Multi-dimensional Discretization Error Estimation for Convergent Apparent Order

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This work presents procedures for estimating the error of numerical solutions of multi-dimensional problems. It is considered that: the numerical error is caused only by truncation errors; error estimations are based on the Richardson extrapolation; and numerical approximations are one-dimensional over uniform grids in each dimension. Two cases are analyzed: when grids are simultaneously refined in all four dimensions (x,y,z,t); and when grid refinement in each dimension is separate from the remaining ones. Examples of uses are presented for problems involving heat transfer and fluid mechanics, which are solved by the finite difference and finite volume methods. It was found that, for the situation in which the apparent order of the estimated error is a monotone convergent one, two values of estimated error can be calculated, which bound the true error.
***Keywords**: discretization error, truncation error, CFD, numerical error, fluid flows*

Introduction

It is still common to find in the relevant literature (Jameson and Martinelli, 1998) works in which the magnitude of the discretization error (Roache, 1998) is assessed only by presenting the numerical results obtained with two or three different grids. Nevertheless, it is already quite common to use Richardson extrapolation (Richardson, 1910) to estimate discretization errors, as, for example, in Roy and Blottner (2001). A variant of the Richardson extrapolation has also been used, the *GCI* estimator (Roache, 1994), for example, in Cadafalch et al. (2002).

For each variable of interest, the error estimation made through Richardson extrapolation uses numerical solutions obtained from two or more different grids, i.e., grids with a different number of volumes, points or elements. Therefore, in a two-dimensional problem, for example, the grids can be refined either simultaneously or separately in both directions (x and y).

The purpose of this work is to present procedures for estimating the error of numerical solutions of multi-dimensional problems when the apparent order (De Vahl Davis, 1983) of the estimated error is a monotone convergent one (Marchi and Silva, 2002). By doing so, one can define the lower and upper limits for the true error. Examples of uses are presented for problems involving heat transfer and fluid mechanics, which are solved by the finite difference and finite volume methods. Furthermore, we have developed our work taking into account the following factors:

1) The theory and the definitions adopted by Marchi and Silva (2002), which deals only with one-dimensional problems.

2) That the numerical error is caused only by truncation errors, i.e., it is either assumed that there are no errors related to iterations, round-off and due to programming (Marchi and Silva, 2002), or, rather, that these errors are very small when compared with truncation errors. In this case, the numerical error is called a discretization error.

3) Estimates of discretization errors are of an *a posteriori* type and are based on Richardson extrapolation (Richardson, 1910; Roache, 1994; Blottner, 1990; Oberkampf and Trucano, 2002), which uses multiple grids.

4) That up to three spatial dimensions (x,y,z) and one temporal (t) dimension are used.

5) That the numerical approximations used for discretizing the mathematical models are one-dimensional (Ferziger and Peric, 1999; Tannehill et al., 1997).

6) That the grids are uniform in each dimension.

7) Estimations of the discretization error can be applied to the dependent variables of the mathematical model or to any variable obtained from them through differentiation, integration or any other mathematical operation.

8) The exact analytical solutions are known for the variables of interest for the problems used as examples in this work. One can therefore compare the estimated error to the true error.

9) The numerical method works in all the grids.

In the next sections a definition of multi-dimensional discretization error and a summary of the significant results from Marchi and Silva (2002) are presented. The procedures used for estimating the true discretization error are shown for grids that are simultaneously refined in all dimensions and for when the refinement is separate in each dimension. Next, examples are presented that include two-dimensional steady-state heat conduction, one-dimensional transient heat conduction and two-dimensional incompressible Navier-Stokes flow. The numerical solutions to such problems are obtained by finite difference and finite volume methods. Finally, a conclusion to this work is presented.

Nomenclature

c = coefficients in the truncation error equation
C = coefficients in the discretization error equation
E = *true* discretization error of the numerical solution
h = grid spacing or distance between two successive grid points
K = coefficients in the numerical solution uncertainty equation
p_L = asymptotic order of the discretization error
p_U = apparent order of the uncertainty
r = grid refinement ratio
t = time
U = uncertainty or estimated error of the numerical solution
U_C = uncertainty of the numerical solution by the convergent estimator
U_{Ri} = uncertainty of the numerical solution by the Richardson estimator
x, y, z = spatial coordinates

Greek Symbols

ε = truncation error
ϕ = numerical solution of the variable of interest
Φ = exact analytical solution of the variable of interest
ϕ_C = convergent numerical solution
ϕ_∞ = estimated analytical solution

Λ = dependent variable

Subscripts

1 fine grid
2 coarse grid
3 supercoarse grid
b base grid
d dimension (1=*x*, 2=*y*, 3=*z*, 4=*t*)

Multi-dimensional Discretization Error

Let us consider the two-dimensional equation of Laplace (Incropera and DeWitt, 1996):

$$\frac{\partial^2 \Lambda}{\partial x^2} + \frac{\partial^2 \Lambda}{\partial y^2} = 0 \qquad (1)$$

where x and y are the independent variables and Λ is the dependent variable. This equation can be discretized with a central difference scheme (Ferziger and Peric, 1999) for each one of its terms, i.e.,

$$\left(\frac{\partial^2 \Lambda}{\partial x^2}\right)_P \approx \frac{(\Lambda_W + \Lambda_E - 2\Lambda_P)}{h_x^2} \qquad (2)$$

$$\left(\frac{\partial^2 \Lambda}{\partial y^2}\right)_P \approx \frac{(\Lambda_S + \Lambda_N - 2\Lambda_P)}{h_y^2} \qquad (3)$$

where

$$h_x = x_P - x_W = x_E - x_P = \ldots = \text{constant 1} \qquad (4)$$

$$h_y = y_P - y_S = y_N - y_P = \ldots = \text{constant 2} \qquad (5)$$

In Eqs. from (2) to (5), the subscripts refer to Fig. 1, in which P represents a generic node in the grid on which numerical approximations are made, and W, E, S and N represent its neighboring nodes. Other numerical approximations can be found in Ferziger and Peric (1999) and Tannehill, Anderson and Pletcher (1997).

Using a Taylor series (Kreyszig, 1999), one can verify that the truncation errors (ε) (Tannehill, Anderson and Pletcher, 1997) of the numerical approximations given in Eqs. (2) and (3) are, respectively,

$$\varepsilon\left(\frac{\partial^2 \Lambda}{\partial x^2}\right)_P = -\left(\frac{\partial^4 \Lambda}{\partial x^4}\right)_P \frac{h_x^2}{12} - \left(\frac{\partial^6 \Lambda}{\partial x^6}\right)_P \frac{h_x^4}{360} - \ldots \qquad (6)$$

$$\varepsilon\left(\frac{\partial^2 \Lambda}{\partial y^2}\right)_P = -\left(\frac{\partial^4 \Lambda}{\partial y^4}\right)_P \frac{h_y^2}{12} - \left(\frac{\partial^6 \Lambda}{\partial y^6}\right)_P \frac{h_y^4}{360} - \ldots \qquad (7)$$

Introducing Eqs. (2) and (3) into Eq. (1), one can obtain

$$\frac{(\Lambda_W + \Lambda_E - 2\Lambda_P)}{h_x^2} + \frac{(\Lambda_S + \Lambda_N - 2\Lambda_P)}{h_y^2} \approx 0 \qquad (8)$$

In this case, the truncation error of Eq. (8) results in the sum of the values of Eqs. (6) and (7). Thus, generalizing, for a four-dimensional differential equation (x,y,z,t) that has many terms in each dimension, with derivatives of several different orders, the truncation error of the discretized differential equation (*DDE*), in each P node of the grid, results in

$$\varepsilon\,(DDE)_P = \sum_{d=1}^{4}\left[\sum_{i=1}^{\infty}\left(c_{i,d}\, h_d^{p_{i,d}}\right)\right] \qquad (9)$$

where d = 1, 2, 3 and 4 represents, respectively, the dimensions x, y, z and t; h_d represents the distance between two consecutive nodes of the grid in each d dimension; i represents each one of the terms of the infinite series, as in Eqs. (6) and (7); $c_{i,d}$ represents coefficients that depend on the derivatives of Λ in each node of the grid, but do not depend on h_d; finally, $p_{i,d}$ are the true orders (Marchi and Silva, 2002) of the truncation error, which are integer and positive numbers. Comments on the different nature of spatial and temporal terms of Eq. (9) and about the own Eq. (9) can be seen in Roache (1998), mainly on pages 125 and 126 and Roache (1994).

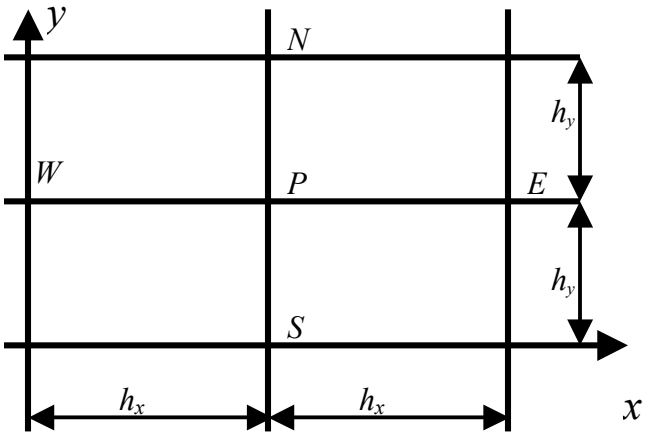

Figure 1. A two-dimensional grid, uniform in each direction.

In analogy (Roache, 1998; Ferziger and Peric, 1999) to the truncation error equation (ε) of Eq. (9), it is possible to assume that the true discretization error (E) of any variable of interest (ϕ) is given by

$$E(\phi) = \sum_{d=1}^{4}\left[\sum_{i=1}^{\infty}\left(C_{i,d}\, h_d^{p_{i,d}}\right)\right] \qquad (10)$$

in which ϕ can be the numerical solution of the dependent variable (Λ) in the differential equation, at a specific coordinate, its average of the whole field, or any other variable obtained from Λ; and the coefficients $C_{i,d}$ and the exponents $p_{i,d}$ may or may not be equal to the coefficients $c_{i,d}$ and $p_{i,d}$ of Eq. (9), depending on ϕ. The true discretization error of the numerical solution (ϕ) can also be defined by

$$E(\phi) = \Phi - \phi \qquad (11)$$

Determining the true discretization error through Eq. (10) or (11) requires knowing the exact analytical solution (Φ). Unfortunately, in practical problems, Φ is unknown. In such

cases, the concept of estimated error (U) is adopted, which is defined by

$$U(\phi) = \phi_\infty - \phi \quad (12)$$

where ϕ_∞ represents an estimation of Φ. To do so, one can use a simplification of Eq. (10), retaining only the first term of each dimension, i.e., the term that prevails over the remaining ones as $h_d \to 0$. Thus, one obtains

$$U(\phi) = K_x h_x^{p_x} + K_y h_y^{p_y} + K_z h_z^{p_z} + K_t h_t^{p_t} \quad (13)$$

in which the coefficients K_d are assumed as constant, i.e., they do not depend on h_d; and p_x, p_y, p_z and p_t are the asymptotic orders (Marchi and Silva, 2002) of the true discretization error of each dimension. Generally speaking, the value of the estimated error (U) is different from the true error (E) due to the simplification made while moving from Eq. (10) to Eq. (13).

Obtaining ϕ_∞ and U in multi-dimensional problems is dealt in this work but first, in the next section, the significant results of Marchi and Silva (2002) are presented because they are the base for the present multi-dimensional problems.

One-dimensional Discretization Error Estimation for Convergent Apparent Order

The Richardson Error Estimator for One-Dimension

For one-dimension, Eq. (13) reduces to

$$U(\phi) = K_L h_L^{p_L} \quad (14)$$

where K_L is a constant, h_L is the grid spacing and p_L is the asymptotic order of the true discretization error. In Eq. (14), instead of using p_L, one can also use the concept of apparent order (p_U) (De Vahl Davis, 1983), i.e.,

$$U(\phi) = K_U h_L^{p_U} \quad (15)$$

where K_U is a constant and

$$p_U = \frac{\log\left(\frac{\phi_2 - \phi_3}{\phi_1 - \phi_2}\right)}{\log(r)} \quad (16)$$

for a constant grid refinement ratio (r), defined by

$$r = \frac{h_{L,2}}{h_{L,1}} = \frac{h_{L,3}}{h_{L,2}} \quad (17)$$

where ϕ_1, ϕ_2 and ϕ_3 are the numerical solutions obtained, respectively, with the fine grid ($h_{L,1}$), coarse grid ($h_{L,2}$) and supercoarse grid ($h_{L,3}$).

It was analyzed the estimate of discretization errors for the situation where the apparent order (p_U) converges monotonically toward the asymptotic order (p_L) as $h_L \to 0$. This happens in two ways that are defined as subconvergent and superconvergent intervals of the apparent order (p_U) or simply denoted as "convergent apparent order". Within the subconvergent interval, p_U converges monotonically to p_L with smaller values than p_L as $h_L \to 0$. Within the superconvergent interval, p_U converges monotonically to p_L with larger values than p_L as $h_L \to 0$.

If the apparent order (p_U) is monotone convergent, then the exact analytical solution (Φ) will be bound between $\phi_\infty(p_L)$ and $\phi_\infty(p_U)$, with

$$\phi_\infty(p_L) = \phi_1 + \frac{(\phi_1 - \phi_2)}{(r^{p_L} - 1)} \quad (18)$$

$$\phi_\infty(p_U) = \phi_1 + \frac{(\phi_1 - \phi_2)}{(r^{p_U} - 1)} \quad (19)$$

Equations (18) and (19) are the generalized Richardson extrapolations (Roache, 1994). Replacing them in Eq. (12), one obtains

$$U_{Ri}(\phi_1, p_L) = \frac{(\phi_1 - \phi_2)}{(r^{p_L} - 1)} \quad (20)$$

$$U_{Ri}(\phi_1, p_U) = \frac{(\phi_1 - \phi_2)}{(r^{p_U} - 1)} \quad (21)$$

which represent the estimated errors of the numerical solution ϕ_1 according to the Richardson error estimator (U_{Ri}). It was demonstrated that

$$\frac{U_{Ri}(\phi_1, p_a)}{E(\phi_1)} \le 1 \le \frac{U_{Ri}(\phi_1, p_b)}{E(\phi_1)} \quad (22)$$

in which p_a and p_b represent the asymptotic order (p_L) or the apparent order (p_U), depending on whether p_U is subconvergent or superconvergent. Within the convergent interval of p_U, this relation worked for all cases and variables of interest: eight linear and non-linear differential equations in fluid dynamics discretized by the finite difference method with uniform one-dimensional grids and with six types of numerical approximations. Outside convergent interval of p_U, this relation can or not works. One has not found a procedure to estimate *a priori* the beginning of the convergent interval of p_U.

An estimated error (U) may be defined as reliable when the ratio between estimated error (U) and true error (E) is larger or equal to unity. According to Eq. (22), the true discretization error of the numerical solution ϕ_1, $E(\phi_1)$, is bound by the estimated errors $U_{Ri}(\phi_1,p_L)$ and $U_{Ri}(\phi_1,p_U)$. Therefore, if the objective is to obtain a reliable estimated error, the numerical solution of the variable of interest (ϕ) should be presented or reported by

$$\phi = \phi_1 + U_{Ri}(\phi_1) \quad (23)$$

where

$$U_{Ri}(\phi_1) = sg(\phi_1 - \phi_2)\, Max\left\{ \left|U_{Ri}(\phi_1, p_L)\right| ; \left|U_{Ri}(\phi_1, p_U)\right| \right\} \quad (24)$$

with $sg(\phi_1-\phi_2)$ representing the sign of the difference between ϕ_1 and ϕ_2, and $Max\{\}$, the maximum between the modules of $U_{Ri}(\phi_1,p_L)$ and $U_{Ri}(\phi_1,p_U)$.

The Convergent Error Estimator for One-Dimension

With the same numerical solutions (ϕ_1, ϕ_2 and ϕ_3) used to obtain the estimated errors provided in Eqs. (20) and (21), it is possible to reduce the true discretization error of the numerical solution, $E(\phi_1)$, through "The Convergent Numerical Solution" (ϕ_C), defined by

$$\phi_C = \frac{\phi_\infty(p_L) + \phi_\infty(p_U)}{2} \tag{25}$$

where $\phi_\infty(p_L)$ and $\phi_\infty(p_U)$ are obtained by the Richardson extrapolation, Eqs. (18) and (19). For ϕ_C, the numerical solution of the variable of interest (ϕ) should be presented or reported by

$$\phi = \phi_C \pm U_C(\phi_C) \tag{26}$$

in which the estimated error of ϕ_C, $U_C(\phi_C)$, is equal to the modulus of half of the interval between $\phi_\infty(p_L)$ and $\phi_\infty(p_U)$, that is,

$$U_C(\phi_C) = \frac{\left|\phi_\infty(p_L) - \phi_\infty(p_U)\right|}{2} \tag{27}$$

Hereafter, U_C is called "The Convergent Error Estimator".

Within the convergent interval of p_U, it is advisable to use the convergent numerical solution (ϕ_C) instead of the calculated numerical solution (ϕ_1) because the true discretization error of ϕ_C, $E(\phi_C)$, is smaller than the true discretization error of ϕ_1, $E(\phi_1)$.

Simultaneous Refinement of a Grid in All Dimensions

Refinement is characterized as simultaneous refinement when the number of nodes, elements or control volumes of all four dimensions (x, y, z, t) vary among the grids used to estimate the discretization error. In a three-dimensional problem, for example, this is done by refining of a grid from 10*10*10 to 15*20*30 control volumes. In the next section, describes the case in which grid refinement in each dimension is separate from that of the remaining ones. Next, two situations will be examined: when the grid refinement ratio is variable in each dimension; and when it is the same.

Variable Grid Refinement Ratio

With Eqs. (12) and (13) designed for five different grids, i.e. with a different number of nodes, elements or control volumes among them in each dimension, indicated by $h_{d,1}$, $h_{d,2}$, $h_{d,3}$, $h_{d,4}$ and $h_{d,5}$, and whose numerical solutions are, respectively, ϕ_1, ϕ_2, ϕ_3, ϕ_4 and ϕ_5, one can obtain

$$\left.\begin{aligned}
\phi_\infty - \phi_1 &= K_x\, h_{x,1}^{p_x} + K_y\, h_{y,1}^{p_y} + K_z\, h_{z,1}^{p_z} + K_t\, h_{t,1}^{p_t} \\
\phi_\infty - \phi_2 &= K_x\, h_{x,2}^{p_x} + K_y\, h_{y,2}^{p_y} + K_z\, h_{z,2}^{p_z} + K_t\, h_{t,2}^{p_t} \\
\phi_\infty - \phi_3 &= K_x\, h_{x,3}^{p_x} + K_y\, h_{y,3}^{p_y} + K_z\, h_{z,3}^{p_z} + K_t\, h_{t,3}^{p_t} \\
\phi_\infty - \phi_4 &= K_x\, h_{x,4}^{p_x} + K_y\, h_{y,4}^{p_y} + K_z\, h_{z,4}^{p_z} + K_t\, h_{t,4}^{p_t} \\
\phi_\infty - \phi_5 &= K_x\, h_{x,5}^{p_x} + K_y\, h_{y,5}^{p_y} + K_z\, h_{z,5}^{p_z} + K_t\, h_{t,5}^{p_t}
\end{aligned}\right\} \tag{28}$$

In this system of equations, all values of h_d, p_d, ϕ_1, ϕ_2, ϕ_3, ϕ_4 and ϕ_5 are known. The unknown values are the four constants K_d and ϕ_∞. After the solution of this system for ϕ_∞ is obtained, one can determine with Eq. (12) the estimated error of each one of the five numerical solutions used in Eq. (28). Only four or three numerical solutions are necessary, respectively, to obtain ϕ_∞ and to calculate the estimated errors in steady-state three-dimensional and two-dimensional problems. In the one-dimensional case, with only two numerical solutions one can obtain ϕ_∞ and U, as has been demonstrated by Roache (1998, 1994), Marchi and Silva (2002) and Blottner (1990).

In the system of Eqs. (28), it is assumed that the asymptotic orders p_x, p_y, p_z and p_t are known based on the numerical approximations used in the discretization of the differential equation. However, they can be left free, i.e., they can be obtained through the concept of apparent order (De Vahl Davis, 1983). Hence, in the four-dimensional case, there will be four other unknown ones and nine numerical solutions will be needed to obtain ϕ_∞. The one-dimensional case has been shown in Marchi and Silva (2002).

Same Grid Refinement Ratio in All Dimensions

Let us consider two different grids, the first, a fine one, characterized by $h_{x,1}$, $h_{y,1}$, $h_{z,1}$ and $h_{t,1}$, and the second, a coarse one, characterized by $h_{x,2}$, $h_{y,2}$, $h_{z,2}$ and $h_{t,2}$. In a particular case of the grid refinement ratio (r) being the same for all dimensions, i.e.

$$r = \frac{h_{x,2}}{h_{x,1}} = \frac{h_{y,2}}{h_{y,1}} = \frac{h_{z,2}}{h_{z,1}} = \frac{h_{t,2}}{h_{t,1}} \tag{29}$$

where r can take on real values greater than the unit value, it is possible to demonstrate that Eq. (13) results in

$$\begin{aligned}
U(\phi) = {} & h_L^{p_L}\,(a_x\, h_L^{p_x - p_L} + a_y\, h_L^{p_y - p_L} \\
& + a_z\, h_L^{p_z - p_L} + a_t\, h_L^{p_t - p_L})
\end{aligned} \tag{30}$$

where

$$p_L = Min\left(p_x, p_y, p_z, p_t\right) \tag{31}$$

and that a_x, a_y, a_z and a_t are constants; p_L represents the minimum value among the asymptotic orders of the four dimensions, according to Eq. (31); and h_L is the dimension of the grid related

to p_L. For $h_L \to 0$, Eq. (30) is reduced to Eq. (14), which together with Eq. (15) represent precisely the one-dimensional case of the previous section. Hence, Eqs. (14) to (27) can be used to obtain the estimated error of numerical solutions in multi-dimensional problems, as long as the grid refinement ratio (r) remains the same in all the dimensions.

Separate Refinement of a Grid in Each Dimension

Refinement is characterized as separate refinement when each (spatial and temporal) dimension is separately refined from the others, with asymptotic orders (p_L) and grid refinement ratios (r) being equal or different from each other in each dimension. The main reason that justifies using separate refinement is the possibility of obtaining error estimations with smaller grids than those required to carry out simultaneous refinement.

Separate refinement is also important because it provides information on the contribution of each dimension to the discretization error. This information can help to determine if the appropriate number of grid points have been used in each dimension. One wants the contribution to the discretization error from each dimension to be nearly the same.

In multi-dimensional problems, there are several possible ways of carrying out separate refinement to estimate the discretization error of a numerical solution, as can be seen in Fig. 2 for a two-dimensional problem. In this figure, $x3$, $x2$ and $x1$ represent, respectively, the number of nodes, elements or control volumes in the direction x, of the supercoarse, coarse and fine grids. The same applies to $y3$, $y2$ and $y1$ in the direction y. The arrows indicate the extrapolation process that allows one to obtain numerical solutions in the x_∞ and y_∞ grids.

The example shown in Fig. 2 relates, as will seen later on, to the case in which the apparent order (p_U) of each dimension is calculated, in which case three grids are necessary in each dimension, according to Eqs. (16), (19) and (21). But in the case of using the concept of asymptotic order (p_L), only two grids are necessary in each dimension, according to Eqs. (18) and (20).

In Fig. 2, the simultaneous refinement, described in the previous section, is characterized by the diagonal line that links the grids ($x3$,$y3$), ($x2$,$y2$) and ($x1$,$y1$), which represent, respectively, the numerical solutions ϕ_3, ϕ_2 and ϕ_1. Using these numerical solutions and the Richardson extrapolation, Eq. (19), ϕ_∞ can be determined, which is represented by the grid (x_∞,y_∞).

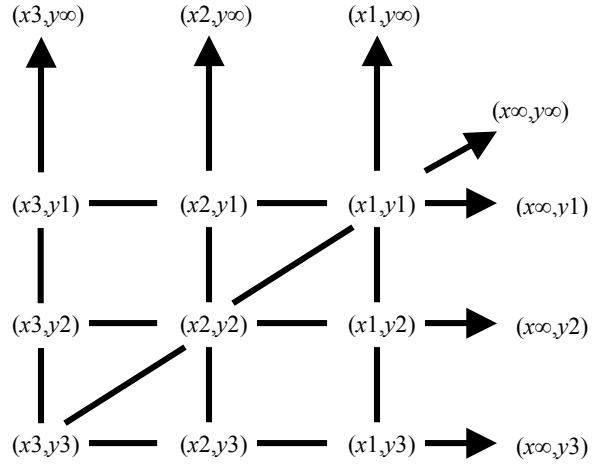

Figure 2. Possibilities for separate refinement in a two-dimensional problem.

The Richardson Error Estimator for Multi-Dimensions

Holding Eq. (13) to be valid and taking the theory of Marchi and Silva (2002) for one-dimensional problems into consideration, the discretization error estimation of the numerical solution can be found for a multi-dimensional problem by using (Roache, 1994)

$$U_b(\phi_b) = \sum_{d=1}^{4} U_d(\phi_b) = U_x(\phi_b) + U_y(\phi_b) + U_z(\phi_b) + U_t(\phi_b) \tag{32}$$

where ϕ_b represents the numerical solution obtained using the grid defined as "the base grid". This grid should be the same one involved in the refinements carried out in all the dimensions. To the example of Fig. 2, if the refinement in the x direction involves the grids ($x3$,$y2$), ($x2$,$y2$) and ($x1$,$y2$), and the refinement in the y direction involves the grids ($x2$,$y3$), ($x2$,$y2$) and ($x2$,$y1$), the base grid is ($x2$,$y2$).

In Eq. (32), $U_b(\phi_b)$ represents the estimated error of the numerical solution ϕ_b. The parameters that appear in Eq. (32) have been calculated through

$$U_d(\phi_b) = sg\left(\phi_{1,d} - \phi_{2,d}\right) Max\left\{\begin{array}{l}\left|\phi_{\infty,d}(p_{L,d}) - \phi_b\right|; \\ \left|\phi_{\infty,d}(p_{U,d}) - \phi_b\right|\end{array}\right\} \tag{33}$$

$$\phi_{\infty,d}(p_{L,d}) = \phi_{1,d} + \frac{(\phi_{1,d} - \phi_{2,d})}{(r_d^{p_{L,d}} - 1)} \tag{34}$$

$$\phi_{\infty,d}(p_{U,d}) = \phi_{1,d} + \frac{(\phi_{1,d} - \phi_{2,d})}{(r_d^{p_{U,d}} - 1)} \tag{35}$$

$$p_{U,d} = \frac{\log\left(\dfrac{\phi_{2,d} - \phi_{3,d}}{\phi_{1,d} - \phi_{2,d}}\right)}{\log(r_d)} \tag{36}$$

$$r_d = \frac{h_{3,d}}{h_{2,d}} = \frac{h_{2,d}}{h_{1,d}} \tag{37}$$

with d = 1, 2, 3 and 4 representing, respectively, the dimensions x, y, z and t; $\phi_{3,d}$, $\phi_{2,d}$ and $\phi_{1,d}$ are the numerical solutions obtained, respectively, using a supercoarse grid ($h_{3,d}$), a coarse grid ($h_{2,d}$) and a fine grid ($h_{1,d}$) in each dimension, which are related through the grid refinement ratio r_d, in Eq. (37); $p_{L,d}$ and $p_{U,d}$ represent the asymptotic and apparent orders of each d dimension.

Let us suppose the apparent order of each dimension ($p_{U,d}$) is convergent, according to the definition of Marchi and Silva (2002), then the true discretization error for the numerical solution ϕ_b, which is $E(\phi_b)$, will be bound by $U_b(\phi_b)$, that is,

$$\frac{U_l(\phi_b)}{E(\phi_b)} \le 1 \le \frac{U_b(\phi_b)}{E(\phi_b)} \tag{38}$$

where $U_I(\phi_b)$ can be obtained through Eq. (32) by substituting *Max* for *Min* in Eq. (33), that is, by reaching the sum of the minimum value of the estimated error in each dimension. In this case, the numerical solution of the variable of interest (ϕ) must be presented or reported by

$$\phi = \phi_b + U_b(\phi_b) \tag{39}$$

The Convergent Error Estimator for Multi-Dimensions

For simultaneous refinement, carried out through Eqs. from (25) to (27), it has been shown that it is possible to reduce the true discretization error (E) using the same set of numerical solutions used to calculate the estimated error (U). This can also be done for separate refinement when Eq. (38) holds true. In this case, adopting the same numerical solutions which are used to calculate $U_b(\phi_b)$, that is, $\phi_{3,d}$, $\phi_{2,d}$ and $\phi_{1,d}$, it is possible to reduce the value of the true discretization error of the numerical solution, $E(\phi_b)$, through

$$\phi_M = \phi_b + \sum_{d=1}^{4} (\phi_{C,d} - \phi_b) \tag{40}$$

$$U_M(\phi_M) = \sum_{d=1}^{4} (U_{C,d}) \tag{41}$$

where (ϕ_M) and (U_M) are called, respectively, "The Convergent Numerical Solution" and "The Convergent Error Estimator" for multi-dimensional problems, and

$$\phi_{C,d} = \frac{\phi_{\infty,d}(p_{L,d}) + \phi_{\infty,d}(p_{U,d})}{2} \tag{42}$$

$$U_{C,d} = \frac{\left|\phi_{\infty,d}(p_{L,d}) - \phi_{\infty,d}(p_{U,d})\right|}{2} \tag{43}$$

in which $\phi_{\infty,d}(p_{L,d})$ and $\phi_{\infty,d}(p_{U,d})$ are provided by Eqs. (34) and (35).

Equations (40) and (41) are equivalent, respectively, to Eqs. (25) and (27) used in simultaneous refinement. For ϕ_M, the numerical solution of the variable of interest (ϕ) should be presented or reported by

$$\phi = \phi_M \pm U_M(\phi_M) \tag{44}$$

The techniques adopted for simultaneous refinement and separate refinement can be used together in the so-called mixed refinement. In a transient two-dimensional problem (x,y,t), for example, simultaneous refinement may be adopted in the x and y directions, while separate refinement is taken up between (x,y) and the time (t).

Results

In this section, numerical results to three problems are shown and described to illustrate how the theory explained in previous sections is applied.

Definition of the Problems

Problem 1 consists of a two-dimensional steady-state heat conduction (Incropera and DeWitt, 1996), described by the Laplace equation (Kreyszig, 1999), Eq. (1). The boundary conditions are of the Dirichlet type at the four sides of a square domain having one unit side, with $\Lambda(x,1) = \sin(\pi x)$ and $\Lambda = 0$ in the other three contours. The analytical solution is

$$\Lambda(x,y) = \sin(\pi x)\frac{\sinh(\pi y)}{\sinh(\pi)} \tag{45}$$

Problem 2 consists of a transient one-dimensional heat conduction (Incropera and DeWitt, 1996), as defined by the equation

$$\frac{\partial \Lambda}{\partial t} = \frac{\partial^2 \Lambda}{\partial x^2} \tag{46}$$

The Dirichlet boundary conditions are $\Lambda(0,t) = \Lambda(1,t) = 0$, and the initial condition is given by $\Lambda(x,0) = \sin(\pi x)$. The analytical solution is

$$\Lambda(x,t) = \sin(\pi x)\, e^{-\pi^2 t} \tag{47}$$

The solution to the problem is obtained for the instant in time t = 0.1 s.

Problem 3 consists of a two-dimensional incompressible Navier-Stokes flow within a square cavity, having a unit side, and with a lid that moves, making the fluid flow along the inside of the cavity. This problem is modeled by the Navier-Stokes equations and described in section 2 of Shih, Tan and Hwang (1989). The mathematical model involves the mass conservation equation and the x- and y-momentum equations, maintaining constant values for viscosity and mass density. A source term is added to obtain an analytical solution to the problem for its three unknown values: two being components of velocity (u, v) and the other pressure. The analytical solution to this problem is provided by Shih, Tan and Hwang (1989).

For Problems 1 and 2, the two variables of interest, that is, the variables for which the true errors and their estimations are being analyzed are the temperature at the center of the solution domain and the average temperature of the field. In the case of Problem 3, the variables of interest are u and v, at the center of the domain, and the mass flow rate (M) that is circulating within the cavity from y = 0 up to y = ½ at x = ½.

The finite difference method was used for Problems 1 and 2, and the finite volume method (Marchi and Maliska, 1994) for Problem 3. In the three problems, the spatial derivatives were given approximated values through the central difference scheme (Ferziger and Peric, 1999). Equation (46) was discretized through the implicit Euler method (Ferziger and Peric, 1999). In Problems 1 and 3, iterations were carried out until the iteration errors reached round-off level to minimize their effects on the discretization errors. The solution to Problem 2 was obtained with one iteration of the TDMA method (Ferziger and Peric, 1999) at each time step.

Same Grid Refinement Ratio in All Dimensions

Adopting simultaneous refinement in the three multi-dimensional problems described above, the same conclusions were reached as those reached in Marchi and Silva (2002) with respect to one-dimensional problems. Some of the results are commented as follows.

Table 1 presents the numerical solutions of Λ(½,½) that were obtained in three different grids for Problem 1. Φ represents the

analytical solution of the variable of interest, that is, the temperature at the center of the solution domain. ϕ_3, ϕ_2 and ϕ_1 represent the numerical solutions. The use of the Richardson error estimator (U_{Ri}), which involves Eqs. from (16) to (24), is shown in the left-hand column of Table 2, where the equation used to calculate each parameter is indicated. The true discretization error (E) is calculated by using Eq. (11). The use of the convergent error estimator (U_C), which involves Eqs. from (25) to (27), is shown in the right-hand column of Table 2.

Table 1. Numerical solutions for Problem 1, Eq. (1), for Λ(½,½).

grid (x*y)	numerical solution	other data
5 * 33	$\phi_3 = 0.206809183$	$r = 2$
9 * 65	$\phi_2 = 0.201144859$	$p_L = 2$
17 * 129	$\phi_1 = 0.199736958$	$\Phi = 0.199268408$

Results for many different grids are presented in Fig. 3. In this figure, for Problem 1, the estimated errors $U_{Ri}(\phi_1)$ and $U_C(\phi_C)$ and the true discretization errors $E(\phi_1)$ and $E(\phi_C)$ of the temperature at the center of the domain are shown. The results refer to grids of 3x3 to 1025x1025 points, where $r = 2$. In this figure, one can see the significant advantage of using ϕ_C, instead of ϕ_1, for reducing the true discretization error. It can also be verified that the estimated error by both the Richardson estimator (U_{Ri}) as well as the convergent estimator (U_C) are reliable for any h_L.

Table 2. Application of the Richardson and Convergent error estimators to the numerical solutions shown in Table 1.

Richardson estimator	Convergent estimator
(Eq. 18) $\phi_\infty(p_L) = 0.199267658$	(Eq. 25) $\phi_C = 0.199269462$
(Eq. 16) $p_U = 2.008358693$	(Eq. 27) $U_C(\phi_C) = \pm 0.000001804$
(Eq. 19) $\phi_\infty(p_U) = 0.199271266$	(Eq. 11) $E(\phi_C) = - 0.000001054$
(Eq. 24) $U_{Ri}(\phi_1) = - 0.000469300$	$U_C(\phi_C) / E(\phi_C) = 1.71$
(Eq. 11) $E(\phi_1) = - 0.000468550$	$U_C(\phi_C) / U_{Ri}(\phi_1) = 0.00384$
$U_{Ri}(\phi_1) / E(\phi_1) = 1.0016$	$U_{Ri}(\phi_1) / U_C(\phi_C) = 260$
(Eq. 23):	(Eq. 26):
$\phi = 0.199736958 - 0.000469300$	$\phi = 0.199269462 \pm 0.000001804$
	$E(\phi_1) / E(\phi_C) = 445$

Table 3 shows the numerical solutions of u(½,½) obtained from three different grids for Problem 3. Φ represents the exact analytical solution of the variable of interest, that is, the component of velocity in the x direction in the center of the solution domain. ϕ_3, ϕ_2 e ϕ_1 represent the numerical solutions. The use of the Richardson error estimator (U_{Ri}), which involves Eqs. from (16) to (24), is shown in the left-hand column of Table 4, where the equation used to calculate each parameter is indicated. The true discretization error (E) is calculated by using Eq. (11). The use of the convergent error estimator (U_C), which involves Eqs. from (25) to (27), is shown in the right-hand column of Table 4.

Table 3. Numerical solutions for Problem 3 for u (½,½).

grid (x*y)	numerical solution	other data
4 * 4	$\phi_3 = - 0.172578576$	$r = 2$
8 * 8	$\phi_2 = - 0.226911929$	$p_L = 2$
16 * 16	$\phi_1 = - 0.243644223$	$\Phi = - ¼$

Table 4. Application of the Richardson and Convergent error estimators to the numerical solutions shown in Table 3.

Richardson estimator	Convergent estimator
(Eq. 18) $\phi_\infty(p_L) = - 0.249221654$	(Eq. 25) $\phi_C = - 0.250155835$
(Eq. 16) $p_U = 1.699202828$	(Eq. 27) $U_C(\phi_C) = \pm 0.000934181$
(Eq. 19) $\phi_\infty(p_U) = - 0.251090015$	(Eq. 11) $E(\phi_C) = 0.000155835$
(Eq. 24) $U_{Ri}(\phi_1) = - 0.007445792$	$U_C(\phi_C) / E(\phi_C) = 5.995$
(Eq. 11) $E(\phi_1) = - 0.006355777$	$U_C(\phi_C) / U_{Ri}(\phi_1) = 0.125$
$U_{Ri}(\phi_1) / E(\phi_1) = 1.171$	$U_{Ri}(\phi_1) / U_C(\phi_C) = 7.97$
(Eq. 23):	(Eq. 26):
$\phi = - 0.243644223 - 0.007445792$	$\phi = - 0.250155835 \pm 0.000934181$
	$E(\phi_1) / E(\phi_C) = - 40.8$

In Tables 2 and 4 one can see the key information: (i) the estimated error by the Richardson estimator (U_{Ri}) is reliable, seeing as $U_{Ri}(\phi_1)/E(\phi_1) > 1$, and it is accurate because $U_{Ri}(\phi_1)/E(\phi_1) \approx 1$; (ii) the relationship of Eq. (22) is met once $\phi_\infty(p_L)$ and $\phi_\infty(p_U)$ bound Φ; and (iii) both the estimated error as well as the true error of the convergent numerical solution (ϕ_C) are much smaller than the calculated numerical solution (ϕ_1) since $U_C(\phi_C)/U_{Ri}(\phi_1)$ and $E(\phi_C)/E(\phi_1) << 1$.

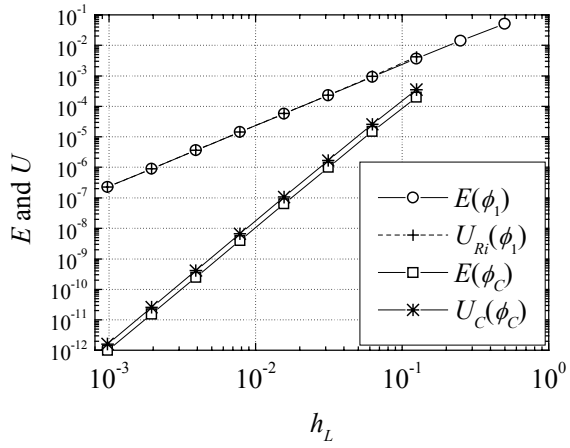

Figure 3. Modules of the estimated error (U) and of the true error (E) for Λ(½,½) in Problem 1.

Table 5 displays the values obtained for apparent order (p_U) of the variables of interest in Problems 1, 2 and 3, using simultaneous refinement and the grid refinement ratio $r = 2$. The expected asymptotic order (p_L) is also shown, which is obtained from the truncation error inferred with the Taylor expansion series on the discretized mathematical model, as shown in Eqs. (6) and (7). The size of the grids displayed in Table 5 refer to finest grids. Hence, to calculate the apparent order (p_U), through Eq. (16), two coarser grids were used in each case. For example, for Problem 3 the grids 256*256, 128*128 and 64*64 were used.

Separate Refinement of a Grid in Each Dimension

The numerical solutions of Problem 2, Eq. (46), are shown in Table 6, for the temperature in the center of the domain. In this case, seeing as it is a two-dimensional problem, the calculation of the estimated error (U_b) involves numerical solutions obtained in five different grids. In this example, the grid 65*750 was chosen

as the grid common to both dimensions, that is, it is the base grid, hence, $\phi_b = \phi_{2,x} = \phi_{2,t}$.

Table 5. Apparent orders (p_U), for r = 2, and asymptotic orders (p_L) for simultaneous refinement.

Problem	variable	grid	p_U	p_L
1	central Λ	1025 * 1025	1.999984	2
1	average Λ	1025 * 1025	1.999903	2
2	central Λ	4097 * 2048	1.000004	1
2	average Λ	4097 * 2048	0.999109	1
3	central u	256 * 256	1.996552	2
3	central v	256 * 256	1.982185	2
3	mass flow rate	256 * 256	2.012358	2

Through analyzing the truncation errors of the numerical approximations used to discretize Eq. (46), it was determined that their asymptotic orders are $p_{L,x} = 2$ and $p_{L,t} = 1$. In this example, the refinement ratio of the grid in the x dimension ($r_x = 2$) is different from the t dimension ($r_t = 1.5$). Through Eqs. from (33) to (36), $p_{L,x}$, $p_{L,t}$ and with the numerical solutions given in Table 6, one can reach the results presented in Table 7. With these results, in turn, one can use the Richardson error estimator (U_b), through Eqs. from (32) to (37) and (39), to find the results shown on the left-hand column of Table 8. It should be noted that $U_b(\phi_b)/E(\phi_b) > 1$, in other words, the estimated error $U_b(\phi_b)$ is reliable for it overestimates the true error $E(\phi_b)$, and it is quite accurate, seeing as $U_b(\phi_b)/E(\phi_b) \approx 1$.

Table 6. Numerical solutions for Problem 2, Eq. (46), for Λ in x = ½ and t = 0.1.

refinement in x ($r_x = 2$)	refinement in t ($r_t = 1.5$)	other data
grid 33*750: $\phi_{3,x} = 0.373245017$	grid 65*500: $\phi_{3,t} = 0.373144380$	$p_{L,x} = 2$
grid 65*750: $\phi_{2,x} = 0.373023555$	grid 65*750: $\phi_{2,t} = 0.373023555$	$p_{L,t} = 1$
grid 129*750: $\phi_{1,x} = 0.372968193$	grid 65*1125: $\phi_{1,t} = 0.372942967$	$\Phi = 0.372707839$

Table 7. Calculation of the components of the estimated error for separate refinement in Problem 2.

Equation	refinement in x	refinement in t
Eq. (34)	$\phi_{\infty,x}(p_{L,x}) = 0.372949739$	$\phi_{\infty,t}(p_{L,t}) = 0.372862379$
Eq. (36)	$p_{U,x} = 2.000091205$	$p_{U,t} = 0.998836779$
Eq. (35)	$\phi_{\infty,x}(p_{U,x}) = 0.372949741$	$\phi_{\infty,t}(p_{U,t}) = 0.372781563$
Eq. (33)	$U_x(\phi_b) = - 0.000073816$	$U_t(\phi_b) = - 0.000241992$

The use of the convergent error estimator (U_M) is shown in the right-hand column of Table 8. To do so, Eqs. from (40) to (44) were used based on the same numerical solutions of Problem 2 given in Table 6 and adopting the parameters provided in Table 7. One can see in Table 8 that $U_M(\phi_M)/E(\phi_M) = 1.00228$, that is, the estimated error $U_M(\phi_M)$ is reliable for it overestimates the value of the true error $E(\phi_M)$. Moreover, there have been significant reductions in both the estimated error as well as the true error of the convergent numerical solution (ϕ_M) with respect to the calculated numerical solution (ϕ_b) seeing as $U_M(\phi_M)/U_b(\phi_b)$ and $E(\phi_M)/E(\phi_b) << 1$.

Table 8. Application of the Richardson and Convergent error estimators to the numerical solutions shown in Table 6.

Richardson estimator	Convergent estimator
(Eq. 32): $U_b(\phi_b) = - 0.000315808$	(Eq. 42) $\phi_{C,x} = 0.372949740$
(Eq. 39) $\phi = 0.373023555 - 0.000315808$	(Eq. 43) $U_{C,x} = \pm 0.000000001$
(Eq. 11): $E(\phi_b) = - 0.000315716$	(Eq. 42) $\phi_{C,t} = 0.372821971$
$U_b(\phi_b) / E(\phi_b) = 1.00029$	(Eq. 43) $U_{C,t} = \pm 0.000040408$
	(Eq. 40) $\phi_M = 0.372748156$
	(Eq. 41) $U_M(\phi_M) = \pm 0.000040409$
	(Eq. 44): $\phi = 0.372748156 \pm 0.000040409$
	(Eq. 11) $E(\phi_M) = - 0.000040317$
	$U_M(\phi_M) / E(\phi_M) = 1.00228$
	$U_M(\phi_M) / U_b(\phi_b) = 0.128$
	$U_b(\phi_b) / U_M(\phi_M) = 7.82$
	$E(\phi_b) / E(\phi_M) = 7.83$

Conclusion

Two procedures were presented to estimate the error of numerical solutions in multi-dimensional problems. Both of the procedures are based on Richardson extrapolation which makes use of multiple grids. In the first procedure, the number of nodes, elements or control volumes of all four dimensions (x, y, z, t) vary among the grids used to estimate the discretization error. In the second procedure, each (spatial and temporal) dimension is separately refined from the others, with asymptotic orders (p_L) and grid refinement ratios (r) being equal or different from each other in each dimension.

These two procedures have been named, respectively, simultaneous refinement and separate refinement. They have been proven to work successfully in the tests carried out, which involved three different problems: two-dimensional steady-state heat conduction, one-dimensional transient heat conduction and two-dimensional incompressible Navier-Stokes flow. The problems were solved by finite difference and finite volume methods for three types of variables of interest: the dependent variables (Λ,u,v), the averages of the dependent variables in the whole field (average Λ) and the integration of a dependent variable (M).

It was shown that the use of simultaneous refinement in multi-dimensional problems is the same as for one-dimensional problems. This occurs if the same grid refinement ratio is used in all dimensions and if the apparent order (p_U) of the estimated error is of the monotone convergent type. In this case, all of the conclusions of Marchi and Silva (2002) prove valid, among which the following are worthy of note: the true discretization error (E) is bound by the estimated values of error found by the Richardson error estimator (U_{Ri}), which are calculated based on the asymptotic (p_L) and apparent (p_U) orders; the true error and the estimated error of the numerical solution can be reduced in a reliable manner by adopting the convergent numerical solution (ϕ_C) and its respective convergent error estimator (U_C); and, outside of the convergent interval of the apparent order (p_U) there is no guarantee as to validity of the two previous conclusions.

The conclusions reached for simultaneous refinement also hold true for separate refinement provided: the apparent order (p_U) of each dimension is of the monotone convergent type and that there is one grid (a base grid) common to all of the refinements carried out in all of the dimensions.

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