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FURTHER DISCUSSION OF NUMERICAL ERRORS IN CFD

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SUMMARY

The methods of estimating numerical errors given in an earlier paper are extended in directions that make them useful in actual CFD applications. In particular, the method of estimating convergence error (the error due to insufficient iteration) is extended to allow the possibility of complex eigenvalues; an ad hoc method that can be applied to any case is also given. For the discretization error, which arises from the numerical approximation of the differential equation(s), methods that can be used on non-uniform drids are presented; they can be extended to unstructured grids as well. The utility of these methods is demonstrated for linear problems as well as solutions of the Navier-Stokes equations. The examples show that the estimation of errors is neither difficult nor expensive.

KEY WORDS: computational fluid dynamics; numerical methods; error

1. INTRODUCTION

In earlier papers,[1,2] one of the authors presented a discussion of sources of errors in computational fluid dynamics and methods for their estimation and control. To summarize, we note that errors arise from the discretization approximations applied to the partial differential equations (*discretization error*) and because the iterative solvers for the resulting equations are not always converged sufficiently (*convergence error*).

The papers referenced above have been criticized because the error estimation methods they suggested may not apply to all cases. Specifically, the estimation method for discretization error is designed for uniform grids (which are not often used in practice) and the convergence error estimator requires the eigenvalues associated with the iteration method to be real (which is often not the case). These deficiencies are sometimes cited to justify not using error estimation. In this paper we shall attempt to overcome some of these objections by generalizing the methods. It is hoped that this will make the use of these methods more commonplace.

2. CONVERGENCE ERROR

2.1. Real eigenvalues

In the iterative solution of a system of equations, convergence error is defined as the difference between the current iterate and the exact solution of the *discretized* equations. We begin by reviewing the method presented in the earlier papers. It should also be noted that this method is much older than

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the cited papers and can be found in the books by Wilkinson[3] and Golub and van Loan[4] as well as still earlier sources.

Any iteration scheme for a linear system can be written as

$$\boldsymbol{\phi}^{(n+1)} = \mathbf{A}\boldsymbol{\phi}^{(n)} + \mathbf{q}, \tag{1}$$

where $\boldsymbol{\phi}^{(n)}$ is the vector representing the solution after the nth iteration, $\mathbf{A}$ is a matrix which depends on the iteration scheme and the problem being solved but may not be known explicitly (it is not the coefficient matrix of the discretized partial differential equation), and $\mathbf{q}$ is a (perhaps modified) source term. The nth iterate is the sum of the converged or exact solution of the discretized equations, $\tilde{\boldsymbol{\phi}}$, and the convergence error $\boldsymbol{\epsilon}^{(n)}$:

$$\boldsymbol{\phi}^{(n)} = \tilde{\boldsymbol{\phi}} + \boldsymbol{\epsilon}^{(n)}. \tag{2}$$

$\boldsymbol{\epsilon}^{(n)}$ obeys the homogeneous form of (1). Convergence of this scheme can be analysed with the help of the eigenvalues λ_k and eigenvectors $\boldsymbol{\psi}_k$ of $\mathbf{A}$ defined by

$$\mathbf{A}\boldsymbol{\psi}_k = \lambda_k \boldsymbol{\psi}_k, \quad k = 1, 2, \ldots, N, \tag{3}$$

where N is the number of equations. The initial error $\boldsymbol{\epsilon}^{(0)}$ may be written as a linear combination of these eigenvectors,

$$\boldsymbol{\epsilon}^{(0)} = \sum_{k=1}^{N} a_k \boldsymbol{\psi}_k, \tag{4}$$

where a_k is a generalized Fourier coefficient. It is not difficult to show that after n iterations

$$\boldsymbol{\epsilon}^{(n)} = \sum_{k=1}^{N} a_k (\lambda_k)^n \boldsymbol{\psi}_k. \tag{5}$$

If the largest eigenvalue (λ_1) is real, then after many iterations the dominant error is the first term in this sum. In this limit, by combining equations (2) and (5), we see that

$$\boldsymbol{\phi}^{(n)} \approx \tilde{\boldsymbol{\phi}} + a_1 (\lambda_1)^n \boldsymbol{\psi}_1. \tag{6}$$

An expression for the convergence error can be derived by using the difference of two successive iterates. From the preceding equation we find

$$\boldsymbol{\chi}^{(n)} = \boldsymbol{\phi}^{(n+1)} - \boldsymbol{\phi}^{(n)} \simeq a_1 (\lambda_1 - 1)(\lambda_1)^n \boldsymbol{\psi}_1. \tag{7}$$

The dominant eigenvalue λ_1 may be estimated by taking the norms of $\boldsymbol{\chi}^{(n)}$ and $\boldsymbol{\chi}^{(n-1)}$ and taking the ratio

$$\lambda_1 \approx |\chi^{(n)}| / |\chi^{(n-1)}|, \tag{8}$$

where $|q|$ represents the L_2-norm of a vector $\mathbf{q}$ or, what is the same thing except for normalization, the root mean square of the components of $\mathbf{q}$.

Once an estimate of the eigenvalue is available, it is not difficult to estimate the convergence error. In fact, by rearranging equation (7), we find

$$\boldsymbol{\epsilon}^{(n)} = \boldsymbol{\phi}^{(n)} - \tilde{\boldsymbol{\phi}} \approx a_1 \lambda_1^n \boldsymbol{\psi}_1 \approx \boldsymbol{\chi}^{(n)} / (\lambda_1 - 1). \tag{9}$$

This error estimate can be computed from the iterates of the solution; the review of the method presented earlier is complete. We note that although the method is designed for linear systems, all systems are essentially linear near convergence; as this is the time when error estimates are most needed, the method can be applied to non-linear systems as well.

2.2. Complex eigenvalues

Unfortunately, iterative methods often must deal with matrices that have complex eigenvalues. When this is the case, the error reduction is not exponential and may not be monotonic. Since the equations are real, complex eigenvalues must occur as conjugate pairs. Their estimation requires an extension of the above procedure. In particular, data from more iterates are required. The basis of the method presented here is again not new and can be found in the works of Golub and van Loan[4] and Wilkinson.[3]

If the eigenvalues of largest magnitude are complex, there are at least two of them. We shall assume that there are exactly two largest eigenvalues which are complex conjugates of each other. Equation (6) must then be replaced by

$$\boldsymbol{\phi}^{(n)} \approx \tilde{\boldsymbol{\phi}} + a_1(\lambda_1)^n \boldsymbol{\psi}_1 + a_1^*(\lambda_1^*)^n \boldsymbol{\psi}_1^*, \tag{10}$$

where a superscript asterisk indicates the conjugate of a complex quantity. As before, we eliminate the contribution of the exact solution by subtracting two successive iterates to obtain $\boldsymbol{\chi}^{(n)}$. If we further let

$$\boldsymbol{\omega} = (\lambda_1 - 1)a_1 \boldsymbol{\psi}_1, \tag{11}$$

(cf. equation (7)), then

$$\boldsymbol{\chi}^{(n)} \approx (\lambda_1)^n \boldsymbol{\omega} + (\lambda_1^*)^n \boldsymbol{\omega}^*. \tag{12}$$

Since the magnitude of the eigenvalue λ_1 is the quantity of greatest interest, we write

$$\lambda_1 = l e^{i\vartheta}. \tag{13}$$

A straightforward calculation then shows that

$$z^{(n)} = \boldsymbol{\chi}^{(n-2)} \cdot \boldsymbol{\chi}^{(n)} - \boldsymbol{\chi}^{(n-1)} \cdot \boldsymbol{\chi}^{(n-1)} = 2l^{2n-2}|\omega|^2[\cos(2\vartheta) - 1], \tag{14}$$

from which it is easy to see that

$$l^2 = z^{(n)}/z^{(n-1)} \tag{15}$$

is an estimate of the square of the magnitude of the eigenvalue.

Estimation of the error requires further approximations. The complex eigenvalues cause the errors to oscillate and the shape of the error to be dependent on the iteration number, even for large n. To estimate the error, we compute the magnitudes of $\boldsymbol{\chi}^{(n)}$ and l from the expressions given above. Because the eigenvalues and eigenvectors are complex, the results contains terms proportional to the cosine of the phase angle. As we are interested only in magnitudes, we assume that these terms are zero in an average sense and drop them. This allows us to find a simple approximate relationship between the two quantities,

$$|\epsilon^{(n)}| \approx |\chi^{(n)}|/\sqrt{(l^2 + 1)}, \tag{16}$$

which is the desired estimate of the error. Owing to the oscillations in the solution, the estimate may not be accurate on any particular iteration, but, as we shall show below, it is quite good on average.

In order to remove some of the effects of the oscillation, we average the eigenvalue estimates over a number of iterations. Depending on the problem and the number of anticipated iterations, this number varied from one to 50 (about 1% of the total number of iterations) in our test calculations.

2.3. General case

Finally, we want a method that can treat both real and complex eigenvalues. The error estimator for the complex case (16) gives low estimates if the principal eigenvalue (λ_1) is real. Also, the contribution of λ_1 to $z^{(n)}$ drops out, so the eigenvalue estimate is quite poor. However, this fact can be used to determine whether λ_1 is real or complex. If the ratio

$$r = |z^{(n)}|/|\chi^{(n)}|^2 \tag{17}$$

is small, the eigenvalue is probably real; if r is large, the eigenvalue is probably complex. We computed this ratio for cases of both types and found that, with real eigenvalues, r tended to be smaller than 10^{-2} and, for complex eigenvalues, $r \approx 1$. We therefore adopted $r = 0{\cdot}1$ as an indicator of the type of eigenvalue and used the appropriate expression for the error estimator. As the results below show, this seems to produce good results.

3. DISCRETIZATION ERROR

3.1. Uniform grids

Discretization error is the difference between the converged solution to the discretized equations and the exact solution of the continuum problem. If the discretization can be characterized by a single parameter, h, the discretized equations may be written as

$$\mathscr{L}_h(\boldsymbol{\phi}_h) = 0, \tag{18}$$

where $\mathscr{L}_h$ represents the discretized operator, which need not be linear.

The discretization error $\boldsymbol{\epsilon}_h$ is the difference between the exact solution of the discretized equations and the solution of the differential equation(s):

$$\boldsymbol{\epsilon}_h = \boldsymbol{\Phi} - \boldsymbol{\phi}_h. \tag{19}$$

The Richardson method of estimating errors is based on computing the solution on at least two grids with different values of h and is accurate for small h. When the coarse grid spacing is twice the fine grid spacing in all directions, the discretization error estimate is

$$\boldsymbol{\epsilon}_h \approx \frac{\boldsymbol{\phi}_h - \boldsymbol{\phi}_{2h}}{2^p - 1}, \tag{20}$$

where p is the order of the method. If the order is not known or if mixed approximations are used for different terms in the equations, the value of the parameter p can be estimated from the solution on three grids:

$$p = -\frac{\log\left(\dfrac{\boldsymbol{\phi}_{2h} - \boldsymbol{\phi}_{4h}}{\boldsymbol{\phi}_h - \boldsymbol{\phi}_{2h}}\right)}{\log 2}. \tag{21}$$

The method can be extended to non-systematic grid refinement or coarsening; this was analyzed by Roache.[5]

3.2. Non-uniform grids

It is interesting to extend this method to non-uniform (stretched) grids. Many discretization approximations lose their leading-order truncation error term on uniform grids. It has been argued that these schemes become less accurate when the grid is non-uniform. This is true in the sense that for a small region (over which the solution is assumed to be smooth) a uniform grid produces a

smaller error. However, a good numerical method makes the truncation error approximately constant over the solution domain, which requires non-uniformity of the grid. A well-chosen non-uniform grid is superior to a uniform grid.

We shall use the central difference (CD) approximation of the first derivative exclusively here; similar conclusions follow for other approximations and higher derivatives.

Using Taylor series expansions, it is not difficult to show that the first derivative of a variable at a point x_i can be expressed as

$$\left(\frac{\partial\phi}{\partial x}\right)_i = \frac{\phi_{i+1}-\phi_{i-1}}{x_{i+1}-x_{i-1}} - \frac{(x_{i+1}-x_i)^2-(x_i-x_{i-1})^2}{2(x_{i+1}-x_{i-1})}\left(\frac{\partial^2\phi}{\partial x^2}\right)_i - \frac{(x_{i+1}-x_i)^3+(x_i-x_{x-1})^3}{6(x_{i+1}-x_{x-1})}\left(\frac{\partial^3\phi}{\partial x^3}\right)_i + \text{HOT}. \tag{22}$$

The CD approximation uses only the first term on the right-hand side:

$$\left(\frac{\partial\phi}{\partial x}\right)_i \approx \frac{\phi_{i+1}-\phi_{i-1}}{x_{i+1}-x_{x-1}}. \tag{23}$$

The difference between (22) and (23) represents the truncation error:

$$\tau^{\text{CD}} = -\frac{(x_{i+1}-x_i)^2-(x_i-x_{i-1})^2}{2(x_{i+1}-x_{i-1})}\left(\frac{\partial^2\phi}{\partial x^2}\right)_i - \frac{(x_{i+1}-x_i)^3+(x_i-x_{i-1})^3}{6(x_{i+1}-x_{i-1})}\left(\frac{\partial^3\phi}{\partial x^3}\right)_i + \text{HOT}. \tag{24}$$

On uniform grids the scheme has a second-order error, but when the grid is non-uniform, the scheme is formally only first-order accurate. At any point x_i the error is larger when the mesh spacing is not uniform. However, since the discretization error also depends on the derivatives of the variables, a uniform distribution of discretization error is impossible to obtain on a uniform grid and a non-uniform grid can produce a smaller error norm for the same number of points.

Of interest is the rate at which the error is reduced as the grid is refined. We shall show that the error of the CD approximation is reduced in approximately a second-order manner whether the grid is uniform or not.

Let us assume that the grid expands or contracts with a constant factor r_e, i.e.

$$r_e = \frac{x_{i+1}-x_i}{x_i-x_{i-1}}. \tag{25}$$

In the case of this so-called compound interest grid the leading truncation error term of the CD scheme is

$$\tau^{\text{CD}} \approx \frac{1-r_e}{2}(x_i-x_{i-1})\left(\frac{\partial^2\phi}{\partial x^2}\right)_i + \text{HOT}. \tag{26}$$

The leading error term of the backward difference (BD) approximation is

$$\tau^{\text{BD}} = \tfrac{1}{2}(x_i-x_{i-1})\left(\frac{\partial^2\phi}{\partial x^2}\right)_i + \text{HOT}.$$

The first-order term in CD is proportional to $(1-r_e)\Delta x$, while in BD it is proportional to Δx alone. When r_e is close to unity, the CD error is substantially smaller than the BD error.

Now let us see what happens when the grid is refined. We shall consider two possibilities: halving the spacing between adjacent coarse grid points or inserting new points so that the fine grid has a constant ratio of spacings.

In the first case the spacing is uniform around the new points and the expansion factor r_e at the old points is the same as on the coarse grid. After several refinements the grid is uniform everywhere except around the coarsest grid points. The number of points belonging to the latter set is small and the global error decreases just a bit more slowly than in a true second-order scheme.

In the second case the expansion factor of the fine grid is smaller than on the coarse grid. A simple calculation shows that

$$r_{e,h} = \sqrt{r_{e,2h}}, \tag{27}$$

where h represents the refined grid and $2h$ the coarse grid. At a node common to both grids the ratio of the leading truncation error terms on the two grids is (see equation (26))

$$r_\tau = \frac{(1 - r_{e,2h})(x_i - x_{i-1})_{2h}}{(1 - r_{e,h})(x_i - x_{i-1})_h}. \tag{28}$$

The following relations between the mesh spacings on the two grids hold (see Figure 1):

$$(x_i - x_{i-1})_{2h} = (x_i - x_{i-1})_h + (x_{i-1} - x_{i-2})_h = (r_{e,h} + 1)(x_{i-1} - x_{i-2})_h,$$
$$(x_i - x_{i-1})_h = r_{e,h}(x_{i-1} - x_{i-2})_h.$$

When these and equation (27) are inserted in (28), it is found that

$$r_\tau = (1 + r_{e,h})^2 / r_{e,h}. \tag{29}$$

This factor has the value $r_\tau = 4$ when $r_e = 1$, i.e. when the grid is uniform. When $r_e > 1, r_\tau > 4$, which means that the error due to the first-order term decreases faster than the second-order error term. For $r_e < 1$ we need only change x to $-x$, i.e. reverse the sign of the co-ordinate, and we see that the results are the same as if the ratio was $1/r_e$. Since, in this method, $r_e \to 1$ as the grid is refined, the convergence becomes second-order asymptotically.

Similar analysis can be applied to other schemes but is more difficult. An example of the application of this method is shown below.

On unstructured grids, if the new grid is obtained by dividing the coarse grid, the Richardson method can be and has been used. An alternative and more general approach is to interpolate the coarse grid results onto the fine grid and use the difference between the two solutions to form the error estimate. In doing so, one must take care that the interpolation scheme used is more accurate than the discretization.

Soon after this paper was first submitted to this journal, an article on this subject by Roache[6] appeared. He discusses a number of issues related to error estimation and introduces a new grid convergence index (GCI). Although we agree with many of the points Roache makes, we do not believe that the GCI offers significant advantages relative to the standard Richardson approach. His point that the grid must be fine enough for the estimates to be accurate is well taken, but on coarse grids no error estimator will be very accurate.

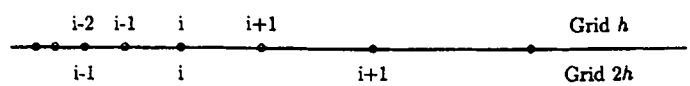

Figure 1. Refinement of a non-uniform grid which expands by a constant factor r_e

4. TEST CASES

In order to test the method of estimating convergence errors, we will first do a linear problem and then non-linear problems from fluid mechanics.

The linear problem is Laplace's equation on the square domain $\{0 < x < 1; 0 < y < 1\}$ with boundary conditions chosen to correspond to the solution $\phi(x, y) = 100xy$. The advantage of this choice is that the second-order central difference approximation to the converged solution is exact for any grid, so the difference between the present iterate and the converged solution is easily computed. The initial guess of the solution is zero everywhere within the domain. We chose SOR as the iterative technique because, if the relaxation parameter is smaller than the optimum value, the dominant eigenvalue is real; for relaxation parameters larger than the optimum value the dominant eigenvalues are complex. For this case the optimum value of the relaxation parameters can be computed;[7] if N is the number of control volumes (CVs) in each direction, for $N = 20, \omega_{opt} = 1{\cdot}729$, while for $N = 40, \omega_{opt} = 1{\cdot}854$.

Results are shown for several cases in Figures 2–4. In each case the norms of the exact convergence error, the error estimate, the difference between two iterates and the residual are shown. Figure 2 shows a case with real eigenvalues which therefore has smooth exponential convergence. The error estimate is almost exact in this case. Figures 3 and 4 shows results for the case in which the eigenvalues of the iteration matrix are complex, which is reflected in the oscillations in the error. As one can see, the comparison of estimated and actual errors is again quite satisfactory.

We next consider a two-dimensional buoyancy-driven cavity flow at Rayleigh number $Ra = 10^5$ and Prandtl number $Pr = 0{\cdot}1$. The vertical walls were kept at constant temperature, while the horizontal walls were adiabatic. Calculations were performed using central differences (CD) on

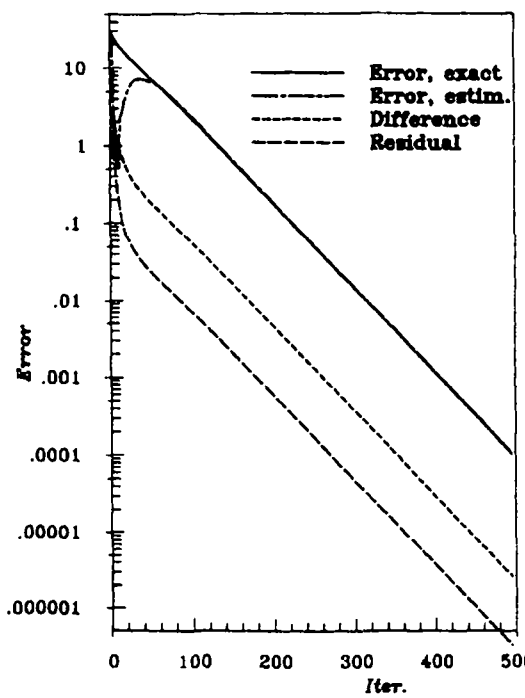

Figure 2. Norms of convergence error, its estimate, difference between two iterates and residual for solution of Laplace's equation by SOR; $\omega = 1{\cdot}6$, 40×40 grid

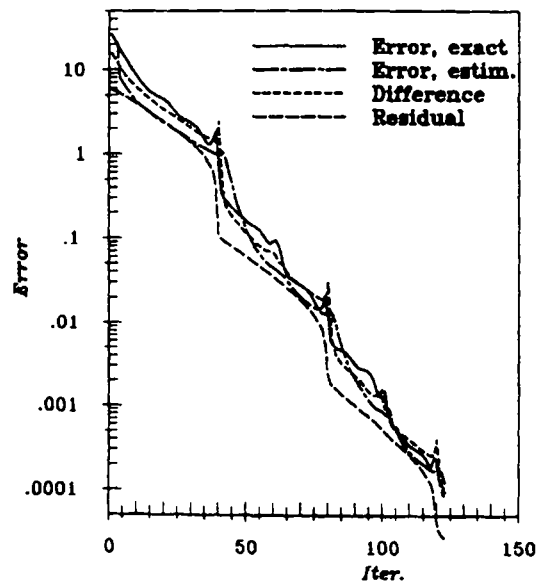

Figure 3. Norms of convergence error, its estimate, difference between two iterates and residual for solution of Laplace's equation by SOR; $\omega = 1{\cdot}9$, 20 x 20 CV grid

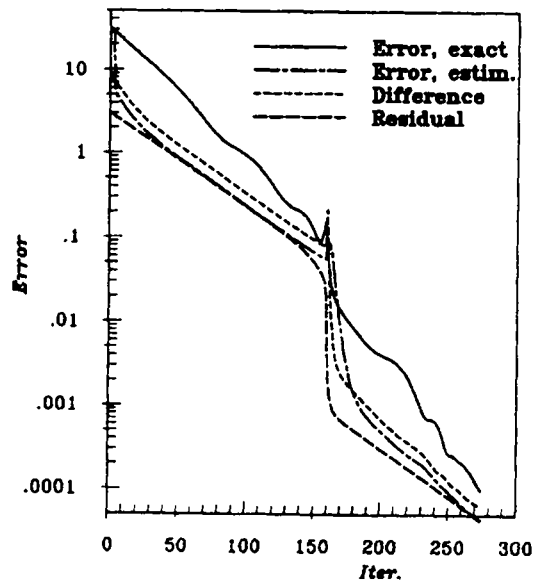

Figure 4. Norms of convergence error, its estimate, difference between two iterates and residual for solution of Laplace's equation by SOR; $\omega = 1{\cdot}95$, 80 x 80 CV grid

various grids. An accurate solution was obtained by iterating until the residual norm became negligibly small (of the order of the round-off error in double precision). Then the calculation was repeated and the convergence error was taken as the difference between the converged and intermediate solutions.

Figure 5 shows the norm of the convergence error, its estimate, the difference between two iterates and the residual for a 32 × 32 control volume (CV) grid using the single-grid (SG) SIMPLE solution algorithm[8] and underrelaxation factors of 0·7 for the velocity components and temperature and 0·3 for the pressure. Similar information is shown for the 64 × 64 grid in Figure 6. Since the SG algorithm needs many iterations to converge, the eigenvalues in the error estimator were averaged over 50 iterations. The initial fields were interpolated from the next coarser grid, which is why the initial error is relatively low, especially on the finer grids.

Figure 7 shows results for the 64 × 64 grid using a multigrid (MG) solution algorithm. The initial solution guess is obtained by interpolating the solution on the next coarser grid (as in Figure 6) and after several iterations on the finest grid a V-MG cycle is performed. Each V-cycle reduces the error substantially, but the fine grid iterations contribute only moderately to the error reduction. The error estimate shows a similar pattern, although the estimate is too low after each V-cycle and needs a few iterations to recover. This is due to the error estimator using information from several iterations. It may be better to estimate the error using only data taken at the ends of multigrid cycles.

Similar results are obtained for lid-driven cavity flow at Reynolds number $Re = 10^3$. These results show that neither the difference between two iterates nor the residual alone is a reliable measure of the convergence error. These quantities decrease with the error but need to be properly normalized to represent the convergence error quantitatively. However, if one knows the initial error approximately (it is the solution itself if zero initial fields are used), then a reliable criterion for stopping the iterations is that the norm of either the difference between two iterates or the residual be reduced by a certain factor. This is justified by the fact that in the figures the curves are nearly parallel.

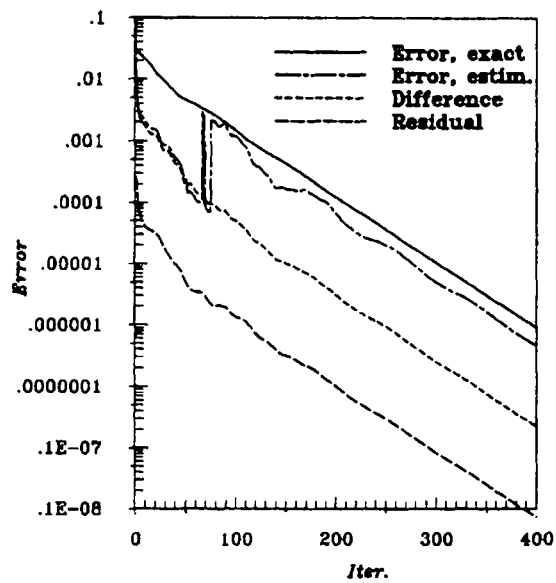

Figure 5. Norms of convergence error, its estimate, difference between two iterates and residual for solution of buoyancy-driven cavity flow; 32 × 32 CV grid, SG algorithm

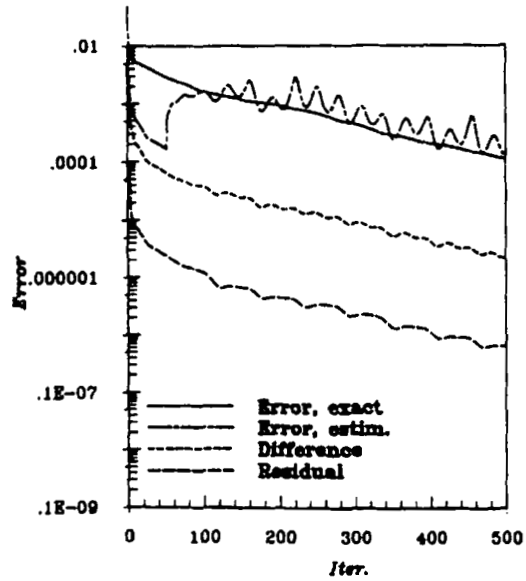

Figure 6. Norms of convergence error, its estimate, difference between two iterates and residual for solution of buoyancy-driven cavity flow; 64 × 64 CV grid, SG algorithm

We look next at the discretization errors in the flow described above. To do this, we performed calculations on uniform and non-uniform grids of 8 × 8 to 256 × 256 control volumes (CVs). The non-uniform mesh expanded with distance from the walls with a constant expansion factor (compound interest grid). On the finer grids the mesh spacing near the walls was halved and other CVs were divided into four, so the expansion factor is constant in both directions. The total heat flux through the isothermal walls is calculated from the converged solution on each grid; this is an integral

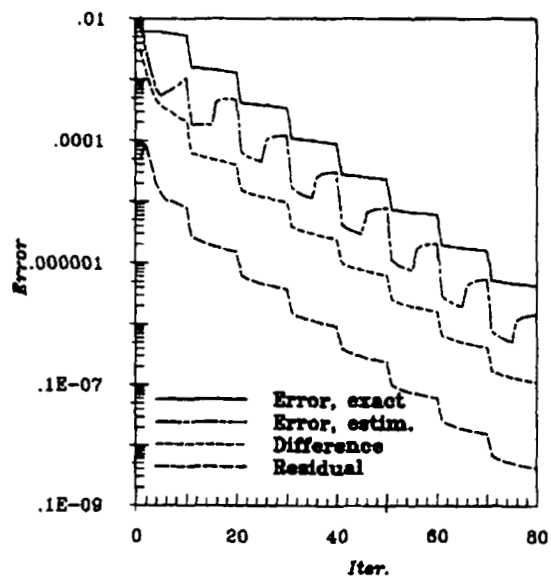

Figure 7. Norms of convergence error, its estimate, difference between two iterates and residual for solution of buoyancy-driven cavity flow; 64 × 64 CV grid, MG algorithm

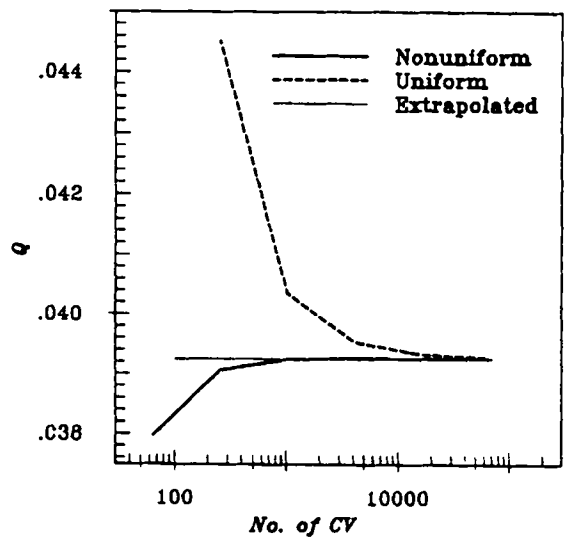

Figure 8. Convergence of total heat flux through isothermal walls in buoyancy-driven cavity flow at $Ra = 10^5$ and $Pr = 0{\cdot}1$ using CD on uniform and non-uniform grids

quantity and its error represents an average error. The strength of the primary eddy is also analysed. Figure 8 shows how these quantities vary as the number of grid points is increased. In Figure 9 the estimated errors in the heat flux and strength of the primary eddy are plotted against the reference mesh spacing, taken as unity on the coarsest grid and reduced by a factor of two on each subsequent grid. Since the exact solution is not known, Richardson extrapolation based on the two finest grid solutions is used to determine the 'exact' values. The CD scheme shows second-order convergence on

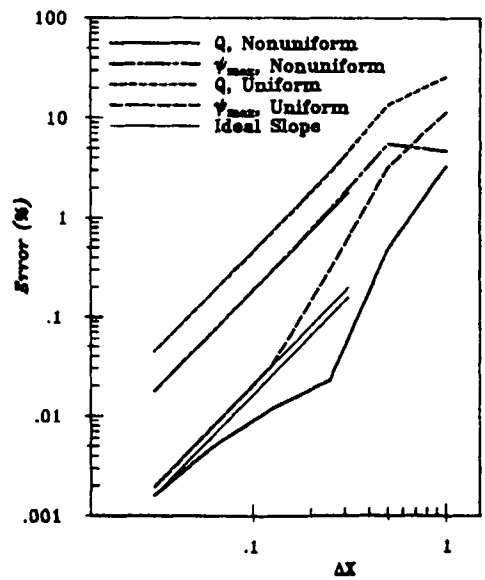

Figure 9. Error in predicted values of Q and ψ_{max} on uniform and non-uniform grids as a function of mean mesh spacing

both the uniform and non-uniform grids, in accordance with the analysis presented earlier. Although the errors on the uniform and non-uniform grids differ by almost an order of magnitude, Richardson extrapolation gives the same result (to five significant figures) when applied to the three finest grids of both types. However, a solution of prescribed accuracy is obtained with much less effort on a non-uniform grid. For several quantities the uniform and non-uniform grid solutions approach the limit from different sides; also, the convergence is not always monotonic, which is why the dependence of the error on Δx shown in Figure 9 is irregular. The order of convergence estimated using equation (21) is valid only when the convergence is monotonic, i.e. for sufficiently fine grids. Thus it is essential to perform calculations on at least three grids to be able to reasonably estimate the discretization errors.

5. CONCLUSIONS

Convergence errors can be accurately estimated from data generated during an iteration process at essentially no additional cost. Although convergence error is the best stopping criterion for an iterative process, reduction of the residual or the difference between successive iterates can be used if normalized properly.

Discretization errors may be reliably estimated provided that solutions on at least two grids of sufficiently different size are available. Care must be taken that these solutions are not contaminated by convergence error.

Although central difference schemes become formally first-order-accurate on non-uniform grids, the error is reduced in nearly a second-order manner as the grid is refined.

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