing an uncertainty estimate to be obtained at all points regardless of local convergence rates.

$$p_{glb} = \frac{1}{N} \sum_{i=1}^{N} \min\left(\max\left(0.05, \hat{p}_i\right), p_f\right)$$
(13)

where N is the number of grid cells or nodes. The global average uncertainty estimator is

$$U_{GCI-glb} = 1.25 \left| \bar{\epsilon}_h \left(p_{glb} \right) \right| \tag{14}$$

and the error estimator is $E_{glb} = \bar{\epsilon}_h (p_{glb})$.

2.3 Correction Factor Method (CF)

The Correction Factor method (CF) developed by Stern et al. [10] and later modified by Wilson et al. [13] is defined as

$$U_{CF} = \begin{cases} \left[9.6(1-CF)^2 + 1.1\right] |\bar{\mathbf{e}}_h(p_{CF})|, \ 0.875 < CF \le 1.125\\ \left[2|1-CF|+1\right] |\bar{\mathbf{e}}_h(p_{CF})|, & 0 < CF \le 0.875\\ \left[2|1-CF|+1\right] |\bar{\mathbf{e}}_h(p_{CF})|, & CF > 1.125 \end{cases}$$
(15)

where

$$CF = \frac{r^{\hat{p}} - 1}{r^{p_f} - 1}.$$
(16)

The correction factor method removes the choice of factor of safety based on the implementers judgement required by the GCI method by writing the factor of safety as a function of the correction factor term CF. This term is used to indicate how far from asymptotic convergence the solution is in a way that is independent of the formal order of accuracy. The asymptotic factor of safety is 1.1 which occurs when CF = 1.

The method is modified for this study to allow uncertainty estimates at all points by adding a lower limit to the observed order of accuracy $p_{CF} = max(0.5, \hat{p})$ and setting $p_{CF} = 0.5$ for oscillatory solutions. The correction factor is also modified so that $CF = (r^{p_{CF}} - 1)/(r^{p_f} - 1)$. Stern at al. [10] prescribed different treatment for oscillatory converging solutions where the uncertainty is half the difference between the maximum and minimum solution values

$$U_{CF} = \frac{1}{2} \left| \max(u_h, u_{rh}, u_{r^2h}) - \min(u_h, u_{rh}, u_{r^2h}) \right|.$$
(17)

2.4 Factor of Safety Method (FS)

The Factor of Safety method (FS) developed by Xing and Stern [8] varies the factor of safety as a function of the normalized order of accuracy $P = \hat{p}/p_f$ which, similar to the *CF* method, is used to indicate how far from asymptotic convergence the solution is in a formal order of accuracy independent manner. The FS method is defined as

$$U_{FS} = \begin{cases} [FS_1P + FS_0(1-P)] |\bar{\mathbf{e}}_h(p_{FS})|, \ 0 < P \le 1\\ [FS_1P + FS_2(P-1)] |\bar{\mathbf{e}}_h(p_{FS})|, \ P > 1 \end{cases}$$
(18)

where $FS_0 = 2.45$, $FS_1 = 1.6$, and $FS_2 = 14.8$. The asymptotic factor of safety is 1.6 which occurs when P = 1. Observed orders of accuracy greater than the formal order are not limited to the formal order because the *FS* method includes treatment for such cases but the method is modified for this study by adding a lower limit $p_{FS} = max(0.5, \hat{p})$ and setting $p_{FS} = 0.5$ for oscillatory solutions. Also $P = p_{FS}/p_f$. Xing and Stern [8] also proposed the discretization error estimator $E_{FS} = P|\bar{\varepsilon}_h(p_{FS})|$.

2.5 Least Squares Method (LSQ-09, LSQ-10)

Eça and Hoekstra [14, 15] developed a least squares approach to smooth the variations in local observed order of accuracy. Using Eq. 3, an error function is created

$$S(\bar{u},\alpha,\tilde{p}) = \left(\sum_{k=1}^{n_g} \left[u_k - \left(\bar{u} + \alpha h_k^{\tilde{p}}\right)\right]^2\right)^{1/2}$$
(19)

where \tilde{p} is the least squares observed order of accuracy, u_k is the k^{th} solution on a grid with spacing h_k , and n_g is the total number of grids. The derivatives of *S* with respect to \bar{u} , α , \tilde{p} are set to zero resulting in a set of three equations solved using the false-position root finding method

$$\alpha = \frac{n_g \sum_{k=1}^{n_g} u_k h_k^{\tilde{p}} - \left(\sum_{k=1}^{n_g} u_k\right) \left(\sum_{k=1}^{n_g} h_k^{\tilde{p}}\right)}{n_g \sum_{k=1}^{n_g} h_k^{2\tilde{p}} - \left(\sum_{k=1}^{n_g} h_k^{\tilde{p}}\right) \left(\sum_{k=1}^{n_g} h_k^{\tilde{p}}\right)}$$
(20)

$$\bar{u} = \frac{\sum_{k=1}^{n_g} u_k - \alpha \sum_{k=1}^{n_g} h_k^{\tilde{p}}}{n_g}$$
(21)

$$\sum_{k=1}^{n_g} u_k h_k^{\tilde{p}} ln(h_k) - \bar{u} \sum_{k=1}^{n_g} h_k^{\tilde{p}} ln(h_k) - \alpha \sum_{k=1}^{n_g} h_k^{2\tilde{p}} ln(h_k) = 0.$$
(22)

The least squares approach requires at least four solutions. The discretization error and uncertainty estimator, labeled LSQ-09, are subject to different conditions depending on the value of \tilde{p} for $p_f = 2$

$$U_{LSQ-09} = \begin{cases} 1.25|\epsilon_{LSQ}| + U_s, & 0.95 \le \tilde{p} \le 2.05\\ \min(1.25|\epsilon_{LSQ}| + U_s, 1.25\Delta_M), & 0 < \tilde{p} \le 0.95\\ \max(1.25|\epsilon_{LSQ}| + U_s, 1.25\Delta_M), & \tilde{p} \ge 2.05\\ \Delta_M, & for all other values \end{cases}$$
(23)

where $\varepsilon_{LSQ} = \alpha h_1^{\tilde{p}}$, U_s is the RMS of the fit, and

$$\Delta_M = max(|u_i - u_j|), \ 1 \le i \le n_g, \ 1 \le j \le n_g.$$

$$\tag{24}$$

The least squares method was modified in Eça [16] to correct some of the deficiencies in the LSQ-09 method. This method labeled LSQ-10 estimates the discretization uncertainty using two additional error functions based on fixed-exponent power series expansions. The additional error functions were added to account for cases where the least squares observed order of accuracy is greater than the formal order $\varepsilon_{LSQ}^2 = \alpha h_k^2$, and where the least squares observed order of accuracy is not near the formal order of accuracy $\varepsilon_{LSQ}^{12} = \alpha_1 h_k + \alpha_2 h_k^2$. If observed order of accuracy does not fit the above conditions then $\varepsilon_{\Delta M} = \Delta_M / (r^{p_m} - 1)$ is used where $p_m = 1$ for $p_f = 2$. Uncertainty estimation for $p_f = 2$ is outlined in Ref. [16] as

$$U_{LSQ-10} = \begin{cases} 1.25|\epsilon_{LSQ}| + U_s, & 0.95 \le \tilde{p} \le 2.05\\ \min(1.25|\epsilon_{LSQ}| + U_s, 3|\epsilon_{LSQ}^{12}| + U_s^{12}), \ 0 < \tilde{p} \le 0.95\\ \max(1.25|\epsilon_{LSQ}| + U_s, 3|\epsilon_{LSQ}^{2}| + U_s^{2}), \ \tilde{p} \ge 2.05\\ 3|\epsilon_{\Delta M}|, & for all other values, \end{cases}$$
(25)

where U_s^{12} and U_s^2 are the RMS of the least squares fit for ε_{LSQ}^{12} and ε_{LSQ}^2 , respectively.

3 Analysis

3.1 Reliability Metrics

To provide an assessment of the accuracy of the discretization error and uncertainty estimates, the effectivity index [17] for each solution variable is computed as

$$\boldsymbol{\theta}_{L_2} = \frac{||\boldsymbol{\bar{\varepsilon}}_h||_{L_2}}{||\boldsymbol{\varepsilon}_h||_{L_2}}.$$
(26)

The discrete L_2 -norm is computed using

$$||f||_{L_2} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} f_i^2}$$
(27)

where f is any vector of length N. The L_2 -norms in this paper are computed for a data set which is composed of a local solution variable on the computational domain with N grid nodes. The effectivity index should converge to one as the grid is refined for an accurate error estimate.

The primary metric for reliability of the uncertainty estimators is conservativeness where an uncertainty estimate is considered conservative if the estimate is greater than the absolute value of the exact error

$$U > |\varepsilon_h|. \tag{28}$$

The generally accepted goal of conservativeness for a discretization uncertainty estimator is that 95 percent of all estimates should be conservative. To compare how accurately the uncertainty estimate compares to the exact error, an equivalent effectivity index is computed in a manner similar to the effectivity index for discretization error

$$\Psi_{L_2} = \frac{||U||_{L_2}}{||\varepsilon_h||_{L_2}}.$$
(29)

The uncertainty effectivity index is meant to compare how closely the uncertainty estimates bound the exact error. Conservativeness is the most important metric; however, choosing a factor of safety of 1000 may result in a 100 percent conservative uncertainty estimator but would not provide meaningful information about the uncertainty. The over-estimation of the uncertainty would be reflected in the uncertainty effectivity index. As a point of reference, the ideal uncertainty estimator should have a conservativeness greater than 95 percent and an uncertainty effectivity index approaching one as the mesh is refined.

3.2 Distance from the Asymptotic Range

To assess the reliability of the discretization error and uncertainty estimators suitable for many simulations of varying complexity, the reliability metrics should be plotted versus a metric which can be correlated to the confidence in the error or uncertainty estimate. The primary metric for confidence is the observed order of accuracy, where an exact estimate results when $\hat{p} = p_f$ with a high degree of confidence and with degrading confidence as the difference between observed order and formal order increases. This metric is referred to as a distance metric, and ideally, the metric should correlate the reliability metrics for a wide range of problems so that for a given distance from asymptotic convergence the estimates can be said to be reliable. Some possible metrics not based on order of accuracy include cell size or cell count used by Phillips and Roy [11] since these values are commonly used as the absicca for discretization error or order of accuracy plots for a grid convergence study. Cell size and cell count are specific only to the set of systematically refined grids for a given application so make a poor choice for correlating reliability metrics for several applications. The correction factors making *CF* a poor choice. Other possible distance metrics considered include the global order of accuracy defined in Eq. 13, the FS method parameter *P*, the global deviation from the formal order developed by Phillips and Roy [18], and the percent of monotonically converging nodes. The FS method parameter *P* is modified for this study by averaging over the local estimates

$$\bar{P} = \frac{1}{N} \sum_{i=1}^{N} P_i.$$
(30)

The global deviation from the formal order of accuracy computes the average distance from the formal order of accuracy averaged over the entire domain

$$\Delta \bar{p} = \min\left(\frac{1}{N}\sum_{i=1}^{N}\min\left(\left|p_{f} - \hat{p}_{i}\right|, 4p_{f}\right), 0.95p_{f}\right).$$
(31)

The observed order of accuracy \hat{p}_i for this distance metric is an empirically modified calculation of the observed order of accuracy using absolute values to include the effects of oscillatory converging nodes

$$\hat{p} = \frac{ln\left(\left|\frac{u_{r2h} - u_{rh}}{u_{rh} - u_{h}}\right|\right)}{ln(r)}.$$
(32)

The percent of Richardson nodes as defined in Section 2.2 was used by Cadafalch et al. [7] as a measure of reliability. This definition includes monotonically diverging nodes which are not asymptotic, so instead monotonically diverging nodes are excluded and only the percent of monotonically converging nodes is considered as a distance metric instead. That is the percentage of all nodes for a given solution variable with a convergence ratio in the range 0 < R < 1.



Fig. 1. Comparison of data for two different uncertainty estimators with quadratic fit and bounds for less scatter (top row) and more scatter (bottom row)

3.3 Data representation

The reliability metrics are computed for over 700 data points for six different discretization error estimators and six different uncertainty estimators. To more clearly present the data, a quadratic regression fit of the reliability metrics versus the distance metric is computed for each error and uncertainty estimator. The purpose of the regression fit is to capture how the reliability metrics behave as solutions approach the asymptotic range. Equally important, is how much scatter is present in the reliability metrics where more scatter indicates less predicatibility from application to application and a less reliable error or uncertainty estimator. To represent the scatter in the data, the 95 percent confidence bound for the quadratic regression fit is computed. The confidence bounds on the regression fit are meant only for comparison purposes to compare the asymptotic behavior and scatter in the reliability metrics for each error and uncertainty estimator. For the error and uncertainty effectivity index, the regression fit is computed for the inverse effectivity index versus the distance metric. This is done because of the range of the data. Several different plotting styles were compared and the inverse of the effectivity index presented the data best with the most accurate regression fit and confidence bounds. For illustrative purposes only, Fig. 1 shows the raw data for the inverse uncertainty effectivity index and the conservativeness of the uncertainty estimator along with the resulting quadratic fit and confidence bounds for two different uncertainty estimators. The distance metric used is the global deviation from the formal order. The inverse uncertainty effectivity index for two different uncertainty estimators have similar asymptotic behavior but have different amounts of scatter in the data. For conservativeness, only the lower bound is needed because the upper bound is not meaningful. Both the asymptotic behavior and scatter in the data are accurately represented by the confidence bounds.

4 Applications

Solutions to various applications are computed using three different finite volume solvers with a formal order of accuracy of two. The solvers include an in-house 2D, structured, Euler solver; Loci-Chem, a 3D, unstructured, Reynolds Averaged Navier-Stokes (RANS) solver [19]; and PARNASSOS, a 3D, structured, incompressible RANS solver [20]. All simulations were performed in double precision and the iterative residuals were converged to machine zero, thus round-off and iterative error may be neglected. The finite volume solution is piecewise constant over a cell so the solution is assumed to be located at the geometric cell center which is a second-order approximation and a local fourth-order least squares curve-fit is used to interpolate the cell-centered values to the nodes. The discretization error and uncertainty is estimated at every coincident node for a given grid triplet (or grid quadruplet for the LSQ methods) for local solution variables (e.g. density, pressure, and velocity). A summary of all solutions and grid triplets are given in Table 1.

Table 1. Summary of Numerical Solutions				
Application	Equation Set	Variables	Grid Triplets	Total Estimates
Subsonic MMS	Euler	<i>ρ</i> , <i>p</i> , <i>u</i> , <i>v</i>	11	44
Supersonic MMS	Euler	<i>ρ</i> , <i>p</i> , <i>u</i> , <i>v</i>	11	44
Ringleb's Flow	Euler	ρ, <i>p</i> , <i>u</i> , <i>v</i>	7	28
Supersonic Vortex Flow	Euler	<i>ρ</i> , <i>p</i> , <i>u</i> , <i>v</i>	11	44
Loci-Chem MMS	RANS BSL-ke	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
(hexahedral cube	RANS BSL-kω	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
and curvilinear)	Euler	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS: Extrapolation BC	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS: Farfield BC	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS: Inflow BC	ρ, p, u, v, w	4	20
Loci-Chem MMS	RANS BSL-ke	<i>ρ</i> , <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
(prismatic cube	RANS BSL-kw	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
and curvilinear)	Euler	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS: Extrapolation BC	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS: Farfield BC	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS: Inflow BC	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
Loci-Chem MMS	RANS BSL-ke	<i>ρ</i> , <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
(tetrahedral cube	RANS BSL- <i>k</i> ω	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
and curvilinear)	Euler	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS: Extrapolation BC	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS: Farfield BC	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS: Inflow BC	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
Loci-Chem MMS	RANS BSL-ke	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
(hybrid cube,	RANS BSL-kω	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	3	15
curvilinear, and)	Euler	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
highly curvilinear)	NS	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS: Extrapolation BC	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS: Farfield BC	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
	NS: Inflow BC	ρ, <i>p</i> , <i>u</i> , <i>v</i> , <i>w</i>	4	20
PARNASSOS MMS (Cartesian)	INS BSL-kω	<i>p</i> , <i>u</i> , <i>v</i>	6	18
PARNASSOS MMS (stretched)	INS BSL-kω	<i>p</i> , <i>u</i> , <i>v</i>	6	18
PARNASSOS MMS (non-orthogonal)	INS BSL-kω	<i>p</i> , <i>u</i> , <i>v</i>	6	18
Turbulent Flat Plate	RANS Spalart-Allmaras	ρ, <i>p</i> , <i>u</i> , <i>v</i>	2	8

4.1 Euler Solver

4.1.1 Manufactured Solutions

Two applications include the supersonic and a subsonic manufactured solution used in Ref. [21]. The basic manufactured solution function is

$$f(x,y) = a_0 + a_1 \sin\left(\frac{b_1 x \pi}{L} + c_1 \pi\right) + a_2 \sin\left(\frac{b_2 y \pi}{L} + c_2 \pi\right)$$
(33)

where the coefficients *a*, *b*, *c* are coefficients to control the magnitude, period, and phase shift of the solution and *L* is the reference length of one. The magnitude a_0 for density, x-velocity, y-velocity, and pressure are $1.0 kg/m^3$, 800.0 m/s, 800.0 m/s, and 100,000.0 Pa for the supersonic manufactured solution and $1.0 kg/m^3$, 70.0 m/s, 90.0 m/s, and 100,000.0 Pa for the supersonic manufactured solution and 2.0 for all solution variables.

Two sets of grids for each manufactured solution are also used to investigate the effect of refinement factor on error and uncertainty estimation. The finest grid for the first grid set is 513x513. This grid is successively coarsened by a factor of two to create seven grid levels where the coarsest is 17x17. The second set includes the first nine grids in the first set plus an additional set which when combined with the first set results in refinement factors of 4/3 and 3/2 instead of refinement factors of two and two between the fine and medium and medium and coarse grids, e.g. 513x513, 385x385, and 257x257 instead of 513x513, 257x257, and 129x129.

4.1.2 Supersonic Vortex Flow

Supersonic vortex flow [22] consists of a flow around a 90 degrees annulus

$$\rho(r) = \rho_i \left(1 + \frac{\gamma - 1}{2} M_i^2 \left(1 - \frac{R_i^2}{r^2} \right) \right)^{\frac{1}{\gamma - 1}}$$

$$u(y, r) = \frac{yU}{r}, \qquad v(x, r) = -\frac{xU}{r}, \qquad P = \frac{\rho^{\gamma}}{\gamma},$$

$$U_i = M_i \rho_i^{\frac{\gamma - 1}{2}}, \qquad U = \frac{U_i R_i}{r}.$$
(34)

The flow field is defined as a function of variables at the inner radius of the annulus denoted by the subscript *i*. The inner radius R_i is 2.0*m*, the outer radius is 3.0*m*, the inner density ρ_i is $1.0 kg/m^3$, and the inner Mach number M_i is 2.0. The finest grid is 513x257 and is successively coarsened by a factor of two to generate a family of grids where the coarsest is 9x5. A second intermediate grid set was also created in the same manner as for the manufactured solutions.

4.1.3 Ringleb's Flow

Ringleb's flow is an inviscid flow around a 180 degree turn [23]. The flow can be supersonic, subsonic, or both depending on the domain chosen. For this study, a supersonic-only region was chosen. Ringleb's flow is governed by the stream function

$$\Psi = \frac{1}{q} \sin(\theta) \tag{35}$$

where θ is the flow angle and *q* is the normalized velocity. A total of six grids were generated for Ringleb's flow from the finest grid of 257x257 using a refinement factor of two to create five grid levels. An intermediate grid set was also created.

4.2 PARNASSOS

4.2.1 Manufactured Solutions

A manufactured solution is used from the 2006 and 2008 Lisbon uncertainty analysis workshops [24]. The manufactured solution is for the BSL-kw RANS turbulence model

$$u = erf(\eta)$$

$$v = \frac{1}{\sigma\sqrt{\pi}} \left(1 - e^{\eta^{2}}\right)$$

$$C_{p} = 0.5ln \left(2x - x^{2} + 0.25\right) ln \left(4y^{3} - 3y^{2} + 1.25\right)$$

$$v_{t} = 0.25 (v_{t})_{max} \eta_{v}^{4} e^{2 - \eta_{v}^{2}}$$

$$k = k_{max} \eta_{v}^{2} e^{1 - \eta_{v}^{2}}$$
(36)



Fig. 2. PARNASSOS Cartesian, stretched, and non-orthogonal grids

where C_p is the coefficient of pressure, $\eta = \sigma y/x$, $\eta_v = \sigma_v y/x$, $\sigma = 4$, $\sigma_v = 2.5\sigma$, $k_{max} = 0.001$, $(v_t)_{max} = 10^3 v$, and $\omega = k/v_t$. The manufactured solution is designed to resemble a boundary layer and is computed on three different grid topologies shown in Fig. 2. Each grid topology has 16 grid levels with grids created in increments of 20 (i.e. 101x101, 121x121, ..., 401x401). The grids are combined to created a total of 6 grid triplets per grid topology with three variables per solution. In total, there are 54 grid triplets included in the data set with discretization error estimated for x-velocity, y-velocity, and pressure.

4.3 Loci-CHEM

4.3.1 Manufactured Solutions

Several manufactured solutions are used to compute 3D, steady-state solutions to the Euler, Navier-Stokes, and RANS equations with two-equation turbulence models. The manufactured solutions used for code verification of Loci-CHEM are discussed in [25, 26]. The manufactured solutions include one Euler solution, BSL- $k\omega$ and BSL- $k\varepsilon$ RANS solutions, and four Navier-Stokes solutions which include extrapolation, farfield, and inflow boundary conditions. Three different grid topologies are used with two different levels of complexity. These grid topologies include hexahedral, tetrahedral, and prismatic grid cells plus a hybrid combination of each on a Cartesian domain, a curvilinear domain, and a highly skewed curvilinear domain [26]. A few examples are shown in Fig. 3. The grid sizes are 65x65x65, 33x33x33, 17x17x17, and 9x9x9. There are a total of two grid triplets per grid topology for seven manufactured solutions with 5 solution variables each for a total of 555 grid triplets.



Fig. 3. Samples of the Loci-CHEM computational grids showing the (a) Cartesian tetrahedral grid, (b) curvilinear prismatic grid, (c) highly skewed curvilinear hexahedral grid, and (d) the curvilinear hybrid grid

4.3.2 Turbulent Flat Plate

A numerical benchmark solution computed for a zero pressure gradient, turbulent flat plate for the RANS equations computed using the Spalart-Allmaras turbulence model [27] is used to evaluate the error and uncertainty estimators in place of an exact solution. The flat plate has a non-dimensional length L of 2 and the Reynolds number at L = 1 is 5,000,000. The



Fig. 4. Turbulent flat plate setup and the 69x49 grid

domain and boundary conditions are shown in Fig. 4. The finest grid used for error and uncertainty estimation is 545x385 and is successively coarsened by a factor of two to create a total of five grids. A numerical benchmark was created by Phillips et al. [21] using the same computational domain and grid topology as the grids used for error and uncertainty estimation. The numerical benchmark grid dimensions are 2177x1537 nodes and computed using Loci-CHEM. The benchmark solution was created using the guidelines included in Phillips et al. [21] which require for a benchmark solution that (1) the numerical benchmark has been shown to be in the asymptotic convergence range and (2) that the code used to generate the benchmark solution has passed all order of accuracy code verification tests for all options exercised in the benchmark problem. Both of these conditions were satisfied for the numerical benchmark and documented by Phillips et al. [21]. The numerical benchmark was developed with the purpose of evaluating discretization error and uncertainty estimates. The error due to the presence of discretization error in the benchmark solution is estimated by propagating the estimated discretization error in the numerical benchmark through the discretization error estimate calculations discussed in this paper. The error in error effectivity index computed using Richardson extrapolation with the formal order of accuracy is about 0.1. The numerical benchmark discretization error has negligible effect on all other computational grids coarser than the 545x385 grid.

5 Results

5.1 Distance Metric

The global observed order of accuracy, the FS method distance metric, global deviation from the formal order, and percent of monotonically converging nodes are compared in Fig. 5. The error effectivity index for Richardson extrapolation using the formal order of accuracy (Eq. 4) for all local solution variables in the test data set is plotted for each distance metric.

The effectivity index should approach one as the solutions become more asymptotic. For the four distance metrics considered, an asymptotic solution occurs at zero for the global deviation from the formal order, 100 percent for the percent of monotonically converging nodes, the formal order of accuracy (two for all cases) for the global order of accuracy, and P = 1 for the Factor of Safety method parameter. The ideal distance metric should show decreasing scatter in the data centered about an inverse effectivity index of one as the data approaches the asymptotic range. Shown in Fig. 5, the global deviation from the formal order, percent of monotonically converging nodes, and the global order of accuracy resemble to varying degrees the expected trend. The distance metric \bar{P} does not show a clear trend. This is because p_{FS} is not limited to a maximum of p_f , and results in the average of P roughly clustering around $\bar{P} = 1$. Of the three other distance metrics that have the particular trend sought, the global deviation from the formal order shows the clearest trend in inverse effectivity index with significantly reduced scatter as the distance metric approaches zero and no scatter at $\Delta \bar{p} = 0$ which is preferred. The percent of monotonically converging nodes and global order of accuracy still have some scatter at asymptotic solution convergence (i.e. 100 percent monotonically converging nodes and $p_{elb} = p_f$). The reason that the global deviation from the formal order performs the best is because orders of accuracy greater than one and less than one are treated as equally far from the asymptotic range. This treatment is prefered since observed orders of accuracy greater than the formal order and less than the formal order are equally non-asymptotic. The difference is that the signs of the higher order terms allow for error cancelation or error addition. For an observed order of accuracy greater than the formal order, the first two terms of the higher order terms will tend to have the same sign, and for orders of accuracy lower than the formal order, the first two terms will tend to have the opposite signs. The percent of monotonically converging nodes is good but not the best choice because observed orders of accuracy greater than the formal order are considerably non-asymptotic but are counted as asymptotic allowing for a misleading more asymptotic distance metric. In a similar manner, the calculation of the global observed order limits orders of accuracy greater than the formal order to equal the formal order. This again allows for a misleading more asymptotic distance metric. Comparison of the distance metric with the uncertainty effectivity index and conservativeness showed similar trends.



Fig. 5. Comparison of the effectivity index for Richardson extrapolation versus various distance measures

5.2 Discretization Error Estimates

Discretization error estimators are compared in Fig. 6 comparing Richardson extrapolation using a) the formal order of accuracy, b) the observed order of accuracy, c) observed order of accuracy modifications p_{OR} , d) globally averaged observed order of accuracy, e) observed order of accuracy modifications p_{CF} , f) and the discretization error estimator proposed by Xing and Stern [8]. The least-square fit confidence bounds, computed as described in Section 3.3, for all seven applications are compared for a total of about 1.6 million error estimates combined into a total of 777 error effectivity index data points. The use of Richardson extrapolation using the formal order of accuracy is the most accurate error estimator where the data is symmetric about an inverse effectivity index of one for the full range of $\Delta \bar{p}$. The scatter in the data decreases resulting in more reliable discretization error estimates as solutions approach the asymptotic range (i.e. as $\Delta \bar{p}$ approaches zero). The other five error estimators use an observed order of accuracy which results in an overestimate of the discretization error due to the observed order of accuracy factor of safety. The observed order factor of safety refers to the implicit factor of safety due to the use of the observed order of accuracy $\bar{\epsilon}_h(p) = FS_p \bar{\epsilon}_h(p_f)$ where $FS_p = \frac{r^p f - 1}{r^p - 1}$. (Note that FS_p is the inverse of *CF*.) The use of the different orders of accuracy results in varying differences in the inverse effectivity index. There are negligible differences between error estimates which use \hat{p} , p_{OR} , and p_{CF} . The use of p_{elb} results in slightly more accurate error estimates compared to $\varepsilon_h(\hat{p})$ as well as reduced scatter. The reduced scatter is due to use of a single value of order of accuracy and observed order factor of safety instead of point-wise variations in the observed order. No error estimator was given for the CF method; however, Richardson extrapolation using the observed order of accuracy p_{CF} is included to compare the effects of not limiting the observed order of accuracy to the formal order. There is no noticable difference between limiting the observed order to the formal order or not limiting the observed order. The same order of accuracy is used for the FS method as the CF method; however, the use of P compensates for the underestimate of discretization error when $p_{FS} > p_f$ and the overestimate of discretization error when $p_{FS} < p_f$. The use of P results in more accurate error estimates compared to $\varepsilon_h(\hat{p})$ and is the second most accurate error estimator compared.

5.3 Discretization Uncertainty Estimation

The inverse uncertainty effectivity index and the conservativeness are shown in Fig. 7 for the discretization uncertainty estimators. The inverse uncertainty effectivity index for the GCI-2g method is the same as the error effectivity index for $\bar{\epsilon}_h(p_f)$ (Fig. 6a), except that it is shifted by a factor of a third due to the presence of the factor of safety (FS = 3). Similarly, the other uncertainty estimators also approach their inverse factor of safety as $\hat{p} \rightarrow p_f$. The use of the observed order of accuracy results in a similar trend as the discretization error estimators which overestimate the uncertainty for non-asymptotic solutions. The GCI-OR, CF, and FS method all have nearly identical observed orders of accuracy. The differences in these methods is due almost exclusively to the choice of factor of safety. The most conservative uncertainty estimators are the LSQ methods which are very similar; however, the uncertainty effectivity index for the LSQ-10 method is significantly improved over the LSQ-09 method and results in a much more accurate uncertainty estimate. The LSQ-10 uncertainty estimator still overestimates the uncertainty considerably more than any of the other uncertainty estimators except the LSQ-



Fig. 6. Error effectivity indices for discretization error estimators



Fig. 7. Uncertainty effectivity index and conservativeness for discretization uncertainty estimators

09. The FS, GCI-OR, and GCI-2g uncertainty estimators are the next most conservative estimators. The FS and GCI-OR methods have very similar trends regarding the uncertainty effectivity index but the FS method is slightly more conservative. The GCI-2g uncertainty estimator is less conservative than both the FS and GCI-OR methods and the uncertainty is also overestimated for more asymptotic solutions. The variable factor of safety used both by the FS and GCI-OR method offer an advantage over a constant factor of safety of three at the cost of one additional solution. The next best uncertainty estimator is the GCI-glb method which does not compare well to the conservativeness goal of 95 percent for solutions far from the asymptotic range. The poor performance of the method is due primarily to the use of a constant factor of safety of 1.25 where increasing the factor of safety would significantly improve performance. It is important to note that the use of the global observed order of accuracy compared to the local observed order of accuracy for the same constant factor of safety improves the conservativeness for non-asymptotic solutions and results in an uncertainty effectivity index closer to one (results not shown). The use of a global observed order of accuracy could be used with any of the other uncertainty estimators to likewise improve both the accuracy and conservativeness. The uncertainty estimator which performs the worst for conservativeness is the CF method; however, the CF method has an uncertainty effectivity index closest to one as $\Delta \bar{\rho}$ approaches zero.

To add an additional level of comparison between the conservativeness of each uncertainty estimator, the overall conservativeness is computed for every uncertainty estimate included in the study for approximately 1.6 million estimates and is independent of the distance measure. The results are shown in Table 2 and are sorted from the highest conservativeness to the lowest. The conservativeness of the absolute value of Richardson extrapolation using the formal order of accuracy is also

Estimator	All Data	$\hat{p} > 0.5$ only
# Data	1.6 Million	1.3 Million
LSQ-09	97.7%	_
FS	97.5%	97.4%
LSQ-10	97.0%	—
GCI-OR	95.8%	95.3%
GCI-2g	95.2%	97.0%
GCI-glb	92.6%	92.4%
CF	89.7%	90.3%
$ \mathbf{\epsilon}_h(p_f) $	49.8%	52.4%

Table 2. Overall conservativeness of each uncertainty estimator

included for comparison and is expected to be 50 percent as discussed by Roache [5] and Oberkampf and Roy [9]. The LSQ, FS, GCI-OR, and GCI-2g methods all meet the 95 percent conservativeness goal. To show the effects of the modifications to the observed order of accuracy (setting oscillatory nodes to 0.5 and limiting orders of accuracy to a minimum of 0.5) that were implemented to estimate the uncertainty at diverging and oscillatory nodes, the uncertainty estimators were applied to only the data with $\hat{p} > 0.5$. This represents about 83 percent of all the data. The FS, GCI-OR, and GCI-glb methods show a very slight decrease in conservativeness and the CF method shows a very slight increase in conservativeness. The most significant change is in the GCI-2g method which had an increased conservativeness of almost two percent points making it one of the better performers with 97 percent conservativeness. The lack of change between including and excluding the specific data supports our modifications to the uncertainty estimators for oscillatory nodes. Furthermore, it also supports our hypothesis that local solutions are, in practice, non-asymptotic and uncertainty estimates for monotonically converging nodes are as reliable as diverging, oscillatory converging or oscillatory diverging nodes.

The CF method was the only uncertainty estimator other than the LSQ methods which specified treatment for oscillatory nodes given in Eq. 17. All other GCI methods were modified for this study to assign a value of 0.5 to the order of accuracy of oscillatory nodes to compute an uncertainty estimate. The lower limit of 0.5 was applied to the CF method to compare the two different treatments of oscillatory nodes. The resulting overall conservativeness for the CF method was 91.5 percent which is only a slight increase in percent over Eq. 17. There was little change in the overall trends of the uncertainty effectivity index.

6 Conclusion

Richardson extrapolation-based discretization error and uncertainty estimators were applied to several different applications with a focus on uncertainty estimation for local solution quantities. The estimators were applied to all coincident grid nodes including diverging and oscillating nodes. All nodes were included to thoroughly investigate the behavior of each estimator because it is not always possible to have local solutions in the asymptotic range; however, a conservative estimate of discretization uncertainty is still desirable, and as demonstrated herein, is possible. The reliability of the error and uncertainty estimates was quantified using the error effectivity index, the uncertainty effectivity index, and the overall conservativeness of the uncertainty estimates. The global deviation from the formal order of accuracy was the distance measure used to correlate the effectivity indices and conservativeness. A total of 777 grid triplets and a total of 1.6 million local estimates were examined.

Overall there was a general trade-off between the accuracy of the error and uncertainty estimates and the conservativeness. The most accurate uncertainty estimator (e.g. effectivity index closest to one) was the CF method but it was also the least conservative. The LSQ methods were the most conservative but significantly overestimated the uncertainty compared to the other methods. The LSQ-10 was much more accurate than the LSQ-09 method with nearly identical conservativeness and should be used instead of the LSQ-09 method. The LSQ-10 and the FS method were very similar in terms of conservativeness. The LSQ-10 method was more conservative for less asymptotic solutions but the overall conservativeness of the FS method was 0.5 percent better. The FS method was more accurate than the LSQ-10 with an uncertainty effectivity index closer to one and had significantly less scatter in the metrics. The LSQ and the FS methods perform similarly and either could be applied successfully for accurate uncertainty estimation; however, the FS method requires only three solutions and is easier to implement than the LSQ methods which require at least four solutions. If only two solutions are available, the GCI-2g method should be used as the overall conservativeness met the 95 percent conservativeness goal for this data set and has been reliably applied to a wide range of applications.

It was also observed that the use of a global order of accuracy improved the conservativeness and accuracy of the uncertainty estimator and decreased the scatter in the data in the effectivity index. While the GCI-glb did not perform well compared to the other uncertainty estimators due to the constant factor of safety of 1.25, the use of a global order of accuracy for local estimates would improve the overall performance of the other uncertainty estimators considered.

The uncertainty estimators were evaluated using simple Euler and Navier-Stokes solutions which are relatively easy to reach the asymptotic range. The uncertainty estimators should be evaluated further using more realistic problems; however, the lack of exact solutions makes the evaluation of the uncertainty estimators more ambiguous and is a current topic of research.

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