Perspective: A Method for Uniform Reporting of Grid Refinement Studies

P. J. Roache
Ecodynamics Research Associates, Inc.,
P.O. Box 9229,
Albuquerque, N.M. 87119

This paper proposes the use of a Grid Convergence Index (GCI) for the uniform reporting of grid refinement studies in Computational Fluid Dynamics. The method provides an objective asymptotic approach to quantification of uncertainty of grid convergence. The basic idea is to approximately relate the results from any grid refinement test to the expected results from a grid doubling using a second-order method. The GCI is based upon a grid refinement error estimator derived from the theory of generalized Richardson Extrapolation. It is recommended for use whether or not Richardson Extrapolation is actually used to improve the accuracy, and in some cases even if the conditions for the theory do not strictly hold. A different form of the GCI applies to reporting coarse grid solutions when the GCI is evaluated from a "nearby" problem. The simple formulas may be applied a posteriori by editors and reviewers, even if authors are reluctant to do so.

Introduction

"If you want a new idea, read an old book." (Anon.)

The Computational Fluid Dynamics community is currently in the midst of a "reform movement" in regard to quantification of uncertainty (e.g., Mehta, 1991; Celik et al., 1993). Progressive journals are now explicit in their requirement for grid convergence studies or other uncertainty estimation (e.g., Roache et al., 1986; Freitas, 1993; AIAA, 1994). However, there is no uniformity in the performance of these studies, nor even more basically in the *reporting* of the results.

This paper proposes the use of a Grid Convergence Index (GCI) for the uniform reporting of grid refinement studies in Computational Fluid Dynamics and related disciplines. There are other possible techniques for the quantification of numerical uncertainty, but systematic grid refinement studies are the most common, most straightforward and arguably the most reliable. The motivation for the proposed uniform Grid Convergence Index is the inconsistent and confusing reporting of grid refinement studies in the engineering and scientific literature. The following hypothetical examples will suffice.

One paper states that the grid density was increased by 50 percent, resulting in a difference in some solution norm of 4 percent (of the fine grid solution) using a first-order accurate method. In another paper, grid density was doubled, resulting in a difference of 6 percent, using a second-order method. Which fine grid solution is more reliable?, i.e., better converged? More important, can the reader have any reasonable expectation that these numbers represent a "percent accuracy error band", i.e., that the fine-grid calculations are probably accurate to within 4 or 6 percent of the true solution of the continuum equations?

Note that we are concerned herein with verification of a particular calculation, i.e., estimating the grid convergence accuracy of a particular discretized solution. We assume that the code itself has already been verified for the same class of problems (so that coding errors are not an issue and, if done properly, the order of accuracy has been verified; e.g., see Steinberg and Roache, 1985; Blottner, 1990). Nor are we concerned with code validation, e.g., that a turbulence model is adequate. See Blottner (1990) for discussion of validation, or "solving right governing equations" versus verification, or "solving governing equations right." (In the present author's opinion, a code and a particular calculation can be verified, and not with excessive difficulty. However, a code cannot be validated in any general sense, i.e., by comparison with experimental values. Rather, only a particular calculation or narrow range of calculations can be validated.) Also, it is always worth noting that this paper and similar grid refinement studies address only "ordered" discretization errors, which by definition vanish as grid spacing $h \to 0$. Specifically, the errors introduced by the use of far-field computational boundaries must be assessed separately (e.g., see Roache, 1972). Further, I consider herein only *a posteriori* error estimation, being of the opinion that useful *a priori* estimation is not possible for fluids engineering problems.

Richardson Extrapolation

Richardson Extrapolation, also known as "h^2 extrapolation" and "the deferred approach to the limit" and "iterated extrapolation," was first used by Richardson in 1910, and later embellished in 1927. The discrete solutions f are assumed to have a series representation, in the grid spacing h, of

Contributed by the Fluids Engineering Division for publication in the JOURNAL OF FLUIDS ENGINEERING. Manuscript received by the Fluids Engineering Division September 11, 1993; revised manuscript received June 6, 1994. Associate Technical Editor: O. Baysal.

$$f = f[\text{exact}] + g_1 h + g_2 h^2 + g_3 h^3 + \ldots \quad (1)$$

The functions g_1, g_2, etc. are defined in the continuum and do not depend on any discretization. For infinitely differentiable solutions, they are related to all orders to the solution derivatives through the elementary Taylor series expansions, but this is not a necessary assumption for Richardson Extrapolation, nor is the infinite series indicated in Eq. (1). It is only necessary that Eq. (1) be a valid definition for the order of the discretization. Thus, the extrapolation may be valid for finite element solutions, etc.

For a second-order method, $g_1 = 0$. Then the idea is to combine two separate discrete solutions f_1 and f_2, on two different grids with (uniform) discrete spacings of h_1 (fine grid) and h_2 (coarse grid), so as to eliminate the leading order error terms in the assumed error expansion, i.e. to solve for g_2 at the grid points in Eq. (1), substitute this into Eq. (1) and obtain a more accurate estimate of f[exact]. The result is the original statement (Richardson, 1927) for h^2 extrapolation.

$$f[\text{exact}] = (h_2^2 f_1 - h_1^2 f_2)/(h_2^2 - h_1^2) + \text{H.O.T.} \quad (2)$$

where H.O.T. are higher-order terms. Using the grid refinement ratio $r = h_2/h_1$, this can be conveniently expressed in terms of a correction to the fine grid solution f_1, dropping H.O.T.

$$f[\text{exact}] = f_1 + (f_1 - f_2)/(r^2 - 1) \quad (3)$$

The most common use of this method is with a grid doubling, or halving. (These are *identical*. Both use two grids, one twice as fine as the other, i.e., we have a coarse grid and a fine grid. Whether we "doubled" or "halved" just depends on which calculation came first!) With $r = 2$, Eq. (3) becomes

$$f[\text{exact}] = 4/3 f_1 - 1/3 f_2. \quad (4)$$

It is often stated that Eq. (4) is fourth-order accurate if f_1 and f_2 are second-order accurate. Actually, as known by Richardson, this is true only if odd powers are absent in the expansion (1), which he achieved by assuming the exclusive use of second-order centered differences. If uncentered differences are used, e.g., upstream weighting of advection terms, even if these are second-order accurate (3-point upstream), the h^2 extrapolation is third-order accurate, not fourth. As a practical limitation, even extrapolations based on centered differences do not display the anticipated fourth-order accuracy until the cell Reynolds number Rc is reduced; for the 1-D advection-diffusion equation with Dirichlet boundary conditions, Rc < 3 is required (Roache and Knupp, 1993).

Although Richardson Extrapolation is most commonly applied to grid doubling, and is often stated to be only applicable to integer grid refinement (e.g., Conte and DeBoor, 1965) this is not required. In order to use Eq. (3) it is necessary to have values of f_1 and f_2 at the same points, which would seem to require commonality of the discrete solutions, and therefore integer grid refinement ratios r (grid doubling, tripling, etc.). However, even in his 1910 paper, Richardson looked forward to defining a continuum f_2 by higher-order interpolation, and in the 1927 paper had a specific approach worked out. Ferziger (1993) alludes to this approach with less detail but more generality. Similarly, Richardson Extrapolation is commonly applied only to obtaining a higher-order estimate on the coarse grid with $h_2 = 2h_1$, but Roache and Knupp (1993) show how to obtain fourth-order accuracy on all fine-grid points by simple second-order interpolation, not of the solution values f_2, but of the extrapolated *correction* from Eq. (4), i.e., by second-order interpolation of 1/3 $(f_1 - f_2)$. The use of simple second-order interpolation avoids complexities with nonuniform grids and near-boundary points.

Richardson (1910, 1927) also considered sixth-order extrapolation (using 3 grid solutions to eliminate g_2 and g_4), parabolic and elliptic equations, staggered grids (then called "interpenetrating lattices"), rapid oscillations and the $2h$ wavelength limit, *a priori* error estimates, singularities, integral equations, statistical problems, Fourier coefficients, and other noncalculus problems. For example, Richardson (1927) showed the power of the method in an elegant example of extrapolating two very crude approximations to a circle, namely an inscribed square and an inscribed hexagon, to get an estimate of π with three-figure accuracy.

The usual assumptions of smoothness apply, as well as the assumption (often verified) that the local error order is indicative of the global error order. The extrapolation must be used with considerable caution, since it involves the additional assumption of monotone truncation error convergence in the mesh spacing h. This assumption may not be valid for coarse grids. Also, the extrapolation magnifies machine round-off errors and incomplete iteration errors (Roache, 1972). In spite of these caveats, the method is extremely convenient to use compared to forming and solving direct fourth-order discretizations, which involve more complicated stencils, wider bandwidth matrices, special considerations for near-boundary points and non-Dirichlet boundary conditions, additional stability analyses, etc., especially in nonorthogonal coordinates which generate cross-derivative terms and generally complicated equations. Such an application was given by the present author in Roache (1982).

The method is in fact oblivious to the equations being discretized and to the dimensionality of the problem, and can easily be applied as a postprocessor (Roache, 1982) to solutions on two grids with no reference to the codes, algorithms or governing equations which produced the solutions, as long as the original solutions are indeed second-order accurate.[1] The difference between the second-order solution and the extrapolated fourth-order solution is itself a useful diagnostic tool, obviously being an error estimator (although it does not provide a true *bound* on the error except possibly for certain trivial problems). It was used very carefully, with an experimental determination rather than an assumption of the *local* order of convergence, by de Vahl Davis (1983) in his classic benchmark study of a model free convection problem. See Nguyen and Maclaine-Cross (1988) for application to heat exchanger pressure drop coefficients. Zingg (1993) applied the Richardson error estimator to airfoil lift and drag calculations in body-fitted grids. (Zingg's work demonstrates the necessity of grid convergence testing even when experimental data are available. In 4 of 7 cases, experimental agreement was better with *coarse* grid calculations than with fine. Also, his data indicate that Richardson Extrapolation can be applied to the estimation of far-field boundary errors, with the error being first order in the inverse of distance to the boundary.) Blottner (1990) has used the same procedure to estimate effects of artificial dissipation terms in hypersonic flow calculations.

An important aspect of Richardson Extrapolation is that it applies not only to point-by-point solution values, but also to solution functionals, e.g., lift coefficient C_L for an aerodynamics problem or integrated discharge for a groundwater flow problem, provided that consistent or higher-order methods are used in the evaluations (e.g., second or higher-order quadratures for lift) as well as the basic assumption that the "order" of the method applies globally as well as locally. If Richardson Extrapolation is applied to produce (say) fourth-order accurate grid values, one could in principle calculate a fourth-order accurate functional like C_L from the grid values, but it would require careful implementation of fourth-order accurate quadratures. It is much simpler to apply the extrapolation directly to the C_L's obtained in each grid, requiring only second-order

[1] I use the common but somewhat abusive terminology of "second-order accurate solution" to mean a solution obtained by a verified second-order accurate method applied in the asymptotic range of grid spacing.

quadratures. Indeed, this is a major attraction of Richardson Extrapolation compared to using fourth-order accurate stencils solved either directly or by deferred corrections. (Note, however, that the two approaches yield different answers, although both are fourth-order accurate if done properly.)

A very significant yet overlooked *disadvantage* of Richardson Extrapolation is that the extrapolated solution generally is not "conservative" in the sense of maintaining conservation properties (e.g., Roache, 1972). This could well dictate that Richardson Extrapolation not be used. For example, if it were used on the ground-water flow simulations for the Waste Isolation Pilot Plant (WIPP PA Dept., 1992), it would be "more accurate" in some norm, but would introduce additional nonconservative (i.e., lack of conservation property) source terms into the radionuclide transport equation. It is also noteworthy that Richardson (1927) pointed out that the accuracy of the extrapolation does not apply to arbitrarily high derivatives of the solution. The extrapolation can introduce noise to the solution which, although low level, may decrease the accuracy of the solution higher derivatives.

Thus, it is not advocated here that Richardson Extrapolation necessarily be used to improve the reported solution, since that decision involves these considerations and possibly others. What is advocated is that, regardless of whether Richardson Extrapolation is used to improve the solution, the proposed Grid Convergence Index (defined herein and based on the generalized theory of Richardson Extrapolation) be used to uniformly *report* grid convergence tests.

A Generalization of Richardson Extrapolation

Without assuming the absence of odd powers in the expansion of Eq. (1), we can generalize Richardson Extrapolation to pth order methods and r-value of grid ratio, again eliminating the leading term in the error expansion, as follows.

$$f[\text{exact}] = f_1 + (f_1 - f_2)/(r^p - 1). \tag{5}$$

If the next term in the series is zero, e.g., if centered differences were used, then the extrapolation is $(p + 2)$ order accurate. But generally, and notably if upstream-weighted methods for advection have been used, the extrapolation is $(p + 1)$ order accurate.

It may easily be verified that Eq. (5) is valid for multidimensions in any coordinates, including space and time, provided that the same grid refinement ratio r is applied, and the order p is uniform, in all space and time directions.

In Eq. (5), the correction to the fine grid solution f_1 is obviously an error estimator of the fine grid solution. Expressing this as an Estimated fractional error E_1 for the fine grid solution f_1, we have

$$E_1[\text{fine grid}] = \epsilon/(r^p - 1) \tag{6}$$

$$\epsilon = (f_2 - f_1)/f_1. \tag{7}$$

Defining the Actual fractional error A_1 of the fine-grid solution as usual,

$$A_1 = (f_1 - f[\text{exact}])/f[\text{exact}] \tag{8}$$

and using Eqs. (5)–(8) and the binomial expansion gives

$$A_1 = E_1 + 0(h^{p+l}, E_1^2) \tag{9}$$

where $l = 1$ generally or $l = 2$ if centered differences have been used. Thus, E_1 is an *ordered error estimator*, i.e., an ordered approximation to the actual fractional error of the fine grid solution. E_1 is a good approximation when the solution is of reasonable accuracy, i.e., when $E_1 \ll 1$.

This is generally *not* true of ϵ in Eq. (7), which is the quantity commonly reported in grid refinement studies. That is, ϵ is not always an error estimator since it does not take into account r or p. For $r < 2$ and $p = 1$, ϵ alone is optimistic, underestimating the grid convergence error compared to E_1 (by a factor of 2 for $r = 1.5$). For $r = 2$ and $p = 2$, ϵ alone is conservative, over-estimating the grid convergence error compared to E_1 (by a factor of 3). Note that ϵ can be made (almost) arbitrarily small, just by choosing $r \approx 1$. (The only qualification is that r is limited by the integer character of the number of grid points, so the smallest $r = N/(N - 1)$ where N is the number of grid points in each direction of the fine grid.) This is analogous to the situation wherein an arbitrarily small tolerance on *iterative* convergence can always be met by using an arbitrarily small relaxation factor, belying the adequacy of such an iterative convergence criterion (Roache, 1972; Ferziger, 1993).

E_1 may of course be expressed as a percent, and like any *relative* error indicator it will become meaningless when f_1 or f[exact] is zero or small relative to $(f_2 - f_1)$, in which case the denominator of Eq. (7) should be replaced with some suitable normalizing value for the problem at hand, as would the usual definition of actual relative error A_1 in Eq. (8).

As described earlier, one may choose to not use Richardson Extrapolation for good reasons, e.g., due to concern over the actual order of the method, or accumulation of round-off error, or incomplete iterative convergence error, or uncertainty that the asymptotic range has been reached, or lack of the conservation property in the extrapolated results, etc. But whether or not one chooses to use or report the results of the extrapolation, one can still use the theoretical basis to *consistently* report the results of the grid refinement study.

Grid Convergence Index for the Fine Grid Solution

Although the error estimator E_1 of Eq. (6) is based on a rational and consistent theory, it is certainly not a *bound* on the error. (Nor is a reliable and practically tight bound on solution error for nonlinear problems likely to be forthcoming, in the author's opinion.) What is generally sought in engineering calculations is not a true "error bound" but just an "error band," i.e., a tolerance on the accuracy of the solution which may in fact be exceeded, but in which the reader/user can have some practical level of confidence. The error estimator E_1 itself does not provide a very good confidence interval. (One might expect that it is equally probable that E_1 be optimistic as conservative, i.e., it is just as likely that the actual error A_1 be greater than E_1 as less than E_1. This would correspond roughly to a 50 percent confidence band.) A well-founded probability statement on the error estimate, such as a statistician would prefer (e.g., a two-sigma limit) is not likely forthcoming for practical CFD problems. However, based on cumulative experience in the CFD community, at least a marginal confidence level exists for the ϵ of Eq. (7) obtained using a grid doubling and a verified second-order accuracy code.

That is, for a grid doubling with a second-order method, and some indication that the calculations are within the asymptotic range of convergence, most CFD practitioners would accept the ϵ of Eq. (7) as a reasonable error band, in the flavor of a statistician's 2-σ range or an experimentalist's 20:1 odds (Kline and McClinstock, 1953). An ϵ of (say) 6 percent would be taken to indicate (not absolutely, but with reasonable confidence) that the fine grid solution was within 6 percent of the asymptotic answer. This confidence is well justified by the theory of Richardson Extrapolation, which shows, from Eqs. (6) and (7) with $r = 2$ and $p = 2$, that the error estimate E_1 is only 1/3 of this error band, or 2 percent.

The idea behind the proposed Grid Convergence Index is to approximately relate the ϵ of Eq. (7) obtained by whatever grid refinement study is performed (whatever p and r) to the ϵ that would be expected from a grid refinement study of the same problem with the same fine grid using $p = 2$ and $r = 2$, i.e., a grid doubling with a second-order method. The relation is based on equality of the error estimates. Given an ϵ from an actual grid convergence test, the GCI is derived by calculating

the error estimate E_1 from Eqs. (6) and (7), then calculating an *equivalent* ϵ that would produce approximately the same E_1 with $p = 2$ and $r = 2$. The absolute value of that *equivalent* ϵ is the proposed Grid Convergence Index for the fine grid solution, which is conveniently expressed as

$$\text{GCI[fine grid]} = 3|\epsilon|/(r^p - 1) \tag{10}$$

where ϵ is defined in Eq. (7).

We note immediately that for a grid doubling ($r = 2$) with a second-order method ($p = 2$), we obtain GCI $= |\epsilon|$, as intended.

The purpose of the proposed GCI is not to preclude more convincing grid convergence tests (such as using Richardson Extrapolation over several grid refinements, e.g., Shirazi and Truman, 1989; Blottner, 1990). The modest purpose herein is just to get minimal two-calculation grid refinement exercises onto a uniform reporting basis.

The GCI, like the theory of Richardson Extrapolation on which it is based, is equally applicable not only to grid values, but also to solution functionals (e.g., C_L) and to plotted curves, wherein ϵ may be read visually or calculated from interpolated tabular values. Thus it may be used to produce plots of the estimated error band about a fine grid solution by post-processing the results of any two grid solutions. Nonphysical oscillations in the solutions ("wiggles", e.g., see Roache, 1972) are of course a cue that the solutions are not in the asymptotic range, Richardson Extrapolation is not accurate, E_1 of Eq. (6) is not a valid error estimator, and confidence in the GCI as an error band is not justifiable.

Applying Eq. (10) to the hypothetical cases in the second paragraph of the introduction, we see that a 4 percent difference from a grid refined by 50 percent using a first-order method gives a fine-grid GCI = 24 percent, whereas a 6 percent difference from a doubled grid using a second-order method gives a fine-grid GCI = 6 percent. Even though the first paper's reported raw deviation ϵ from coarse to fine grid calculations might appear at first glance to be better than that reported in the second paper (4 percent compared to 6 percent), it is in fact not nearly as well converged (24 percent compared to 6 percent), as indicated by the proposed Grid Convergence Index.

For a less hypothetical example, consider the grid convergence results reported by the present author (Roache, 1982) for benchmark calculations of weakly separated flows obtaining using Richardson Extrapolation applied with grid doubling. The reported quantification of convergence was the maximum fractional deviation ϵ_4 between the fine-grid second-order and the extrapolated fourth-order solution f_4 from Eq. (4),

$$\epsilon_4 = (f_1 - f_4)/f_4 \tag{11}$$

The values reported were $\epsilon_4 = 0.17$ percent for wall vorticity and 0.13 percent for a velocity profile at a longitudinal station traversing the separation bubble. This ϵ_4 is easily related to the ϵ of Eq. (7); combining Eqs. (4), (7), and (11) shows

$$\epsilon = 3 - 3/(1 + \epsilon_4) = 3\epsilon_4 + 0(\epsilon_4^2). \tag{12a}$$

$$\text{GCI[fine grid]} \simeq 9\epsilon_4 \tag{12b}$$

The reported grid convergence criteria (Roache, 1982) of 0.17 percent for wall vorticity and 0.13 percent for velocity would now be replaced by the much more conservative GCI[fine grid] = 1.53 and 1.17 percent.

In such cases wherein Richardson Extrapolation is actually used to produce a higher order accurate solution, rather than just to estimate the error of the fine grid solution, the GCI of Eq. (10) (or (12*b*)) appears to be unfairly conservative. The solution used is the (say) fourth-order accurate solution, but the reported GCI would be the same even if only the second-order accurate fine grid solution were used. That is, E_1 and GCI are respectively the error estimator and Grid Convergence Index for the fine grid second-order solution, not for the fourth-order solution. Although we expect the extrapolated solution to be more accurate than the fine grid solution, we would need additional information (a solution on a third grid) to estimate the error of the extrapolated solution itself. Such a third grid solution could be used in principle (possibly not in practice, for nonlinear fluids engineering problems) to extrapolate a sixth order accurate solution. That is, the error estimate (and therefore the GCI) will always lag the best solution estimate. This is quite conservative when the conditions for validity of Richardson Extrapolation have been convincingly demonstrated by numerical experiments (e.g., Roache, 1982; Shirazi and Truman, 1989; Blottner, 1990; Roache and Knupp, 1993). A heuristic extension for such situations is to report the GCI for the extrapolated solution based on Eq. (10) with ϵ replaced by ϵ_4 from Eq. (11), giving GCI[ext. sol.] $\simeq |E_1$ [fine grid]$| = |\epsilon|/(r^p - 1)$.

On the other extreme, it is recognized that ostensibly second-order algorithms may fail to attain second-order performance in a particular calculation, due to coding quirks or errors, subtleties in nonlinear problems, overly strong grid stretching, failure to attain the asymptotic range, etc. (see, e.g., de Vahl Davis, 1983; Steinberg and Roache, 1985; Shirazi and Truman, 1989; Roache et al., 1990.) Unless the author has convincingly verified that the code actually attains the theoretical order, at least on a "nearby" problem, the more conservative value of $p = 1$ should be used in reporting the GCI in Eq. (10).

Two calculations of the same problem with the same value of GCI, say a first-order calculation on a finer grid and a second-order calculation on a coarser grid, are not quite indifferent as to the uncertainty of the calculations. The GCI of the first-order calculations is based on an only second-order accurate error estimator, whereas the GCI of the second-order calculations is based on a third or fourth-order accurate error estimator. Thus, even with the same GCI, the second-order calculations have less uncertainty (in their uncertainty estimates) than the first-order calculations.

Grid Convergence Index for the Coarse Grid Solution

Ostensibly, if we have a fine grid and a coarse grid solution, we would be expected to use the fine grid solution, so reporting of the above fine-grid GCI of Eq. (10) would apply. However, a practical scenario occurs for which the contrary situation applies, i.e., we use the coarse grid solution.

Consider a parametric study in which hundreds of variations are to be run. (For example, consider a 3-D time-dependent study of dynamic stall, with perhaps 3 Mach numbers, 6 Reynolds numbers, 6 airfoil thickness ratios, 3 rotor tip designs, and 2 turbulence models: a total of 648 combinations.) A scrupulous approach would require a grid refinement study for each case, but most engineers would be satisfied with one or a few good grid refinement tests, expecting, e.g., that a grid adequate for a NACA 0012 airfoil could be assumed to be adequate for a NACA 0015 airfoil. (In fact, this is often not justified by experience, e.g., stall characteristics can be quite sensitive to thickness ratio.) So for the bulk of the stack of calculations, we would be using the coarse grid solution, and we want a Grid Convergence Index for it. That is, we derive a Grid Convergence Index from Eq. (5), not as the correction to the fine grid solution f_1, but as the correction to the coarse grid solution f_2. In this case, the error estimate changes and must be less optimistic.

$$f[\text{exact}] \simeq f_2 + (f_1 - f_2)r^p/r^p - 1). \tag{13}$$

The coarse-grid GCI is then

$$\text{GCI[coarse grid]} = 3|\epsilon|r^p/(r^p - 1). \tag{14}$$

$$\text{GCI[coarse grid]} = r^p \cdot \text{GCI[fine grid]}. \tag{15a}$$

$$\text{GCI[coarse grid]} = \text{GCI[fine grid]} + 3|\epsilon|. \tag{15b}$$

Table 1 Grid convergence index (GCI) calculated from Eqs. (10) and (14) for common values of grid ratios (r) and orders of the basic numerical method (p), for both coarse grid solutions and fine grid solutions, normalized to $\epsilon = 1$ percent

	Fine grid GCI				Coarse grid GCI		
	$r = 2$	1.5	1.1		$r = 2$	1.5	1.1
p				p			
1	3.00%	6.00%	30.00%	1	6.00%	9.00%	33.00%
2	1.00%	2.40%	14.29%	2	4.00%	5.40%	17.29%
3	0.43%	1.26%	9.06%	3	3.43%	4.26%	12.06%
4	0.20%	0.74%	6.46%	4	3.20%	3.74%	9.46%

Applying this equation to the hypothetical cases in the second paragraph, we see that a 4 percent difference from a grid refined by 50 percent using a first-order method gives a coarse-grid GCI = 36 percent, whereas a 6 percent difference from a doubled grid using a second-order method gives a coarse-grid GCI = 24 percent. Note that the higher-order method appears to be working against us here, because we are coarsening, rather than refining, the grid. In actuality, the ϵ for the higher order method will be smaller for the same grid refinement close to convergence.

GCI values for some common combinations of r and p, normalized to $\epsilon = 1$ percent, are given in Table 1.

Should the Coefficient be "1" or "3"?

The functional form of the definition of the GCI (Eqs. (10), (14), (15)) is rational and objective, but the coefficient "3" is a judgment call. It could arguably be "1", or conceivably "1.5" or "2" or something else between 1 and 3.

The value "3" is possibly too conservative. As the quality and rigor of the grid convergence study increases, so does the conservatism of using the coefficient "3" in the definition of the GCI. However, consider practical complications such as rapidly varying coefficients from turbulent eddy viscosities or strong grid stretching, nonlinear systems, nonuniform behavior of various error norms, experimental determination of spatially varying p (e.g., see de Vahl Davis, 1983), nonmonotonic convergence (e.g., see Celik and Zhang, 1993). Such complications, while not contradicting the ultimate applicability of Richardson Extrapolation (i.e., in the asymptotic range) do increase the uncertainty associated with the error estimate for practical engineering fluid dynamics calculations. Likewise, if the grid convergence exercise is only performed for a representative "nearby" problem, uncertainty is increased. These considerations provide additional rationale for retaining "3" as the coefficient, in the sense of a "factor of safety".

As noted above, using the value "3" makes grid doubling with second-order methods into the standard of comparison. This is not intended to make second-order methods the goal, only the standard. (Like an IQ of 100, it is not meant to discourage genius.) It just means that for $p = 2$ and $r = 2$, we obtain GCI [fine grid] = ϵ. That is, it does not change what authors who use grid doubling with a second-order method already have been reporting, namely ϵ.

Using the value "1" would make the GCI equal the error estimator obtained from Richardson Extrapolation. As noted earlier, since this is the best estimate we can make given only the information from calculations on two grids, we can only expect equal probability that the true answer is inside or outside of this band. Also, simple tests on the steady-state Burgers equation will quickly demonstrate that "1" is *not* usually conservative. Is <50 percent probability acceptable for an error band? I think not. Perhaps most damning, the use of "1" makes grid doubling with first order methods into the standard of comparison, i.e., for $p = 1$ and $r = 2$, the GCI [fine grid] calculated using "1" would = ϵ. Clearly, we do not want first order methods to be the standard of comparison! (See, e.g., Freitas, 1994.)

A 50 percent "factor of safety" over the Richardson error estimator would be achieved with the value "1.5", or the naieve value of "2" might prove to be a neat and reasonable compromise. But much experimentation would be required over an ensemble of problems to determine a near-optimum value and to establish the correspondence with statistical measures such as the 2-σ band. Note that a true optimum would likely depend upon the family of numerical methods (e.g., medium-order FVM, high-order FDM or FEM, etc.) and upon the family of problems (e.g., turbulence, transonic, free surface, etc.)

All things considered, and after discussions solicited from many (on the order of 200) CFD practitioners, I recommend use of the value "3" in the definition of the GCI, even though it will be too conservative for high quality grid convergence studies. Of course, there is nothing to preclude an author from reporting *both* the GCI and the Richardson Error estimator E_1.

Noninteger Grid Refinement

Although it is generally assumed that grid doubling is preferable, it is argued here that, especially for the computer limitations frequently encountered in practice for multidimensional problems, it may be better to use a smaller change in grid resolution, say 10 percent. Consider a base grid, and refine or coarsen. If engineering intuition or studies on related ("nearby") problems have led to a good (economical, yet adequately accurate) grid selection for the base grid, then we are likely in the asymptotic range, but perhaps just barely. If we can afford to double the grid, we will certainly get more accurate answers, but the cost can be large. With an optimal numerical solution method, e.g., a good multigrid method, in which the computing cost is merely proportional to the number of unknowns, doubling a grid in three space dimensions and time will increase the cost over the base grid calculation by a factor of 16; if suboptimal methods are used, the penalty is worse. If we coarsen the grid instead, the economics work for us, i.e., the coarse grid solution is only 1/16 as expensive as the base grid; however, the coarse grid solution may be out of the asymptotic range. This situation is especially evident in turbulent boundary layer calculations, wherein we need $y^+ < 1$ for the first grid point off the wall. See, e.g., Shirazi and Truman (1989) or Wilcox (1993). This applies only when the turbulence equations are integrated to the wall. Different requirements apply if wall functions are used; e.g., see Celik and Zhang (1993) or Wilcox (1993).

Since the theory of generalized Richardson Extrapolation is valid for noninteger r, it is easier to use a small value (unless the computor is confident that the coarse grid with $r = 2$ will still be in the asymptotic range). However, there are practical limits to small r. For example, increasing the number of grid points by one in a base grid calculation of a 100 × 100 grid gives $r = 1.01$, and the theory is still valid. (Indeed, it would still be better than no grid refinement study at all.) But the results will now be obscured by other error sources, e.g., the "noise" of incomplete iterative convergence and machine round-off error. That is, as we reduce the change in the discretization error by using $r \to 1$, the leading truncation error term may be swamped by noise. As an intuitive engineering guess, a minimum 10 percent change ($r = 1.1$) is recommended. Of course, provided that the coarse grid is within the asymptotic range, the estimates are more reliable for larger r, for grid *refinement*.

A reviewer has expressed skepticism that one really can learn anything about grid convergence by changing the resolution by only 10 percent. It is intuitively obvious that the error estimates are more reliable for larger r, *for grid refinement*. It is perhaps less obvious that the opposite is true for grid coarsening, i.e., when we keep the answers of the finer grid.

Then it should be clear that there is *more* additional information, and therefore sharper error estimates, available for $r \sim 1$ than for $r \gg 1$ (limited only by noise pollution from round-off and incomplete iteration errors). For example, consider a fine grid using 100 nodes. A coarse grid calculation using 90 nodes ($r = 1.1111 \ldots$) contains more information (and is more expensive) than a coarse grid calculation using 50 nodes ($r = 2$). A set of easily reproduced calculations was performed on the steady-state Burgers equation with $u(0) = 1$ and $u(1) = 0$ (suggestive of stagnation flow), Re = 10, and $p = 2$, with a fine grid of 100 interior nodes and coarse grids from 25 to 99 nodes. The error estimator for $f = du/dx$ at $x = 1$ obtained using the coarse grid of 90 nodes ($r = 1.1111$, or a factor of 0.9 coarsening) is 3.2 times *more* accurate than the error estimator obtained using the coarse grid of 50 nodes ($r = 2$, or a factor of 0.5 coarsening).

Independent Coordinate Refinement and Mixed Order Methods

The simplest mode in which to apply the proposed Grid Convergence Index is to use a single parameter r to refine/coarsen the grid in all coordinates, space and time. However, there are often good reasons for not doing this. In boundary layer calculations (whether using boundary layer equations, full Navier-Stokes equations, or something intermediate) it is often the case that grid convergence is easy to establish in the longitudinal direction (being essentially dictated by the free-stream flow, which is not sensitive to Reynolds number) but is more problematical in the transverse direction, being sensitive to Re. Also, in time-dependent problems, it is much easier to develop a code that is solution-adaptive in the time-step than in the spatial grid, so that time discretization errors might be independently controlled (e.g., see Roache, 1991, 1992A, 1993) and the systematic grid refinement test would be restricted to the spatial grid.

In such a case, the multidimensional theory indicates that the error estimates can be obtained orthogonally. (The functions g_1, g_2, etc. in Eq. (1) for the x direction now depend on Δy, and a constant (in x) term appears, but it may be verified that these do not affect the algebra of solving for g_1, even with cross derivatives present from nonorthogonal grids, at least for $p = 1$ or 2.) In each coordinate direction, Eq. 10 or 14 is applied separately, with $r_t \neq r_x \neq r_y$, etc., and the resulting Grid Convergence Indexes are added.

$$\text{GCI} = \text{GCI}_t + \text{GCI}_x + \text{GCI}_y + \text{GCI}_z, \text{ etc.} \qquad (16)$$

The additional error made by this "alternating direction Richardson extrapolation," compared to refinement in all directions at once, is not merely heuristic but is ordered (it improves for fine grids and for $r \sim 1$) and small enough for the procedure to be practical. It is important to note that the procedure must be performed globally, i.e., with complete global solutions obtained for each refinement in independent coordinate directions; attempts to apply the extrapolation procedure by lines do not produce ordered or usable error estimates.

Consistent Richardson Extrapolation error estimators cannot be obtained from just two calculations (a coarse and a fine grid calculation) when different r are used in different coordinate directions, because there is no basis for separating out the directional contributions. In this case, a conservative GCI should be used, based on the smallest directional r. For example, in a 2-D steady flow calculated in a fine grid of 100 $\times$ 100 cells and a coarse grid of 50 $\times$ 75 cells, unless other theoretical considerations apply, we would have to conservatively attribute the change in solution to the more modest grid refinement, and use $r = 4/3$ to calculate the fine-grid GCI from Eq. (10).

A similar situation occurs with mixed-order methods, e.g., the not uncommon situation of a method with first-order time accuracy, and second-order space accuracy. A conservative approach would be to use $p = 1$ in Eq. (10), but a better estimate would be obtained using separate grid convergence studies in space and time, using $p = 1$ for the time contribution and $p = 2$ for the space contribution from Eq. (10), and simply adding the results as in Eq. (16). For hybrid methods that shift locally to two-point upstream differencing for large cell Re, the conservative $p = 1$ must be used. For methods which use higher order stencils for advection than for diffusion, the error will be dominated asymptotically by the lower order term. For example, for solutions calculated by Leonard's ULTIMATE method (Leonard, 1991) which is third order for advection, the GCI would have to be reported conservatively using $p = 2$ in Eq. (10) or (14).

Non-Cartesian Grids, Boundary Fitted Grids, Unstructured Grids, Adaptive Grids

The procedures for calculating GCI definitely apply to non-cartesian grids, with special considerations and caveats.

The Taylor series basis of Richardson Extrapolation applies to stretched orthogonal and nonorthogonal grids as long as the stretching is analytical. It is cleanest to apply in the transformed plane (ξ, η, ζ) where r is defined as above. The order of the extrapolation accuracy will now be affected by the order and iterative convergence of the grid generation equations. Shirazi and Truman (1989) found a surprising sensitivity of the error estimates to discretization of metrics and Jacobians, and to incomplete iterative convergence. For another example, if strong exponential source terms are used (e.g., near trailing edges of airfoils) which depend strongly on h (e.g., see Thompson et al., 1985) then a refined-grid generation will pollute the Richardson Extrapolation.

However, even if the grid generation equations are not converged, making the actual Richardson Extrapolation less dependable, it is still recommended that the proposed uniform GCI be reported rather than the simple raw data of ϵ.

Solution-adaptive grid generation codes may have their own internal *local* error estimators. More often, solution adaptive grid generation of the redistribution or enrichment types (Thompson et al., 1985; Knupp and Steinberg, 1993) is not based on any error estimator but on solution behavior (gradient, curvature, or simply resolution requirement) which is only loosely related to *local* error (which in turn is very loosely related to the *global* error of interest herein). In such a case, the GCI reporting procedure recommended herein can be applicable if the solution-adaptive procedure is used only to obtain the base grid solution. This grid can then be changed nonadaptively, perhaps refined by a higher-order interpolation or coarsened by simply removing every other point as in Zingg (1993) and the GCI of Eqs. (10) or (14) applied to this new grid. However, practical coding difficulties exist for time-dependent solution-adaptive grids, and it is not clear how to perform meaningful *global* error estimation nor uniform grid convergence reporting in this important situation. (See also remarks on unstructured grids below.)

Another difficulty occurs for unstructured grids. If the base grid is unstructured, the GCI procedure would still apply if one used a systematic method of grid refinement or coarsening, e.g., refining each base grid triangle into four new triangles gives $r = 2$ for use in Eq. (10). However, if the coarsening/refinement is also unstructured, as occurs in some algorithms and in user-interactive grid generation codes, there is no systematic and quantifiable grid refinement index like r to use in Eq. (10). Such grid refinement FEM studies are customarily reported simply in terms of the total number of elements used in the coarse (N_2) and fine (N_1) grids. Use in Eq. (10) of an

$$\text{effective } r = (N1/N2)^{1/D}, \qquad (17)$$

where D is the dimensionality of the problem, and reporting the GCI is clearly preferable to simply reporting ϵ. But it does not have the firm basis of a structured grid refinement, and may significantly underestimate or overestimate the accuracy, depending on whether the grid refinement algorithm (or the intuition of the interactive user) refined the grid in the critical areas or not.

For unstructured grid refinement and (structured or unstructured) grid adaption, I suppose it should be the burden of the algorithm developer to convince the reader/user that the local grid adaptivity process (sometimes based on a *local* error estimator) can be usefully correlated with a meaningful engineering *global* error estimate, which is the real interest. This is very difficult to accomplish convincingly for any problem which a fluid dynamicist would consider non-trivial (mainly because local truncation errors are advected downstream) but it can be done; see Schonauer et al., 1981).

Shocks, Discontinuities, Singularities

In both his 1910 and 1927 papers, Richardson already considered the effect of singularities on the extrapolation procedure. These cases must be considered individually. If the form of the singularity is known *a priori*, it may be removed analytically. If unknown, its presence may be detected by checking to see if the asymptotic range has been reached (see below). Shocks and other discontinuities (e.g., contact surfaces) invalidate the Taylor series basis of Richardson Extrapolation, but unless the flow contains large numbers of complex shock patterns, the GCI procedure herein would still seem to have validity and be recommended. As pointed out by Ferziger (1993), a more appropriate error measure here might be the shock position. (Further experience with complex shocked flows is needed.)

Note also that Blottner (1990) has shown how the concept of Richardson Extrapolation can be applied to systematically estimating the error due to artificial dissipation terms used in hypersonic shock calculations. The contribution of these terms to the proposed GCI must also be calculated orthogonally to the other terms. If these terms are not estimated separately, the grid convergence tests will be polluted, since the (nonlinear) shock dissipation terms depend on h, and therefore the continuum problem being approximated changes from grid to grid. See also Kuruvila and Anderson (1985). (This is the same difficulty that can appear with grid generation equations, noted above.)

Also, the theory of Richardson Extrapolation is not applicable to nonlinear flux limiters, but again we expect these to be local applications, and still recommend the reporting of GCI over simply reporting the raw data for ϵ, but also recommend more detailed investigation, e.g., perhaps 3 grids (see below). The point is that the presence of shocks, other discontinuities or singularities can complicate grid convergence studies whether or not the proposed GCI is used for reporting the results, so these complications do not constitute a criticism of the proposed GCI.

Achieving the Asymptotic Range

The theory of Richardson Extrapolation, and therefore of the proposed Grid Convergence Index, depends on the assumption that the Taylor series expansion (or at least, the definition of the order of the discretization implied by Eq. (4)) is valid asymptotically, and that the two grids are within the asymptotic range. For smooth elliptic problems, this is easy to achieve. (A second-order accurate discretization of a Laplace equation with smooth boundary values is well behaved over virtually all discretizations.) For Reynolds numbers $\gg 1$, it is more problematic, and more than two grid solutions are required. The methodology proposed herein does allow for detecting this situation in a straightforward manner, provided that the order of the method, p, is uniform.

If an exact solution is known to a model problem, we can monitor

$$E_p = \text{error}/h^p \tag{18}$$

as h is refined. Then the (approximate) constancy of E_p is a faithful verification of the order p and an indication that the asymptotic range is achieved (e.g., see Richardson, 1927; Steinberg and Roache, 1985; Roache et al., 1990; Blottner, 1990; Roache and Knupp, 1993). In the practical case wherein the exact solution is not known, we perform at least three grid solutions and calculate two GCI, from fine grid to intermediate (GCI_{12}) and from intermediate to coarse grid (GCI_{23}). Then the (approximate) constancy of $E_p \simeq GCI/(3h^p)$, or

$$GCI_{23} \simeq r^p\, GCI_{13} \tag{19}$$

indicates that the asymptotic range is achieved.

This indication that the asymptotic range has been achieved is usually faithful, in the author's experience (Roache, 1982; Roache et al., 1990; Roache and Knupp, 1993). But an exception (and unfortunately, an important one) occurs in problems with multiple scales of solution variation wherein a finer scale of the problem variation has been completely missed in the grid refinements. For example, in dual-continuum models of transport in porous media (WIPP PA Dept., 1992) the time scale for diffusion and storage in the material matrix blocks may be orders of magnitude less than the time scale for essentially advective transport in the fracture system. Time-step refinement may indicate no substantial change in the results (i.e., a false indication of convergence) if the time step is of the order of the advective time scale. Similar situations occur in turbulent boundary layer studies where some minimal viscous sublayer resolution is required (see Wilcox, 1993; Shirazi and Truman, 1989) and in chemically reacting flows which can have more time scales than species. Adaptive ODE solvers are good at detecting multiple time scales, but in multidimensional flows, at present there seems to be no substitute for an independent estimate (from theory or experiment) of the physical scales of interest.

Since so many authors are reluctant to perform even the most minimal grid convergence tests with two grids (Roache, et al., 1986; Roache, 1990), it may seem scrupulous to recommend *three* grids as a matter of course. In fact, it is required to be sure that the calculations are in the asymptotic range, if this is not already inferred from experience with a "nearby" calculation as in, e.g., Nguyen and Maclaine-Cross (1988) or Blottner (1990). But the presently proposed GCI is an easier improvement over the simplistic reporting of raw data on ϵ.

G. de Vahl Davis (1983), in his classic benchmark calculations of a buoyancy-driven cavity, indicated local convergence rates of *less* than first order for the relatively coarse grids used, even though the method was asymptotically second-order accurate. In the absence of such meticulous work as that of de Vahl Davis, the reporting of a GCI based on the assumed $p = 2$ would be preferable to simplistic reporting the raw data of ϵ, but if there is any indication of less-than-theoretical convergence rates, the more conservative estimate with GCI evaluated from Eq. (10) or (14) using $p = 1$ should be reported.

Method of Characteristics and Spectral Methods

It is not clear how or if the proposed GCI would be applicable to calculations obtained by the classic method of characteristics, as used in gas dynamics, because of the possibly discontinuous solutions and the irregular gridding. The various Modified Method of Characteristics (e.g., see references in Roache, 1992b) will produce more systematic grid refinement, but the concept of "order" is more tenuous for the Flux-Based

MMOC (as evidenced by the fact that the accuracy *improves* as the Courant number increases above 1), and the GCI may not be applicable. Similarly, for spectral and pseudo-spectral methods, and certainly for spectral elements, different extrapolation procedures would be required. It is not known at this time how well the GCI would apply or could be extended.

Nonsmooth Property Variation

In aerodynamics problems, one typically deals with smooth property variations over modest ranges, if not with constant property problems. In groundwater flow and transport calculations, uncertainty is much greater, and sensitivity studies are often performed with Monte Carlo techniques used to generate property variations of orders of magnitude, even from one grid block (finite volume) to the next (WIPP PA Dept., 1992). Geologic layering produces discontinuous variations in properties of several orders of magnitude.

In these situations, it is not advisable to use noninteger grid refinement parameters r, because additional errors would be introduced by interpolation of properties. This confusion would be aggravated by the common use of harmonic averaging for properties (e.g., Roache, 1991, 1992A, 1993). Likewise, grid coarsening is not advisable if a coarsened grid would not resolve the scale of the property variations (often the case for expensive two-phase flow calculations, e.g., WIPP PA Dept., 1992). The only approach applicable is a brute-force grid refinement by a factor of 2, which avoids any necessity for interpolation of properties.

The GCI proposed herein still has two contributions to such problems, (*a*) in including the effect of the order of the method p in Eq. (10), and (*b*) in economizing a consistent treatment of *further* grid refinement. That is, a third grid (second refinement) need not involve the expense of another grid doubling (to a quadrupling of the base grid resolution) but can be done on a tripled grid, and reported consistently with the proposed GCI. The difference in computer time between calculating the sequence (base h_0, $1/2h_0$, $1/4h_0$) and the sequence (base h_0, $1/2h_0$, $1/3h_0$) can be significant. Consider an *optimal* method with base-case computer time $= T_2$ in 2-D and T_3 in 3-D, and time-step resolution increased in proportion to the spatial grid resolution. The quadrupling sequence costs $73T_2$ in 2-D while the tripling sequence costs $36T_2$; in 3-D, the costs are $273T_3$ and $98T_3$, respectively. The savings of a factor of 2 in 2D and somewhat less than 3 in 3D will be greatly amplified if *suboptimal* direct solution methods are used (WIPP PA, 1992).

A more fundamental question arises when geostatistical methods are used to generate particular realizations of grid-block property variations with specified statistical parameters. Only the statistical results are of interest, not the solutions of the individual realizations. The question is then, should the grid refinement studies be performed separately from the geostatistical realizations? That is, should the solution of the partial differential equations be converged on finer grids with the assumed continuum property variation fixed at a geostatistically generated coarse-grid distribution, or should the geostatistical generation also change as the grid is refined? This is not a trivial question, and although definition of a fixed continuum problem for the grid refinement studies is conceptually easier, it is clear that substantial computer savings could accrue to the combined convergence approach. In either case, the grid increments should be less than (be able to partially resolve) the correlation length of the property variation.

Example

A reviewer has requested a simple example of the calculation of a Grid Convergence Index. I choose the easily reproduced case of a steady-state Burger's equation

$$-uu_x + u_{xx}/\mathrm{Re} = 0, \quad u(0) = 1, \quad u(1) = 0 \tag{20}$$

for Re = 1000 solved with second-order centered differences on a uniform grid, and evaluate the quantity $f = du/dx$ at $x = 1$. Using a fine grid calculation with 2000 cells, we obtain $f_1 = -529.41$. Then we coarsen the grid to 1600 cells ($r = 1.25$) and obtain $f_2 = -544.48$. The quantity typically reported (from Eq. (7)) would be $|\epsilon| = 100$ percent $\cdot (f_2 - f_1)/f_1 = 2.85$ percent. The factor $(r^p - 1)$ is $(1.25^2 - 1) = 0.5625$. The magnitude of the Richardson Extrapolation error estimator for the fine grid solution from Eq. (6) is $|E_1| = |\epsilon|/(r^p - 1) = 2.85$ percent/0.5625 = 5.07 percent. The fine grid value of the Grid Convergence Index from Eq. (10) is GCI[fine grid] $= 3|\epsilon|/(r^p - 1) = 3 \cdot 2.85$ percent/0.5625 = 15.20 percent. Comparison with the exact solution $f_{\text{exact}} = -500.00$ indicates that the exact magnitude of the fine-grid error A_1 is 100 percent $\cdot |(f_2 - f_{\text{exact}})/f_{\text{exact}}| = 100$ percent $\cdot |-529.41 + 500.00|/500.00 = 5.88$ percent. As is typical, the Richardson Extrapolation error estimator E_1 is not conservative (5.07 < 5.88 percent), whereas the GCI is conservative and quite so (15.20 > 5.88 percent), in the spirit of a 2σ error band.

If the coarse grid solution (or the coarse grid solution to a nearby problem) were to be used, the Richardson Extrapolation error estimator would be increased to $|E_1| + |\epsilon| = 5.07 + 2.85$ percent = 7.92 percent. The GCI would be increased by $3|\epsilon|$ as in Eq. (15*b*) to GCI[coarse grid] = 15.20 + 3 • 2.85 percent = 23.75 percent. The actual magnitude of the coarse grid error is 100 percent $\cdot |(f_2 - f_{\text{exact}})/f_{\text{exact}}| = 100$ percent $\cdot |-544.48 + 500.00|/500.00 = 8.90$ percent. Again, the Richardson Extrapolation error estimator E1 is not conservative for the coarse grid (7.92 < 8.90 percent), whereas the GCI is conservative (23.75 > 8.90 percent).

Conclusion

The quantification of uncertainty in CFD publications has been noticeably improving, with minimal grid refinement studies becoming more common. Unfortunately, it has not always been possible to uniformly interpret these studies.

In this paper, it has been proposed that the results of systematic grid refinement studies be uniformly reported using the Grid Convergence Index of Eq. (10) or (14), which is based upon a grid refinement error estimator derived from the theory of the generalized Richardson Extrapolation. While not answering all questions involved with verification of a calculation, this proposed method at least enforces some uniformity in the reporting and is based upon an objective asymptotic estimate of the grid convergence error, although the GCI is not a true error bound.

Since the GCI will often be less optimistic than the simplistic ϵ of Eq. (7), especially for the all-too-popular first-order methods, some reluctance of authors may be anticipated. Fortunately, the formulas are simple enough to be applied *a posteriori* by editors and reviewers. It is urged that they do so in the review process to continue improving the quality of CFD papers. To quote Ferziger (1993), "... *the frequently heard argument 'any solution is better than none' can be dangerous in the extreme. The greatest disaster one can encounter in computation is not instability or lack of convergence but results that are simultaneously good enough to be believable but bad enough to cause trouble.*"

Acknowledgments

This work was partially supported by Sandia National Laboratories and the United States Department of Energy under Contract DE-AC04-76DP00789, Dr. M. G. Marietta, Technical Monitor, and the United States Army Aviation Systems Command, Aeroflightdynamics Directorate under Contract NAS2-13618, Dr. W. J. McCroskey, Technical Monitor. The author appreciates the significant suggestions of Dr. F. G.

Blottner, Dr. M. Fewell, Dr. P. M. Gresho, Dr. P. M. Knupp, Dr. B. P. Leonard, Dr. S. L. Steinberg, Dr. C. R. Truman, Dr. D. C. Wilcox, and two anonymous reviewers, and the opening quotation from Dr. S. Piacsek.

References

AIAA, 1994, "Editorial Policy Statement on Numerical Accuracy and Experimental Uncertainty," *AIAA Journal*, Vol. 32, No. 1, Jan., p. 3.

Blottner, F. G., 1990, "Accurate Navier-Stokes Results for the Hypersonic Flow over a Spherical Nosetip," *Journal Spacecraft and Rockets*, Vol. 27, No. 2, pp. 113–122.

Celik, I., Chen, C. J., Roache, P. J., and Scheuerer, G., 1993, *Symposium on Quantification of Uncertainty in Computational Fluid Dynamics*, FED Vol. 158, ASME Fluids Engineering Division Summer Meeting, Washington, DC, June 20–24.

Celik, I., and Zhang, W-M., 1993, "Application of Richardson Extrapolation to Some Simple Turbulent Flow Calculations," *FED Vol. 158, Symp. on Quantification of Uncertainty in Computational Fluid Dynamics*, ASME Fluids Engineering Division Summer Meeting, Washington, DC, June 20–24, pp. 29–38.

Conte, S. D., and de Boor, C., 1965, *Elementary Numerical Analysis: An Algorithmic Approach*, McGraw-Hill, New York, p. 313.

de Vahl Davis, G., 1983, "Natural Convection of Air in a Square Cavity: A Bench Mark Numerical Solution," *Int. J. for Numerical Methods in Fluids*, Vol. 3, No. 3, pp. 249–264.

Ferziger, J. H., 1981, *Numerical Methods for Engineering Application*, Wiley, New York, NY.

Ferziger, J. H., 1993, "Estimation and Reduction of Numerical Error," *FED Vol. 158, Symp. on Quantification of Uncertainty in Computational Fluid Dynamics*, ASME Fluid Engineering Division, Summer Meeting, Washington, D.C., June 20–24, pp. 1–8.

Freitas, C. J., 1993, "Editorial," ASME JOURNAL OF FLUIDS ENGINEERING, Vol. 115, No. 3, Sept., pp. 339–340.

Kline, S. J., and McClinstock, F. A., 1953, "Describing Uncertainties in Simple-Sample Experiments," *Mechanical Engineering*, Jan., pp. 3–8.

Knupp, P. M., and Steinberg, S. L., 1993, *Fundamentals of Grid Generation*, CRC Press, Boca Raton, FL.

Kuruvila, G., and Anderson, J. D., 1985, "A Study of the Effects of Numerical Dissipation on the Calculation of Supersonic Separated Flows," AIAA Paper 85-0301, Jan.

Leonard, B. P., 1991, "The ULTIMATE Conservative Difference Scheme Applied to Unsteady One-Dimensional Advection," *Computational Methods in Applied Mechanics and Engineering*, Vol. 88, pp. 17–74.

Mehta, U. B., 1991, "Some Aspects of Uncertainty in Computational Fluid Dynamics Results," ASME JOURNAL OF FLUIDS ENGINEERING, Vol. 113, No. 4, Dec., pp. 538–543.

Nguyen, T. V., and Maclaine-Cross, I. L., 1988, "Incremental Pressure Drop Number in Parallel-Plate Heat Exchangers," ASME JOURNAL OF FLUIDS ENGINEERING, Vol. 110, pp. 93–96, March 1988.

Richardson, L. F., 1910, "The Approximate Arithmetical Solution by Finite Differences of Physical Problems Involving Differential Equations, with an Application to the Stresses in a Masonry Dam," *Transactions of the Royal Society of London*, Series A, Vol. 210, pp. 307–357.

Richardson, L. F., 1927, "The Deferred Approach to the Limit," *Transactions of the Royal Society of London*, Series A, Vol. 226, pp. 299–361. "Part I. Single Lattice," "Part II. Interpenetrating Lattices" by J. A. Gaunt.

Roache, P. J., 1972, *Computational Fluid Dynamics*, Hermosa Publishers, Albuquerque, NM. First Edition.

Roache, P. J., 1982, "Scaling of High-Reynolds-Number Weakly Separated Channel Flows," *Numerical and Physical Aspects of Aerodynamic Flows*, T. Cebeci, ed., Chapter 6, Springer Verlag, NY, pp. 87–98.

Roache, P. J., Ghia, K. N., and White, F. M., 1986, "Editorial Policy Statement on the Control of Numerical Accuracy," ASME JOURNAL OF FLUIDS ENGINEERING, Vol. 108, No. 1, p. 2.

Roache, P. J., 1990, "Need for Control of Numerical Accuracy," *Journal of Spacecraft and Rockets*, Vol. 27, No. 2, pp. 98–102, Mar.–Apr.

Roache, P. J., Knupp, P. M., Steinberg, S., and Blaine, R. L., 1990, "Experience with Benchmark Test Cases for Groundwater Flow," ASME FED Vol. 93, *Benchmark Test Cases for Computational Fluid Dynamics*, I. Celik and C. J. Freitas, eds., Book No. H00598, pp. 49–56, June.

Roache, P. J., 1991, "Computational Fluid Dynamics Algorithms and Codes Developed for WIPP Site Simulations," in *Computational Mechanics*, Cheung, Y. K., Lee, J. H. W., and Leung, A. Y. T., eds., *Proc. Asian Pacific Conf. on Computational Mechanics*, A. A. Balkema, Rotterdam, Vol. 2, pp. 1325–1335, Hong Kong, 11–13 Dec.

Roache, P. J., 1992, "Computational Fluid Dynamics Algorithms Developed for WIPP Site Simulations," in Russell, T. F., et al., eds., *Proc. IX International Conference on Computational Methods in Water Resources*, Denver, CO, June 9–12, Elsevier Applied Science, New York, pp. 375–382.

Roache, P. J., 1992, "A Flux-Based Modified Method of Characteristics," *International Journal for Numerical Methods in Fluids*, Vol. 15, pp. 1259–1275.

Roache, P. J., and Knupp, P. M., 1993, "Completed Richardson Extrapolation," *Communications in Numerical Methods in Engineering*, Vol. 9, pp. 365–374.

Roache, P. J., 1993, "The SECO Suite of Codes for Site Performance Assessment," *Proc. 1993 Int. High-Level Radioactive Waste Management Conf.*, Las Vegas, NV, Apr. 26–30.

Schonauer, W., Raith, K., and Glotz, G., 1981, "The Principle of the Difference of Difference Quotients as a Key to the Self-Adaptive Solution of Nonlinear Partial Differential Equations," *Computer Methods in Applied Mechanics and Engineering*, Vol. 28, No. 3, pp. 327–359.

Shirazi, S. A., and Truman, C. R., 1989, "Evaluation of Algebraic Turbulence Models for PNS Predictions of Supersonic Flow Past a Sphere-Cone," *AIAA Journal*, Vol. 27, No. 5, pp. 560–568.

Steinberg, S. L., and Roache, P. J., 1985, "Symbolic Manipulation and Computational Fluid Dynamics," *J. of Computational Physics*, Vol. 57, pp. 251–284.

Thompson, J. F., Warsi, Z. U. A., and Mastin, C. W., 1985, *Numerical Grid Generation Foundations and Applications*, North-Holland, NY.

Wilcox, D. C., 1993, *Turbulence Modeling for CFD*, DCW Industries, Inc., La Canada, CA.

WIPP PA Dept. (1992), *Annual Performance Assessment for the Waste Isolation Pilot Plant, Dec. 1992, Vol. 1 Preliminary Comparison with 40 CFR 191, Subpart B Vol. 2: Technical Basis*, Performance Assessment Department, Sandia National Laboratories, Albuquerque, NM.

Zingg, D. W., 1993, "Grid Studies for Thin-Layer Navier-Stokes Computations of Airfoil Flowfields," *AIAA Journal*, Vol. 30, No. 10, pp. 2561–2564.