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CENTRAL DIFFERENCE METHOD OF $O(\Delta x^6)$ IN SOLUTION OF THE CDR EQUATION WITH VARIABLE COEFFICIENTS AND ROBIN CONDITION

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Abstract: This paper aims to extend the Taylor series obtaining expressions for the discretization of the derivatives of first and second order accurate $O(\Delta x^6)$ using central differences. The convection-diffusion-reaction (CDR) equation with variable coefficients and Robin boundary conditions was chosen, aiming several numerical comparisons and analysis of some special points in the computational domain, the derivative of the first order (convective term) was extended through the backward and forward differences, both $O(\Delta x^3)$. Two numerical applications with analytical solution using the L_∞ norm validate the computational code and facilitate the analysis of results.

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1. Introduction

In the last decades, heat transfer and fluid mechanics problems have been analyzed in terms of different numerical schemes. Of these, the Finite Element Method retains flexibility and ease in dealing with complex domains, which, to be divided often generates a non-ordered matrix causing a high computational time (see [2]; [4]), and the high computational cost caused by the calculation of integrals that generate the coefficients of the main matrix (see [5]; [6]). Now, the Finite Difference Method replace the partial derivatives that appear in the governing equations by the algebraic difference quotients yielding an ordered matrix which can be resolved by any linear system solution method, using only non-zero coefficients of the matrix, usually highly sparse (see [7]).

In this work, a special contribution is the Taylor series expansion of the derivatives of the first and second order, the convective and diffusive terms, respectively, with the accuracy of $O(\Delta x^6)$, for solving convection-diffusion-reaction problems with variable coefficients and with Robin condition, notably in convective situations that have dominant oscillations in the numerical majority of numerical methods in the literature, when unrefined meshes are used.

2. Finite Difference Method

Numerical simulation methods based on partial differential equations form an important part of contemporary science and are widely used in engineering and scientific applications. In this paper, the Finite Difference Method is used, in which the main feature is the approximation of the temporal and spatial partial derivatives in the governing equation with finite differences that relate the values of the unknown function at a set of neighboring grid points at various time levels. This approximation replaces the partial differential equations with a finite difference equation.

Considering a function $T(x)$ and its derivative at point x,

$$\frac{\partial T(x)}{\partial x} = \lim_{\Delta x \to 0} \frac{T(x+\Delta x) - T(x)}{\Delta x}. \tag{1}$$

If $T(x+\Delta x)$ is expanded in Taylor series around x, we get

$$T(x+\Delta x) = T(x) + \Delta x \frac{\partial T(x)}{\partial x} + \frac{(\Delta x)^2}{2}\frac{\partial^2 T(x)}{\partial x^2} + \frac{(\Delta x)^3}{3!}\frac{\partial^3 T(x)}{\partial x^3} + \dots \tag{2}$$

Substituing the equation (2) in the equation (1), results

$$\frac{T(x+\Delta x) - T(x)}{\Delta x} = \frac{\partial T(x)}{\partial x} + \frac{\Delta x}{2}\frac{\partial^2 T(x)}{\partial x^2} + \dots = \frac{\partial T(x)}{\partial T} + O(\Delta x) \tag{3}$$

that is first order approximation, i.e., the truncation error is $O(\Delta x)$.

Writing T in Taylor series at $x_{i+1} = x_i + \Delta x$ and $x_{i-1} = x_i - \Delta x$, we have (see [1]),

$$T_{i+1} = T_i + \Delta x \left(\frac{\partial T}{\partial x}\right)_i + \frac{\Delta x^2}{2}\left(\frac{\partial^2 T}{\partial x^2}\right)_i + \frac{\Delta x^3}{3!}\left(\frac{\partial^3 T}{\partial x^3}\right)_i + \ldots \tag{4a}$$

$$T_{i-1} = T_i - \Delta x \left(\frac{\partial T}{\partial x}\right)_i + \frac{\Delta x^2}{2}\left(\frac{\partial^2 T}{\partial x^2}\right)_i - \frac{\Delta x^3}{3!}\left(\frac{\partial^3 T}{\partial x^3}\right)_i + \ldots \tag{4b}$$

Rearranging the equation (4-a), we arrive at the *forward difference*:

$$\left(\frac{\partial T}{\partial x}\right)_i = \frac{T_{i+1} - T_i}{\Delta x} + O(\Delta x). \tag{5}$$

Similarly, from the equation (4-b), we have the *backward difference*:

$$\left(\frac{\partial T}{\partial x}\right)_i = \frac{T_i - T_{i-1}}{\Delta x} + O(\Delta x). \tag{6}$$

Now, subtracting the equation (4-b) from equation (4-a), we obtain the *central difference*

$$\left(\frac{\partial T}{\partial x}\right)_i = \frac{T_{i+1} - T_{i-1}}{2\Delta x} + O(\Delta x^2). \tag{7}$$

Finally, by adding the equation (4-a) and equation (4-b), we get the expression of the *central difference for second derivative of* T:

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_i = \frac{T_{i+1} - 2T_i + T_{i-1}}{2\Delta x} + O(\Delta x^2). \tag{8}$$

For the forward and backward finite difference, [1] has the following formula with an accuracy of $O(\Delta x^2)$ for the first derivative of T:

$$\text{Forward:} \quad \left(\frac{\partial T}{\partial x}\right)_i = \frac{-3T_i + 4T_{i+1} - T_{i+2}}{2\Delta x} + O(\Delta x^2), \tag{9a}$$

$$\text{Backward:} \quad \left(\frac{\partial T}{\partial x}\right)_i = \frac{3T_i - 4T_{i-1} + T_{i-2}}{2\Delta x} + O(\Delta x^2). \tag{9b}$$

Whereas, for the central difference of $O(\Delta x^4)$, shows following formulas:

$$\left(\frac{\partial T}{\partial x}\right)_i = \frac{-T_{i+2} + 8T_{i+1} - 8T_{i-1} + T_{i-2}}{12\Delta x} + O(\Delta x^4), \tag{10a}$$

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_i = \frac{-T_{i+2} + 16T_{i+1} - 30T_i + 16T_{i-1} - T_{i-2}}{12\Delta x^2} + O(\Delta x^4). \tag{10b}$$

A special contribution of this work is to construct approximations of $O(\Delta x^3)$ for the forward and backward finite difference and $O(\Delta x^6)$ for central differences from the Taylor series. Using the same philosophy of the equation (4-a,b) to $i-2$ and $i-3$, the result is

$$T_{i-2} = T_i - 2\Delta x \left(\frac{\partial T}{\partial x}\right)_i + 2\Delta x^2 \left(\frac{\partial^2 T}{\partial x^2}\right)_i - \frac{4\Delta x^3}{3}\left(\frac{\partial^3 T}{\partial x^3}\right)_i + \dots \quad (11a)$$

$$T_{i-3} = T_i - 3\Delta x \left(\frac{\partial T}{\partial x}\right)_i + \frac{9\Delta x^2}{2} \left(\frac{\partial^2 T}{\partial x^2}\right)_i - \frac{9\Delta x^3}{2}\left(\frac{\partial^3 T}{\partial x^3}\right)_i + \dots \quad (11b)$$

Using the equation (4-b), (11-a,b), we construct the following expression:

$$\begin{aligned} aT_i + bT_{i-1} + cT_{i-2} + dT_{i-3} &= (a+b+c+d)T_i \\ -\Delta x(b+2c+3d)\left(\frac{\partial T}{\partial x}\right)_i &+ \frac{\Delta x^2}{2}(b+4c+9d)\left(\frac{\partial^2 T}{\partial x^2}\right)_i \\ &- \frac{\Delta x^3}{6}(b+8c+27d)\left(\frac{\partial^3 T}{\partial x^3}\right)_i + \dots \end{aligned} \quad (12)$$

From equation (15), to find an expression for the first derivative of T we find the following system:

$$\begin{cases} a+b+c+d=0 \\ b+2c+3d=-1 \\ b+4c+9d=0 \\ b+8c+27d=0 \end{cases} \Longrightarrow \begin{cases} a=11/6 \\ b=-3 \\ c=3/2 \\ d=-1/3 \end{cases}.$$

Thus an expression for the first derivative of T with backward finite difference of $O(\Delta x^3)$ will be:

$$\left(\frac{\partial T}{\partial x}\right)_i = \frac{11T_i - 18T_{i-1} + 9T_{i-2} - 2T_{i-3}}{6\Delta x} + O(\Delta x^3). \quad (13)$$

Similarly, an expression for finite difference forward of $O(\Delta x^3)$ will be:

$$\left(\frac{\partial T}{\partial x}\right)_i = \frac{-11T_i + 18T_{i+1} - 9T_{i+2} + 2T_{i+3}}{6\Delta x} + O(\Delta x^3). \quad (14)$$

To find expressions for the central difference of $O(\Delta x^6)$ is must expand the Taylor series for points $i+2$ and $i+3$ as follows:

$$T_{i+2} = T_i + (2\Delta x)\left(\frac{\partial T}{\partial x}\right)_i + \frac{(2\Delta x^2)}{2}\left(\frac{\partial^2 T}{\partial x^2}\right)_i + \frac{(2\Delta x^3)}{3!}\left(\frac{\partial^3 T}{\partial x^3}\right)_i + \dots \quad (15a)$$

$$T_{i+3} = T_i + (3\Delta x)\left(\frac{\partial T}{\partial x}\right)_i + \frac{(3\Delta x^2)}{2}\left(\frac{\partial^2 T}{\partial x^2}\right)_i + \frac{(3\Delta x^3)}{3!}\left(\frac{\partial^3 T}{\partial x^3}\right)_i + \dots \quad (15b)$$

From equations (4-a,b), (11-a,b), (15-a,b), we arrive at the expression:

$$\begin{aligned} aT_{i+3} + bT_{i+2} + cT_{i+1} + dT_i + eT_{i-1} + fT_{i-2} + gT_{i-3} = \\ (a+b+c+d+e+f+g)T_i + \Delta x(3a+2b+c-e-2f-3g)\left(\frac{\partial T}{\partial x}\right)_i \\ +\frac{\Delta x^2}{2}(9a+4b+c+e+4f+9g)\left(\frac{\partial^2 T}{\partial x^2}\right)_i \\ +\frac{\Delta x^3}{3!}(27a+8b+c-e-8f-27g)\left(\frac{\partial^3 T}{\partial x^3}\right)_i \\ +\frac{\Delta x^4}{4!}(81a+16b+c+e+16f+81g)\left(\frac{\partial^4 T}{\partial x^4}\right)_i \\ +\frac{\Delta x^5}{5!}(243a+32b+c-e+32f-243g)\left(\frac{\partial^5 T}{\partial x^5}\right)_i \\ +\frac{\Delta x^6}{6!}(729a+65b+c+e+64f+729g)\left(\frac{\partial^6 T}{\partial x^6}\right)_i \ldots \end{aligned} \tag{16}$$

From equation (16), to establish an expression for the first derivative of T, we get the following linear system:

$$\begin{cases} a+b+c+d+e+f+g=0 \\ 3a+2b+c-e-2f-3g=1 \\ 9a+4b+c+e+4f+9g=0 \\ 27a+8b+c-e-8f-27g=0 \\ 81a+16b+c+e+16f+81g=0 \\ 243a+32b+c-e+32f-243g=0 \\ 729a+64b+c+e+64f+729g=0 \end{cases} \Longrightarrow \begin{cases} a=1/60 \\ b=-15/100 \\ c=3/4 \\ d=0 \\ e=-3/4 \\ f=15/100 \\ g=-1/60 \end{cases}$$

which leads the following expression

$$\left(\frac{\partial T}{\partial x}\right)_i = \frac{T_{i+3} - 9T_{i+2} + 45T_{i+1} - 45T_{i-1} + 9T_{i-2} - T_{i-3}}{60\Delta x} + O(\Delta x^6). \tag{17}$$

Again using the equation (16) to obtain an expression for the second derivative of T, we have, then, the following system:

$$\begin{cases} a+b+c+d+e+f+g=0 \\ 3a+2b+c-e-2f-3g=0 \\ 9a+4b+c+e+4f+9g=2 \\ 27a+8b+c-e-8f-27g=0 \\ 81a+16b+c+e+16f+81g=0 \\ 243a+32b+c-e+32f-243g=0 \\ 729a+64b+c+e+64f+729g=0 \end{cases} \Longrightarrow \begin{cases} a=1/90 \\ b=-15/100 \\ c=3/2 \\ d=-49/18 \\ e=3/2 \\ f=-15/100 \\ g=1/90 \end{cases}$$

which leads the following expression

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_i = \frac{1}{180\Delta x^2}(2T_{i+3} - 27T_{i+2} + 270T_{i+1} - 490T_i + 270T_{i-1} \\ -27T_{i-2} + 2T_{i-3}) + O(\Delta x^6). \qquad (18)$$

3. Model Equation

As indicated in the introduction, to demonstrate the efficacy of discretization from the expressions given by equation (13), (14), (17) and (18) is presented the convection-diffusion-reaction problem with variable coefficients and Robin boundary conditions as follows:

$$k(x)\frac{\partial^2 T(x)}{\partial x^2} + u(x)\frac{\partial T(x)}{\partial x} + D(x)T(x) = f(x) \quad \text{in} \quad \Omega = [0,1], \qquad (19a)$$

$$AT + B\frac{\partial T(0)}{\partial x} = C, \qquad (19b)$$

$$ET + G\frac{\partial T(1)}{\partial x} = H. \qquad (19c)$$

4. Formulation

For numerical solution of the problem described in equation (19a-c), four formulations have been proposed and are described below.

Case 1: Dividing the domain into *NNodes* nodes and considering $\Delta x = 1/(NNodes - 1)$, we have:

Node 1: Forward difference $O(\Delta x^2)$ (boundary condition in $x = 0$):

$$\left(A - \frac{3B}{2\Delta x}\right)T_i + \left(\frac{2B}{\Delta x}\right)T_{i+1} + \left(-\frac{B}{2\Delta x}\right)T_{i+2} = C.$$

Node 2: Forward difference $O(\Delta x^2)$ in the first derivative and Central difference $O(\Delta x^2)$ in the second derivative:

$$\left(\frac{k}{\Delta x^2}\right)T_i + \left(-\frac{2k}{\Delta x^2} - \frac{3u_2}{2\Delta x} + D\right)T_{i+1} \\ + \left(\frac{k}{\Delta x^2} + \frac{2u_2}{\Delta x}\right)T_{i+2} + \left(-\frac{u_2}{2\Delta x}\right)T_4 = f_{i+1}.$$

Node 3 to $NNodes-2$: Forward difference $O(\Delta x^2)$ in the first derivative and Central difference $O(\Delta x^4)$ in the second derivative:

$$\left(\frac{-k}{12\Delta x^2}\right)T_{i-2}+\left(\frac{4k}{3\Delta x^2}\right)T_{i-1}+\left(\frac{-5k}{2\Delta x^2}-\frac{3u_i}{2\Delta x}+D\right)T_i$$
$$+\left(\frac{4k}{3\Delta x^2}+\frac{2u_i}{\Delta x}\right)T_{i+1}+\left(-\frac{k}{12\Delta x^2}-\frac{u_i}{2\Delta x}\right)T_{i+2}=f_i.$$

Node $NNodes-1$: Backward difference $O(\Delta x^2)$ in the first derivative and Central difference $O(\Delta x^4)$ in the second derivative:

$$\left(\frac{u_{NNodes-1}}{2\Delta x}\right)T_{NNodes-3}+\left(\frac{k}{\Delta x^2}-\frac{2u_{NNodes-1}}{\Delta x}\right)T_{NNodes-2}$$
$$+\left(\frac{-2k}{\Delta x^2}+\frac{3u_2}{2\Delta x}\right)T_{NNodes-1}+\left(\frac{k}{\Delta x^2}\right)T_{NNodes}=f_{NNodes-1}.$$

Node $NNodes$: Backward difference $O(\Delta x^2)$ (boundary condition in $x=1$):

$$\left(\frac{G}{2\Delta x}\right)T_{NNodes-2}+\left(-\frac{2G}{\Delta x^2}\right)T_{NNodes-1}+\left(E+\frac{3G}{2\Delta x}\right)T_{NNodes}=H.$$

Case 2: This case is different from the previous central nodes (3 to $NNodes-2$), the first derivative of T used in the central differences of $O(\Delta x^4)$ as follows:

$$\left(\frac{-k}{12\Delta x^2}\right)T_{i-2}+\left(\frac{4k}{3\Delta x^2}-\frac{2u_i}{3\Delta x}\right)T_{i-1}+\left(\frac{-5k}{2\Delta x^2}+D\right)T_i$$
$$+\left(\frac{4k}{3\Delta x^2}+\frac{2u_i}{3\Delta x}\right)T_{i+1}+\left(-\frac{k}{12\Delta x^2}-\frac{u_i}{12\Delta x}\right)T_{i+2}=f_i.$$

Case 3: In this case the formulation will be applied $O(\Delta x^3)$ for forward and backward differences and $O(\Delta x^6)$ in this central difference as follows:
Node 1: Forward difference $O(\Delta x^3)$ (boundary condition in $x=0$):

$$\left(A-\frac{11B}{6\Delta x}\right)T_1+\left(\frac{3B}{2\Delta x}\right)T_2+\left(-\frac{3B}{2\Delta x}\right)T_3+\left(\frac{B}{3\Delta x}\right)T_4=C.$$

Node 2: Forward difference $O(\Delta x^3)$ in the first derivative and Central difference $O(\Delta x^2)$ in the second derivative:

$$\left(\frac{k}{\Delta x^2}\right)T_1+\left(-\frac{2k}{\Delta x^2}-\frac{11u_2}{6\Delta x}+D\right)T_2+\left(\frac{k}{\Delta x^2}+\frac{3u_2}{\Delta x^2}\right)T_3$$
$$+\left(-\frac{3u_2}{2\Delta x}\right)T_4+\left(\frac{u_2}{3\Delta x}\right)T_5=f_2.$$

Node 3: Forward difference $O(\Delta x^3)$ in the first derivative and Central difference $O(\Delta x^4)$ in the second derivative:

$$\begin{aligned}&\left(-\frac{k}{12\Delta x^2}\right)T_1+\left(\frac{4k}{3\Delta x^2}\right)T_2+\left(-\frac{5k}{2\Delta x^2}-\frac{11u_3}{6\Delta x}+D\right)T_3\\&+\left(\frac{4k}{3\Delta x^2}+\frac{3u_3}{\Delta x}\right)T_4+\left(-\frac{k}{12\Delta x^2}-\frac{3u_3}{2\Delta x}\right)T_5+\left(\frac{u_3}{3\Delta x}\right)T_6=f_3.\end{aligned}$$

Node 4 to $NNodes-3$: Forward difference $O(\Delta x^3)$ in the first derivative and Central difference $O(\Delta x^6)$ in the second derivative:

$$\begin{aligned}&\left(\frac{k}{90\Delta x^2}\right)T_{i-3}+\left(-\frac{3k}{20\Delta x^2}\right)T_{i-2}+\left(\frac{3k}{2\Delta x^2}\right)T_{i-1}\\&+\left(-\frac{49k}{18\Delta x^2}-\frac{11u_i}{6\Delta x}+D\right)T_i+\left(\frac{3k}{2\Delta x^2}+\frac{3u_i}{\Delta x}\right)T_{i+1}\\&+\left(-\frac{3k}{20\Delta x^2}-\frac{3u_i}{2\Delta x}\right)T_{i+2}+\left(\frac{k}{90\Delta x^2}+\frac{u_i}{3\Delta x}\right)T_{i+3}=f_i.\end{aligned}$$

Node $NNodes-2$: Forward difference $O(\Delta x^3)$ in the first derivative and Central difference $O(\Delta x^4)$ in the second derivative:

$$\begin{aligned}&\left(-\frac{u_{NNodes-2}}{3\Delta x}\right)T_{NNodes-5}+\left(-\frac{k}{12\Delta x^2}+\frac{3u_{NNodes-2}}{2\Delta x}\right)T_{NNodes-4}\\&+\left(\frac{4k}{3\Delta x^2}-\frac{3u_{NNodes-2}}{\Delta x}\right)T_{NNodes-3}\\&+\left(-\frac{5k}{2\Delta x^2}+\frac{11u_{NNodes-2}}{6\Delta x}+D\right)T_{NNodes-2}\\&+\left(\frac{4k}{3\Delta x^2}\right)T_{NNodes-1}+\left(-\frac{k}{12\Delta x^2}\right)T_{NNodes}=f_{NNodes-2}.\end{aligned}$$

Node $NNodes-1$: Forward difference $O(\Delta x^3)$ in the first derivative and Central difference $O(\Delta x^2)$ in the second derivative:

$$\begin{aligned}&\left(-\frac{u_{NNodes-1}}{3\Delta x}\right)T_{NNodes-4}+\left(-\frac{3u_{NNodes-1}}{2\Delta x}\right)T_{NNodes-3}\\&+\left(\frac{k}{\Delta x^2}-\frac{3u_{NNodes-1}}{2\Delta x}\right)T_{NNodes-2}\\&+\left(-\frac{2k}{\Delta x^2}+\frac{11u_{NNodes-1}}{6\Delta x}+D\right)T_{NNodes-1}\\&+\left(\frac{k}{\Delta x^2}\right)T_{NNodes}=f_{NNodes-1}.\end{aligned}$$

Node $NNodes$: Forward difference $O(\Delta x^3)$ (boundary condition in $x = 1$):

$$\left(-\frac{G}{3\Delta x}\right) T_{NNodes-3} + \left(\frac{3G}{2\Delta x}\right) T_{NNodes-2} + \left(-\frac{3G}{\Delta x}\right) T_{NNodes-1} + \left(\frac{11G}{6\Delta x} + E\right) T_{NNodes} = H.$$

Case 4: This case is different from the previous central nodes, Node 4 to $NNodes - 3$, where the first derivative is discretized using central difference of $O(\Delta x^6)$ in this manner:

$$\left(\frac{k}{90\Delta x^2} - \frac{u_i}{60\Delta x}\right) T_{i-3} + \left(\frac{-3k}{20\Delta x^2} + \frac{3u_i}{20\Delta x}\right) T_{i-2} + \left(\frac{3k}{2\Delta x^2} - \frac{3u_i}{4\Delta x}\right) T_{i-1} + \left(-\frac{49k}{18\Delta x^2} + D\right) T_i + \left(\frac{3k}{2\Delta x^2} + \frac{3u_i}{4\Delta x}\right) T_{i+1} + \left(\frac{-3k}{20\Delta x^2} - \frac{3u_i}{20\Delta x}\right) T_{i+2} + \left(\frac{k}{90\Delta x^2} + \frac{u_i}{60\Delta x}\right) T_{i+3} = f_i.$$

5. Numerical Application

A *FORTRAN* computational code to investigate the problem given by equation (23a-c) was built with the mesh generated internally. For solving the linear system *IMSL* library routine, *DLSARG*, was used. For the error analysis the L_∞ norm, which is the maximum error in the domain compared with the analytical solution, was used and too the *convergence rate (CR)* (see [3]):

$$CR = \frac{log(E_1/E_2)}{log(\Delta x_1/\Delta x_2)}, \tag{20}$$

where E_1 and E_2 are *average absolute errors (AAE)* correspond to grids with mesh sizes Δx_1 and Δx_2, respectively.

Here, two applications will be proposed. In the first it is a convective-diffusive case which will be varied in the convection coefficient in order to analyze the efficiency of the method in highly convective situations. Finally, a second application in the case of convection-diffusion with variable coefficients and Robin condition will be tested and analyzed.

5.1. Application 1: Convection-Diffusion with Dominant Convection

In this case, the following equation and boundary conditions are employed:

$$\gamma\frac{dT}{dx}-\frac{d^2T}{dx^2}=0 \quad \text{in} \quad \Omega=[0,1], \quad T(0)=5 \quad \text{and} \quad \frac{dT(1)}{dx}=10$$

which analytical solution is given by $T(x) = (c/\gamma)exp(\gamma x) + d$, where $c = 10/exp(\gamma)$ and $d = 5 - (c/\gamma)$.

In this application, for convection coefficient values at $\gamma = 1, 10$ and 100, was fixed the thermal conductivity value in $k = 1$. For $\gamma = 1$ we have a diffusion dominant case. For this situation, considering rough meshes with $\Delta x = 1/10, \Delta x = 1/20$ or $\Delta x = 1/40$, all cases showed reasonable results according to Table 1, destacking the cases 3 and 4, the which to $\Delta x = 1/20$, already have results of about 10^{-4}. However, such as the problem it becomes dominant, Tables 2 and 3, the results for rough meshes are unsatisfactory.

Δx	**Case 1**	**Case 2**	**Case 3**	**Case 4**
1/10	2,92E-02	7,06E-02	2,19E-03	2,51E-03
1/20	7,42E-03	1,68E-02	2,59E-04	3,21E-04
1/40	1,86E-03	4,10E-03	3,12E-05	4,02E-05
1/80	4,66E-04	1,01E-03	3,82E-06	5,03E-06
1/100	2,98E-04	6,45E-04	1,94E-06	2,57E-06
1/200	7,46E-05	1,60E-04	2,41E-07	3,21E-07
1/500	1,19E-05	2,56E-05	1,56E-08	2,11E-08
1/1000	2,98E-06	5,38E-06	4,36E-09	3,56E-09

Table 1: L_∞ norm of error in solution of $T(x)$ for $\gamma = 1$.

Δx	**Case 1**	**Case 2**	**Case 3**	**Case 4**
1/10	5,04E-01	3,19E-01	9,81E-02	1,87E-01
1/20	1,52E-01	9,29E-02	2,28E-02	3,86E-02
1/40	4,11E-02	2,37E-02	3,21E-03	5,94E-03
1/80	1,04E-02	5,75E-03	3,82E-04	7,89E-04
1/100	6,71E-03	3,63E-03	1,90E-04	4,06E-04
1/200	1,67E-03	8,77E-04	2,20E-05	5,11E-05
1/500	2,67E-04	1,36E-04	1,32E-06	3,26E-06
1/1000	6,67E-05	3,37E-05	1,61E-07	4,07E-07

Table 2: L_∞ norm of error in solution of $T(x)$ for $\gamma = 10$.

According to Table 2, cases 1 and 2 only reach an accuracy of about 10^{-4} to $\Delta x = 1/500$, while for cases 3 and 4 this is can be noted to $\Delta x = 1/80$

Δx	**Case 1**	**Case 2**	**Case 3**	**Case 4**
1/10	divergence	6,73E-01	divergence	4,39E-01
1/20	divergence	3,02E-01	divergence	2,19E-01
1/40	divergence	1,26E-01	divergence	8,88E-02
1/80	7,21E-02	4,58E-02	divergence	2,88E-02
1/100	5,06E-02	3,19E-02	divergence	1,87E-02
1/200	1,52E-02	9,28E-03	2,27E-03	3,86E-03
1/500	2,65E-03	1,51E-03	1,63E-04	3,13E-04
1/1000	6,71E-04	3,63E-04	1,90E-05	4,05E-05

Table 3: L_∞ norm of error in solution of $T(x)$ for $\gamma = 100$.

Δx	**Case 1**	**Case 2**	**Case 3**	**Case 4**
1/10	-	-	-	-
1/20	1,73	1,78	2,11	2,28
1/40	1,89	1,97	2,83	2,70
1/80	1,98	2,04	3,07	2,91
1/100	1,96	2,06	3,13	2,98
1/200	2,01	2,05	3,11	2,99
1/500	2,00	2,03	3,07	3,00
1/1000	2,00	2,01	3,04	3,00

Table 4: Order of convergence rate (CR) of the results in Table 2.

i.e., to meshes about 6 times less refined. In particular, deserves mention in this application in which case $\gamma = 100$ (Table 3). For cases 1 and 3 which use forward differences in the first derivative at the internal points on computational mesh, had distinct results for rough meshes. Emphasizing the case 3 in which the results only began to converge on a mesh with $\Delta x = 1/200$. For these meshes in which the results were different the Gauss-Seidel method for solving the linear system and divergence in the results were still observed. Note again in Table 3, the results obtained in cases 2 and 4 are more stable, even with rough meshes, demonstrating that the use of central differences in the first and second derivatives resulted in well-posed linear system, and no difference was observed in the results. Because the case is highly convective, only achieved an accuracy of about 10^{-4} for a mesh with $\Delta x = 1/1000$ for cases 1 and 2 and $\Delta x = 1/500$ for cases 3 and 4. Table 4 shows the convergence rate of the results presented in Table 2. Note it is significantly higher in cases 3 and 4.

5.2. Application 2: Convection-Diffusion with Variables Coefficients and Robin Condition

For this case we adopt the following equation and boundary conditions:

$$k\frac{d^2T}{dx^2} + \left(\frac{1}{1+x}\right)\frac{dT}{dx} = x+1 \quad \text{in} \quad \Omega = [0,1],$$
$$T(0) - k\frac{dt(0)}{dx} = 1 \quad \text{and} \quad T(1) = \frac{dT(1)}{dx} = 1$$

which analytical solution is given by

$$T(x) = \frac{(x+1)^3}{3(2k+1)} + D\left(\frac{(x+1)^{1-\frac{1}{k}}}{k-1} - \left(\frac{2^{1-\frac{1}{k}}}{k-1} - \frac{2^{-\frac{1}{k}}}{k}\right)\right) + \left(1 - \frac{20}{3(2k+1)}\right),$$

where $D = \dfrac{(19+3k)/(3(2k+1))}{((1-2^{1-\frac{1}{k}})/(k-1) - 2^{-\frac{1}{k}}/k) - 1}$.

Δx	**Case 1**	**Case 2**	**Case 3**	**Case 4**
1/10	6,10E-04	7,38E-04	2,51E-04	2,45E-04
1/20	1,60E-04	1,97E-04	3,69E-05	3,55E-05
1/40	4,10E-05	5,09E-05	5,03E-06	4,78E-06
1/80	1,03E-05	1,29E-05	6,59E-07	6,20E-07
1/100	6,66E-06	8,29E-06	3,40E-07	3,20E-07
1/200	1,67E-06	2,08E-06	4,33E-08	4,06E-08
1/500	2,68E-07	3,35E-07	2,85E-09	2,67E-09
1/1000	6,71E-08	8,37E-08	5,65E-10	5,42E-10

Table 5: L_∞ norm of error in solution of $T(x)$ for $k = 2$.

Δx	**Case 1**	**Case 2**	**Case 3**	**Case 4**
1/10	1,34E-01	1,08E-01	5,99E-02	5,50E-02
1/20	4,24E-02	2,99E-02	1,15E-02	9,78E-03
1/40	1,18E-02	7,54E-03	1,80E-03	1,41E-03
1/80	3,13E-03	1,85E-03	2,52E-04	1,86E-04
1/100	2,02E-03	1,17E-03	1,32E-04	9,65E-05
1/200	5,15E-04	2,88E-04	1,72E-05	1,22E-05
1/500	8,34E-05	4,55E-05	1,13E-06	7,89E-07
1/1000	2,09E-05	1,13E-05	1,42E-07	9,84E-08

Table 6: L_∞ norm of error in solution of $T(x)$ for $k = 2 \times 10^{-1}$.

Δx	**Case 1**	**Case 2**	**Case 3**	**Case 4**
1/10	1,79E+00	1,82E+00	1,59E-00	1,55E-00
1/20	1,18E+00	1,17E+00	9,43E-01	9,34E-01
1/40	6,20E-01	5,68E-01	3,97E-01	3,86E-01
1/80	2,49E-01	2,02E-01	1,09E-01	1,00E-01
1/100	1,76E-01	1,37E-01	6,67E-02	5,93E-02
1/200	5,40E-02	3,63E-02	1,17E-02	9,42E-03
1/500	9,65E-03	5,62E-03	9,18E-04	6,54E-04
1/1000	2,49E-03	1,35E-03	1,22E-04	8,25E-05

Table 7: L_∞ norm of error in solution of $T(x)$ for $k = 2 \times 10^{-2}$.

Δx	**Case 1**	**Case 2**	**Case 3**	**Case 4**
1/10	-	-	-	-
1/20	1,66	1,85	2,38	2,49
1/40	1,85	1,99	2,68	2,79
1/80	1,91	2,03	2,84	2,92
1/100	1,96	2,05	2,90	2,94
1/200	1,97	2,02	2,94	2,98
1/500	1,99	2,01	2,97	2,99
1/1000	2,00	2,01	2,99	3,00

Table 8: Order of convergence rate (CR) of the results in Table 6.

Here, the convective and source terms are variable and the Robin boundary conditions, where the condition at $x = 0$ depends on the conductivity coefficient k, which, in this application, varies for values $2, 2\times10^{-1}$ and 2×10^{-2}. For $k = 2$, Table 5, we have a situation like the one presented in Table 1, i.e, the diffusive dominant case. Note that for a mesh with $\Delta x = 1/10$ is possible to achieve a standard order error of 10^{-4}. When $k = 2 \times 10^{-1}$ does not happen, since the problem becomes convection dominant, increase the number of oscillations so that a mesh with $\Delta x = 1/10$ the accuracy is only $10^{-4}(k = 2)$ to 10^{-1} for $k = 2 \times 10^{-1}$, in cases 1 and 2, Table 6. In Table 7, where $k = 2 \times 10^{-2}$ to $\Delta x = 1/10, \Delta x = 1/20, \Delta x = 1/40$ and $\Delta x = 1/80$ the numerical oscillations are very significant in four cases. From Table 7, an accuracy of order 10^{-4} was only achieved by cases 3 and 4 in a mesh with $\Delta x = 1/500$, the same is not true in cases 1 and 2 in the meshes proposed in this paper. Table 8 shows the convergence rate of the results presented in Table 6. Note that it is significantly higher in cases 3 and 4, the same had already occurred in an application 1.

6. Conclusions

In this work, four formulations using the Finite Difference Method have been proposed. In general, in all cases, the diffusion dominant problems, good results were achieved. However, the dominant convective problems, cases 3 and 4 had the best results. It is noteworthy that cases 1 and 3 showed divergence in their results in an application, in which case, in which meshes used unrefined form. The literature shows that convection dominant problems cause numerical oscillations especially for unrefined meshes. However, in this work, the use of central differences in the first and second derivative, cases 2 and 4, showed reasonable results even for coarse meshes, to the point that, in case 4, have accuracy of order 10^{-2} (for $\Delta x = 1/40$). In future work, this technique will be implemented for two and three-dimensional and nonlinear problems.

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References

[1] T.J. Chung, *Computational Fluid Dynamics*, Cambridge University Press, Cambridge (2002).

[2] N. Camprub, I. Colominas, F. Navarrina, M. Casteleiro, Least-Squares and G.L.S. numerical approaches for convective-diffusive transport problems in engineering, In: *Proceedings of the European Congress on Computational Methods in Applied Sciences and Engineering, ECCOMAS* (2000).

[3] G. Gürarslan, Numerical modelling of linear and nonlinear diffusion equations by compact finite difference method, *Applied Mathematics and Computation*, **216** (2010), 2472-2478.

[4] A. Hannukainen, S. Korotov, M. Krezek, Nodal $O(h^4)$-Superconvergente in 3D by averaging piecewise linear, bilinear, and trilinear FE approximations, *Journal of Computational Mathematics*, **28**, No. 1 (2010), 1-10.

[5] E.C. Romão, L.F.M. Moura, J.B.C. Silva, Analysis of error in the solution of the 2-D diffusion equation by finite element methods, *TEMA Tend. Mat. Apl. Comput.*, **9**, No. 2 (2008), 287-298.

[6] E.C. Romão, M.D. Campos, L.F.M. Moura, Application of Galerkin and least-squares finite element method in the solution of 3D Poisson and Helmholtz equations, *Computers and Mathematics with Applications*, **62** (2011), 4288-4299.

[7] W.F. Spotz, G.F. Carey, A high-order compact formulation for the 3D Poisson equation, *Numerical Methods Partial Differential Equations*, **12** (1996), 235-243.