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Numerical solution of parabolic differential equations using finite differences: a comparative study

Solução numérica de equações diferenciais parabólicas usando diferenças finitas: um estudo comparativo

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Resumo

Neste trabalho, aplicou-se o método das diferenças finitas para equações diferenciais parabólicas com o objetivo de comparar resultados numéricos de problemas que envolvem difusão térmica. A solução numérica é obtida através da utilização dos métodos numéricos explícito, implícito e implícito de Crank-Nicolson. São descritos os critérios de estabilidade e da consistência de cada método analisado. Os resultados numéricos mostraram que as formulações implícitas superam as condições de estabilidade do método explícito, possibilitando a utilização de passos maiores na malha. As aproximações, no entanto, são mais satisfatórias quando esses passos tendem para zero. Levando em consideração os critérios de convergência, as formulações apresentadas nesse trabalho apresentam soluções numéricas confiáveis dos problemas. Os métodos implícito e de Crank-Nicolson são, consideravelmente, melhores em relação ao método explícito.
Palavras-chave: Equações Diferenciais Parabólicas. Soluções numéricas. Diferenças Finitas.

Abstract

In this work, the finite difference method was applied to parabolic differential equations in order to compare numerical results of problems involving thermal diffusion. The numerical solution is obtained by using the explicit, implicit and implicit numerical methods of Crank-Nicolson. The stability and consistency criteria of each method are described. The numerical results showed that the implicit formulations outweigh the stability conditions of the explicit method, making it possible to use larger steps in the mesh. The approximations, however, are more satisfactory when those steps tend to zero. Taking into account the convergence criteria, the formulations presented in this paper present reliable numerical solutions of the problems. The implicit and Crank-Nicolson methods are considerably better in relation to the explicit method.
Keywords: Differential Parabolic Equations. Numerical solutions. Finite Differences.

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1 Introduction

The modeling of many problems related to several areas of knowledge, such as Physics, Biology, Economics, Engineering and Geometry has resulted in complex equations. From the effort of great mathematicians, many important contributions to the solution of these problems have arisen. Many researchers are currently working on finding solution methods. However, with the great evolution of computing, enormously increasing the capacity of data processing, the computer has become a very powerful tool for the solution of these equations and the problems mentioned.

In the past, studies of physical phenomena and nature were based on two scientific methods: theoretical and practical. The theoretical method develops principles, laws, equations, and physical theories of problems. The practical method deals with observations and experiments. Nowadays, scientific studies have benefited enormously from the technological advances and connected the practical and theoretical methods, thus being able to work with a new method: the numerical one.

The use of numerical techniques for simulation has been possible thanks to the development of algorithms for solving complex problems by making large number of calculations in short times. In this way, the main advantages of using a numerical method are: fast results, low cost, less effort with large number of hand-made calculations, solve complex processes and complex geometries, etc. However, the numerical methods present some disadvantages that influence on the study as errors of approximations, instability, memory cost of the computer. In this work, attention is focused on the study of formulations for solving problems that result in parabolic partial differential equations (PDE). These equations represent non-stationary problems and, in addition, they have the great advantage of not propagating discontinuities, that is, the solution of a parabolic equation is always smooth within its solution domain, even when the initial condition is not. Parabolic equations model phenomena that evolve over time. Thus, one of the variables always has a temporal character that distinguishes it from the others.

In the study, we will work with problems that model the heat flow in the bar. The mathematical descriptions of the processes of heat flow in bar, known as diffusion equations, began to be proposed in the nineteenth century by Joseph Fourier, who published in 1822 the mathematical classic Théorie Analytique de la Chaleur (The Analytical Theory of Heat) [1].

The diffusion equation is a partial parabolic differential equation which, in one-dimensional case, has constant coefficients. The exact solution to this problem can be found by the method of separating variables without too many complications. Although in the literature there are different methods used to determine the exact solutions of partial differential equations, most of the time we know only of their existence without it being possible to determine them. In this case, numerical methods can be used to determine approximate solutions to problems.

At present, there are different numerical techniques and formulas to determine the solution of one (PDE). Here, in this work, we will deal with processes that involve finite differences. This technique allows the present derivatives of the EDP to be replaced by numerical values of a function, in discretized domain. In this technique, explicit and implicit formulations may be made.

At the present time, a difficulty of finite difference techniques is its explicit formulation, since it requires a large number of computational cycles and can consume a large amount of memory, occupying a large space for storage and high processing time. These problems occur when the mesh is refined and the combined values of the steps require that the time step be small enough, increasing the number of calculations required by the method. When the time step is not small enough, the method becomes unstable. That is, the numerical solution accumulates errors of the previous cycles and loses its physical meaning. An alternative to this problem is to use implicit formulations.

The use of implicit methods for PDE was initiated when Crank and Nicolson, in 1947, used an unconditionally stable method for the diffusion equation. Since then, several researchers have been proposing modifications in the formulation and applying in several EPDs that model the most varied problems. In addition to its favorable stability, the implicit method allows to advance in the temporal step using larger steps, whithout instabilities. Clearly, this does not mean that it will lead to better approximations.

Given the importance and employability of the cited numerical methods, the main objectives of this work are to analyze and compare the numerical results obtained by the explicit, implicit and Crank-Nicolson formulations, applied to the diffusion equation.

2 Theoretical Grounding

2.1 Partial differential equations (PDEs)

Partial differential equations are those involving partial derivatives of a function. They are classified into three categories: Parabolic (evolution problems), Elliptic (equilibrium problems) and Hyperbolic (problems involving propagation or discontinuity). The problem addressed in this work is evolutionary, known as the diffusion or heat equation, which is a parabolic PDE, given by:

$$\phi_t = \alpha^2 \phi_{xx}, \tag{1}$$

under the Dirichlet contour conditions, which specifies the value of the function in the contour.

The value α^2 represents the thermal diffusivity of the material. For more details on the heat equation see ref. [2].

2.2 Analytical solution

In order to find the necessary solutions, it is assumed that $\phi(x, t)$ is a product of two other functions X and T which depend respectively on x and t. Thus, there will be two ordinary differential equations that can be solved without any complication, by analyzing the intervals of interest.

In this way, the method of separating variables is applied, the exact solving of the problem (1) is given by

$$\phi_n(x, t) = X_n(x) \cdot T_n(t) = c \cdot e^{\frac{-\alpha^2 n^2 \pi^2}{l} t} \cdot sen\left(\tfrac{n\pi x}{l}\right),$$

for some real constant c. Using series of Fourier see [2] [p.126-129], it is possible to show that the solution ϕ of problem (1) is given by

$$\phi(x, t) = \sum_{i=1}^{\infty} c_n \cdot sen\left(\frac{n\pi x}{l}\right) \cdot e^{\frac{-\alpha^2 n^2 \pi^2}{l} t}, \tag{2}$$

with

$$\psi(x) = \phi(x, 0) = \sum_{i=1}^{\infty} c_n \cdot sen\left(\tfrac{n\pi x}{l}\right),$$

and

$$c_n = \tfrac{2}{l} \int_0^l \psi(x) \cdot sen\left(\tfrac{n\pi x}{l}\right) dx, \quad n = 1, 2, \ldots$$

The method of separating variables for the diffusion equation is presented in detail in ref. [2] and [3].

2.3 Discretization

To solve a differential equation computationally, it is fundamental to express the domain (region) where the problem will be solved properly. Usually, it is not possible to obtain numerical solutions in continuous regions, due to their infinity of points. First, the domain is discretized. The concept of discretizing springs from the transformation of the continuous problem into a discrete and finite.

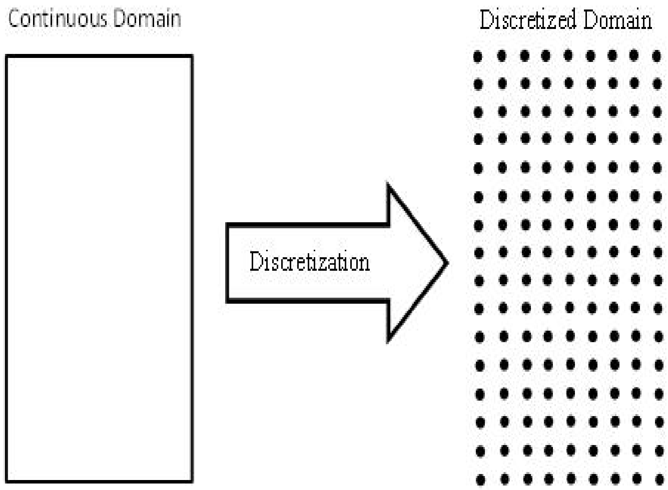

Figura 1: Domain Discretization

In the points of this discretized domain solutions are obtained for the problem. It is intuitively noticed that the higher the number of points, the greater the computational effort.

2.4 Finite differences

The techniques of finite differences consist of replacing the derivatives of the differential equation (DE) with approximations involving numerical values of functions. Thus we will discretize the derivative in the time of (1), obtaining the following notation:

$$\phi_{i,j} = \phi(x,t); \phi_{i,j+1} = \phi(x, t + \Delta t). \tag{3}$$

In the explicit method, the equations are independent, which allows direct solutions.This method is quite simple and fast, but it presents stability problems. Implicit methods show favorable stabilities, however, the resulting difference equations require system resolutions for each resolution cycle, which may slow the method.

Applying the finite formulas for the derivatives of (1), the following formulations are obtained:

Explicit Method:

$$\phi_{i,j+1} = \phi_{i,j} + \sigma\left(\phi_{i-1,j} - 2\phi_{i,j} + \phi_{i+1,j}\right), \tag{4}$$

Implicit method:

$$\phi_{i,j-1} = \phi_{i,j} - \sigma\left(\phi_{i-1,j} - 2\phi_{i,j} + \phi_{i+1,j}\right). \tag{5}$$

Crank and Nicolson Method:

$$\phi_{i,j+1} = \phi_{i,j} + \frac{\sigma}{2}\left(\phi_{i-1,j} + \phi_{i-1,j+1} - 2\left(\phi_{i,j} + \phi_{i,j+1}\right) + \phi_{i+1,j} + \phi_{i+1,j+1}\right), \tag{6}$$

to $\sigma = \frac{\alpha^2 \Delta t}{\Delta x^2}$.

Complete theory of finite difference techniques in ref. [3] and ref. [4].

2.5 Consistency of numerical methods

The consistency of a numerical method is related to its order of convergence. The order of convergence is given by the order of the error caused by the approximation and the exact solution defined above. A method that has higher order, for same step sizes, produces more accurate approximations.

Definition I: *A numerical method is consistent related to a given equation if the truncation error of this method for this equation is at least $O(\Delta x)$.*

For the diffusion equation (1) the methods present the following order of convergences:

Explicit Method: $O(\Delta t + \Delta x^2)$.

Implicit method: $O(\Delta t + \Delta x^2)$.

Crank and Nicolsom method: $O(\Delta t^2 + \Delta x^2)$.

2.6 Stability of numerical methods

To find the approximate solution to a problem, one must have a number of calculations depending on Δx and Δt. That is, the smaller the values the greater the number of steps to arrive at the approximate solution. This can lead to an uncontrolled accumulation of errors, and in that case, the applied method is said to be stable or unstable. A numerical method can be interpreted as a procedure of producing numbers from the initial data. However, these initial data may contain errors (for example, computer rounding), and if amplified, in a short time the error growth will dominate the solution produced and it will lose its meaning.

Definition II: *A numeric method is stable if the associated difference equation does not amplify errors from the previous steps.*

In general, a numerical method can be classified as:

Conditionally Stable: the methods that must satisfy a condition so that they obtain stable solutions

Unconditionally Stable: Methods that are not required to meet stability conditions.

Unconditionally unstable: There are no criteria for solutions to be stable.

2.6.1 Method of Von Newmann

The Von Neumann criterion is widely used to determine the stability of a finite difference method. The difference equation is expanded using the Fourier series expansion, where the decay or growth of the amplification factor indicates the stability of the method.

Suppose the error of a numeric method can be expanded as follows:

$$E_i = \sum_{n=0}^{N} \psi_n \cdot e^{I\alpha_n ih}, \quad i = 0, 1, \ldots, N \tag{7}$$

in that E_i is the global error at each point along the line, $\alpha_n = \frac{n\pi}{L}$ is the wave number in the direction of x, L is the length of the x-axis, $I = \sqrt{-1}$, ψ_n, n is the amplitude in the time axis t in n, α_t is a complex number and $Nh = L$.

Representing the error in the initial step, to analyze the subsequent ones it is enough to analyze the propagation of a generic harmonic,

$$\psi_n e^{I\zeta i} e^{\gamma j}, \tag{8}$$

Where $\zeta \in \mathbb{R}$ and $\gamma \in \mathbb{C}$, both arbitrary. Note that it already acts as the power of e^{γ}. Then the evolution in time explodes if $e^{\gamma} > 1$ or if it tends to zero.

In practice, the difference equation can be applied as follows.

$$\Phi_{i,j} = e^{\gamma j} e^{I\zeta i}, \tag{9}$$

analogously,

$$\begin{aligned} \Phi_{i+1,j} &= e^{\gamma j} e^{I\zeta(i+1)}, \\ \Phi_{i,j+1} &= e^{\gamma(j+1)} e^{I\zeta i}. \end{aligned}$$

Recital $\Phi \approx \phi$.
An equation of differences will be stable if it satisfies the condition of ψ_n does not grow with time, therefore , the ratio

$$\left| \frac{\psi_{n+1}}{\psi_n} \right| \leq 1,$$

for every ζ. This condition of stability is necessary for convergence of a numerical method, but not sufficient.

Further details on the Neumann method and the other stability criteria in ref. [4].

In this work, the stability of the numerical formulas was evaluated by Neuman´s criterion . Therefore, for the explicit, implicit and Crank and Nicolson methods, for the diffusion equation (1), we have:

I Explicit Method is conditionally stable if $\sigma \leq \frac{1}{2}$ ref. [5];

Demonstration: Applying (9) to (4), yields

$$e^{\gamma(j+1)} e^{I\zeta i} = e^{\gamma j} e^{I\zeta i} + \sigma \left(e^{\gamma j} e^{I\zeta(i-1)} - 2e^{\gamma j} e^{I\zeta i} + e^{\gamma j} e^{I\zeta(i+1)} \right),$$

$$e^{\gamma} = 1 + \sigma \left(e^{-I\zeta i} - 2 + e^{I\zeta i} \right),$$

as $e^{-I\zeta i} + e^{I\zeta i} = cos(-\zeta) + Isen(-\zeta) + cos(\zeta) + Isen(\zeta) = 2cos(\zeta)$, then

$$e^{\gamma} = 1 + \sigma\left(-2 + 2cos(\zeta)\right).$$

For the method to be stable, as presented in section 2.6.1, one must assume that $\left|e^{\lambda}\right| \leq 1$ and impose that $e^{\lambda} \geq -1$. Thus we have

$$1 + \sigma\left(-2 + 2cos(\zeta)\right) \geq -1,$$

thus,

$$\sigma \leq \tfrac{1}{1-cos(\zeta)},$$

therefore,

$$\sigma \leq \frac{1}{2}. \tag{10}$$

II Implicit method is unconditionally stable;

Demonstration: Following the same idea of the explicit method, from (9) to (5), we have the following development:

$$\begin{aligned}
e^{\gamma(j-1)}e^{I\zeta i} &= e^{\gamma j}e^{I\zeta i} - \sigma\left(e^{\gamma j}e^{I\zeta(i-1)} - 2e^{\gamma j}e^{I\zeta i} + e^{\gamma j}e^{I\zeta(i+1)}\right)\\
e^{\gamma j}e^{-\gamma}e^{I\zeta i} &= e^{I\zeta i}e^{\gamma j}\left[1 - \sigma\left(e^{-I\zeta} - 2 + e^{I\zeta}\right)\right]\\
e^{-\gamma} &= 1 - \sigma\left(e^{-I\zeta} - 2 + e^{I\zeta}\right)\\
e^{-\gamma} &= 1 - \sigma\left(cos(-\zeta) + Isen(-\zeta) - 2 + cos(\zeta) + Isen(\zeta)\right)\\
e^{-\gamma} &= 1 + 4\sigma\left(\frac{cos(\zeta) - 1}{2}\right)\\
e^{-\gamma} &= 1 + 4\sigma sen^2\frac{\zeta}{2},
\end{aligned}$$

so,

$$e^{\gamma} = \frac{1}{1 + 4\sigma sen^2\frac{\zeta}{2}}. \tag{11}$$

It is easy to note that (11) is always smaller than for all σ. In this case, the method is said to be unconditionally stable.

III The Implicit Method of Crank-Nicolson is unconditionally stable.;

Demonstration: From (9) to (6), follows

$$
\begin{aligned}
e^{\gamma(j+1)}e^{I\zeta i} &= e^{\gamma j}e^{I\zeta i}+\frac{\sigma}{2}(e^{\gamma j}e^{I\zeta(i-1)}+e^{\gamma(j+1)}e^{I\zeta(i-1)}-2e^{\gamma j}\left(e^{I\zeta i}+e^{\gamma}e^{I\zeta i}\right)+\\
&\quad +e^{\gamma j}e^{I\zeta(i+1)}+e^{\gamma(j+1)}e^{I\zeta(i+1)})\\
e^{\gamma} &= 1+\frac{\sigma}{2}(e^{-I\zeta}+e^{\gamma}e^{-I\zeta}-2-2e^{\gamma}+e^{I\zeta}+e^{\gamma}e^{I\zeta})\\
e^{\gamma} &= \frac{1+\frac{\sigma}{2}(e^{-I\zeta}-2+e^{I\zeta})}{1-\frac{\sigma}{2}\left(e^{-I\zeta}-2+e^{I\zeta}\right)}\\
e^{\gamma} &= \frac{1+\frac{\sigma}{2}(2cos(\zeta)-2)}{1-\frac{\sigma}{2}\left(2cos(\zeta)-2\right)},
\end{aligned}
$$

Therefore,

$$
e^{\gamma}=\frac{1-2\sigma sen^2\frac{\zeta}{2}}{1+2\sigma sen^2\frac{\zeta}{2}}. \tag{12}
$$

Clearly (12) is always less than for all σ. In this way, this method is unconditionally stable.

2.7 Convergence of numerical method

The method presented here is defined for well-placed problems.

Definition III: *A problem is called well-placed if it has only solution that depends continuously on the initial data or border or both.*

The analysis of the convergence of a numerical method is extremely important because it is expected that the numerical solution produces a solution as close as possible to that of the analytical solution of the problem. A relation between consistency, stability and convergence is associated with the Theorem of Lax.

The Lax Theorem: *A necessary and sufficient condition for convergence of a method, when applied to a well-placed initial value problem, is that the discretization scheme is consistent and stable.*

3 Implementation:

The Python language was used for the implementation of the formulas 4, 5 and 6 that are presented in ref. [6]. See ref. [7] and ref. [8] for MATLAB implementations.

The formulation 4, because only arithmetic operations is simple implementation. since formulations 5 and 6 present operations with tridiagonal matrices (see [3]) that an auxiliary algorithm known as the Thomas Algorithm is required (see [8])

The fact of solving these matrices makes processing and the loops of the implicit method codes slower than the explicit method code. In this way, the data presented in the next subsections is considered the compilation time for analysis.

3.1 Problem I

Suppose a metal bar, thermally insulated on its side surface, with constant diffusivity at $\alpha^2 = 1$ and length $x = 1$, with its ends in contact with blocks of ice at $0\,°C$, and being heated by a torch, so that the heat at $t = 0$ obeys the function.

$$\phi(x, 0) = 100 \cdot sen(\pi x).$$

Consider all units of measure according to the International System of Units.

The objective is to know the temperature at each point x, as we advance in time, that is, to know $\phi(x, t)$ describing the temperature at x at time t.

Thus, the problem can be modeled by the following equation and boundary conditions. The variable T is considered the end time of the problem.

$$\begin{aligned} \phi_t &= \phi_{xx}, \quad \alpha > 0, \quad 0 \le x \le 1, \quad t \ge 0 \\ \phi(x,0) &= 100 \cdot sen(\pi x), \quad 0 \le x \le 1 \\ \phi(0,t) &= 0, \quad t > 0 \\ \phi(l,T) &= 0, \quad t > 0 \end{aligned} \tag{13}$$

whose exact solution is $\phi(x, t) = 100 \cdot e^{-\pi^2 t} \cdot sen(\pi x)$.

Here we denote by E^* the mean error of the method and P the processing time of the algorithm for the solution at the points and η the standard deviation of the errors in relation to the analytical solution.

For this problem, we consider the mesh $[0, 1] \times [0, 0.5]$, so that $\Delta x = 0.1$ and $\Delta t = 1/200$, for the first simulation.

$$\sigma = \frac{1 \cdot 0.005}{0.1^2}$$

thereby,

$$\sigma = \frac{1}{2}$$

It is observed that the $\sigma = \frac{1}{2} \le \frac{1}{2}$ that satisfies the stability condition of the explicit method described in section 2.6. Table 1 presents the numerical results of the exact and approximate solutions by the Explicit, Implicit and Implicit method of Crank-nicolson, respectively.

Tabela 1: Numerical results for $\Delta x = 0.1$ and $\Delta t = 1/200$

Exact solution × Numerical results				
(x,t)	Exact	Explicit	Implicit	Nicolson
(0.0, 0.0)	0.0	0.0	0.0	0.0
(0.1, 0.5)	0.222242	0.204463	0.259880	0.242789
(0.2, 0.5)	0.422730	0.388912	0.494322	0.461813
(0.3, 0.5)	0.581838	0.535291	0.680376	0.635631
(0.4, 0.5)	0.683992	0.629273	0.799829	0.747229
(0.5, 0.5)	0.719192	0.661656	0.840990	0.785683
(0.6, 0.5)	0.683992	0.629273	0.799829	0.747229
(0.7, 0.5)	0.581838	0.535291	0.680376	0.635631
(0.8, 0.5)	0.422730	0.388912	0.494322	0.461813
(0.9, 0.5)	0.222243	0.204463	0.259880	0.242789
(1.0, 0.5)	0.0	0.0	0.0	0.0
E^*	–	$-4.00 \cdot 10^{-2}$	$9.00 \cdot 10^{-2}$	$4.67 \cdot 10^{-2}$
η	–			
P	–	0.008	0.008	0.012

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The explicit method expressed by equation (4) is computationally simple in relation to the methods described by equations (5) and (6), however, the restriction of the stability of the method greatly limits the time step Δt. For the results presented in table 1, it can be observed that, with the satisfied condition, the mean error modulus of the explicit method was better than the other methods.

In order to improve the average error E^* of the methods we refine the mesh so that Δt is the part of the applied one earlier, thereby , $\Delta t = 1/600$. See $\sigma \approx 0.167$ satisfies the stability condition of (4). observe the results in table 2.

Tabela 2: Numerical results for $\Delta x = 0.1$ and $\Delta t = 1/600$

Exact solution × Numerical results				
(x, t)	Exact	Explicit	Implicit	Nicolson
$(0.0, 0.0)$	0.0	0.0	0.0	0.0
$(0.1, 0.5)$	0.222242	0.222261	0.240739	0.235197
$(0.2, 0.5)$	0.422730	0.422766	0.457913	0.447372
$(0.3, 0.5)$	0.581838	0.581888	0.630263	0.615754
$(0.4, 0.5)$	0.683992	0.684050	0.740919	0.723863
$(0.5, 0.5)$	0.719192	0.719253	0.779048	0.761114
$(0.6, 0.5)$	0.683992	0.684050	0.740919	0.723863
$(0.7, 0.5)$	0.581838	0.581888	0.630263	0.615754
$(0.8, 0.5)$	0.422730	0.422766	0.457913	0.447372
$(0.9, 0.5)$	0.222243	0.222261	0.240739	0.235197
$(1.0, 0.5)$	0.0	0.0	0.0	0.0
E^*	–	$4.29 \cdot 10^{-5}$	$4.20 \cdot 10^{-2}$	$3.00 \cdot 10^{-2}$
η	–			
P	–	0.017	0.013	0.040

There have been improvements in the error of all methods, it can be verified that the best was the implied method. Refining the mesh of the problem, now at x, we reduce the size of Δx by half, $\Delta x = 0.05$ and keep the step $\Delta t = 1/600$ fixed. Now we have $\sigma \approx 0.667$, that is $\sigma > \frac{1}{2}$, which is outside the condition of (4). The results are presented in table 3.

Tabela 3: Numerical results for $\Delta x = 0.05$ and $\Delta t = 1/600$

Exact solution × Numerical results				
(x, t)	Exata	Explícito	Implícito	Nicolson
$(0.0, 0.0)$	0.0	0.0	0.0	0.0
$(0.1, 0.5)$	0.222242	1.056e+50	0.233664	0.228197
$(0.2, 0.5)$	0.422730	2.008e+50	0.444456	0.434056
$(0.3, 0.5)$	0.581838	2.765e+50	0.611742	0.597427
$(0.4, 0.5)$	0.683992	3.250e+50	0.719145	0.702317
$(0.5, 0.5)$	0.719192	3.418e+50	0.756154	0.738460
$(0.6, 0.5)$	0.683992	3.251e+50	0.719145	0.702317
$(0.7, 0.5)$	0.581838	2.766e+50	0.611741	0.597426
$(0.8, 0.5)$	0.422730	2.010e+50	0.444456	0.434056
$(0.9, 0.5)$	0.222243	1.057e+50	0.233664	0.228197
$(1.0, 0.5)$	0.0	0.0	0.0	0.0
E^*	–	e+50	$2.6 \cdot 10^{-2}$	$1.4 \cdot 10^{-2}$
η	–			
P	–	$1.2 \cdot 10^{-2}$	$2.0 \cdot 10^{-2}$	$4.3 \cdot 10^{-2}$

Clearly, the solution of the explicit method was dominated by accumulated errors, making it a so-called spurious solution. This instabilization of the solution for values Δx and Δt justifies the importance of the study of the stability of a numerical method. Note that, from the physical point of view, the numerical results do not present reasonable solutions. However, for the implicit and implicit method of Crank-Nicolson, the solutions improved due to the decrease of the error. In this way, we will refine the mesh in order to further reduce the average error of the implicit and implicit method of Crank-Nicolson. Let's refine the mesh by changing the partition on both axes. In the space axis, let $\Delta x = 0.025$ and, in the time axis, $\Delta t = 1/1000$. Then we will make $\Delta x = 0.025$ and $\Delta t = 1/10000$. The results are presented in results 4 and 5, respectively. As for these values the combination of the partitions Δx and Δt is outside the stability of (4), the numerical solutions of the explicit method will not be presented in the table.

Tabela 4: Numerical results for $\Delta x = 0.025$ and $\Delta t = 1/1000$

Exact solution × Numerical results				
(x,t)	Exata	Explícito	Implícito	Nicolson
(0.0, 0.0)	0.0	0.0	0.0	0.0
(0.1, 0.5)	0.222242	–	0.228256	0.225006
(0.2, 0.5)	0.422730	–	0.434169	0.427986
(0.3, 0.5)	0.581838	–	0.597583	0.589072
(0.4, 0.5)	0.683992	–	0.702500	0.692496
(0.5, 0.5)	0.719192	–	0.738653	0.728133
(0.6, 0.5)	0.683992	–	0.702500	0.692496
(0.7, 0.5)	0.581838	–	0.597583	0.589072
(0.8, 0.5)	0.422730	–	0.434169	0.427986
(0.9, 0.5)	0.222243	–	0.228256	0.225006
(1.0, 0.5)	0.0	0.0	0.0	0.0
$E*$	–	–	$1.4 \cdot 10^{-2}$	$6.3 \cdot 10^{-3}$
η	–			
P	–	–	$3.8 \cdot 10^{-2}$	$1.2 \cdot 10^{-2}$

Tabela 5: Numerical results for $\Delta x = 0.01$ e $\Delta t = 1/10000$

Exact solution × Numerical results				
(x,t)	Exata	Explícito	Implícito	Nicolson
(0.0, 0.0)	0.0	0.0	0.0	0.0
(0.1, 0.5)	0.222242	–	0.222873	0.222551
(0.2, 0.5)	0.422730	–	0.423930	0.423317
(0.3, 0.5)	0.581838	–	0.583490	0.582646
(0.4, 0.5)	0.683992	–	0.685933	0.684942
(0.5, 0.5)	0.719192	–	0.721233	0.720190
(0.6, 0.5)	0.683992	–	0.685933	0.684942
(0.7, 0.5)	0.581838	–	0.583490	0.582646
(0.8, 0.5)	0.422730	–	0.423930	0.423317
(0.9, 0.5)	0.222243	–	0.222873	0.222551
(1.0, 0.5)	0.0	0.0	0.0	0.0
E^*	–	–	$1.4 \cdot 10^{-3}$	$7.0 \cdot 10^{-4}$
η	–			
P	–	–	$9.2 \cdot 10^{-1}$	2.25

Note that the methods presented their improvements with the refinements of the meshes. That is, the more$\Delta x, \Delta t \to 0$, respecting the stability criteria of the method, the error $E^* \to 0$.

3.2 Problem II

Consider the diffusion equation

$$\begin{aligned} u_t &= u_{xx}, \quad \alpha > 0, \quad 0 \leq x \leq 1, \quad t \geq 0 \\ u(x,0) &= 2x(1-x), \quad 0 \leq x \leq 1 \\ u(0,t) &= 0, \quad t > 0 \\ u(1,T) &= 0, \quad t > 0 \end{aligned} \tag{14}$$

In that using the procedure presented in (2.2), we find the analytical solution,

$$u(x,t) = \frac{16}{\pi^3}\sum_{n=0}^{\infty}\frac{sen((2n+1)\pi x)\cdot e^{-(2(2n+1)^2\pi^2)t}}{(2n+1)^3}. \quad (15)$$

Let us select some times in the solution $t = 0$, t = 0.05 e $t = 0.10$. See picture 2

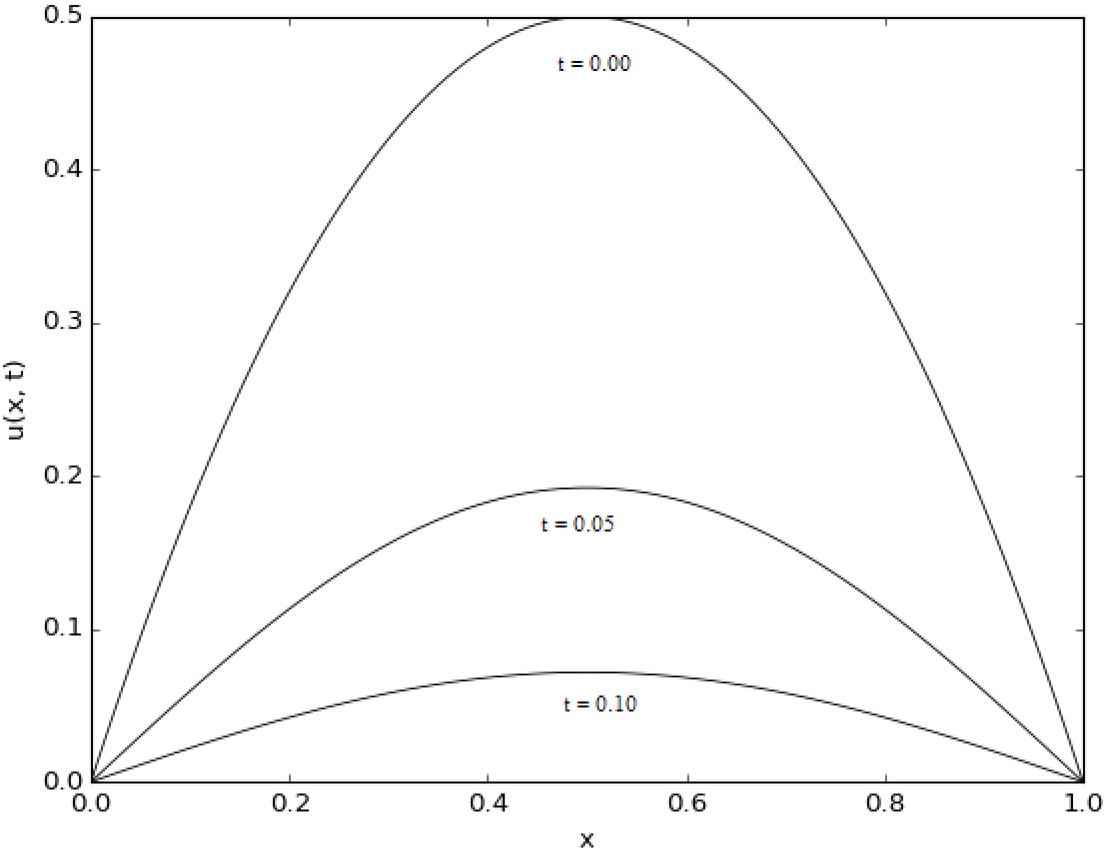

Figura 2: Graph of the analytical solution at times $t = 0$, $t = 0.05$ and $t = 0.10$ of problem II.

Using the steps $\Delta x = 0.01$ and $\Delta t = 1/100000$ and applying the explicit method to find the approximate solutions for $t = 0$, $t = 0.05$ and $t = 0.10$, we have the data of figure 3. Only the multiple steps of 0.1 in the space axis are separated for better visualization. Note that the results are excellent, although it requires a lot of computational effort. The implemented algorithm ran at a time $P = 14.25$ seconds, while the implicit and Crank-Nicolson method processed, with the same steps, at time $P = 2.157$ seconds and $P = 5.122$ seconds, respectively. Furthermore, choosing the combination of the steps Δx and Δt so that the stability condition (10) is satisfied is fundamental to good approximations.

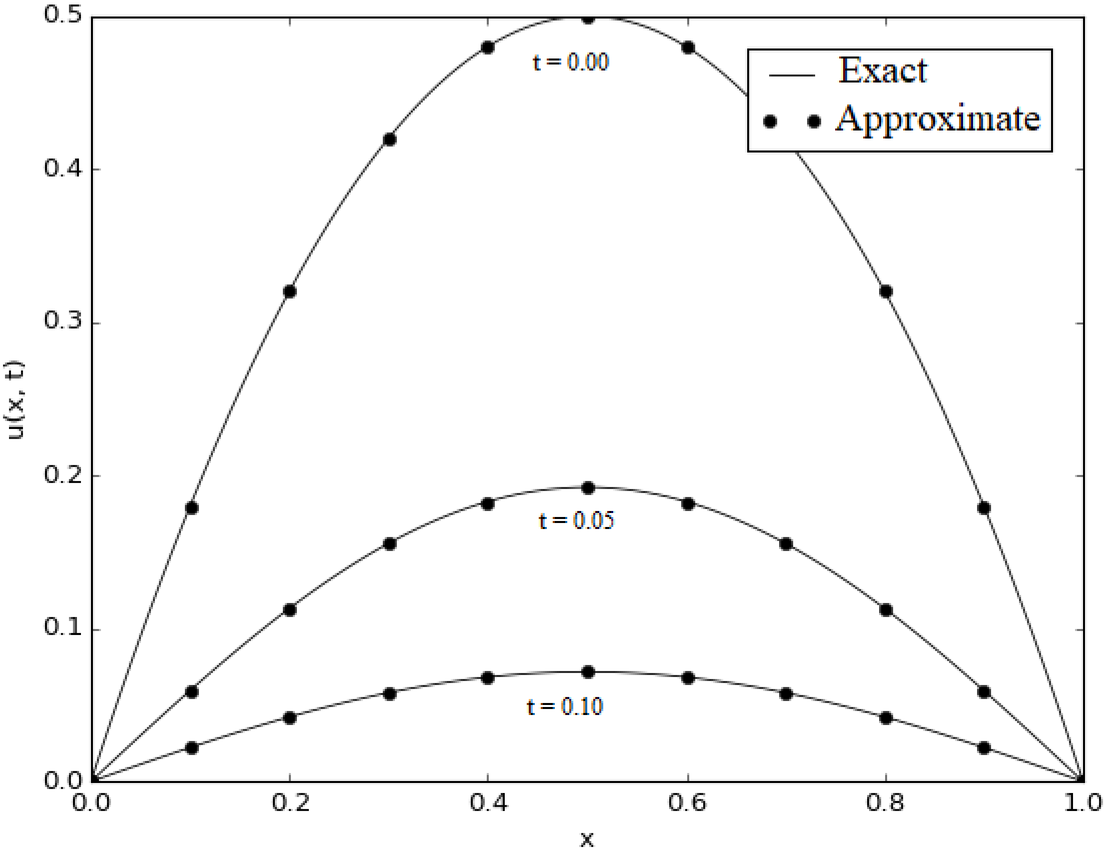

Figura 3: Graph of the approximate solution by the explicit method at times $t = 0$, $t = 0.05$ and $t = 0.10$ of problem II.

Now the implicit method is applied for steps $\Delta x = 0.01$ and $\Delta t = 1/1000$. Graph 4 shows good approximations, not bad for an economy in the time step of 100 times. Although the method solves systems, the fact of being unconditionally stable makes it possible to use larger steps, reducing the loops due to $N \times N$ matrix resolution.

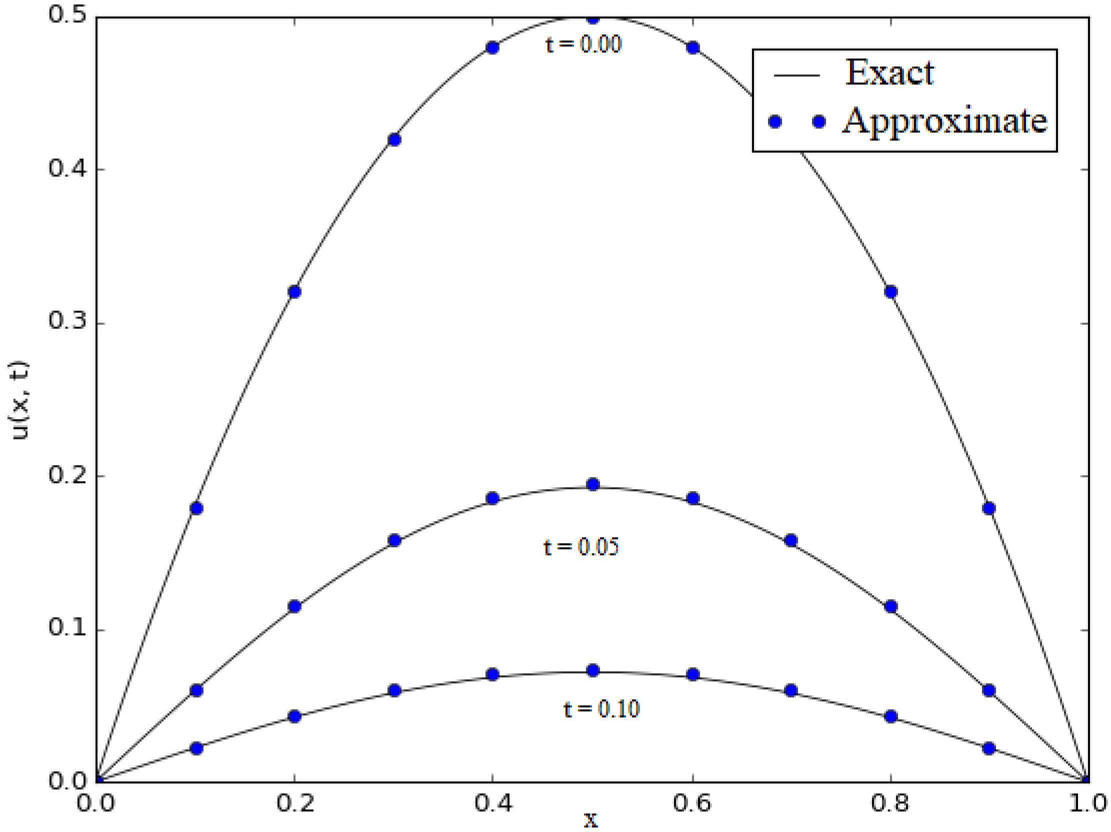

Figura 4: Graph of the approximate solution by the implicit method at time $t = 0$, $t = 0.05$ e $t = 0.10$ of problem II.

By further increasing the time step Δt, so that $\Delta t = 1/800$ and $\Delta x = 0.1$, and applying the Crank-Nicolson method, figure 5, the approximations were also interesting. This is because this method, besides being unconditionally stable, is $O(\Delta t^2 + \Delta x^2)$. That is, it has its order 2 consistency. This means that convergence is faster. Therefore, in addition to allowing larger steps, the implicit method of Crank-Nicolson has greater order of convergence allowing larger steps to be used than those used in the implicit method.

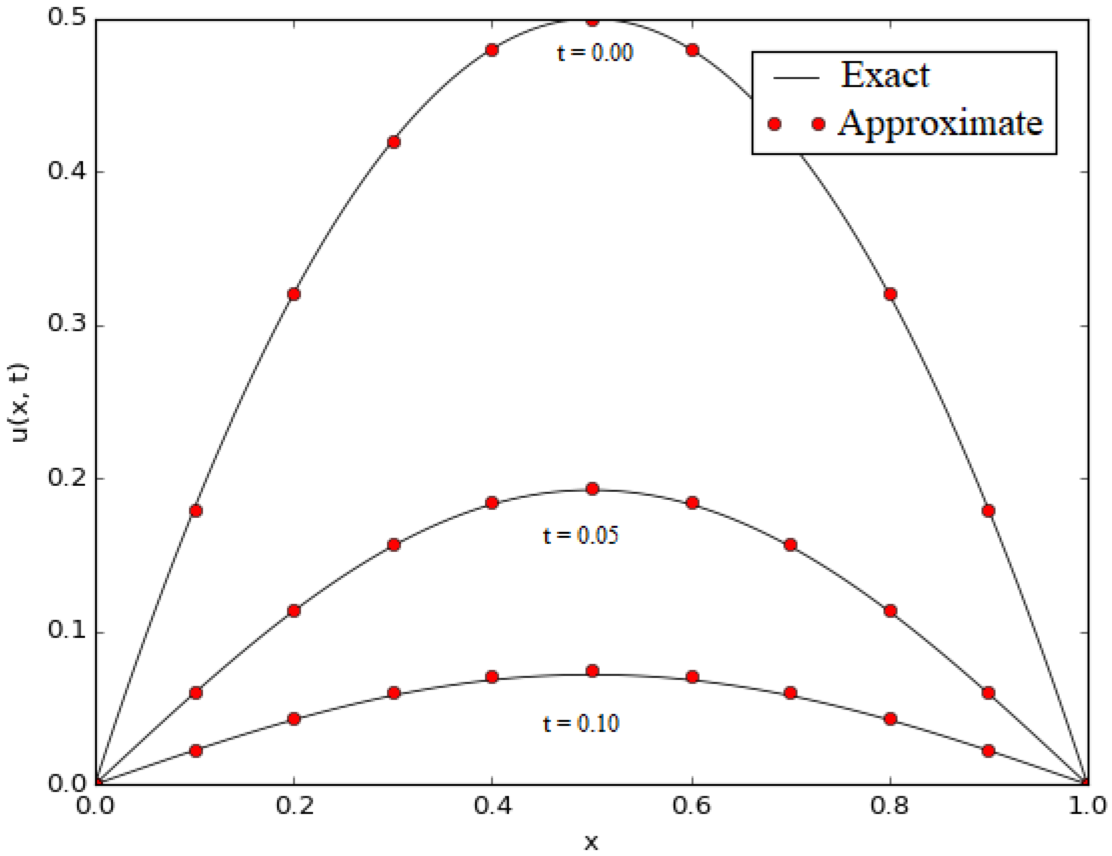

Figura 5: Graph of the approximate solution solution by the Crank-Nicolson method at times $t = 0$, $t = 0.05$ e $t = 0.10$ of problem II.

4 Conclusion

The experiments of the explicit method presented satisfactory results within the interval $\sigma \leq \frac{1}{2}$. The analytical and experimental validations prove the ability of this formulation to solve problems for low values of Δt with a sufficiently large Δx. However, the search for values that satisfy the stability condition can be tedious and the computational cost, due to having a small Δt, is large.

Numerical results showed that implicit formulations outweigh the stability conditions of the explicit method, and larger steps within the mesh may be used. However, the approximations are more satisfactory when $\Delta x, \Delta t \to 0$, keeping the point (x, t) fixed. On the other hand, the implicit Crank-Nicolsom formulations, because of their greater order of consistency, show a faster convergence than the implicit and explicit method, thus allowing even greater steps in the time axis.

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