



Highly accurate numerical solutions with repeated Richardson extrapolation for 2D laplace equation



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ABSTRACT

A theoretical basis is presented for the repeated Richardson extrapolation (RRE) to reduce and estimate the discretization error of numerical solutions for heat conduction. An example application is described for the 2D Laplace equation using the finite difference method, a domain discretized with uniform grids, second-order accurate approximations, several variables of interest, Dirichlet boundary conditions, grids with up to $8,193 \times 8,193$ nodes, a multigrid method, single, double and quadruple precisions and up to twelve Richardson extrapolations. It was found that: (1) RRE significantly reduces the discretization error (for example, from $2.25E-07$ to $3.19E-32$ with nine extrapolations and a $1,025 \times 1,025$ grid, yielding an order of accuracy of 19.1); (2) the Richardson error estimator works for numerical results obtained with RRE; (3) a higher reduction of the discretization error with RRE is achieved by using higher calculation precision, a larger number of extrapolations, a larger number of grids and correct error orders; and (4) to obtain a given value error, much less CPU time and RAM memory are required for the solution with RRE than without it.

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1. Introduction

It is important to improve techniques that allow for reduction of the numerical error in order to diminish the computational cost (CPU time and RAM memory) involved in obtaining numerical solutions. Some of the ways to reduce numerical errors caused by discretization errors are: (a) refine the grid, with the attending disadvantage of increasing the computational cost; (b) increase the order of accuracy of numerical approximations, with the disadvantage of increasing the complexity of the numerical model; and (c) use extrapolation techniques, one of which is the Richardson extrapolation (RE) [1–5]. To use RE requires having the numerical solution of the variable of interest on two grids with different numbers of nodes. RE is also used as an estimator of the discretization error [6] or it serves as the basis for other estimators such as the GCI (Grid Convergence Index) [7]. Reference [8] describes a comprehensive study on extrapolation processes in numerical analysis, most of which are based on RE or on variants thereof.

Repeated Richardson extrapolation (RRE) [5] consists of applying the Richardson extrapolation successively. Therefore, to use RRE requires having the numerical solution of the variable of interest in three or more grids with different numbers of

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nodes, thus allowing for two or more REs. In other areas [4,5], RRE is used with many REs, but this is not the case in CHT (Computational Heat Transfer) and CFD (Computational Fluid Dynamics). The authors of references [2,9] applied RRE with two REs to two-dimensional problems (2D) of heat conduction. RRE was applied with up to three REs by [10–13] in the solution of 2D Navier–Stokes equations. However, in CHT and CFD it is more common to apply RE than RRE; for example: [14] in various types of 1D problems; [15,16] in the 2D Poisson equation; in the 2D advection–diffusion equation [17] and 3D [18]; in 2D Navier–Stokes equations [19]; in 2D natural convection [20]; and in 2D turbulent flows [19,21,22]. Therefore, to date, RE and particularly RRE have been little used in CHT and CFD to reduce the discretization error, probably due to the difficulties reported by [2–4,7,12,14,19,21–26].

Based on [27–30] and on this work, the main advantages of using RRE are: (1) it greatly reduces the discretization error; (2) it is a simple post-processing method, i.e., it does not interfere directly in obtaining the numerical solution in a given grid h ; (3) its computational cost is very low in terms of CPU time and RAM memory; (4) it can be applied to existing computational codes or to results already obtained; (5) it is applicable to several numerical methods, numerical approximations and variables of interest; (6) it does not depend on a priori analyses or on knowledge of the analytical solution to the problem; and (7) even with numerical solutions without RRE, which are of low order (one or two), one obtains numerical solutions with RRE that are of extremely high order (higher than ten). As will be shown in this paper, RRE can be used in two ways; the first, to obtain the same discretization error with a grid containing far fewer nodes, thus reducing the computational cost. This way is especially recommended for practical applications and validations. The second way allows for a reduction of the discretization error in a grid with the same number of nodes, resulting in much smaller errors and greater reliability of the solution. Using RRE in this way is especially indicated for generating benchmarks.

The objectives of this work are as follows: (i) present a theoretical basis of RRE aimed at reducing and estimating the discretization error in heat conduction; (ii) show that the use of RRE is extremely effective in reducing the error; (iii) test an error estimator for RRE; (iv) show the effects on RRE caused by the type of numerical approximation, type of variable of interest, precision of the calculations, number of extrapolations, number of grids and orders of the error; and (v) show the computational cost of RRE. To achieve these objectives, the RRE theory is applied to the solution of the 2D Laplace equation with up to twelve REs. A paper with preliminary results contained in present work was published at CILAMCE/2008 [28].

2. Mathematical model

The mathematical model considered here is the two-dimensional Laplace equation with Dirichlet boundary conditions, defined by

$$\begin{cases} \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0, & 0 < x, y < 1, \\ T(x, 1) = \sin(\pi x), & T(x, 0) = T(0, y) = T(1, y) = 0, \end{cases} \quad (1)$$

where x and y are the coordinate directions and T represents the temperature. Physically, this equation can model a problem of heat conduction on a flat plate with constant properties, in a steady state, as well as several other physical phenomena. The analytical solution for Eq. (1) is $T(x, y) = \sin(\pi x) \sinh(\pi y) / \sinh(\pi)$.

The variables of interest in this work, i.e., the variables to which the RRE theory are applied, are: (i) the temperature at the center of the domain, i.e., at $x = y = 1/2$, represented by T_c ; (ii) the temperature profile at $x = 1/2$, represented by T_y ; (iii) the mean of the temperature field, represented by T_m ; (iv) the mean of the l_1 norm of the numerical error, represented by L ; and the heat transfer rates at the boundaries of $x = 1$ (v) and $y = 1$ (vi), represented, respectively, by Q_e and Q_n . The justification for the choice of these variables is presented in the next section.

The variables T_m and Q_e are defined mathematically by

$$T_m = \frac{1}{A} \int_0^1 \int_0^1 T(x, y) dx dy, \quad (2)$$

$$Q_e = -kZ \int_0^1 \left(\frac{\partial T}{\partial x} \right)_{x=1} dy, \quad (3)$$

where A is the heat transfer area, k is the thermal conductivity of the material and Z is the heat transfer length in z direction, all with a unitary value.

3. Numerical model

3.1. Numerical solution without extrapolation

Eq. (1) is discretized with the finite difference method [31], uniform grids and the CDS (Central Differencing Scheme) scheme of second-order accuracy, resulting in

$$\frac{(T_{i-1j} - 2T_{ij} + T_{i+1j})}{h^2} + \frac{(T_{ij-1} - 2T_{ij} + T_{ij+1})}{h^2} = 0, \quad (4)$$

where i and j represent each node in the grid, and h is the distance between two consecutive nodes of the grid in each direction.

Writing Eq. (4) for all the N nodes in the grid, one has a system of algebraic equations which is solved by means of the *Modified Strongly Implicit* (MSI) method [32]. To hasten the convergence, a geometric multigrid method [33] was employed with the *Full Approximation Scheme* (FAS), V-cycle, restriction by injection, prolongation by bilinear interpolation and coarsening ratio of two.

The null value was used as the initial estimate of the solution for each problem. The number of times the V-cycle of the multigrid method is repeated is called external iterations. The iterative process was repeated until the machine round-off error for the numerical solution of the variables T_c and T_m was reached, aiming to eliminate the contribution of the iteration error to the numerical error.

Three computational programs were implemented in Fortran 95 language, version 9.1 of Intel, one using single precision (Real*4), another with double precision (Real*8) and the third with quadruple precision (Real*16). The simulations were performed in a core of a microcomputer equipped with an Intel Xeon Quad Core X5355 processor, 2.66 GHz, 16 GB RAM and 64-bit Windows XP operating system.

The numerical solution of variable T_c was obtained directly from the central node of each grid after obtaining the numerical solution of Eq. (4), since grids with an odd number of nodes were always used. The numerical solution of variable T_y was obtained directly from 15 nodes equally spaced in the grid after obtaining the numerical solution of Eq. (4) for grids with 17×17 nodes or larger. The numerical solution of Eq. (2) for T_m was obtained by means of numerical integration by the trapezoidal rule [34]. The numerical solution of Eq. (3) for Q_e was obtained by means of numerical integration by the trapezoidal rule preceded by the use of the UDS (*One-sided Differencing Scheme*) scheme [31] of second-order accuracy on each boundary node. Variable Q_n was obtained analogously to Q_e .

Variables T_c and T_y were chosen to verify the effect of the Richardson extrapolation on 15 specific nodes in the grids and because they are variables dependent on the differential equation of the problem, Eq. (1), i.e., the primary variable of the problem, whose solution involves two numerical approximations of the CDS type, as indicated in Eq. (4). Variable L was chosen to monitor, through a single variable, the behavior of the numerical error of the whole field of T with the decrease of h . Variables T_m , Q_e and Q_n were used to verify the effect of the Richardson extrapolation on secondary variables, i.e., obtained from T , and involving one and two numerical approximations in addition to those used to obtain T .

The numerical solution (ϕ) without extrapolation of each above described variable of interest was obtained by using a set of grids $g = [1, G]$, where $g = 1$ is the coarsest grid, which has the highest h , and $g = G$ is the finest grid, with the lowest h .

3.2. Numerical solution with multiple extrapolations

For each variable of interest, the numerical solution (ϕ) in grid g with m Richardson extrapolations is given by

$$\phi_{g,m} = \phi_{g,m-1} + \frac{\phi_{g,m-1} - \phi_{g-1,m-1}}{r^{p_{m-1}} - 1}, \quad (5)$$

where $r = h_{g-1}/h_g$ is the grid refinement ratio, and the variable p_m represents the true orders [6] of the discretization error, which can be obtained as explained in the next Section 4. Eq. (5) is valid for $g = [2, G]$ and $m = [1, g - 1]$. Eq. (5) was obtained by extending to the case of $m > 1$ the works of [1,2,6,7], which present equations equivalent to the case of $m = 1$.

It should be noted that to obtain each value of $\phi_{g,m}$ requires having two numerical solutions ϕ in two grids (g and $g - 1$) at $m - 1$. For any g , $m = 0$ represents the numerical solution of ϕ without any extrapolation, which is obtained as described in the previous Section 3.1. For $m = 1$, one has the standard or single Richardson extrapolation, which is commonly used to estimate the discretization error [6] or to improve the solution of each grid g [16]. For a given value of g , Eq. (5) can be applied up to $g - 1$ times, performing m Richardson extrapolations.

4. The numerical error and its estimate

For a given variable of interest, the numerical error (E) of the numerical solution (ϕ) can be defined by

$$E(\phi) = \Phi - \phi, \quad (6)$$

where Φ is the exact analytical solution of the variable of interest. In the present work, we consider that the numerical error is caused by four sources [6]: discretization, iteration, round-off and programming errors.

When the numerical error is caused only by the discretization error, one has [5,8]

$$E(\phi) = C_0 h^{p_0} + C_1 h^{p_1} + C_2 h^{p_2} + \dots = \sum_{m=0}^{\infty} C_m h^{p_m}, \quad (7)$$

where C_0, C_1, C_2, \dots are the coefficients that depend on Φ and its derivatives, as well as on the independent variables, but are independent of h ; and p_0, p_1, p_2, \dots are the true orders of $E(\phi)$, whose set is represented by p_m .

The values of p_m are generally positive integer numbers [8] with $0 < p_0 < p_1 < p_2 < \dots$, which constitute an arithmetic progression of ratio $q = p_1 - p_0$. In addition, p_0 is called the asymptotic order or the order of accuracy of $E(\phi)$ or of the

numerical solution ϕ . The values of p_m can be obtained a priori with a procedure that uses the Taylor series [31], or a posteriori as explained in the next Section 4.1.

The theoretical order of accuracy of the numerical solution of ϕ , with p_m orders constituting an arithmetic progression, and m extrapolations is

$$p_m = p_0 + m(p_1 - p_0), \tag{8}$$

where this equation is valid for $g = [1,G]$ and $m = [0,g - 1]$.

4.1. Obtaining error orders

The values of p_m obtained a priori can be confirmed a posteriori with the concept of effective order (p_E) [35] of the discretization error, which, generalized for repeated Richardson extrapolation, is given by

$$(p_E)_{g,m} = \frac{\log \left[\frac{E(\phi_{g-1,m})}{E(\phi_{g,m})} \right]}{\log(r)}, \tag{9}$$

where E is calculated by Eq. (6).

Eq. (9) is valid for $g = [2,G]$ and $m = [0,g - 2]$. The other definitions in Section 3.2 apply here. It should be noted that to obtain each value of p_E it is necessary to know the error of the numerical solution in two grids. In theory, as $h \rightarrow 0$, the values of $(p_E)_{g,m}$ should tend toward the true order (p_m) given by Eq. (8). Eq. (9) was obtained by extending to the case of $m \geq 1$ the work of [35], which presents an equation equivalent to the case of $m = 0$.

According to Eq. (9), p_E is a function of the error of the variable of interest. Hence, this equation cannot be applied to problems whose analytical solution is unknown. Moreover, Eq. (9) should not be used when one intends to confirm a posteriori the values of p_m obtained a priori and without using numerical solutions extrapolated from the same values of p_m that were obtained a priori. In such cases, one can use the concept of apparent or observed order (p_U) [10,36,20,21,3,6] of the estimated discretization error, which, generalized to repeated Richardson extrapolation, is given by

$$(p_U)_{g,m} = \frac{\log \left[\frac{\theta_{g-1,m} - \theta_{g-2,m}}{\theta_{g,m} - \theta_{g-1,m}} \right]}{\log(r)}, \tag{10}$$

where variable θ is explained below. Eq. (10) was obtained by extending to the case of $m \geq 1$ the works [10,36,20,21,3,6], which present an equation equivalent to the case of $m = 0$.

Eq. (10) is valid for $g = [3,G]$, $m = [0, \text{Int}((g - 3)/2)]$ and constant r among the three grids, i.e., $r = h_{g-2}/h_{g-1} = h_{g-1}/h_g$, where $\text{Int}(a)$ represents the integer part of a . The remaining definitions in Section 3.2 apply here. It is also possible to obtain p_U for variable r among three grids; this case is addressed in [3,35]. As $h \rightarrow 0$, the values of $(p_U)_{g,m}$ should tend toward the true order (p_m) of the respective level of extrapolation (m) of Eq. (7), independently of any a priori analysis. These values of p_m , obtained a posteriori, should be used in Eq. (5).

It should be noted that to obtain each value of p_U in Eq. (10) requires numerical solutions related to three grids. These solutions are not obtained with Eq. (5) because it admits that the values of p_m are known. To obtain p_m a posteriori independently of p_m a priori, instead of using variable ϕ , obtained with Eq. (5), one uses the new variable θ , which is calculated by

$$\theta_{g,m} = \theta_{g,m-1} + \frac{\theta_{g,m-1} - \theta_{g-1,m-1}}{r^{(p_U)_{g,m-1}} - 1}. \tag{11}$$

Eq. (11) is valid for $g = [3,G]$ and $m = [1, \text{Int}((g - 1)/2)]$. The other definitions in Section 3.2 apply here. In addition, for $m = 0$, Eq. (11) does not apply; in this case, one has $\theta_{g,0} = \phi_{g,0}$, where $\phi_{g,0}$ is the numerical solution obtained without any extrapolation, as described in Section 3.1.

To adequately characterize the series of values of p_m , ideally one should determine at least the first three orders: p_0, p_1 and p_2 . If this is not possible, one can simply determine p_0 and p_1 , since the values of p_m normally constitute an arithmetic progression and the remaining values are a function of these first two orders of the series. When only p_0 is determined, one can determine the remaining values arbitrarily. Lastly, if no value is determined, one can use the series with the lowest values: 1, 2, 3, ... The impact of the arbitrary choice of the values of p_m will be addressed in the Results section.

In the present work, the values of p_m used in Eq. (5) are obtained from $(p_U)_{g,m}$ of Eq. (10) for $m = [0,2]$. These are positive integer numbers that are extracted, for each level of extrapolation (m), from the tendency of the values of $(p_U)_{g,m}$ when $h \rightarrow 0$.

4.2. Error estimator

For any variable of interest, an estimate (U) of the discretization error of the numerical solution (ϕ) in the grid g , with m Richardson extrapolations, is given by

$$U(\phi_{g,m}) = \frac{\phi_{g,m} - \phi_{g-1,m}}{r^{p_m} - 1}. \tag{12}$$

Eq. (12) is valid for $g = [2, G]$ and $m = [0, g - 2]$. The other definitions of Section 3.2 apply here. Eq. (12) was obtained by extending to the case of $m > 1$ the works of [1,2,6,7], which present equations equivalent to the case of $m = 1$.

5. Results

Using double precision (Real*8), numerical solutions were obtained for the variables of interest in grids containing 3×3 , 5×5 , 9×9 , ... up to $8,193 \times 8,193$ nodes; thus, $G = 13$ grids. On the other hand, with single (Real*4) and quadruple (Real*16) precision, the finest grid had $4,097 \times 4,097$ nodes; therefore, $G = 12$ grids. Although 50 and 20 external iterations were performed with double and quadruple precision, respectively, the machine round-off error was reached with only six and twelve external iterations, respectively. To reach the machine round-off error, the maximum CPU time was 20 min and 1 h 5 min, respectively, for double and quadruple precision. The number of significant digits of numerical solutions without extrapolation is at least 12 and 30, respectively, for double and quadruple precision; this means that in these digits the solutions have no round-off error. To measure the numerical error with Eq. (6), the analytical solution (Φ) of each variable of interest was obtained using Maple software with 30 and 64 digits, respectively, for the numerical solutions obtained with double and quadruple precision. Presented below are some of the results of this work. The omitted results exhibited the same qualitative behavior as the ones given below.

5.1. Error reduction and estimation with RRE

Figs. 1–3, respectively, present the modulus of the following results for the variables Tc , Tm and Qe as a function of grid size (h), obtained with quadruple precision and $G = 12$ grids:

- Eh , calculated with Eq. (6), which is the error of the numerical solution of ϕ without any extrapolation ($m = 0$) and obtained as described in Section 3.1 for $g = [1, G]$.
- Uh , calculated with Eq. (12) for $g = [2, G]$ and $m = 0$, which is the estimate of Eh .
- $Em2$, calculated by Eq. (6), which is the error of numerical solution of ϕ with extrapolation, obtained as described in Section 3.2 by means of Eq. (5) for $g = [3, G]$ and $m = g - 2$.
- $Um2$, calculated with Eq. (12) for $g = [3, G]$ and $m = g - 2$, which is the estimate of $Em2$.
- $Em1$, calculated with Eq. (6), which is the error of numerical solution of ϕ with extrapolation, obtained as described in Section 3.2 by means of Eq. (5) for $g = [2, G]$ and $m = g - 1$.
- $d\phi = \phi_{g,m} - \phi_{g-1,m}$, which is the numerator of Eq. (12), where $\phi_{g,m}$ is obtained by Eq. (5), as described in Section 3.2, for $g = [2, G]$ and $m = g - 2$.

The error of numerical solutions obtained with RRE can only be estimated in the second coarsest grid at each level of extrapolation m . Therefore the results of $Em2$ and $Um2$ are presented. Although its error cannot be estimated consistently, the result of $Em1$ is presented to show the effect of the level of extrapolation for the same grid h .

In these three figures one can see that, in general: (i) Uh coincides visually with Eh in any h ; (ii) $Um2$ is close to $Em2$ in any h , with values slightly lower than $Em2$; (iii) $Em1$ is a little lower than $Em2$; (iv) $d\phi$ is much higher than $Em2$; and (v) $Em1$ and

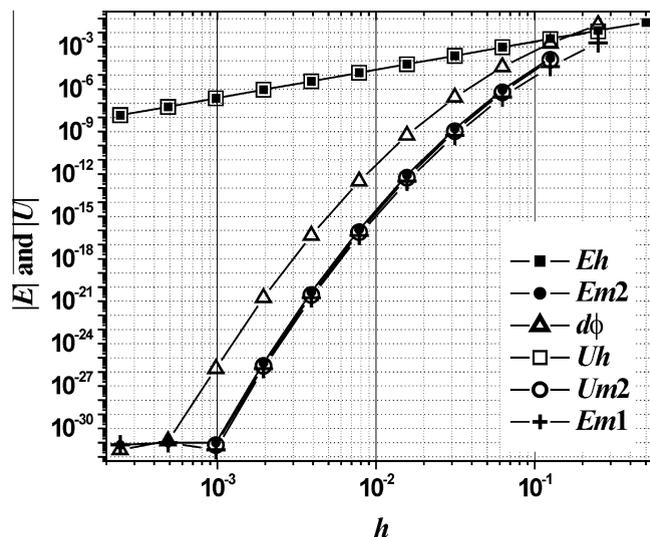


Fig. 1. Errors (E) and their estimates (U) as a function of grid size (h) for Tc (Real*16).

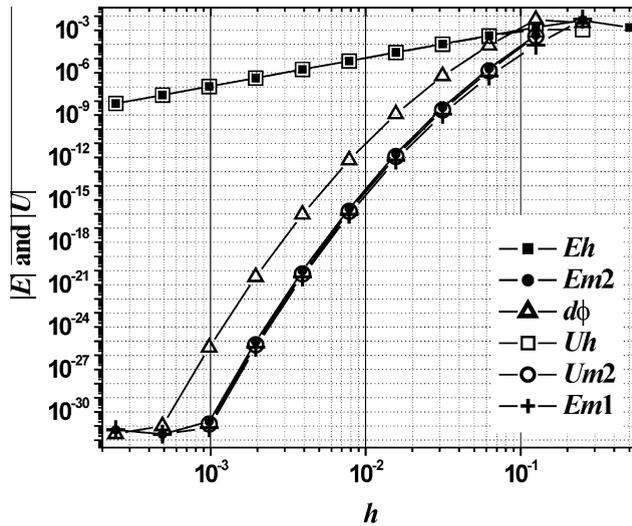


Fig. 2. Errors (E) and their estimates (U) as a function of grid size (h) for Tm (Real*16).

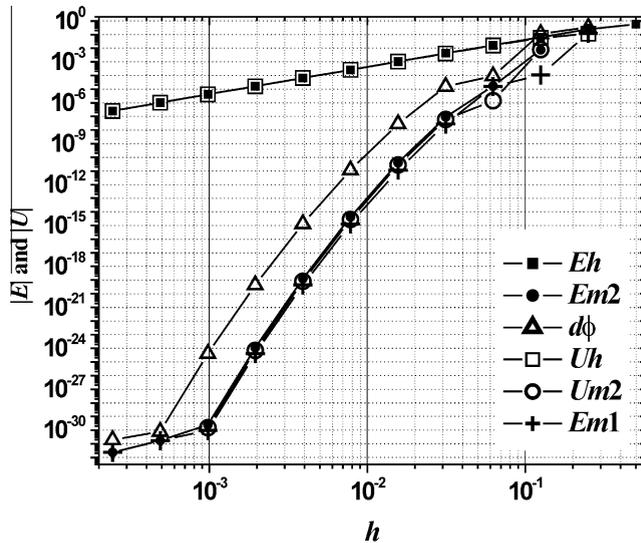


Fig. 3. Errors (E) and their estimates (U) as a function of grid size (h) for Qe (Real*16).

$Em2$ are very much lower than Eh and become progressively lower in relation to Eh the lower h is. Moreover, in the finer grids, i.e., lower h , because the round-off error ($E\pi$) is higher than the discretization error: RRE loses its effect of reducing the error; $Um2$, i.e., Eq. (12) is useless; and $d\phi$ can be used as an estimator for $Em1$ and $Em2$.

Based on these results, it can be concluded that: (a) RRE is extremely efficient to reduce the discretization error, except in the case of very coarse grids; (b) in each grid g with spacing h , the lowest error with RRE occurs for $m = g - 1$, i.e., $Em1$; (c) RRE reduces the error of primary or secondary variables equally efficiently, regardless of the number of numerical approximations used; (d) the Richardson estimator given by Eq. (12) is accurate to predict the discretization error of numerical solutions obtained by Eq. (5) with RRE; (e) $d\phi$ can be used as a reliable estimator of Em , although it overestimates it considerably; it can also be used even when E is dominated by $E\pi$ instead of Em , as can be seen in Figs. 1–3; and (f) round-off errors affect the performance of RRE in very fine grids when they prevail over the discretization errors.

Tables 1 and 2 help demonstrate the efficiency of RRE in reducing the error of variable Tc , obtained with quadruple precision. For three specific grids, Table 1 shows the effect of RRE on the reduction of the discretization error, measured by the ratio $Eh/Em1$, upon refining the grid and increasing the number of extrapolations (m). For example, even in a grid as coarse as 17×17 , the error is already reduced more than three thousand times with only three extrapolations ($m = 3$). Hence, RRE can be used to obtain benchmark solutions.

Table 1
Reduction of the T_c error for specific grids (Real*16).

| Grid | 17×17 | 129×129 | $1,025 \times 1,025$ |
|------------------|----------------|------------------|----------------------|
| h | 6.25E-02 | 7.81E-03 | 9.77E-04 |
| $ E_h $ | 9.20E-04 | 1.44E-05 | 2.25E-07 |
| $ E_{m1} $ | 2.71E-07 | 4.56E-17 | 3.19E-32 |
| m of E_{m1} | 3 | 6 | 9 |
| $ E_h / E_{m1} $ | 3.39E+03 | 3.16E+11 | 7.05E+24 |

Table 2
Reduction of grid nodes for specific T_c errors (Real*16).

| Error level | $5.00E-03$ | $5.00E-05$ | $5.00E-07$ |
|--|--------------|----------------|----------------------|
| E_h grid | 9×9 | 65×65 | $1,025 \times 1,025$ |
| $ E_h $ | 3.65E-03 | 5.76E-05 | 2.25E-07 |
| E_{m1} grid | 5×5 | 9×9 | 17×17 |
| $ E_{m1} $ | 1.92E-03 | 3.84E-05 | 2.71E-07 |
| m of E_{m1} | 1 | 2 | 3 |
| Ratio of the number of nodes of E_h and E_{m1} grids | 3.24E+00 | 5.22E+01 | 3.64E+03 |

For three specific error levels, Table 2 shows the effect of RRE in reducing the number of nodes of a grid to obtain the same discretization error. For example, for the error level $5.00E-07$, it is necessary to use the $1,025 \times 1,025$ grid to reach this error level without RRE and the 17×17 grid with RRE. Thus, a grid more than three thousand times smaller is required with RRE than without RRE. This ratio between the number of nodes of E_h and E_{m1} grids indicates the level of reduction of the computational cost (CPU time and RAM memory) achieved by using RRE compared to not using RRE. Hence, RRE can be employed with great computational efficiency.

5.2. Effect of calculation precision

Fig. 4 presents the value of the E_h modulus of the numerical solutions without extrapolation obtained with single (Real*4), double (Real*8) and quadruple (Real*16) precision for variable T_c as a function of grid size (h). This figure also presents the value of the E_{m1} modulus of the numerical solutions extrapolated and obtained with the same three precisions for variable T_c . E_h and E_{m1} follow the same definitions of Section 5.1. This figure presents results for the $g = [1, G = 12]$ grids.

In Fig. 4, note that: (i) the round-off error ($E\pi$) becomes the main source of the numerical error below a value of h , which depends on the precision used in the calculations and on whether the numerical solution was obtained with or without extrapolation; (ii) numerical solutions with extrapolation are much more affected by $E\pi$ than without extrapolation [24], i.e., the value of h below which the extrapolations are affected by $E\pi$ is much higher than the h of the numerical solutions

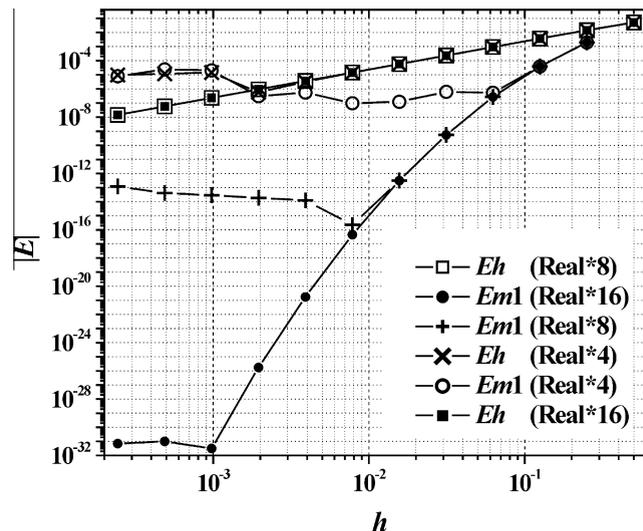


Fig. 4. Effect of calculation precision on the T_c error as a function of grid size (h).

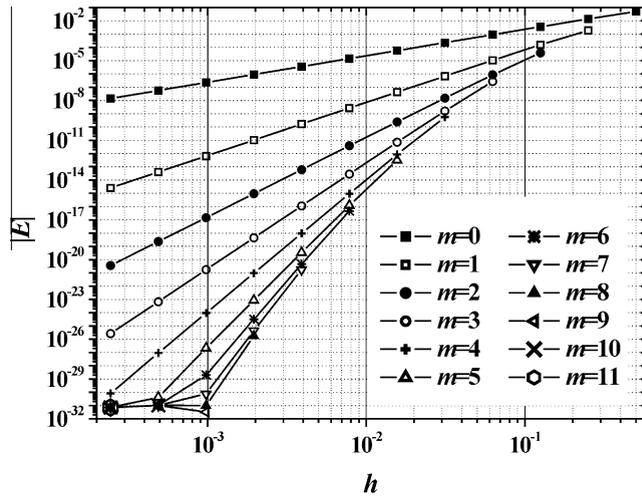


Fig. 5. Effect of the number of extrapolations (m) on the T_c error as a function of grid size (h) (Real*16).

without extrapolation; and (iii) the higher the precision used in the calculations the greater the efficiency of RRE in reducing the discretization error.

5.3. Effect of the number of extrapolations (m)

Fig. 5 shows the effect of the number of extrapolations (m) on the modulus of the T_c error as a function of grid size (h) for results obtained with quadruple precision (Real*16). This figure presents results for the $g = [1, G = 12]$ grids. Each curve represents a level of extrapolation $m = [0, g - 1]$. It should be kept in mind that $m = 0$ refers to results of the T_c error without extrapolation, obtained as described in Section 3.1; and for $m \geq 1$ the results of the T_c error with extrapolation, obtained as described in Section 3.2 with Eq. (5).

It is evident, in Fig. 5, that the higher m is for the same h , the greater the efficiency of RRE in reducing the discretization error. In addition, for the same m , the lower h is the smaller the error; this result is well known for $m = 0$. However, in the finer grids, i.e., those with the lowest values of h , which in this case occurs for $m \geq 5$, E_π reduce the efficiency of RRE. The lowest error ($3.19E-32$) was obtained with $m = 9$ at its highest h , i.e., in the $1,025 \times 1,025$ grid ($g = 10$).

Fig. 6 shows the effective order (p_E) of the T_c error as a function of grid size (h) and number of extrapolations (m) corresponding to the errors in Fig. 5. The p_E values were calculated from Eq. (9), as described in Section 4.1, for $g = [2, G]$ and $m = [0, g - 2]$. Each curve represents a level of extrapolation m . The highest value of p_E (17.4) was obtained with $m = 8$ at its highest h , i.e., in the $1,025 \times 1,025$ grid ($g = 10$). In the finer grids, i.e., the ones with the lowest values of h , which in this

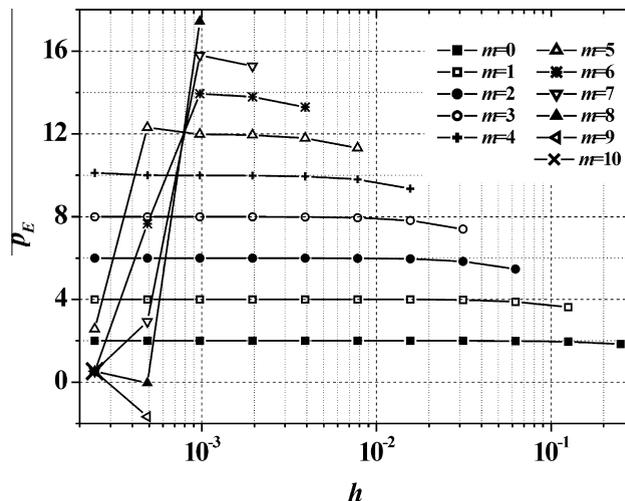


Fig. 6. Effective order (p_E) of the T_c error as a function of grid size (h) and number of extrapolations (m) (Real*16).

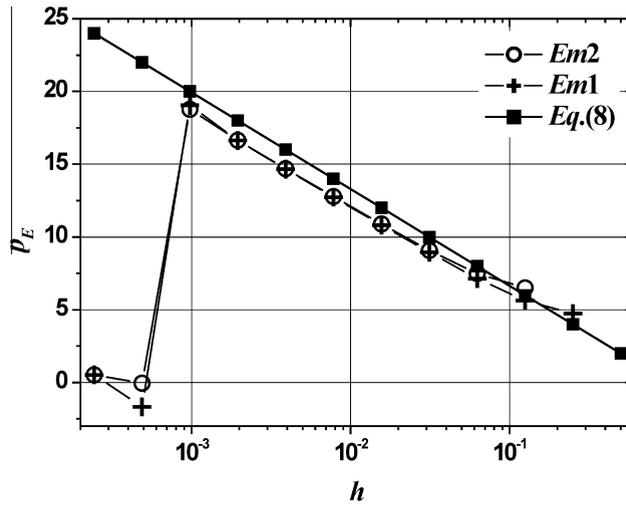


Fig. 7. Effective order (p_E) of the $Em1$ and $Em2$ curves of T_c as a function of grid size (h) (Real*16).

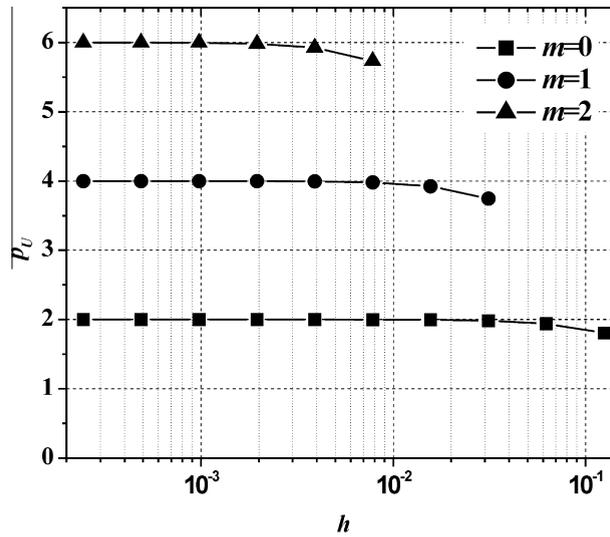


Fig. 8. Apparent order (p_U) of the estimated T_c error as a function of grid size (h) and number of extrapolations (m) (Real*16).

case occurs for $m \geq 4$, $E\pi$ affects the calculation of p_E , resulting in values that should be disregarded. This figure clearly shows the following values of p_m : 2, 4, 6, 8, 10 and 12; and the curves show a tendency toward the values 14 and 16.

Fig. 7 presents the effective order (p_E) of the T_c error as a function of grid size (h) for the $Em2$ and $Em1$ curves in Fig. 1. This figure also shows the theoretical order curve given by Eq. (8), with $p_0 = 2$ and $p_1 = 4$. Disregarding the two lowest values of h in which $E\pi$ dominates the error, one can see that the performance of RRE generally follows that theoretical curve, with a difference of 0.35 to 1.38 in each h . The highest value of p_E (19.1) was obtained between $m = 8$ and 9 in the $1,025 \times 1,025$ grid ($g = 10$).

5.4. Verification and effect of error orders

Fig. 8 illustrates the apparent order (p_U) of the estimated T_c error as a function of grid size (h). The T_c values were obtained with Eq. (11) and quadruple precision, and those of p_U with Eq. (10), according to the theory described in Section 4.1. The figure shows results for $g = [3,12]$ and levels of extrapolation $m = 0, 1$ and 2. With these results, it is clear that as $h \rightarrow 0$, the values of p_U tend toward the orders 2, 4 and 6.

Fig. 9 shows the effect of the arbitrary choice of the values of p_m on the performance of RRE. Aiming to serve as a reference, this figure presents the Eh and $Em1$ (denote as $p_m = 2,4,6\dots$ correct) curves of Fig. 1 again, for the variable T_c obtained with quadruple precision. It also shows the $Em1$ curves that were obtained with three series of arbitrary values for p_m . The use of

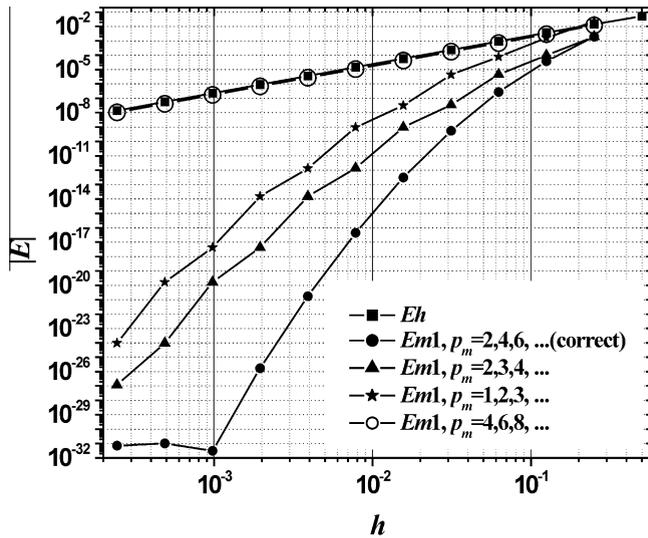


Fig. 9. T_c errors (E) as a function of grid size (h) and values of error orders (Real*16).

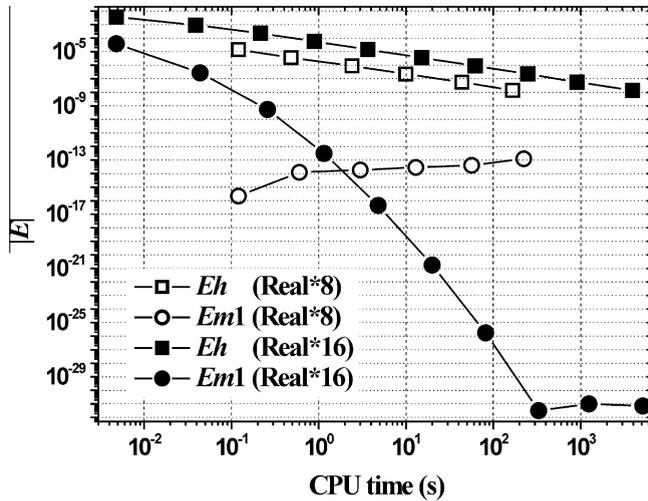


Fig. 10. T_c errors (E) as a function of CPU time and calculation precision.

these arbitrary values reduces the efficiency of RRE considerably in relation to the correct curve, until the effect of RRE is virtually eliminated when $Em1$ almost coincides with Eh .

5.5. Computational efficiency of RRE

Fig. 10 presents the modulus of the error versus the CPU time (in seconds) needed to obtain the solution of variable T_c until the machine round-off error ($E\pi$) is reached. This figure clearly shows that the errors (Eh) of the solutions without extrapolation decrease almost linearly with the increase in CPU time. For the same value of h , Eh with Real*16 is equal to Eh with Real*8, but the CPU time of Eh with Real*16 is about 20 times longer than with Real*8. However, the number of iterations to reach $E\pi$ with Real*16 is twice that of Real*8. Hence, per iteration, the CPU time of the solution with Real*16 is approximately 10 times longer than with Real*8.

In Fig. 10, the CPU time of the error with RRE (Em) in a given grid is the sum of the CPU times of all the coarsest grids, since they are necessary to obtain Em . For example, the CPU time plotted in the figure and corresponding to Em in the $1,025 \times 1,025$ grid also includes the CPU time of the grids 513×513 , 257×257 down to 3×3 , i.e., 10 grids. For $Em1$ with Real*8, the figure shows the results of CPU time only for 129×129 grid and larger ones, in which $E\pi$ already exceeds the discretization error; the CPU time in the smaller grids did not be measured because it was too brief.

As can be seen in Fig. 10, the increment in CPU time with the reduction of $Em1$ (Real*16) decreases as the smaller the error is. This behavior is better than that of the Eh curves. Moreover, for a given error value, the CPU time of $Em1$, even with Real*16, is much shorter than that of Eh , even if one uses the smallest of these values (Real*8). For example, for the error level of $2E-7$, the solution with RRE is obtained with a 200 times shorter CPU time than without RRE. Another example: for the error level of $5E-10$ (which required extrapolating the Eh curve), the solution with RRE is obtained with a 26 thousand times shorter CPU time than without RRE. Hence, in terms of CPU time, the efficiency of RRE increases as the error value decreases.

As can be seen in Fig. 10, for a given value of CPU time, the error with RRE ($Em1$), even with Real*16, is much lower than without RRE (Eh). For example, for a CPU time of 1 s, the solution with RRE has a more than $3E+6$ times lower error than without RRE. Another example: for a CPU time of 100 s, the solution with RRE has a more than $8E+17$ times lower error than without RRE. Hence, the efficiency of RRE in reducing the error increases with increasing CPU time.

In terms of RAM memory, the computational cost of using RRE is almost the same as without RRE for a given grid.

6. Conclusion

This paper presented a theoretical basis for performing repeated Richardson extrapolation (RRE) in heat conduction. RRE was applied to reduce and estimate the discretization error of the numerical solution of the 2D Laplace equation. This work was performed using the finite difference method, a square calculation domain discretized with uniform grids, second-order accurate approximations, several variables of interest, Dirichlet boundary conditions, grids with up to millions of nodes, a multigrid method, single, double and quadruple precisions, a sufficient number of iterations to reach the machine round-off error, and up to twelve Richardson extrapolations.

It was found that:

- (1) RRE is extremely efficient in reducing the discretization error of primary and secondary variables, regardless of the number of numerical approximations employed.
- (2) The Richardson estimator is accurate in predicting the discretization error of numerical solutions obtained with RRE.
- (3) A greater reduction of the discretization error with RRE is achieved by using higher precision in the calculations, a larger number of extrapolations (m), a larger number of grids, and correct error orders.
- (4) To obtain a given error value, much less CPU time and RAM memory are required for the solution with RRE than without RRE.
- (5) When the round-off error is higher than the discretization error, RRE loses its effect of reducing the error; moreover, the Richardson estimator does not work, so $d\phi$ can be used instead.

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