

ERROR ANALYSIS IN THE NUMERICAL SOLUTION OF 3D CONVECTION-DIFFUSION EQUATION BY FINITE DIFFERENCE METHODS

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ABSTRACT

In this work an error analysis for numerical solution of 3D convection-diffusion equation by finite difference methods has been done. The backward, the forward and the central difference schemes are applied for three applications: a case with diffusion dominant corresponding to high diffusion coefficients and two cases with convection dominant or with low diffusion coefficients. In the second application the convective coefficients are function only of the diffusion coefficient that in dimensionless form is named Reynolds numbers. In the third application the convective coefficients are function of both the Reynolds number and of the space. The three applications have analytical solutions to facilitate numerical comparisons of the solutions.

Keywords: Finite Difference Method, Error Analysis, Reynolds Numbers, Convection-Diffusion.

NOMENCLATURE

x, y, z	space coordinates
f	source
u	temperature
L_2	Global norm
L_∞	Maximum error
\mathfrak{R}	real numbers
Re	Reynolds number

Greek symbols

Ω	three-dimensional domain
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Subscripts

$i, i+1$	position of node in discretization
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1. INTRODUCTION

The Finite Difference Method (FDM) is a powerful tool to solve fluid mechanics and heat transfer problems. Several authors already presented excellent results from the application of FDM in 1D, 2D and 3D problems of Fluid mechanics and Heat Transfer.

In Hsu (2006) the 3D inverse non-Fourier heat conduction problem are solved by Finite Difference Method and showing excellent results because it is purely diffusive problems. Excellent results are also

presented in Yang et al (2002), were one particular integral formulations are presented for 2D and 3D transient potential flow (heat conduction) analysis. The results of the analysis are compared with an alternative formulation developed using the volume integral conversion approach, obtained excellent results.

Among them Gupta and Zhang (2000) utilized an explicit fourth order finite difference scheme for the solution of 3D convection-diffusion equation. In Romão et al (2008) a FDM was applied to numerical solution of 1D transient diffusion equation obtaining good results. In Chung (2002) several problems of Fluid Mechanics were solved by the application of FDM, including solution of the Laplace and the Burgers equations. In Hon and Chen (2003) a numerical solution of a convection-diffusion equation by the *Boundary Knot Method* is compared with its analytical solution.

In this work, three variants of the Finite Difference Method (FDM) are applied to an error analysis in the solution of the convection-diffusion equation. They are the backward, the forward and central difference schemes. Three applications are considered: one with diffusion predominant and the other two with convection predominant, a case with convective coefficients function only of the Reynolds number and another with convective coefficients depending on the Reynolds number and the position.

The performance of each scheme is analyzed and discussed.

In this work we consider the solution of a 3D convection-diffusion problem modeled by the general equation:

$$a \frac{\partial^2 u}{\partial x^2} + b \frac{\partial^2 u}{\partial y^2} + c \frac{\partial^2 u}{\partial z^2} + d \frac{\partial u}{\partial x} + e \frac{\partial u}{\partial y} + g \frac{\partial u}{\partial z} + hu = f(x, y, z) \quad (1)$$

with $a = a(x, y, z)$, $b = b(x, y, z)$, $c = c(x, y, z)$, $d = d(x, y, z)$, $e = e(x, y, z)$, $g = g(x, y, z)$, $h = h(x, y, z)$ and $u = u(x, y, z)$.

2. FINITE DIFFERENCE METHOD

The basic idea of finite difference methods is simple: derivatives in differential equations are written in terms of discrete quantities of dependent and independent variables, resulting in simultaneous algebraic equations with all unknowns prescribed at discrete mesh points for the entire domain.

In this item, we present three variants of the finite difference method (Chung (2002), Smith (1971) and Fortuna (2000)) for deriving equations.

2.1 Taylor Series – Finite Difference Methods

Consider a function $u(x)$ and its derivative at point x ,

$$\frac{\partial u(x)}{\partial x} = \lim_{\Delta x \rightarrow 0} \frac{u(x + \Delta x) - u(x)}{\Delta x} \quad (2)$$

If $u(x + \Delta x)$ is expanded in Taylor Series around $u(x)$, we obtain

$$u(x + \Delta x) = u(x) + \Delta x \frac{\partial u(x)}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 u(x)}{\partial x^2} + \dots \quad (3)$$

Substituting (3) into (2) yields

$$\frac{\partial u(x)}{\partial x} = \lim_{\Delta x \rightarrow 0} \left(\frac{\partial u(x)}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 u(x)}{\partial x^2} + \dots \right) \quad (4)$$

Or it is seen from (3) that

$$\begin{aligned} \frac{u(x + \Delta x) - u(x)}{\Delta x} &= \frac{\partial u(x)}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 u(x)}{\partial x^2} + \dots \Rightarrow \\ \frac{u(x + \Delta x) - u(x)}{\Delta x} &= \frac{\partial u(x)}{\partial x} + O(\Delta x) \end{aligned} \quad (5)$$

The derivative $\partial u(x)/\partial x$ in (5) is of first order in Δx , indicating that the truncation error $O(\Delta x)$ goes

to zero like the first power in Δx . The finite difference form given by (2), (4) and (5) is said to be of the first order accuracy.

We may write u in Taylor series at $i+1$ and $i-1$,

$$u_{i+1} = u_i + \Delta x \left(\frac{\partial u}{\partial x} \right)_i + \frac{\Delta x^2}{2} \left(\frac{\partial^2 u}{\partial x^2} \right)_i + \frac{\Delta x^3}{3!} \left(\frac{\partial^3 u}{\partial x^3} \right)_i + \dots \quad (6)$$

$$u_{i-1} = u_i - \Delta x \left(\frac{\partial u}{\partial x} \right)_i + \frac{\Delta x^2}{2} \left(\frac{\partial^2 u}{\partial x^2} \right)_i - \frac{\Delta x^3}{3!} \left(\frac{\partial^3 u}{\partial x^3} \right)_i + \dots \quad (7)$$

Rearranging Eq. (6) and after neglecting terms of order greater than 2, we arrive at the **forward difference**:

$$\left(\frac{\partial u}{\partial x} \right)_i = \frac{u_{i+1} - u_i}{\Delta x} + O(\Delta x) \quad (8)$$

Likewise, from (7), we have the **backward difference**:

$$\left(\frac{\partial u}{\partial x} \right)_i = \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x) \quad (9)$$

A **central difference** is obtained by subtracting (7) from (6):

$$\left(\frac{\partial u}{\partial x} \right)_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + O(\Delta x^2) \quad (10)$$

It is seen that the truncation errors for the forward and backward differences are first order, whereas the central difference yields a second order truncation error (Chung, 2000).

Finally, by adding (6) and (7), we have

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} = \left(\frac{\partial^2 u}{\partial x^2} \right)_i + \frac{(\Delta x)^2}{12} \left(\frac{\partial^4 u}{\partial x^4} \right)_i + \dots \quad (11)$$

This leads to the finite difference formula for the second derivative with second order accuracy,

$$\left(\frac{\partial^2 u}{\partial x^2} \right)_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + O(\Delta x^2) \quad (12)$$

3. DERIVATION OF FINITE DIFFERENCE SCHEME EQUATIONS

In that follows, the mathematical formulation by FDM in three considered variants is presented for the convection-diffusion Equation (1).

3.1 Forward Difference Scheme - FDS

By substitution of Eqs. (8) and (12) in Eq. (1), we obtain the forward difference scheme as

$$\begin{aligned} & \left(\frac{a}{\Delta x^2} + \frac{d}{\Delta x} \right) u_{i+1,j,k} + \left(\frac{b}{\Delta y^2} + \frac{e}{\Delta y} \right) u_{i,j+1,k} + \\ & \frac{b}{\Delta y^2} u_{i,j-1,k} + \left(\frac{c}{\Delta z^2} + \frac{g}{\Delta z} \right) u_{i,j,k+1} + \frac{a}{\Delta x^2} u_{i-1,j,k} + \\ & \frac{b}{\Delta y^2} u_{i,j-1,k} + \left(\frac{c}{\Delta z^2} + \frac{g}{\Delta z} \right) u_{i,j,k+1} + \frac{a}{\Delta x^2} u_{i-1,j,k} + \\ & \frac{c}{\Delta z^2} u_{i,j,k-1} + \left(-\frac{2a}{\Delta x^2} - \frac{2b}{\Delta y^2} - \frac{2c}{\Delta z^2} - \frac{d}{\Delta x} - \right. \\ & \left. \frac{e}{\Delta y} - \frac{g}{\Delta z} + h \right) u_{i,j,k} = f(x, y, z) \end{aligned} \quad (13)$$

3.2 Backward Difference Scheme - BDS

In a similar way, by substituting the Eqs. (9) and (12) in (1), we obtain the backward difference scheme

$$\begin{aligned} & \frac{a}{\Delta x^2} u_{i+1,j,k} + \frac{b}{\Delta y^2} u_{i,j+1,k} + \frac{c}{\Delta z^2} u_{i,j,k+1} + \\ & \left(\frac{a}{\Delta x^2} - \frac{d}{\Delta x} \right) u_{i-1,j,k} + \left(\frac{b}{\Delta y^2} - \frac{e}{\Delta y} \right) u_{i,j-1,k} + \\ & \left(\frac{c}{\Delta z^2} - \frac{g}{\Delta z} \right) u_{i,j,k-1} + \left(-\frac{2a}{\Delta x^2} - \frac{2b}{\Delta y^2} - \frac{2c}{\Delta z^2} + \frac{d}{\Delta x} + \right. \\ & \left. \frac{e}{\Delta y} + \frac{g}{\Delta z} + h \right) u_{i,j,k} = f(x, y, z) \end{aligned} \quad (14)$$

3.3 Central Difference Scheme - CDS

The central difference scheme is obtained by combination of Esq. (10), (12) and Eq. (1)

$$\begin{aligned} & \left(\frac{a}{\Delta x^2} + \frac{d}{2\Delta x} \right) u_{i+1,j,k} + \left(\frac{b}{\Delta y^2} + \frac{e}{2\Delta y} \right) u_{i,j+1,k} + \\ & \left(\frac{c}{\Delta z^2} + \frac{g}{2\Delta z} \right) u_{i,j,k+1} + \left(\frac{a}{\Delta x^2} - \frac{d}{2\Delta x} \right) u_{i-1,j,k} + \left(\frac{b}{\Delta y^2} - \right. \\ & \left. \frac{e}{2\Delta y} \right) u_{i,j-1,k} + \left(\frac{c}{\Delta z^2} - \frac{g}{2\Delta z} \right) u_{i,j,k-1} + \left(-\frac{2a}{\Delta x^2} - \frac{2b}{\Delta y^2} - \right. \\ & \left. \frac{2c}{\Delta z^2} + h \right) u_{i,j,k} = f(x, y, z) \end{aligned} \quad (15)$$

4. NUMERICAL APPLICATIONS

The numerical solution of the linear Equations (13), (14) and (15) was obtained by the utilization of the Gauss-Seidel Method with error $\leq 10^{-7}$ (Barroso *et. al.*, 1987). In the utilization of this method only the non zeroes coefficients of the matrix need to be stored. In all applications the delta are all of the same size: $\Delta x = \Delta y = \Delta z = h$, and the domain will be an hexahedra of unitary side.

The first application is a case of convection-diffusion equation in which all coefficients are unitary constants in the whole domain. The L_2 -norm of the error is calculated (Dhatt and Touzot (1984), Romão *et al.* (2008)) in order to analyze the errors in the numerical solution. Also the maximum error is analyzed by the evaluation of the L_∞ -norm. The L_2 norm of the error was defined like in (Zlimal, 1978):

$$\|e\| = \left[\left(\sum_{i=1}^{N_{nost}} e_i^2 \right) / N_{nost} \right]^{1/2}.$$

In this equation, N_{nost} is the total number of nodes in the mesh and $e_i = |T_{(num)_i} - T_{(an)_i}|$, where $T_{(num)}$ is the result from the numerical solution and $T_{(an)}$ is the result from the analytical solution respectively. The L_2 norm presented a overview of error, while the L_∞ norm a view point of error.

The same is done in the second and third applications, but the coefficients of the convective terms are functions of number Reynolds, so that the third application the coefficients also depend on the space. The results of second application are compared with results from Gupta and Zhang (2000). The same size h of discretization of Gupta was used in this work. The applications 1 at 3 are defined in domain $\Omega = [0,1]^3$, with $\Omega \in \mathfrak{R}$.

Application 1. In this case, the convection-diffusion equation simplifies to:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + \frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} + \frac{\partial u}{\partial z} = 0$$

subject to the Dirichlet boundary condition.

The analytical solution for the above equation is (Hon and Chen, 2003),

$$u(x, y, z) = e^{-x} + e^{-y} + e^{-z}$$

The calculated norms are presented in Tables 1 and 2. The first column of the tables is the size the spatial discretization; the second column show the number of non zeros coefficients in the linear system; the third the number of points in the domain and the last three columns are the norms of the errors.

Table 1. L₂-norm of the errors in the numerical solutions of the three FDM considered.

h	NCNN	Nnodes	L ₂ Norm		
			FDS	BCS	CDS
1/5	600	216	2,87E-03	3,74E-03	1,08E-04
1/8	2787	729	2,16E-03	2,55E-03	4,90E-05
1/10	5705	1331	1,83E-03	2,09E-03	3,29E-05
1/16	25163	4913	1,25E-03	1,36E-03	1,43E-05
1/20	50415	9261	1,02E-03	1,10E-03	1,00E-05
1/32	214683	35937	6,68E-04	7,03E-04	6,84E-06
1/64	1774907	274625	3,34E-04	3,68E-04	1,46E-05
1/100	6852095	1030301	1,70E-04	2,82E-04	5,57E-05

By inspection of tables 1 and 2, as expected, the mesh refinement reduce the value of the error, the central difference yielding to better results which with h = 0,2 already presents a maximum error and a L₂-norm of order 10⁻⁴. In this first application convection and diffusion are of the same order of importance. In the next two applications the convection is predominant in order to analyze the robustness of the methods. Convective dominant problems present difficulties to numerical methods in general.

Table 2. L_∞-norm of the errors in the numerical solutions of the three FDM considered.

h	NCNN	Nnodes	L ₂ Norm		
			FDS	BCS	CDS
1/5	600	216	8,62E-03	1,13E-02	3,27E-04
1/8	2787	729	5,70E-03	6,76E-03	1,29E-04
1/10	5705	1331	4,78E-03	5,47E-03	8,60E-05
1/16	25163	4913	3,12E-03	3,39E-03	3,62E-05
1/20	50415	9261	2,51E-03	2,69E-03	2,55E-05
1/32	214683	35937	1,59E-03	1,67E-03	1,85E-05
1/64	1774907	274625	7,69E-04	8,66E-04	4,25E-05
1/100	6852095	1030301	3,58E-04	6,88E-04	1,62E-04

In the routine used to solve the linear system, only non zero coefficients (NCNN – number of coefficients non nulls) need to be storage. For example, in a mesh with h = 0,05, NCNN = 50.415 and Nnodes = 9.261 (Nnodes = number of nodes) if a full matrix was assembled, for the linear systems (13), (14) and (15) one would have in a 9.261x9.261, 85.766.121 coefficients to be storage. Storing only the nonzero elements, the number of coefficients to be storage reduces to 50.415, less than 1 percent of the full matrix, with a significant reduction in the computational cost.

We also noted in tables 1 and 2, that when using a mesh with h = 1/100, the results begin to be less than the precision of mesh h = 1/64, though not presented in this work, for a mesh h = 1/200 precision now falls to values close to 10⁻³, demonstrating that excessive

refinement do not always have better results (for CDS).

Application 2. In this application the convective coefficients are function of the Reynolds numbers and the equation considered is of the form:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} - (\text{Re} \cos \alpha \cos \beta) \frac{\partial u}{\partial x} - (\text{Re} \cos \alpha \sin \beta) \frac{\partial u}{\partial y} - (\text{Re} \sin \alpha) \frac{\partial u}{\partial z} = f(x, y, z)$$

with α = 35°, β = 45° and subject to the Dirichlet boundary condition.

The analytical solution is (Gupta and Zhang, 2000),

$$u(x, y, z) = \sin \pi \cdot x \cdot \sin \pi \cdot y \cdot \sin \pi \cdot z .$$

Table 3. Maximum error to Re = 1.

h	FDS	BDS	CDS	Gupta 2000, standard upwind
1/16	2,15E-02	1,44E-02	3,43E-03	1,45E-02
1/32	9,85E-03	8,10E-03	7,97E-04	8,09E-03
1/64	4,67E-03	4,31E-03	1,62E-04	4,28E-03

Table 4. Maximum error to Re = 10.

h	FDS	BDS	CDS	Gupta 2000, standard upwind
1/16	1,70E-01	1,27E-01	4,32E-03	1,28E-01
1/32	7,88E-02	6,81E-02	3,50E-04	6,82E-02
1/64	3,79E-02	1,19E-02	2,66E-04	3,54E-02

Table 5. Maximum error to Re = 100.

h	FDS	BDS	CDS	Gupta 2000, standard upwind
1/16	8,47E-01	2,71E-01	6,11E-03	2,71E-01
1/32	1,11E-01	1,48E-01	1,52E-03	1,48E-01
1/64	8,87E-02	7,82E-02	3,81E-04	7,82E-02

Tables 3 to 5 show the results of the present simulation compared with the analytical solution from Gupta (2000). Although, the present results are less accurated than the results from Gupta (2000), we have used only first order discretization (FDS and BDS) and second order discretization (CDS), while Gupta has used an upwind scheme with identical

results to those presented this work backward scheme.

In tables 3 to 5, it can be observed that when the Reynolds number increases the errors of the present simulations are of the same (or better) order of accuracy of the results from Gupta (2000), being better at CDS. For this Reynolds number the convection already predominate over the diffusion.

Table 6. L₂ Norm of error to Re = 1.

h	FDS	BDS	CDS
1/16	6,97E-03	4,68E-03	1,04E-03
1/32	3,33E-03	2,74E-03	2,69E-04
1/64	1,61E-03	1,49E-03	5,56E-05

Table 7. L₂ Norm of error to Re = 10.

h	FDS	BDS	CDS
1/16	5,38E-02	4,03E-02	1,34E-03
1/32	2,59E-02	2,25E-02	1,08E-03
1/64	1,27E-02	3,53E-02	8,68E-05

Table 8. L₂ Norm of error to Re = 100.

h	FDS	BDS	CDS
1/16	1,04E-01	8,17E-02	1,96E-03
1/32	6,30E-02	4,63E-02	5,11E-04
1/64	2,76E-02	2,47E-02	1,30E-04

In tables 6 to 8, one notes that the average error introduced by the L₂ norm is around the same order of accuracy of the maximum error introduced by the L_∞ norm.

Application 3. In this application the convective coefficients are function of the Reynolds number as well as of the space (x, y, z) and the equation is of the form:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + (\text{Re sen y sen z cos x}) \frac{\partial u}{\partial x} + (\text{Re sen x sen z cos y}) \frac{\partial u}{\partial y} + (\text{Re sen x sen y cos z}) \frac{\partial u}{\partial z} = f$$

with $f = f(x, y, z)$. The analytical solution is,

$$u(x, y, z) = \cos(4x + 6y + 8z).$$

Table 9. Maximum error to Re = 1.

h	FDS	BDS	CDS
1/8	6,52E-02	9,33E-02	7,72E-02
1/16	1,44E-02	2,81E-02	1,90E-02
1/32	2,99E-03	9,49E-03	4,72E-03
1/64	1,67E-03	3,67E-03	1,15E-03

Table 10. L₂ Norm of error to Re = 1.

h	FDS	BDS	CDS
1/8	2,36E-02	3,42E-02	2,87E-02
1/16	5,18E-03	1,06E-02	7,69E-03
1/32	1,00E-03	3,53E-03	2,00E-03
1/64	4,78E-04	1,31E-03	5,09E-04

In tables 9, 11 and 13 are presented the norms L_∞ of error while tables 10, 12 and 14 are presented L₂ norms of error for values of h equal to 1/8, 1/16, 1/32 and 1/64 for the three schemes proposed in this paper. Again, the CDS stands before the other two schemes, but for the L₂ norm the FDS has order of accuracy consistent with the results of the CDS in almost all the refinements.

Table 11. Maximum error to Re = 10.

h	FDS	BDS	CDS
1/8	1,34E-01	3,52E-01	9,28E-02
1/16	8,44E-02	1,39E-01	2,27E-02
1/32	4,76E-02	6,10E-02	5,74E-03
1/64	2,53E-02	2,86E-02	1,42E-03

Table 12. L₂ Norm of error to Re = 10.

h	FDS	BDS	CDS
1/8	3,43E-02	9,40E-02	3,37E-02
1/16	2,28E-02	3,93E-02	9,04E-03
1/32	1,36E-02	1,79E-02	2,35E-03
1/64	7,46E-03	8,57E-03	6,02E-04

The highlight negative is that the BDS, using the Gauss-Seidel to solve the linear system, showed no convergence results for meshes with h equal to 1/8 and 1/16 for a Re = 100. For meshes with h equal to 1/32 and 1/64, in turn, the method converged normally.

Table 13. Maximum error to Re = 100.

h	FDS	BDS	CDS
1/8	5,01E-01	Not converge	2,14E-01
1/16	2,72E-01	Not converge	4,98E-02
1/32	1,48E-01	2,06E-01	1,25E-02
1/64	7,79E-02	8,87E-02	3,13E-03

Table 14. L₂ Norm of error to Re = 100.

h	FDS	BDS	CDS
1/8	1,57E-01	Not converge	7,02E-02
1/16	9,35E-02	Not converge	1,81E-02
1/32	5,15E-02	6,15E-02	4,67E-03
1/64	2,72E-02	2,95E-02	1,19E-03

For this case, was tested meshes with h equal to 1/100 and 1/200, but the results are worse than the precision shown for the mesh h = 1/64 for the three variations of the Reynolds number, thus showing that not always the constant refinement of the mesh always present better results.

5. CONCLUSIONS AND FUTURE WORK

The Finite Difference method is a powerful tool in solution of convection-diffusion problems. The numerical solution of this kind of problem generally is affected by numerical oscillations when the Reynolds number increases. The obtained results demonstrated that for error of order 10^{-2} or 10^{-3} , discretization of first or second order already can be satisfactory. With this order of error the simulations are relatively of low cost and of easy implementation, for example, in Fortran language.

In next works, more general problems to which analytical solutions are not known will be analyzed. With computers of great capacity of RAM, more refined meshes shall be considered and more realistic problems where the velocity field needs to be obtained also will be considered.

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