Multi-dimensional Discretization Error Estimation for Convergent Apparent Order

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, and time) 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 $G_{CI}$ 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 Valdi 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 $\text{a posteriori}$ 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 (Perziger 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

- $c_\text{r}$ = coefficients in the truncation error equation
- $c_\text{d}$ = coefficients in the discretization error equation
- $E = \frac{c_\text{d}}{c_\text{r}}$ = discretization error of the numerical solution
- $h$ = grid spacing or distance between two successive grid points
- $k$ = coefficients in the numerical solution uncertainty equation
- $p_\text{as}$ = asymptotic order of the discretization error
- $\rho_\text{a}$ = apparent order of the uncertainty
- $r_\text{ef}$ = grid refinement ratio
- $t$ = time
- $U$ = uncertainty or estimated error of the numerical solution
- $U_\text{ce}$ = uncertainty of the numerical solution by the convergent estimator
- $U_\text{re}$ = uncertainty of the numerical solution by the Richardson estimator
- $x, y, z$ = spatial coordinates

Greek Symbols

- $\varepsilon$ = truncation error
- $\Phi$ = numerical solution of the variable of interest
- $\Phi^*$ = exact analytical solution of the variable of interest

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References

- De Valdi Davis, 1983
- Roache, 1998
- Roy and Blottner, 2001
- Marchi and Silva, 2002

Keywords: Discretization error, truncation error, CFD, numerical error, fluid flows

\[ \phi = \text{convergent numerical solution} \]

\[ \phi_e = \text{estimated analytical solution} \]

\[ \Lambda = \text{dependent variable} \]

**Subscripts**

1. fine grid
2. coarse grid
3. super coarse grid
4. base grid
5. dimension \((1 = x, 2 = y, 3 = z, 4 = \gamma)\)

**Multi-Dimensional Discretization Error**

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

\[ \frac{\partial^2 \Lambda}{\partial x^2} + \frac{\partial^2 \Lambda}{\partial y^2} = 0 \]  

(1)

where \(x\) and \(y\) are the independent variables and \(\Lambda\) 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.,

\[ \left( \frac{\partial^2 \Lambda}{\partial x^2} \right)_p = \frac{(\Lambda_n + \Lambda_n - 2\Lambda_p)}{h_x^2} \]  

(2)

\[ \left( \frac{\partial^2 \Lambda}{\partial y^2} \right)_p = \frac{(\Lambda_n + \Lambda_n - 2\Lambda_p)}{h_y^2} \]  

(3)

where

\[ h_x = x_{p+1} - x_p = x_{x-1} - x_p = \ldots = \text{constant 1} \]  

(4)

\[ h_y = y_{p+1} - y_p = y_{y-1} - y_p = \ldots = \text{constant 2} \]  

(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 \(x\), \(y\), \(z\) and \(\gamma\) 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 \(\varepsilon\) (Tannehill, Anderson and Pletcher, 1997) of the numerical approximations given in Eqs. (2) and (3) are, respectively,

\[ \varepsilon = \left( \frac{\partial^2 \Lambda}{\partial x^2} \right)_p = \frac{\partial^2 \Lambda}{\partial x^2} \frac{h_x^2}{12} \left( \frac{\partial^6 \Lambda}{\partial x^6} \right)_p 360 \]  

(6)

\[ \varepsilon = \left( \frac{\partial^2 \Lambda}{\partial y^2} \right)_p = \frac{\partial^2 \Lambda}{\partial y^2} \frac{h_y^2}{12} \left( \frac{\partial^6 \Lambda}{\partial y^6} \right)_p 360 \]  

(7)

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

\[ \left( \frac{(\Lambda_n + \Lambda_n - 2\Lambda_p)}{h_x^2} \right) + \left( \frac{(\Lambda_n + \Lambda_n - 2\Lambda_p)}{h_y^2} \right) = 0 \]  

(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 \((\Lambda_{x,y,z,\gamma})\) that has many terms in each dimension, with derivatives of several different orders, the truncation error of the discretized differential equation \((\Lambda_{x,y,z,\gamma})\), in each node of the grid, results in

\[ \varepsilon_{DDE} = \sum_{\gamma} \sum_{\lambda} \left( \frac{(\Lambda_n + \Lambda_n - 2\Lambda_p)}{h_x^2} \right) \]  

(9)

where \(\gamma = 1, 2, 3, 4\) represents, respectively, the dimensions \(x, y, z, \gamma\) and \(\lambda, \mu, \nu, \rho\) represents the distance between two consecutive nodes of the grid in each \(\lambda\) dimension. \(\lambda\) represents each one of the terms of the infinite series, as in Eqs. (6) and (7); \(c_{\lambda,\mu,\nu,\rho}\) represent coefficients that depend on the derivatives of \(\Lambda\) in each node of the grid, but do not depend on \(h_x, h_y, h_z, h_{\gamma}\), which 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.](image)

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

\[ \varepsilon(\phi) = \sum_{\gamma} \sum_{\lambda} \left( \frac{(\Lambda_n + \Lambda_n - 2\Lambda_p)}{h_x^2} \right) \]  

(10)

in which \(\phi\) can be the numerical solution of the dependent variable \(\Lambda\) in the differential equation, at a specific coordinate, its average of the whole field, or any other variable obtained from \(\Lambda\); and the coefficients \(c_{\lambda,\mu,\nu,\rho}\) and the exponents \(p, q, r, s\) may or may not be equal to the coefficients \(x, y, z, \gamma\) of Eq. (9), depending on \(\phi\). The true discretization error of the numerical solution \((\phi)\) can also be defined by

\[ \varepsilon(\phi) = \Phi - \phi \]  

(11)

Determining the true discretization error through Eq. (10) or (11) requires knowing the exact analytical solution \((\Phi)\). Unfortunately, in practical problems, \(\Phi\) is unknown. In such cases, the concept of estimated error \((\varepsilon)\) is adopted, which is defined by

\[ \varepsilon(\phi) = \phi - \phi \]  

(12)
where \( \phi_e \) represents an estimation of \( \Phi \). 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 \( h \rightarrow 0 \). Thus, one obtains

\[
U(\phi) = K_1 h_1^{p_x} + K_2 h_2^{p_y} + K_3 h_3^{p_z} + K_4 u_x^{p_x} + K_5 u_y^{p_y} + K_6 u_z^{p_z} \tag{13}
\]

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

Obtaining \( \phi_e \) 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

\[
U(\phi) = K_U h_1^{p_x} \tag{14}
\]

where \( K_U \) is a constant and \( h_1 \) is the grid spacing and \( p_x \) is the asymptotic order of the true discretization error. In Eq. (14), instead of using \( p_x \), one can also use the concept of apparent order \( (p_a) \) (De Vahl Davis, 1983), i.e.,

\[
U(\phi) = K_U h_1^{p_a} \tag{15}
\]

where \( K_U \) is a constant and

\[
p_a = \log_{0.1} \left( \frac{\phi_2 - \phi_1}{\phi_1 - \phi_2} \right) \tag{16}
\]

for a constant grid refinement ratio \( (\varepsilon) \), defined by

\[
\varepsilon = \frac{h_{1,2}}{h_{1,1}} = \frac{h_{1,3}}{h_{1,2}} \tag{17}
\]

where \( \phi_1, \phi_2 \), and \( \phi \) are the numerical solutions obtained, respectively, with the fine grid \( (h_{1,1}) \), coarse grid \( (h_{1,2}) \) and supercoarse grid \( (h_{1,3}) \).

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

If the apparent order \( (p_a) \) is monotonically convergent, then the exact analytical solution \( (\Phi) \) will be bound between \( \phi_a(p_a) \) and \( \phi_{e_p}(p) \), with

\[
\phi_a(p_a) = \phi_a(p) \tag{18}
\]

\[
\phi_{e_p}(p) = \phi_{e_p}(p) \tag{19}
\]

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

\[
U_a(\phi_1, p_x) = \frac{\phi_1 - \phi_2}{(\varepsilon - 1)} \tag{20}
\]

\[
U_a(\phi_1, p_y) = \frac{\phi_1 - \phi_2}{(\varepsilon - 1)} \tag{21}
\]

which represent the estimated errors of the numerical solution \( \phi \) according to the Richardson error estimator \( (U_a) \). It was demonstrated that

\[
\frac{U_a(\phi_1, p_x)}{U_a(\phi_1, p_y)} \leq 1 \leq \frac{U_a(\phi_1, p_y)}{U_a(\phi_1, p_x)} \tag{22}
\]

in which \( p_x \) and \( p_y \) represent the asymptotic order \( (p) \) or the apparent order \( (p_a) \) depending on whether \( p_x \) is subconvergent or superconvergent. Within the convergent interval of \( p_x \), 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 \( p_x \), this relation can or not works. One has not found a procedure to estimate a priori the beginning of the convergent interval of \( p_x \).

An estimated error \( (\varepsilon) \) may be defined as reliable when the ratio between estimated error \( (\varepsilon) \) and true error \( (\varepsilon) \) is larger or equal to unity. According to Eq. (22), the true discretization error of the numerical solution \( \phi_e \), \( \varepsilon(\phi_e) \), is bound by the estimated errors \( U_a(\phi_1, p_x) \) and \( U_a(\phi_1, p_y) \). Therefore, if the objective is to obtain a reliable estimated error, the numerical solution of the variable of interest \( (\phi) \) should be presented or reported by

\[
\phi = \phi_1 + U_a(\phi_1) \tag{23}
\]

where

\[
U_a(\phi_1) = U_a(\phi_1, p_x) \max \left\{ \left| \frac{\phi_1 - \phi_2}{(\varepsilon - 1)} \right| \right\} \tag{24}
\]

with \( \varepsilon(\phi_1 - \phi_2) \) representing the sign of the difference between \( \phi_1 \) and \( \phi_2 \), and \( \max \{ \} \), the maximum between the modules of \( U_a(\phi_1, p_x) \) and \( U_a(\phi_1, p_y) \).

**The Convergent Error Estimator for One-Dimension**

With the same numerical solutions \( (\phi, \phi_1, \phi_2 \) and \( \phi \) 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, \( g(\phi) \), through "The Convergent Numerical Solution" \( (\phi) \), defined by

\[
\phi = \frac{\phi_a(p_a) + \phi_{e_p}(p)}{2} \tag{25}
\]
where \( \phi_{0}(p) \) and \( \phi_{\infty}(p) \) are obtained by the Richardson extrapolation, Eqs. (18) and (19). For \( \phi_{c} \), the numerical solution of the variable of interest \( \phi \) should be presented or reported by

\[
\phi = \phi_{c} \pm U_{c}(\phi_{c})
\]

(26)

in which the estimated error of \( \phi_{c} \), \( U_{c}(\phi_{c}) \), is equal to the modulus of half of the interval between \( \phi_{0}(p) \) and \( \phi_{\infty}(p) \), that is,

\[
U_{c}(\phi_{c}) = \frac{|\phi_{\infty}(p) - \phi_{0}(p)|}{2}
\]

(27)

Hereafter, \( U_{c} \) is called "The Convergent Error Estimator."

Within the convergent interval of \( p \), it is advisable to use the convergent numerical solution \( \phi_{c} \) instead of the calculated numerical solution (\( \phi_{0} \)) because the true discretization error of \( \phi_{c} \) is smaller than the true discretization error of \( \phi_{0} \).

**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 \( 10 \times 10 \times 10 \) to \( 20 \times 20 \times 20 \) 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 \( h_{x,1}, h_{x,2}, h_{y,1}, h_{y,2}, h_{z,1}, h_{z,2}, h_{t,1}, h_{t,2} \) and \( h_{x,3}, h_{x,4}, h_{y,3}, h_{y,4}, h_{z,3}, h_{z,4}, h_{t,3}, h_{t,4} \), and whose numerical solutions are, respectively, \( \phi_{1}, \phi_{2}, \phi_{3}, \phi_{4} \) and \( \phi_{5} \), one can obtain

\[
\begin{align*}
\phi_{5} - \phi_{1} & = K_{11} h_{x,1}^{p_{x,1}} + K_{12} h_{x,2}^{p_{x,2}} + K_{13} h_{x,3}^{p_{x,3}} + K_{14} h_{x,4}^{p_{x,4}} \\
\phi_{5} - \phi_{2} & = K_{21} h_{x,1}^{p_{x,1}} + K_{22} h_{x,2}^{p_{x,2}} + K_{23} h_{x,3}^{p_{x,3}} + K_{24} h_{x,4}^{p_{x,4}} \\
\phi_{5} - \phi_{3} & = K_{31} h_{x,1}^{p_{x,1}} + K_{32} h_{x,2}^{p_{x,2}} + K_{33} h_{x,3}^{p_{x,3}} + K_{34} h_{x,4}^{p_{x,4}} \\
\phi_{5} - \phi_{4} & = K_{41} h_{x,1}^{p_{x,1}} + K_{42} h_{x,2}^{p_{x,2}} + K_{43} h_{x,3}^{p_{x,3}} + K_{44} h_{x,4}^{p_{x,4}}
\end{align*}
\]

(28)

In this system of equations, all values of \( p_{x}, p_{y}, p_{z}, p_{t}, q_{x}, q_{y}, q_{z}, q_{t} \) and \( \phi_{5} \) are known. The unknown values are the four constants \( K_{51}, K_{52}, K_{53}, K_{54} \) and \( \phi_{5} \). After the solution of this system for \( \phi_{5} \), \( \phi_{5} \) 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 \( \phi_{5} \) 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 \( \phi_{5} \) and \( U_{c} \), 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 \( p_{x}, p_{y}, p_{z}, p_{t}, q_{x}, q_{y}, q_{z}, q_{t} \) 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 \( \phi_{5} \). 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 \( h_{x,1}, h_{x,2}, h_{y,1}, h_{y,2} \), and the second, a coarse one, characterized by \( h_{x,1}, h_{x,2}, h_{y,1}, h_{y,2} \). In a particular case of the grid refinement ratio \( \lambda \) being the same for all dimensions, i.e.

\[
\begin{align*}
\lambda_{x} &= \frac{h_{x,2}}{h_{x,1}} = \frac{h_{y,2}}{h_{y,1}} = \frac{h_{z,2}}{h_{z,1}} = \lambda_{1}
\end{align*}
\]

(29)

where \( \lambda_{1} \) can take on real values greater than one unit, it is possible to demonstrate that Eq. (13) results in

\[
U(\phi) = \lambda_{1}^{p_{L}} (a_{x} h_{x,1}^{p_{x,1}} + a_{y} h_{y,1}^{p_{y,1}} + a_{z} h_{z,1}^{p_{z,1}})
\]

(30)

where

\[
p_{L} = \text{Min} \left( p_{x}, p_{y}, p_{z}, p_{t} \right)
\]

(31)

and that \( a_{x}, a_{y}, a_{z}, a_{t} \) 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 \( h_{L} \rightarrow 0 \), 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 \( \lambda \) 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 \( q_{x}, q_{y}, q_{z}, q_{t} \) and grid refinement ratios \( \lambda_{x}, \lambda_{y}, \lambda_{z}, \lambda_{t} \) 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, \( s_{x}, s_{y} \) and \( s_{z} \) 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 \( s_{y}, s_{z}, s_{t} \) and \( s_{z}, s_{t} \) in the direction \( y \). The arrows indicate the extrapolation process that allows one to obtain numerical solutions in the \( \lambda_{x}, \lambda_{y}, \lambda_{z}, \lambda_{t} \) grids.

The example shown in Fig. 2 relates, as will be seen later on, to the case in which the apparent order \( q_{x} \) 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 \( p_m \), 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 \((s_1, 2s_2, 2s_3)\), \((2s_1, s_2, 2s_3)\) and \((2s_1, 2s_2, s_3)\), which represent, respectively, the numerical solutions \(\phi_1\), \(\phi_2\) and \(\phi_3\). Using these numerical solutions and the Richardson extrapolation, Eq. (19), \(\phi_w\) can be determined, which is represented by the grid \((s_1, 2s_2, 2s_3)\).

\[
\phi_{w,1}(p_{U,w}) = \phi_w + \frac{\phi_{u,1}(p_{U,w}) - \phi_{u,2}(p_{U,w})}{\left(\frac{s_1}{s_1} - 1\right)}
\]

with \(j = 1, 2, 3\) and 4 representing, respectively, the dimensions \(x, y, z\) and \(i\); \(\phi_{u,1}, \phi_{u,2}, \phi_{u,3}\) and \(\phi_{u,4}\) are the numerical solutions obtained, respectively, using a supercoarse grid \((s_1, s_2, s_3)\), a coarse grid \((2s_1, s_2, s_3)\) and a fine grid \((s_1, 2s_2, 2s_3)\) in each dimension, which are related through the grid refinement ratio \(r_{s,1}\) in Eq. (37); \(p_{U,1}\) and \(p_{U,2}\) represent the asymptotic and apparent orders of each \(s\) dimension.

Let us suppose the apparent order of each dimension \((s_{i,j})\) is convergent, according to the definition of Marchi and Silva (2002), then the true discretization error for the numerical solution \(\phi_s\), which is \(\varepsilon(\phi_s)\), will be bound by \(u_s(\phi_s)\), that is,

\[
\frac{\varepsilon(\phi_s)}{E(\phi_m)} \leq 1 \leq \frac{u_s(\phi_s)}{E(\phi_m)}
\]

where \(u_s(\phi_s)\) can be obtained through Eq. (32) by substituting \(M_{max}\) for \(M_{nit}\) 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 \(\phi\) must be presented or reported by

\[
\phi = \phi_s + u_s(\phi_s)
\]

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 (Rouche, 1994)

\[
u_s(\phi) = \frac{4}{s_1} \nu_s(\phi) = \nu_s(\phi) + \nu_s(\phi) + \nu_s(\phi)
\]

where \(\phi_s\) 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 \(y\) direction involves the grids \((s_1, 2s_2, 2s_3)\), \((2s_1, s_2, 2s_3)\) and \((2s_1, 2s_2, s_3)\), and the refinement in the \(x\) direction involves the grids \((s_1, 2s_2, 2s_3)\), \((s_1, 2s_2, 2s_3)\) and \((s_1, 2s_2, s_3)\), the base grid is \((s_1, 2s_2, 2s_3)\).

In Eq. (32), \(u_s(\phi)\) represents the estimated error of the numerical solution \(\phi_s\). The parameters that appear in Eq. (32) have been calculated through

\[
u_s(\phi) = \nu_s(\phi) + \nu_s(\phi) + \nu_s(\phi)
\]

where \(\phi_{u,1}\) and \(\phi_{u,2}\) are called, respectively, "The Convergent Numerical Solution" and "The Convergent Error Estimator" for multi-dimensional problems, and

\[
\phi_{u,1}(p_{U,1}) = \frac{\phi_{u,2}(p_{U,2}) - \phi_{u,3}(p_{U,3})}{2}
\]

\[
\phi_{u,2}(p_{U,2}) = \frac{\phi_{u,3}(p_{U,3}) - \phi_{u,4}(p_{U,4})}{2}
\]
Multi-dimensional Discretization Error Estimation for Convergent Apparent Order

in which $\phi_n(y_{ij})$ and $\phi_n(x_{ij})$ are provided by Eqs. (34) and (35). Equations (40) and (41) are equivalent, respectively, to Eqs. (25) and (27) used in simultaneous refinement. For $\phi_n$, the numerical solution of the variable of interest ($\phi$) should be presented or reported by

$$
\phi = \phi_n \pm u_n(\phi_n)
$$

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 ($\phi(y_{ij})$), for example, simultaneous refinement may be adopted in the $x$ and $y$ directions, while separate refinement is taken up between ($x_{ij}$) and the time ($t_j$).

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 (Kreyzig, 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

$$
\lambda(x, 1) = \sin(\pi x)
$$

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

$$
\frac{\partial \lambda}{\partial t} = \frac{\partial^2 \lambda}{\partial x^2}
$$

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

$$
\lambda(x, t) = \sin(\pi x)e^{-t}
$$

The solution to the problem is obtained for the instant in time $\tau = 0.1$. 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 variables: two being components of velocity ($u_x, u_y$) 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 $u_x$ and $u_y$, at the center of the domain, and the mass flow rate ($\psi$) through that cavity, which is circularly within the cavity from $r = 0$ up to $r = 0.5$ at $\psi = 0.5$.

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

Adapting 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 $\lambda(x, 1)$ that were obtained in three different grids for Problem 1. $\phi$ represents the analytical solution of the variable of interest, that is, the temperature at the center of the solution domain. $\phi_n$, $\phi_0$, and $\phi_1$ represent the numerical solutions. The use of the Richardson error estimator ($\psi_n$), 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 ($\epsilon_n$) is calculated by using Eq. (11). The use of the convergent error estimator ($\psi_n$), which involves Eqs. from (25) to (27), is shown in the right-hand column of Table 2.

<table>
<thead>
<tr>
<th>Grid</th>
<th>$\lambda_n$</th>
<th>$\lambda_0$</th>
<th>$\lambda_1$</th>
<th>$\psi_n$</th>
<th>$\psi_0$</th>
<th>$\psi_1$</th>
<th>$\epsilon_n$</th>
<th>$\epsilon_0$</th>
<th>$\epsilon_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5*33</td>
<td>0.199267658</td>
<td>0.199267658</td>
<td>0.199267658</td>
<td>0.00001804</td>
<td>0.00001804</td>
<td>0.00001804</td>
<td>0.00001804</td>
<td>0.00001804</td>
<td>0.00001804</td>
</tr>
<tr>
<td>9*65</td>
<td>0.199267658</td>
<td>0.199267658</td>
<td>0.199267658</td>
<td>0.00001804</td>
<td>0.00001804</td>
<td>0.00001804</td>
<td>0.00001804</td>
<td>0.00001804</td>
<td>0.00001804</td>
</tr>
<tr>
<td>17*129</td>
<td>0.199267658</td>
<td>0.199267658</td>
<td>0.199267658</td>
<td>0.00001804</td>
<td>0.00001804</td>
<td>0.00001804</td>
<td>0.00001804</td>
<td>0.00001804</td>
<td>0.00001804</td>
</tr>
</tbody>
</table>

Results for many different grids are presented in Fig. 1. In this figure, for Problem 1, the estimated errors $\psi_n(\phi)$ and $\psi_0(\phi)$ and the true discretization errors $\epsilon_n(\phi)$ and $\epsilon_0(\phi)$ of the temperature at the center of the domain are shown. The results refer to grids of 3x3 to 1025x1025 points, where $\tau = 2$. In this figure, one can see the significant advantage of using $\psi_0$, instead of $\psi_n$, for reducing the true discretization error. It can also be verified that the estimated error by both the Richardson estimator ($\psi_0$) as well as the convergent estimator ($\psi_1$) are reliable for any $k$. The Richardson and Convergent estimators for the numerical solutions are shown in Table 2.

<table>
<thead>
<tr>
<th>Richardson estimator</th>
<th>Convergent estimator</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(\phi_0)$</td>
<td>$(\phi_0)$</td>
</tr>
<tr>
<td>$(\phi_1)$</td>
<td>$(\phi_1)$</td>
</tr>
<tr>
<td>$(\phi_2)$</td>
<td>$(\phi_2)$</td>
</tr>
<tr>
<td>$(\phi_3)$</td>
<td>$(\phi_3)$</td>
</tr>
</tbody>
</table>

Table 1. Numerical solutions for Problem 1, Eq. (1), for $\lambda_n(1, 1)$.

Table 2. Application of the Richardson and Convergent estimators to the numerical solutions shown in Table 1.
Table 3 shows the numerical solutions of $u(\frac{1}{2}, \frac{1}{2})$ obtained from three different grids for Problem 3. $\Phi$ 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. $\phi_0$, $\phi_1$ represent the numerical solutions. The use of the Richardson error estimator ($e_0$) for $\phi$, 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 ($e_0$) is calculated by using Eq. (11). The use of the convergence error estimator ($e_0$) for $\phi$, which involves Eqs. from (25) to (27), is shown in the right-hand column of Table 4.

<table>
<thead>
<tr>
<th>Table 3. Numerical solutions for Problem 3 for $u(\frac{1}{2}, \frac{1}{2})$.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid</td>
</tr>
<tr>
<td>------</td>
</tr>
<tr>
<td>4*4</td>
</tr>
<tr>
<td>8*8</td>
</tr>
<tr>
<td>16*16</td>
</tr>
</tbody>
</table>

The numerical solutions of $u(\frac{1}{2}, \frac{1}{2})$ are 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 ($p_a$), 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 ($e_0$) 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, $\phi = \frac{\phi}{\phi_0} = \phi$. Solution Refinement Table 5. Apparent orders ($p_a$) for $r = 2$, and asymptotic orders ($p_b$) for simultaneous refinement.

<table>
<thead>
<tr>
<th>Problem</th>
<th>Variable</th>
<th>Grid</th>
<th>$p_a$</th>
<th>$p_b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>central $\Lambda$</td>
<td>1025 × 1025</td>
<td>1.999694</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>average $\Lambda$</td>
<td>4007 × 2048</td>
<td>1000009</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>central $\lambda$</td>
<td>256 × 256</td>
<td>1.999652</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>central $\kappa$</td>
<td>256 × 256</td>
<td>1.982185</td>
<td>2</td>
</tr>
</tbody>
</table>

Through analysis, the truncation errors of the numerical approximations used to discretize Eq. (46), it was determined that their apparent orders are $p_a = r - 2$ and $p_b = 1$. In this example, the refinement ratio of the grid in the $x$ dimension ($r = 2$) is different from the $y$ dimension ($r = 1.5$). Through Eqs. (31) to (36), $p_a$ and $p_b$, and with the numerical solutions given in Table 6, one can use the Richardson error estimator ($e_0$) through Eqs. from (32) to (39), to find the results shown on the left-hand column of Table 7. It should be noted that $U_0(\phi_0) > 1$ in other words, the estimated error $U_0(\phi_0)$ is reliable for it underestimates the true error $e_0(\phi_0)$, and it is quite accurate, as $U_0(\phi_0) > 1$.

### Table 6. Numerical solutions for Problem 2, Eq. (46), for $A$ in $\times = \frac{1}{2}$ and $t = 0.1$.

<table>
<thead>
<tr>
<th>Problem</th>
<th>Refinement in $x$</th>
<th>Refinement in $y$</th>
<th>Other data</th>
</tr>
</thead>
<tbody>
<tr>
<td>grid 55*750</td>
<td>2 × 2</td>
<td>1.5</td>
<td>$p_a = 2$</td>
</tr>
<tr>
<td>$\phi = 0.373245017$</td>
<td>$\phi = 0.373144380$</td>
<td>$\phi = 0.373203555$</td>
<td>$\phi = 0.3732942967$</td>
</tr>
<tr>
<td>grid 65*750</td>
<td>1.5</td>
<td>1</td>
<td>$p_b = 1$</td>
</tr>
</tbody>
</table>

To calculate the refined values of the component of the estimated error for separate refinement in Problem 2.

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

<table>
<thead>
<tr>
<th>Equation</th>
<th>Refinement in $x$</th>
<th>Refinement in $y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi = 0.3732949739$</td>
<td>$\phi = 0.3732862379$</td>
<td>$\phi = 0.3732949739$</td>
</tr>
<tr>
<td>$\phi = 0.3732949741$</td>
<td>$\phi = 0.3732781563$</td>
<td>$\phi = 0.3732949739$</td>
</tr>
<tr>
<td>$\phi = 0.3732949741$</td>
<td>$\phi = 0.3732781563$</td>
<td>$\phi = 0.3732949739$</td>
</tr>
</tbody>
</table>

The use of the convergence error estimator ($e_0$) is shown in the right-hand column of Table 3. 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 $v_u(\phi)/v_c(\phi) = 1.00228$, that is, the estimated error $v_u(\phi)$ is reliably for it overestimates the value of the true error $v(\phi)$. Moreover, there have been significant reductions in both the estimated error as well as the true error of the convergent numerical solution ($\phi$) with respect to the calculated numerical solution ($\phi$) seeing as $v_u(\phi)/v_c(\phi) < 1$.

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

<table>
<thead>
<tr>
<th>Richardson estimator</th>
<th>Convergent estimator</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Eq. 32) $v_u(\phi) = -0.000315808$</td>
<td>(Eq. 42) $v_u(\phi) = -0.02949740$</td>
</tr>
<tr>
<td>(Eq. 39) $v_c(\phi) = -0.000315855$</td>
<td>(Eq. 43) $v_c(\phi) = -0.000000001$</td>
</tr>
<tr>
<td>(Eq. 11) $v(\phi) = -0.000315716$</td>
<td>(Eq. 42) $v(\phi) = 0.02821971$</td>
</tr>
<tr>
<td>$v(\phi)/v(\phi) = 1.00029$</td>
<td>$v(\phi)/v(\phi) = 1.02228$</td>
</tr>
<tr>
<td>$v(\phi)/v(\phi) = 1.02228$</td>
<td>$v(\phi)/v(\phi) = 1.02228$</td>
</tr>
<tr>
<td>$v(\phi)/v(\phi) = 1.02228$</td>
<td>$v(\phi)/v(\phi) = 1.02228$</td>
</tr>
<tr>
<td>$v(\phi)/v(\phi) = 7.82$</td>
<td>$v(\phi)/v(\phi) = 7.82$</td>
</tr>
<tr>
<td>$v(\phi)/v(\phi) = 7.82$</td>
<td>$v(\phi)/v(\phi) = 7.82$</td>
</tr>
</tbody>
</table>

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 ($p_i$) and grid refinement ratios ($\lambda_i$) 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 problems. The problems were solved by finite difference and finite volume methods for three types of variables of interest: the dependent variables (solenoidal), the averages of the dependent variables in the whole field (average $A$) and the integration of a dependent variable ($\phi$).

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 ($p_i$) of the estimated error is of the monotone convergent type. In this case, all of the conclusions of Marchi and Silva (2002) proved valid, among which the following are worthy of note: the true discretization error ($v(\phi)$) is bounded by the estimated values of error found by the Richardson error estimator ($v_u(\phi)$), which are calculated based on the asymptotic ($p_i$) and apparent ($p_i$) 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 ($\phi$) and its respective convergent error estimator ($v_c(\phi)$) and, outside of the convergent interval of the apparent order ($p_i$), 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 ($p_i$) 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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