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A COMPARISON OF TIME DISCRETIZATION SCHEMES IN THE SOLUTION OF A CONVECTION-DIFFUSION EQUATION

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Abstract. The aim of this work is to present in a didactic way a comparison of analytical and numerical solutions of a transient one-dimensional heat transfer problem. So, the solution of a parabolic equation of convection-diffusion type has been done with discretization in space by the Central Finite Difference method and in the time by five schemes: two explicit and three implicit. From the analytical and the numerical results the L_2 norm and the L-infinity norm are evaluated as measures of the error. Some numerical applications are presented and discussed.

1 INTRODUCTION

In this work, a transient one-dimensional problem of heat transfer governed by a parabolic equation is considered for comparison of five time discretization schemes. One-dimensional problem is considered because the focus of this work is the comparison of time discretization schemes. For one-dimensional problems the space discretization and the bookkeeping of the nodes number and their coordinates is a simple task.

In this way, for the simple problem considered the time dependent temperature varies in the space, only in one spatial direction (Incropera et al. 2006). In the open literature, this problem of convection-diffusion type has been treated by several authors.

Arpaci (1966), present a sequence of formulation of conduction problems and procedures of solution. A vast discussion about analytical techniques of solution such separation of variables and superposition methods among others are presented by Özisik (1980).

Several applications of heat transfer with internal generation temperature dependent are considered by Bejan (1993) and the Integral Method is used.

For the numerical solution of diffusion type problems the finite difference method is amply utilized due to its simplicity and efficiency in this kind of problem.

In the classical finite difference method the difference equations are obtained by expanding the derivative terms in Taylor series yielding to algebraic equations that can be solved by appropriated numerical techniques from the linear algebra.

Different options of the finite difference method can be developed. In this work the Central Difference Scheme which is second order accurate $O(\Delta x^2)$ (Smith, 1986; Wendlande, 2003) has been applied. Also, several times discretization schemes can be employed: explicit which may be unstable depending on the time step or implicit schemes, generally, stables independently of the time step. Two explicit schemes are used: Forward and the Dufort-Frankel and three implicit: Laasonen, Crank-Nicolson and β schemes (Chung, 2002).

The numerical results from the five time discretization schemes above listed and from the analytical solutions are compared by the evaluation of L_2-norm and the L_∞-norm. This kind of problem has been analyzed in Ortega and Rheinboldt (1970) and Romão et al. (2004) by finite elements methods.

2 MODEL EQUATION

The partial differential equation considered in this study is the following transient convection-diffusion equation:

$$\frac{\partial u(x,t)}{\partial t} = \alpha \frac{\partial^2 u(x,t)}{\partial x^2} + \gamma \frac{\partial u(x,t)}{\partial x} \tag{1}$$

where $x,t \in \Re$, $t > 0$ and α, γ are real constants. For simplicity from now on, it will be utilized the notation u instead $u(x,t)$.

3 SPATIAL DISCRETIZATION METHOD

Before to discretized the second and first order derivative on the right hand side of Eq. (1) it´s convenient to present an expansion in Taylor series of the variable u around a point:

$$\begin{aligned} u_{i+1} &= u_i + \Delta x u_i' + (\Delta x)^2 u_i''/2! + (\Delta x)^3 u_i'''/3! + \cdots \\ u_{i-1} &= u_i - \Delta x u_i' + (\Delta x)^2 u_i''/2! - (\Delta x)^3 u_i'''/3! + \cdots \end{aligned} \tag{2}$$

where Δx is the space subdivision of [0,*L*], $L \in \Re_{+}^{*}$ is the set of non-negative real numbers.

In the central finite difference method, the first order derivative in Eq. (1) is obtained by subtracting the equations bellow:

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + O(\Delta x^2) \tag{3}$$

So, the second order derivative in Eq. (1) is obtained by elimination of the first derivative between the expansions in Taylor series equations. The second derivative is then the expressed as

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

4 TIME DISCRETIZATION SCHEMES

The transient term on the left hand side of Eq. (1) gives a parabolic character to that equation. In reality, the Eq. (1) has nature parabolic due to the transient term, elliptic due to the diffusive term and hyperbolic due to the convective term. The time discretization of the transient term has been done by two explicit and three implicit schemes.

4.1 Explicit Methods

In the explicit methods the solution at a time step *n+1* only depends on the solution at time n. So, known the variables at time *t* the variables at time $t + \Delta t$, where Δt is the time step, can be obtained.

4.1.1 Forward-Time/Central-Space (FTCS) Method

In this scheme the transient term is discretized by the explicit forward difference scheme. The combination of this time discretization with the central difference scheme for space discretization is named FTCS and the resulting discretized equation is:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{\alpha(u_{i+1}^n - 2u_i^n + u_{i-1}^n)}{\Delta x^2} + \frac{\gamma(u_{i+1}^n - u_{i-1}^n)}{2\Delta x}, O(\Delta t, \Delta x^2)$$

or after a rearranging

$$u_i^{n+1} = u_i^n + d(u_{i+1}^n - 2u_i^n + u_{i-1}^n) + A(u_{i+1}^n - u_{i-1}^n) \tag{5}$$

where *d* is named the *diffusion number* defined as

$$d = \frac{\alpha \Delta t}{\Delta x^2} \tag{6}$$

and $A = (\gamma.\Delta t)/(2\Delta x)$.

By a von Neumann analysis of stability (Ortega et al., 1970) this scheme will be stable only when the diffusion number is the range*:* $0 < d \le 1/2$. This method is explicit because the temperature at the *n+1* instant of time depends on only the temperature on the past time *n* as shown in Eq. ((5).

4.1.2 Dufort-Frankel Method

The finite difference equation for this method is given by

$$\frac{u_i^{n+1}-u_i^{n-1}}{2\Delta t}=\frac{\alpha\left(u_{i+1}^{n}-2\dfrac{u_i^{n+1}+u_i^{n-1}}{2}+u_{i-1}^{n}\right)}{\Delta x^2}+\frac{\gamma(u_{i+1}^{n}-u_{i-1}^{n})}{2\Delta x},\quad O(\Delta t^2,\Delta x^2,(\Delta t/\Delta x)^2)$$

or after a rearranging

$$(1+2d)u_i^{n+1}=(1-2d)u_i^{n-1}+2d(u_{i+1}^{n}+u_{i-1}^{n})+B(u_{i+1}^{n}-u_{i-1}^{n}) \tag{7}$$

where $B=(\gamma.\Delta t)/(\Delta x)$

This scheme can be shown to be unconditionally stable by the von Neumann stability analysis.

4.2 Implicit Methods

In the implicit schemes the solution at time level *n+1* may also depends on the solution at the same level as will be shown later.

4.2.1 Laasonen Method

Contrary to the explicit schemes, the solution for implicit schemes involves the variables at more than one nodal point for the time step *(n+1)*, we may write the difference for Eq. (1) in the form

$$\frac{u_i^{n+1}-u_i^{n}}{\Delta t}=\frac{\alpha(u_{i+1}^{n+1}-2u_i^{n+1}+u_{i-1}^{n+1})}{\Delta x^2}+\frac{\gamma(u_{i+1}^{n+1}-u_{i-1}^{n+1})}{2\Delta x},\quad O(\Delta t,\Delta x^2)$$

or in the following form

$$(A+d)u_{i+1}^{n+1}-(1+2d)u_i^{n+1}+(d-A)u_{i-1}^{n+1}=-\frac{1}{\Delta t}u_i^{n} \tag{8}$$

This scheme is unconditionally stable.

4.2.2 Crank-Nicolson Method - CN

An alternative scheme of time discretizing the Eq. (8) is to replace the diffusion term by an average between *n* and *n+1* levels, i.e.,

$$\frac{u_i^{n+1}-u_i^{n}}{\Delta t}=\frac{1}{2}\left[\alpha\frac{(u_{i+1}^{n+1}-2u_i^{n+1}+u_{i-1}^{n+1})}{\Delta x^2}+\gamma\frac{u_{i+1}^{n+1}-u_{i-1}^{n+1}}{2\Delta x}+\alpha\frac{(u_{i+1}^{n}-2u_i^{n}+u_{i-1}^{n})}{\Delta x^2}+\gamma\frac{(u_{i+1}^{n}-u_{i-1}^{n})}{2\Delta x}\right],\qquad O(\Delta t,\Delta x^2)$$

or

$$\frac{(d+A)}{2}u_{i+1}^{n+1}-(1+d)u_i^{n+1}+\frac{(d-A)}{2}u_{i-1}^{n+1}=-\frac{(d+A)}{2}u_{i+1}^{n}-(1-d)u_i^{n}-\frac{(d-A)}{2}u_{i-1}^{n} \tag{9}$$

The scheme is unconditionally stable and is second order accurate.

4.2.3 β-Method

A general form of the finite difference equation for Eq. (1) may be written as

$$\frac{u_i^{n+1}-u_i^n}{\Delta t}=\beta\left[\alpha\frac{(u_{i+1}^{n+1}-2u_i^{n+1}+u_{i-1}^{n+1})}{\Delta x^2}+\gamma\frac{u_{i+1}^{n+1}-u_{i-1}^{n+1}}{2\Delta x}\right]+$$
$$(1-\beta)\left[\alpha\frac{(u_{i+1}^{n}-2u_i^{n}+u_{i-1}^{n})}{\Delta x^2}+\gamma\frac{(u_{i+1}^{n}-u_{i-1}^{n})}{2\Delta x}\right],\ O(\Delta t,\Delta x^2) \tag{10}$$

For $1/2\le\beta\le 1$, the method is unconditionally stable. For $\beta=1/2$, Eq.(10) reduces to the Crank-Nicolson Method, whereas $\beta=0$ is equivalent to the FTCS Method.

5 NUMERICAL APPLICATIONS

In the tables of results the following abbreviators are used: *FT – Forward Time, DF – Dufort Frankel, L – Laasonen, CN- Crank-Nicolson, β – β-Method* and, in all applications, the diffusion number was fixed as d=0,5 (Eq. (6)). We compute the error using the L_2 norm, which is the average error throughout the domain, defined by $\|e\|_2=\left[\left(\sum_{i=1}^{Nnost}e_i^2\right)/Nnost\right]^{1/2}$ (Zlhmal, 1978), where $e_i=|T_{(num)_i}-T_{(an)_i}|$, in which the term $T_{(num)}$ and $T_{(an)}$ is the result from the numerical solution and the result from the analytical solution, respectively, and the L_∞ norm, defined by $\|e\|_\infty=|T_{(num)}-T_{(an)}|$, which is the maximum error in the entire domain.

In the tables below shows the errors in the numerical solutions to facilitate comparisons with the proposed results. A graphical representation of these results was not adopted since d=0,5 and thus Δx and Δt both vary in each case.

5.1 Application 1: Transient Diffusion Case

In the first case only transient diffusion with α=1 is considered. In the Eq. (1), γ=0. In this case the domain, governing equations and the analytical solution are:

Domain: $[0,1]\text{x}[0,t]\subset\Re^2$

Equation: $\frac{\partial u(x,t)}{\partial t}=\frac{\partial^2 u(x,t)}{\partial x^2}$

Boundary Conditions: $\frac{\partial u(0,t)}{\partial x}=0$ and $u(1,t)=0$.

Initial Condition: $u(x,0)=-10$.

Analytical Solution: $u(x,t)=-20\sum_{n=0}^{\infty}\frac{(-1)^n}{\beta_n}e^{-\beta_n^2 t}\cos(\beta_n x)$,

where $\beta_n=\frac{(2n+1)}{2}\pi$, $n=1,2,3,\ldots,\infty$.

The norms of the errors are presented in Table and Table 2 for several combinations of space subdivision Δx and time step discretization Δt. For better results small time steps are required.

Δx Δt	FT	DF	L	CN	β=0,75
2E-01 2E-02	2,73E-01	2,75E-01	3,25E-01	2,03E-01	2,60E-01
2E-02 2E-04	1,00E-02	8,22E-03	1,08E-02	9,44E-03	1,01E-02
2E-03 2E-06	8,97E-04	8,78E-04	9,00E-04	8,92E-04	9,00E-04

Table 1: L_2-norm for Application 1.

Δx Δt	FT	DF	L	CN	β=0,75
2E-01 2E-02	4,30E-01	5,64E-01	6,47E-01	3,70E-01	5,16E-01
2E-02 2E-04	3,02E-02	2,73E-02	3,32E-02	3,02E-02	3,17E-02
2E-03 2E-06	2,93E-03	2,90E-03	2,95E-03	2,93E-03	2,95E-03

Table 2: L_∞-norm for Application 1.

5.2 Application 2: Pure diffusion case with different α.

The influence of variation of the diffusion coefficient has been also analyzed. The range of variation is from $\alpha = 1\times10^{-1}$ to $\alpha = 1\times10^{-3}$. In this case, the domain, governing equations and the analytical solution are:

Domain: $[0,1]x[0,t] \subset \Re^2$

Equation: $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$

Boundary Conditions: $u(0,t) = 0$ and $u(1,t)=e^{-\alpha.t}sen(1)$

Initial Condition: $u(x,0) = sen(x)$

Analytical Solution: $u(x,t) = e^{-\alpha.t} sen(x)$ **.**

Δx Δt	FT	DF	L	CN	β=0,75
2E-01 2E-01	3,88E-02	1,63E-04	2,90E-04	7,62E-05	1,86E-04
2E-02 2E-03	3,93E-04	1,69E-06	3,39E-06	8,48E-07	2,12E-06
5E-03 1,25E-04	2,47E-05	1,06E-07	2,13E-07	5,34E-08	1,33E-07

Table 3: L_2-norm for Application 2 with $\alpha = 1\times10^{-1}$.

Δx Δt	FT	DF	L	CN	β=0,75
2E-01 2E-01	7,90E-02	2,50E-04	4,46E-04	1,17E-04	2,86E-04
2E-02 2E-03	8,06E-04	2,40E-06	4,81E-06	1,20E-06	3,00E-06
5E-03 1,25E-04	5,03E-05	1,50E-07	3,01E-07	7,52E-08	1,88E-07

Table 4: L_∞-norm for Application 2 with $\alpha = 1\times10^{-1}$.

Δx Δt	FT	DF	L	CN	β=0,75
2E-02 2E-02	2,36E-03	2,92E-07	5,82E-07	1,45E-07	3,64E-07
5E-03 1,25E-03	1,48E-04	1,83E-08	3,67E-08	9,19E-09	2,29E-08
2E-03 2E-04	2,37E-05	2,94E-09	5,89E-09	1,47E-09	3,68E-09

Table 5: L_2-norm for Application 2 with $\alpha = 1\times10^{-2}$.

Δx Δt	FT	DF	L	CN	β=0,75
2E-02 2E-02	8,05E-03	4,42E-07	8,81E-07	2,20E-07	5,51E-07
5E-03 1,25E-03	5,09E-04	2,76E-08	5,52E-08	1,38E-08	3,45E-08
2E-03 2E-04	8,14E-05	4,42E-09	8,84E-09	2,21E-09	5,52E-09

Table 6: L_∞-norm for Application 2 with $\alpha = 1\times10^{-2}$.

Δx Δt	FT	DF	L	CN	β=0,75
2E-02 2E-01	1,37E-02	3,29E-08	6,53E-08	1,64E-08	4,09E-08
5E-03 1,25E-02	8,35E-04	2,07E-09	4,13E-09	1,03E-09	2,58E-09
2E-03 2E-03	1,33E-04	3,31E-10	6,63E-10	1,65E-10	4,14E-10

Table 7: L_2-norm for Application 2 with $\alpha = 1\times10^{-3}$.

Δx Δt	FT	DF	L	CN	β=0,75
2E-02 2E-01	7,88E-02	5,22E-08	1,02E-07	2,58E-08	6,43E-08
5E-03 1,25E-02	5,03E-03	3,24E-09	6,48E-09	1,62E-09	4,05E-09
2E-03 2E-03	8,14E-04	5,19E-10	1,03E-09	2,59E-10	6,49E-10

Table 8: L_∞-norm for Application 2 with $\alpha = 1\times10^{-3}$.

For diffusion type problems none problem of convergence has been detected.

5.3 Application 3: Convection-Diffusion case and different α.

In this case the convective term with γ=1 is retained in the Eq. (1). Also, in this case, periodic initial and boundary conditions are considered. So, the domain, governing equations and the analytical solution are:

Domain: $[0,1]x[0,t] \subset \Re^2$

Equation: $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} - \frac{\partial u}{\partial x}$

Boundary Conditions: $u(0,t) = e^{-\alpha.t} sen(-t)$ and $u(1,t) = e^{-\alpha.t}\,\mathrm{sen}(1-t)$

Initial Condition: $u(x,0) = sen(x)$

Analytical Solution: $u(x,t) = e^{-\alpha.t} sen(x-t)$.

When the diffusive coefficient is reduced the problem becomes more convective dominant and in general the solution may be oscillatory or instable. In the Table 9 to Table 18 are presented results for the Application 3.

Δx Δt	FT	DF	L	CN	β=0,75
2E-01 2E-02	4,41E-04	4,40E-04	7,71E-04	1,56E-04	4,61E-04
2E-02 2E-04	4,78E-06	4,78E-06	8,19E-06	1,70E-06	4,94E-06
2E-03 2E-06	4,83E-08	4,82E-08	8,26E-08	1,71E-08	4,99E-08

Table 9: L_2-norm for Application 3 with α = 1.

Δx Δt	FT	DF	L	CN	β=0,75
2E-01 2E-02	6,61E-04	6,60E-04	1,16E-03	2,41E-04	7,02E-04
2E-02 2E-04	6,68E-06	6,68E-06	1,15E-05	2,41E-06	6,95E-06
2E-03 2E-06	6,68E-08	6,67E-08	1,15E-07	2,41E-08	6,95E-08

Table 10: L_∞-norm for Application 3 with α = 1.

Δx Δt	FT	DF	L	CN	β=0,75
2E-01 2E-01	1,47E-01	1,46E-01	1,62E-02	3,56E-03	1,02E-02
2E-02 2E-03	1,47E-02	1,47E-02	1,93E-04	2,44E-05	1,08E-04
2E-03 2E-05	1,33E-05	1,33E-05	1,65E-05	1,49E-05	1,57E-05

Table 11: L_2-norm for Application 3 with $\alpha = 1 \times 10^{-1}$.

Δx Δt	FT	DF	L	CN	β=0,75
2E-01 2E-01	2,17E-02	2,16E-02	2,33E-02	6,43E-03	1,48E-02
2E-02 2E-03	1,99E-04	1,99E-04	2,59E-04	3,75E-05	1,45E-04
2E-03 2E-05	1,80E-05	1,81E-05	1,96E-05	1,81E-05	1,88E-05

Table 12: L_∞-norm for Application 3 with $\alpha = 1 \times 10^{-1}$.

Δx Δt	FT	DF	L	CN	β=0,75
2E-02 2E-02	1,71E-03	1,70E-03	1,71E-03	5,24E-05	8,86E-04
5E-03 1,25E-03	1,06E-04	1,06E-04	1,09E-04	2,25E-06	5,55E-05
2E-03 2E-04	1,69E-05	1,68E-05	1,75E-05	3,52E-07	8,90E-06

Table 13: L_2-norm for Application 3 with $\alpha = 1 \times 10^{-2}$.

Δx Δt	FT	DF	L	CN	β=0,75
2E-02 2E-02	2,38E-03	2,37E-03	2,37E-03	9,24E-05	1,22E-03
5E-03 1,25E-03	1,46E-04	1,46E-04	1,50E-04	3,86E-06	7,62E-05
2E-03 2E-04	2,34E-05	2,33E-05	2,40E-05	6,02E-07	1,21E-05

Table 14: L_∞-norm for Application 3 with $\alpha = 1\times10^{-2}$.

Δx Δt	FT	DF	L	CN	β=0,75
2E-02 4E-02	4,40E+04	4,24E-02	3,34E-03	1,04E-04	1,75E-03
5E-03 2,5E-03	2,87E+180	4,29E-04	2,16E-04	2,46E-06	1,09E-04
2E-03 4E-04	Not convergent	6,87E-05	3,47E-05	3,57E-07	1,75E-05

Table 15: L_2-norm for Application 3, $\alpha = 1\times10^{-2}$ and $d = 1$.

Δx Δt	FT	DF	L	CN	β=0,75
2E-02 4E-02	1,62E+06	1,83E-01	4,64E-03	1,84E-04	2,41E-03
5E-03 2,5E-03	2,24E+181	5,93E-04	2,98E-04	4,21E-06	1,50E-04
2E-03 4E-04	Not convergent	9,48E-05	4,78E-05	6,11E-07	2,40E-05

Table 16: L_∞-norm for Application 3, $\alpha = 1\times10^{-2}$ and $d = 1$.

Δx Δt	FT	DF	L	CN	β=0,75
2E-02 1E-01	1,76E+04	4,24E-02	8,00E-03	4,73E-04	4,39E-03
5E-03 6,5E-03	2,93E+142	2,70E-03	5,37E-04	3,89E-06	2,71E-04
2E-03 1E-03	Not convergent	4,31E-04	8,64E-05	3,94E-07	4,34E-05

Table 17: L_2-norm for Application 3, $\alpha = 1\times10^{-2}$ and d=2.5.

Δx Δt	FT	DF	L	CN	β=0,75
2E-02 1E-01	7,88E+04	8,65E-02	1,10E-02	8,31E-04	6,03E-03
5E-03 6,5E-03	1,05E+143	3,73E-03	7,41E-04	6,67E-06	3,73E-04
2E-03 1E-03	Not convergent	5,94E-04	1,19E-04	6,74E-07	5,97E-05

Table 18: L_∞-norm for Application 3, $\alpha = 1\times10^{-2}$ and d=2.5.

By inspection of the Table 15 to Table 18, it can be observed that for small values of the diffusion coefficient, the FT fails to yield to the convergent solution while for the all other schemes the solution has been obtained.

6 CONCLUSIONS

Different options of time discretization for the Finite Difference Method have been tested in this work. The one-dimensional model equation of convection-diffusion type has been considered as the mathematical model. Two explicit and three implicit schemes were compared. The influences of the sizes of the space discretization and time step were analyzed. The influence of the diffusion coefficient has been also verified. For convection dominant situations some schemes may be diverging as in the case of the FT scheme. In general, the best results were obtained with the Crank-Nicolson scheme, due to its second order of accuracy.

The choice of the method may to result in convergence or not of the solution. In general implicit schemes are convergents, however, they require iterative solutions to avoid matrix inversion. For large problems the explicit schemes may be the only viable option, with appropriated time step sizes discretization for stability.

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