AN ERROR ESTIMATOR FOR CFD APPLICATIONS: THE AES METHOD

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ABSTRACT

A novel method was developed to estimate the discretization error in numerical computations. The aforementioned method avoids the necessity to use the Richardson extrapolation (RE), the traditional method to extrapolate numerical solutions to zero grid size. The idea on which the method is based consists on the existence of a proportional relation between the approximate error and the true error. The proposed method only requires numerical solutions on three grids, compared to the traditional Richardson extrapolation technique that in some cases needs more than four numerical solutions. Besides, it is not necessary to know the order of the scheme used to discretize the governing equations, in fact, the method is capable of determining the discretization order. The method can also be used as an indicator whether the solution is in the asymptotic region or not. It is easily applicable to one-, two-, and three dimensional problems even to integral quantities. The relations used are fully derived from theoretical considerations. The performance of the proposed method was tested using one-dimensional linear and non-linear first order ordinary differential equations and a manufactured solution for a steady one-dimensional scalar transport equation. For all the studied cases, the estimated true errors were found to agree well with the true errors.

RESUMEN

Un método novedoso fue desarrollado para estimar el error de discretización en simulaciones numéricas. El método antes mencionado evita el uso de la extrapolación de Richardson (RE), el método tradicional para extraer las soluciones numéricas a tamaños de malla de cero. La idea en la cual se basa el método consiste en la existencia de una relación proporcional entre el error aproximado y el error verdadero. El método propuesto solamente requiere tres soluciones numéricas en mallas diferentes, comparado con la técnica de extrapolaion de Richardson tradicional que en algunos casos requiere de más de cuatro soluciones numéricas. Además, no es necesario conocer el orden del esquema de discretización utilizado, en realidad, el método es capaz de determinar dicho orden de discretización. El método también se puede usar como un indicador de si la solución numérica se encuentra o no en la región asintótica. El método es fácilmente aplicable a problemas unidimensionales, bidimensionales y tridimensionales y también en cantidades integrales. Las relaciones usadas son derivadas completamente de consideraciones teóricas. El desempeño del método propuesto fue probado utilizando ecuaciones diferenciales ordinarias de primer orden tanto lineal como no lineal y una solución manufacturada para una ecuación estable y unidimensional de transporte de un escalar. Para todos los casos estudiados, los errores verdaderos estimados se asemejaron bastante bien con los errores verdaderos.

1. INTRODUCTION

The solution of differential equations by using discretization schemes implicitly carries errors which come from different sources such as discretization error or grid-convergence error, iteration-convergence error, modeling error, round-off error, interpolation and/or extrapolation errors, among many others. Therefore, as a consequence, the numerical solutions are expected to present uncertainty in a similar manner as happens with experimental work. In order to assess the numerical uncertainty,
it is imperative to count with a method capable to estimate the numerical error.

In this work the efforts are focused on the use of a novel method on three different cases for which the exact solutions are known in order to assess the performance of the method on the estimation of the grid-convergence error which may be dominant over the other sources of errors [1-4]. The proposed method [5, 6] compared to the Richardson extrapolation method [7, 8] is simpler and its use is not restricted to monotonically converging cases as the widely studied Richardson extrapolation is [9-18]. Besides, the method does not require knowing the apparent order of the discretization scheme and only needs the numerical solution on three grids. In fact, the discretization order can be inferred from the method itself.

2. ERROR ESTIMATOR

The method presented in this study named Approximate Error Spline method is a variant of the extrapolation method proposed by Celik et al. [19, 20] and was developed to predict the true error. The main assumption of this method is that the true error, \( E_t \), is proportional to the approximate error, \( E_a \), as given by the following equation

\[
\tilde{E}_t^h = c E_a^h \tag{1}
\]

where the constant \( c \) appearing in Eq. (1) is the global proportionality constant. The true error is defined as

\[
\tilde{E}_t^h \equiv E_t^h = \phi - \phi_h \tag{2}
\]

The approximate error \( E_a^h \), is defined as the difference between the numerical solutions on two consecutive grid densities \( h \) and \( \alpha h \);

\[
E_a^h = \phi_h - \phi_{\alpha h} \tag{3}
\]

where \( \alpha \) is the grid refinement or coarsening factor; i.e. \( \alpha_1 = h_2 / h_1 \), \( \alpha_2 = h_3 / h_2 \), etc. In the present study, \( h_1 < h_2 < h_3 \) means that subscript “1” denotes the smallest grid size (fine grid) and subscript “3” the coarsest grid, and therefore, \( \alpha \) representing the refinement factor (\( \alpha > 1 \)).

In Eq. (2), \( \phi \) represents the exact solution and \( \phi_h \) is the numerical solution on a grid represented by the cell size \( h \). We propose to call the new method Approximate Error Scaling Method (AESM) while Eq. (1) is a scaling and \( \tilde{E}_t^h \) is an estimate of the ‘true error’, \( E_t^h \).

In order to apply Eq. (1), numerical calculations on three different grids (triplet) are needed. By simple algebra, Eq. (3) can be rewritten as

\[
\phi - \phi_h = c_1 (\phi - \phi_2) \tag{4}
\]

\[
\phi - \phi_{\alpha} = c_1 (\phi_2 - \phi_3) \tag{5}
\]

Subtracting Eq. (4) from Eq. (5) and solving for \( c_1 \) yields

\[
c_1 = \frac{\phi_2 - \phi_1}{\phi_3 - 2\phi_2 + \phi_1} \tag{6}
\]

Similarly, the true error on medium and coarse grids can be written as

\[
\phi - \phi_2 = c_2 (\phi_1 - \phi_2) \tag{7}
\]

\[
\phi - \phi_3 = c_2 (\phi_2 - \phi_3) \tag{8}
\]

Subtracting Eq. (7) from Eq. (8) and solving for \( c_2 \) gives

\[
c_2 = \frac{\phi_3 - \phi_2}{\phi_3 - 2\phi_2 + \phi_1} \tag{9}
\]

The post-processing of the numerical calculations on the three grids enables determination of the proportionality constants \( c_1 \) and \( c_2 \) by making use of Eqs. (6) and (9). In a 2D computational domain, \( c_1 \) and \( c_2 \), given by Eqs. (6) and (9), have a 2D distribution, \( \left( c_{i,j} \right) \), and the global constant \( c \), given in Eq. (1), is calculated from the arithmetic average of the local constants;

\[
c = \frac{1}{2} (\bar{C}_1 + \bar{C}_2) \tag{10}
\]

where
The operator \( \| \| \) represents the summation of the absolute value of its argument over the whole computational domain and \( N_3 \) is the number of cells used in the coarsest grid (grid 3) of the triplet.

It must be realized that the dimensions of the variables arrays due to different grid resolutions chosen for the triplet are different. In order to compute Eqs. (6) and (9) it is required that the numerical solutions on the three grids have the same dimensions and same location of the computed values. The approach followed in this study was to interpolate the solutions on the fine grid \( (\phi_1) \) and on the medium grid \( (\phi_2) \) to the coarse grid (grid 3), thus keeping the error incurred by interpolation in its lower value. Therefore, after interpolation, the dimensions of the arrays for \( c_{1,i,j} \) and \( c_{2,i,j} \) are the same as those of the coarsest grid.

Note that Eqs. (6) and (9) represent the proportionality constant using the finest triplet \((1, 2, 3)\) but the method is not limited to the use of that triplet when numerical calculations on more than three grids were performed, however, the same \( \alpha \) between consecutive grids has to be used. The use of the finest triplet is expected to give a more accurate estimation of the true error.

It is important to mention that the methodology described by Eqs. (10), (6) and (9) is not only applicable on 2D problems but also on 1D, 3D and even on integral quantities.

The calculation of the local proportionality constants defined by Eqs. (6) and (9) requires special treatment in the cases where singularities may arise during the evaluation of the denominator in both equations. The approach followed in this study to avoid these singularities is to limit the absolute values of these local proportionality constants to be less than one order of magnitude of their theoretical values in the asymptotic region given by

\[
c_1 = \frac{1}{\alpha^n - 1} \quad \text{and} \quad c_2 = \frac{\| c_{1,i,j} \|_N}{N_3} \quad \text{(11)}
\]

It is important to mention that in the asymptotic range the difference between the proportionality constants \( c_2 \) and \( c_1 \) equals 1 (see Eqns. 12 and 13). Therefore by calculating the difference between this two proportionality constants it can be determined if the numerical solutions are in the asymptotic range without the need to define or establish the order of the discretization scheme.

The equations used to calculate the true error on the fine grid, approximate error between the solutions on the fine and medium grids and the estimated true error are given by

\[
E^{13}_i = \phi^{ana}_{1,i,j} - \phi^{num}_{13}, \quad E^{13}_a = \phi^{num}_{13} - \phi^{num}_{23}, \quad \tilde{E}^{13}_a = \frac{\| \phi^{num}_{13} - \phi^{num}_{23} \|_N}{N_3} \quad \text{(14)}
\]

The binary subscripts/superscripts denote interpolation from the first grid (on the left) to the second grid (on the right). The superscripts \( ana \) and \( num \) stand for analytical and numerical solutions, respectively. Also the subscripts \( a \) and \( t \) represent approximate and true, respectively. The tilde on top of the true error indicates estimated true error.

The estimated true error reported in Eq. (14) uses the same definition given in Eq. (4) but using a global proportionality constant. The reason for using the definition given in Eq. (4) is that the numerical solution on finer grids will give solutions closer to the exact solution.

3. RESULTS

In this section are presented the results for linear and non-linear one-dimensional equations at steady state as well as for a one-dimensional scalar transport equation where the velocity field is prescribed.

3.1. Steady One-Dimensional Linear Equation

The discussion on this case will focus on the solution of the following 1D equation

\[
\frac{d\phi}{dx} = a\phi \quad 0 < x < 1 \quad \text{(15)}
\]

where the selected parameter \( a \) is -25.
Discretization of the governing equation using forward differencing results in the exact finite difference solution given by
\[ \phi_i = (1 + ah) \phi_0 \] (16)
and
\[ \phi_i = \frac{\phi_0}{(1 - ah)} \] (17)
when using backward discretization.

In the two previous equations \( h \) is the grid size and \( \phi_0 \) is the boundary value.

Oscillatory convergence is observed on coarse grids with about 10 nodes or less when forward differencing is used. However with this number of grids, the numerical solutions are not physically acceptable solutions. Acceptable solutions are obtained when more than 25 nodes are used in the numerical simulations and the oscillatory convergence behavior is not present anymore.

The use of backward discretization does not show oscillatory convergence even with coarse grids. The lack of oscillations is due because the numerical solution using backward discretization is more accurate compared with the solution using forward differencing.

The triplet consisting of 30-60-120 grids is used to evaluate the performance of the error estimator when forward differencing was used. In Figure 1, the solution on the three grids mentioned above are presented as well as the true error on the fine grid, the approximate error between the fine and medium grids and the estimated true error.

When using backward differencing, the error estimator method described in this study is evaluated with \( a = -5 \). The selected triplet consisted of 5-10-20 nodes. In Figure 2 the numerical solutions on the three grids mentioned above are presented and compared with the exact solution. The calculated errors using the method proposed in this study are also shown in Figure 2. From Figure 2, it is evident that the estimated true error using the AES closely predicts the true error. For this triplet, the proportionality constants \( C_1 \) and \( C_2 \) are 1.125 and 2.125 respectively. From these two values it can be concluded that the numerical solutions are in the asymptotic range.

3.2. Steady One-Dimensional Non-Linear Equation

The model equation studied in this case is
\[ \frac{d\phi}{dx} = a_1 \phi - a_2 \phi^2 ; \quad 0 \leq x \leq 1 \] (18)
subject to the boundary condition \( \phi(0) = \phi_o \).

The parameters \( a_1 \) and \( a_2 \) are constants, prescribed as 14.5 and 0.0127, respectively.

The exact solution to the one-dimensional equation is
\[ \phi = \frac{a_1 \phi_o}{a_2 \phi_o + (a_1 - a_2 \phi_o) \exp(-a_1 x)} \] (19)

Figure 1 Use of triplet 30-60-120 and forward differencing, (a) numerical solutions and (b) estimated errors.
By using first order forward differencing to discretize the governing equation, the numerical solution takes the form

\[ \phi_i = (1 + a_i h)\phi_{i-1} - a_2 h \phi_{i-1}^2 \]  
(20)

Using central differencing, the discretized equation takes the following form

\[ \phi_{i+1} = \phi_{i-1} + 2a_i h \phi_i - 2a_2 h \phi_i^2 \]  
(21)

The convergence behavior of the numerical solution at \( x = 1.0 \) is highly oscillatory when \( h > 0.072 \) and not physically acceptable solutions are obtained at that location.

Although the convergence is more stable using first order forward differencing, the numerical solutions using this discretization scheme are not as accurate when compared with central differencing discretization (second order). Discretization with 2nd order forward differencing did not provide acceptable solutions since the scheme showed instabilities that led to divergence.

The estimation of the true error is evaluated for both cases, using first order forward differencing and central differencing. The refinement of the grids to conform the triplet was done by doubling the grid. In case of discretization of the governing equation with first order forward differencing (see Figure 3), the AES method did not predict closely the true error. However when the discretization of the first derivative was done using central differencing (Figure 4), the AES method estimates closely the true error.

Figure 2 Use of triplet 5-10-20 and backward differencing with \( a=5 \), (a) numerical solutions and (b) estimated errors

Figure 3 Estimation of the true error with AES method using first order forward differencing to discretize the first derivative (a) \( h_c=0.05 \) and (b) \( h_c=0.01 \)
3.3. Steady One-Dimensional Scalar Transport Equation

The third study case is the application of the proposed method for the solution of a 1D steady scalar transport equation which can be written as

\[ \frac{d}{dx} \left( u\phi \right) = \frac{d}{dx} \left( \Gamma \frac{d\phi}{dx} \right) + S_\phi \]  \tag{22}

The velocity field denoted by \( u \) is prescribed as

\[ u = \bar{u} \cos(\omega x) \]  \tag{23}

The analytical solution to Eq. (22) is given by

\[ \phi = \exp \left( \frac{\mu x}{\Gamma} \right) \]  \tag{24}

In the present study, the average velocity \( \bar{u} = 2.5 \), the frequency \( \omega = \pi \) and the diffusion coefficient \( \Gamma = 1.0 \) are chosen to obtain a definite solution to the problem. The computational domain extends from \( 0 \leq x \leq 1 \) and the boundary conditions are prescribed by evaluating Eq. (24) at the boundaries.

Three successively denser grids (9, 17 and 33 cells) with a grid refinement ratio of 2 were generated to solve the 1D scalar transport equation. These grids will be referred henceforth as coarse, medium and fine grid, respectively. The diffusion and convective terms were discretized using second order central differencing. The analytical solution along with the numerical solution on the three grids is plotted in Figure 5. As it can be seen from the figure, the numerical solution approaches to the analytical solution as the grid is refined (i.e. on fine grid).

Figure 4 Estimation of the true error with AES method using central differencing to discretize the first derivative (a) \( h_c=0.05 \) and (b) \( h_c=0.025 \)

Figure 5 Analytical and numerical solutions of the scalar

Figure 6 illustrates a comparison of true, approximate, and estimated true error, calculated by using the same triplet.

For the triplet used in this case, the calculated proportionality constants \( C_1 \) and \( C_2 \) are 0.37 and 1.38, respectively.
Similar calculations using several triplets along with grid refinement factors of 2 and 3, were performed by discretizing the convective terms with first order upwind and second order central differencing schemes. The grids used in these cases were refined until the solutions were close to or in the asymptotic region. It was observed from these numerical experiments that the calculated proportionality constants approached to their theoretical values in the asymptotic region as the grid is refined as shown in Figures 7 and 8. It was also observed that the difference between the two proportionality constants is also 1.0 when the solutions are in or close to the asymptotic region.

Therefore, aside from its capability to estimate the true error, the methodology presented here, can be used to determine the order of the discretization scheme. Also, the difference of the proportionality constants might be used as an index to evaluate how close the numerical solutions are from being in the asymptotic region. Further studies are underway on this respect.

Figure 6 True error, approximate error and estimated true error

Figure 7 Upwind scheme for convective terms with refinement factors of (a) 2 and (b) 3

Figure 8 Central differencing for convective terms with refinement factors of (a) 2 and (b) 3
4. CONCLUSIONS

A simple error estimation method based on the assumption that the approximate error is proportional to the true error is proposed. This method assumes that, at least, in the asymptotic range the approximate error is proportional to the true error. The proportionality coefficient is estimated as an average value of the local coefficients calculated using a set of three numerical solutions on three different grids. The method is verified on steady one-dimensional linear and non-linear equations and one-dimensional scalar transport. All indications are that this method gives reliable estimates of the error even on relatively coarse grids and on non-monotonic grid convergence cases. In the 1D scalar transport equation case, the calculated proportionality constants showed the theoretical values as the numerical solutions approached to the asymptotic region, therefore, the method presented in this study can be used to determine the order of the discretization scheme used in the numerical simulations. Besides the order of the discretization scheme, the method provides information that allows determining if the numerical solutions are obtained in the asymptotic range without the need to know a priori the order of the method, a task usually difficult to establish.

REFERENCES


