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Review

On some finite difference methods for solving initial-boundary value problems in partial differential equations

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This paper presents some finite difference methods for solving initial-boundary value problems in partial differential equations namely explicit method, implicit method and Crank Nicolson method. Finite difference methods are used to solve partial differential equations by approximating the differential equations over the area of integration by a system of algebraic equations. We discuss the convergence of these methods in the context of the exact solution. Moreover Crank Nicolson method is unconditionally stable, more accurate and converges faster than its two counterparts, the explicit and implicit methods.

Keywords: Accuracy, Convergence, Crank Nicolson Method, Finite Difference Method, Explicit Method, Implicit Method.
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INTRODUCTION

The mathematical formulation of most problems in science involving rates of change with respect to two or more independent variables, usually representing time, often leads to a partial differential equation.

Problems involving time as one independent variable sometimes lead to parabolic partial differential equations, the simplest of which is the diffusion equation, derived from the theory of heat conduction (Ames, 1992). The diffusion equation plays an important role in a broad range of practical applications such as fluid mechanics. Only a limited number of special types of parabolic equation have been solved analytically and the usefulness of these solutions is further restricted to problems involving shapes for which the boundary conditions can be satisfied. In such cases numerical methods are some of the very few means of solution.

The finite difference approximations are one of the simplest and of the oldest methods to solve partial differential equations. It was already known by L. Euler (1707-1783) ca. 1768, in one dimension of space and was probably extended to two dimensions by C. Runge (1856-1927) ca. 1908. The advent of finite difference techniques in numerical applications began in the early 1950s and their development was stimulated by the emergence of computers that offered a convenient framework for dealing with complex problems of science and technology. Theoretical results have been obtained during the last five decades regarding the accuracy, stability and convergence of the finite difference method for partial differential equations.

Crank Nicolson Method for solving parabolic partial

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differential equations was developed by John Crank and Phyllis Nicolson in the mid-20th century. A practical method for numerical evaluation of partial differential equations of the heat conduction type was considered by (Crank and Nicolson, 1996). (Frankel and Du Fort, 1953) modified the simple explicit scheme and proved that it is much more stable than the simple explicit case, enabling larger time steps to be used. (Fadugba, et al., 2012) considered the stability and accuracy of finite difference method for option pricing. However, according to (Britz, 1988), the accuracy of the simple explicit method is barely improved upon.

There are many exhaustive texts on this subject such as (Ames, 1992; Cooper, 1998; Kaw and Garapati, 2011; Morton and Mayers, 1994; Smith, 1965; Vetterling et al., 2007), just to mention few.

In this paper we shall only consider the accuracy of explicit, implicit and Crank Nicolson method in the context of exact formula for solvingpartial differential equations.

Finite Difference Methods

The finite difference methods attempt to solve partial differential equations by approximating the differential equation over the area of integration by a system of algebraic equations. The finite difference approach is one of the premier mathematical tools employed to solve partial differential equations. They are a means of obtaining numerical solutions to partial differential equations.

The most common finite difference methods for the solution of partial differential equation are:

- Explicit method
- Implicit method
- Crank Nicolson Method

These are closely related but differ in stability, accuracy and execution speed. In the formulation of a partial differential equation problem, there are three components to be considered:

• The partial differential equation.

• The region of space-time on which the partial differential equation is required to be satisfied.

• The ancillary boundary and initial conditions to be met.

One of the simple examples of a parabolic PDE is the heat-conduction equation for a metal rod shown in the Figure 1 below;

$$f_{xx} = \frac{1}{\lambda} f_t \tag{1}$$

Where f denotes temperature which is a function of location, x and time, t in which the thermal diffusivity λ is given by

$$\lambda = \frac{k}{\rho C} \tag{2}$$

Where

k = Thermal conductivity of rod material,

ρ = Density of rod material,

C = Specific heat of the rod material

Let us consider the diagram below:

In finite difference methods we replace the partial derivative occurring in the partial differential equations by approximations based on Taylor series expansions of function near the point or points of interest. The derivative we seek is expressed with many desired order of accuracy. For a rod of length L which is divided into $n+1$ nodes, $\delta x = \frac{L}{n}$ and the time is similarly broken into time steps of δt. Hence f_i^n corresponds to the temperature at node i, that is, $x = i\delta x$ and time, $t = n\delta t$, where δt = time step. The time derivative of the right hand side of Equation (2) is approximated by the forward divided difference approximation

$$f_t\big|_{i,j} \cong \frac{f_i^{n+1} - f_i^n}{\delta t} \tag{3}$$

The finite difference form of the heat equation (1) is now given with the spatial second derivative evaluated from a combination of the derivatives at time steps n and $n+1$

$$\frac{1}{\lambda}\left(\frac{f_i^{n+1} - f_i^n}{\delta t}\right) = m\left(\frac{f_{i+1}^n - 2f_i^n + f_{i-1}^n}{(\delta x)^2}\right) + (1-m)\left(\frac{f_{i+1}^{n+1} - 2f_i^{n+1} + f_{i-1}^{n+1}}{(\delta x)^2}\right) \tag{4}$$

Where

i = Node number along the $x-$direction, $i = 0,1,....,k$,

n = Node number along the time,

δx = Distance between nodes.

From the above formula, we have for explicit when $m=1$ and an implicitwhen $m=0$ as shown below in equations (5) and (6) respectively:

$$\frac{1}{\lambda}\left(\frac{f_i^{n+1} - f_i^n}{\delta t}\right) = \left(\frac{f_{i+1}^n - 2f_i^n + f_{i-1}^n}{(\delta x)^2}\right) \tag{5}$$

$$\frac{1}{\lambda}\left(\frac{f_i^{n+1} - f_i^n}{\delta t}\right) = \left(\frac{f_{i+1}^{n+1} - 2f_i^{n+1} + f_{i-1}^{n+1}}{(\delta x)^2}\right) \tag{6}$$

Solving for the temperature at the time node $n+1$ in (5), we have;

$$f_i^{n+1} = f_i^n + \lambda\frac{\delta t}{(\delta x)^2}\left(f_{i+1}^n - 2f_i^n + f_{i-1}^n\right) \tag{7}$$

The expression $\frac{\lambda\delta t}{(\delta x)^2}$ is known as the diffusion number and will be denoted by r, i.e.

$$r = \lambda\frac{\Delta t}{(\Delta x)^2} \tag{8}$$

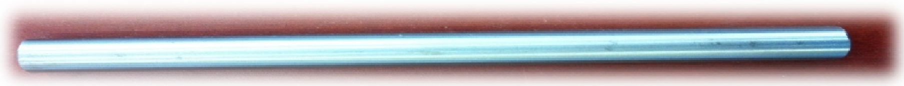

Figure 1 A Metal Rod

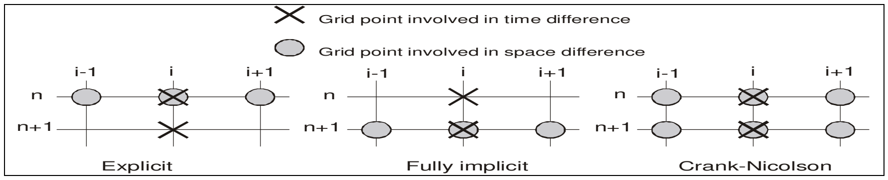

Figure 2 A Computational Diagrams for Explicit, Implicit and Crank Nicolson Methods

Therefore,

$$f_i^{n+1} = f_i^n + r\left(f_{i+1}^n - 2f_i^n + f_{i-1}^n\right) \tag{9}$$

Equation (9) can be solved explicitly because it can be written for each internal location node of the rod for time node $n+1$ in terms of the temperature at time node n. The explicit method does not guarantee stability which depends on the value of the time step, location step and the parameters of the elliptic equation. For the partial differential equation (2) the explicit method is convergent and stable for

$$\frac{\lambda \delta t}{(\delta x)^2} \le \frac{1}{2} \tag{10}$$

These issues are addressed by using the implicit method. Instead of the temperature being found one node at a time, the implicit method results in simultaneous linear equations for the temperature at all interior nodes for a particular time

Similarly, by solving (6), we have that;

$$\frac{f_i^{n+1} - f_i^n}{\delta t} = \lambda \frac{f_{i+1}^{n+1} - 2f_i^{n+1} + f_{i-1}^{n+1}}{(\delta x)^2} \tag{11}$$

So,

$$f_i^n = -rf_{i-1}^{n+1} + (1+2r)f_i^{n+1} - rf_{i+1}^{n+1} \tag{12}$$

Equation (12) is called implicit method which can be written for all nodes (except the external nodes), at a particular time level.

In fact m can be any value between 0 and 1, however a common choice for $m = 0.5$. Therefore we have from (4) that;

$$\frac{1}{\lambda}\left(\frac{f_i^{n+1} - f_i^n}{\delta}\right) = \frac{1}{2}\left(\frac{f_{i+1}^n - 2f_i^n + f_{i-1}^n}{(\delta x)^2}\right) + \frac{1}{2}\left(\frac{f_{i+1}^{n+1} - 2f_i^{n+1} + f_{i-1}^{n+1}}{(\delta x)^2}\right) \tag{13}$$

Equation (13) is the average of explicit and implicit schemes as written above in (5) and (6) respectively. The above equation (13) can be arranged so that the temperatures at the present time step $(n+1)$ are on the left hand side. By applying these equations to all the nodes, we shall obtain a system with tridiagonal coefficient matrix.

$$-\frac{1}{2}\left(\frac{\lambda\delta}{(\delta x)^2}\right)f_{i-1}^{n+1} + \left(1+2\frac{\lambda\delta}{(\delta x)^2}\right)f_i^{n+1} - \frac{1}{2}\left(\frac{\lambda\delta}{(\delta x)^2}\right)f_{i+1}^{n+1} = \frac{1}{2}\left(\frac{\lambda\delta}{(\delta x)^2}\right)f_{i-1}^n + \left(1-2\frac{\lambda\delta}{(\delta x)^2}\right)f_i^n - \left(\frac{\lambda\delta}{(\delta x)^2}\right)f_{i+1}^n \tag{14}$$

So,

$$-\frac{r}{2}f_{i-1}^{n+1} + (1+2r)f_i^{n+1} - \frac{r}{2}f_{i+1}^{n+1} = \frac{r}{2}f_{i-1}^n + (1-2r)f_i^n + rf_{i+1}^n \tag{15}$$

Therefore,

$$-r\left(f_{i-1}^{n+1} + f_{i+1}^{n+1}\right) + 2(1+r)f_i^{n+1} = r\left(f_{i-1}^n + f_{i+1}^n\right) + 2(1-r)f_i^n \tag{16}$$

Equation (16) is called Crank Nicolson method and its associated boundary and initial conditions are as given.

If we divide the $x-$interval $0 \le x \le 1$ into k equal interval, we have $(k-1)$ internal mesh points per time row. Then for $n = 1$ and $i = 1, 2, ..., k-1$, (16) gives a system of $(k-1)$ linear equations for the $(k-1)$ unknown values $f_1^1, f_2^1, f_3^1, ...f_{k-1}^1$ in the first time row in terms of the initial values $f_0^0, f_1^0, f_2^0, ...f_k^0$ and the boundary values $f_0^1 = 0, f_k^1 = 0$. Similarly for $n = 1, n = 2$, and so on; that is for each time row we have to solve such a system of $(k-1)$ linear equations resulting from (16). Equation (16) can be written in a matrix equation as

$$Tf = tb \tag{17}$$

where the unknown $f = f^{n+1}$, the known concentrations $b = f^n$ and T, t are tri-diagonal matrices of coefficients defined as

$$\begin{bmatrix} (2+2r) & -r & 0 & \cdots & 0 \\ -r & 2(1+r) & -r & \cdots & 0 \\ 0 & -r & 2(1+r) & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & -r \\ 0 & 0 & 0 & -r & 2(1+r) \end{bmatrix} \begin{bmatrix} f_1^{n+1} \\ f_2^{n+1} \\ f_3^{n+1} \\ \vdots \\ f_{k-1}^{n+1} \end{bmatrix} = \begin{bmatrix} 2(1-r) & r & 0 & \cdots & 0 \\ r & 2(1-r) & r & \cdots & 0 \\ 0 & r & 2(1-r) & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & r \\ 0 & 0 & 0 & r & 2(1-r) \end{bmatrix} \begin{bmatrix} f_1^n \\ f_2^n \\ f_3^n \\ \vdots \\ f_{k-1}^n \end{bmatrix} \tag{18}$$

Crucial to the convergence of this method is the condition (Turner, 1994)

$r = \dfrac{\lambda \delta t}{(\delta x)^2} \le \dfrac{1}{2}$, this implies that

$$\delta t \le \frac{(\delta x)^2}{2\lambda} \tag{19}$$

Condition (19) is a drawback in practice. Indeed, in order to attain sufficient accuracy, we have to choose δx small, which makes δt very small by (19). This will make the computation exceptionally lengthy, as more time levels will be required to cover the region. A method that imposes no such restriction as $r = \frac{\lambda \delta t}{(\delta x)^2}$ was proposed by Crank and Nicolson in (Smith, 1965)

Stability Analysis of Finite Difference Method (Frankel and Du Fort, 1953)

The two fundamental sources of error are the truncation error in the stock price discretization and in the time discretization. The importance of truncation error is that the numerical scheme solves a problem that is not exactly the same as the problem we are trying to solve.

The three fundamental factors that characterize a numerical scheme are consistency, stability and convergence

- Consistency: A finite difference of a partial differential equation is consistent, if the difference between partial differential equation and finite differential equation vanishes as the interval and time step size approach zero. Consistency deals with how well the finite difference equation approximates the partial differential equation and it is the necessary condition for convergence.
- Stability: For a stable numerical scheme, the errors from any source will not grow unboundedly with time.
- Convergence: It means that the solution to a finite difference equation approaches the true solution to the partial differential equation as both grid interval and time step sizes are reduced. The necessary and sufficient conditions for convergent are consistency and stability.

These three factors that characterize a numerical scheme are linked together by Lax equivalence theorem (Frankel and Du Fort, 1953) which states that given a well posed linear initial value problem and a consistent finite difference scheme, stability is the necessary and sufficient condition for convergence.

In general, a problem is said to be well posed if:

- A solution to the problem exists.
- The solution is unique when it exists.
- The solution depends continuously on the problem data.

A Necessary and Sufficient Condition for Stability (Frankel and Du Fort, 1953)

Let $f_{i+1} = Af_i$ be a system of equations, where A and f_{i+1} are matrix and column vectors respectively. Then

$$\left.\begin{aligned} f_i &= Af_{i-1} \\ &= A^2 f_{i-2} \\ &\vdots \\ &= A^i f_0 \end{aligned}\right\} \tag{20}$$

For $i = 1,2,...,N$ and f_0 is the vector of initial value. We are concerned with stability and we also perturbed the vector of the initial value f_0 to g_0. The exact solution at the i^{th} row is given by

$$g_i = A^i g_0 \tag{21}$$

Let the perturbation or error vector e be denoted by $e = g - f$ and using the perturbation vectors (20) and (21), we have

$$\left.\begin{aligned} e_i &= g_i - f_i \\ &= A^i g_0 - A^i f_0 \\ &= A^i (g_0 - f_0) \end{aligned}\right\}$$

Therefore,

$$e_i = A^i e_0 \tag{22}$$

Hence for compatible matrix and vector norms [9]

$$\|e_i\| \le \|A^i\| \, \|e_0\|$$

Lax and Richmyer defined the difference scheme to be stable when there exists a positive number L such that L is independent of i, δt and δx, then $\|A\| \le L$. This limits the amplification of any initial perturbation and therefore of any arbitrary initial rounding errors, since $\|e_i\| \le L$ $\|e_0\|$ and $\|A^i\| \le \|A\|^i$, then the Lax-Richmyer definition of stability is satisfied when

$$\|A\| \le 1 \tag{23}$$

Hence (20) is the necessary and sufficient condition for the finite difference equations to be stable (Smith, 1965). Since the spectral radius $\rho(A)$ satisfies $\rho(A) \le \|A\|$, it follows from (23) that $\rho(A) \le 1$.

By Lax equivalence theorem, the three finite difference methods are consistent and convergent but in the analysis of their stability, explicit method is quite stable, while the implicit and Crank Nicolson methods are conditionally and unconditionally stable finite difference methods respectively because they calculate small change in the option value for a small change of the initial conditions, converge to the solution of the partial differential equation and calculation error decreases when number of time and price partitions increase.

Numerical Examples and Results

A rod of steel is subjected to a temperature of $100°C$ on the left end and $25°C$ on the right end. If the rod is of

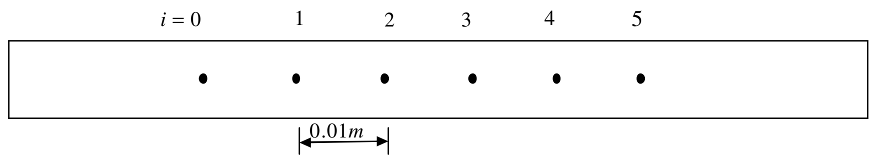

Figure 3 Schematic Diagram showing the node representation in the Model

Table 1 Results Generated from Implicit, Explicit and Crank Nicolson Finite Difference Methods

Temperature at Nodes $T(°C)$	Explicit Method $(°C)$	Implicit Method $(°C)$	Crank Nicolson Method $(°C)$
$n=0, \quad t=3$			
f_0^1	100.0000	100.0000	100.0000
f_1^1	53.9120	39.4510	44.3720
f_2^1	20.0000	24.7920	23.7460
f_3^1	20.0000	21.4380	20.7970
f_4^1	22.1200	21.4770	21.6070
f_5^1	25.0000	25.0000	25.0000
$n=1, \quad t=6$			
f_0^2	100.0000	100.0000	100.0000
f_1^2	59.0730	51.3260	55.8830
f_2^2	34.3750	30.6690	31.0750
f_3^2	20.8990	23.8760	23.1740
f_4^2	22.4420	22.8360	22.7300
f_5^2	25.0000	25.0000	25.0000
$n=2, \quad t=9$			
f_0^3	100.0000	100.0000	100.0000
f_1^3	65.9500	59.0430	62.6040
f_2^3	39.1320	36.2920	37.6130
f_3^3	27.2660	26.8090	26.5620
f_4^3	22.8720	24.2430	24.0420
f_5^3	25.0000	25.0000	25.0000

length $0.05m$, use Crank-Nicolson method to find the temperature distribution in the rod from $t=0$ to $t=9$ seconds. Use $\delta x = 0.01m$ and $\delta t = 3s$.

Given

$$\alpha = 54W(m-K)^{-1}, \qquad \rho = 7800kgm^{-3}, \qquad (24)$$

$$C = 490J(kg-K)^{-1}.$$

The initial temperature of the rod is $20°C$.

Solution

The parabolic heat conduction equation associated with the above problem is given by

$$f_{xx} = \frac{1}{\lambda} f_t \qquad 0 < x < 0.05, \; t > 0 \qquad (25)$$

With boundary conditions

$$f = 100°C \text{ at } x = 0, \; t > 0 \qquad (26)$$

Table 2 Comparison of Temperature obtained at interior nodes $n = 2$ and $i = 1,2,3,4$ using Implicit, Explicit and Crank Nicolson Finite Difference Methods

Temperature at Nodes $T(°C)$	Exact Solution $(°C)$	Explicit Method $(°C)$	Implicit Method $(°C)$	Crank Nicolson Method $(°C)$
f_0^3	100.0000	100.0000	100.0000	100.0000
f_1^3	62.5100	65.9530	59.0430	62.6040
f_2^3	37.0840	39.1320	36.2920	37.6130
f_3^3	25.8440	27.2660	26.8090	26.5620
f_4^3	23.6100	22.8720	24.2430	24.0420

Table 3 Errors Generated from Explicit, Implicit and Crank Nicolson Finite Difference Methods

Temperature at Nodes $T(°C)$	Explicit Method $(°C)$	Implicit Method $(°C)$	Crank Nicolson Method $(°C)$
f_0^3	0.0000	0.0000	0.0000
f_1^3	3.4430	3.4670	0.0940
f_2^3	2.0480	0.7920	0.5290
f_3^3	1.4220	0.9650	0.2820
f_4^3	0.7380	0.6330	0.4320

$f = 25°C$ at $x = 0.05,\ t > 0$ (27)

And initial conditions

$f = 20°C$ at $t = 0,\ 0 < x < 0.05$ (28)

$$\lambda = \frac{\alpha}{\rho C} = \frac{54}{7800 \times 490} = 1.4129 \times 10^{-5}\ m^2/s \quad (29)$$

Then

$$r = \lambda \frac{\delta t}{(\delta x)^2} = 1.412 \times 10^{-5} \frac{3}{(0.01)^2} = 0.4239 \quad (30)$$

The boundary conditions are given below:

$$\left. f_0^n = 100°C,\ f_5^n = 25°C \right\} \text{ for } n = 0,1,2,3 \quad (31)$$

The initial temperature of the rod is $20°C$, that is, all the temperatures of the nodes inside the rod are at $20°C$, $t = 0$ except for the boundary nodes given by (31). This could be represented as

$$f_i^0 = 20°C, \text{ for } i = 1,2,3,4. \quad (32)$$

The initial temperature at the nodes inside the rod (when $t = 0$ second) is given by

$$\left. f_0^0 = 100°C,\ f_5^0 = 25^0 C \right\} \text{ from } (31)$$

$$\left. f_1^0 = 20°C, f_2^0 = 20°C, f_3^0 = 20°C, f_4^0 = 20°C \right\} \text{ from}(32)$$

The temperature at the nodes inside the rod when $t = 3$ seconds, from (31), we have the boundary condition of the form:

$$\left. f_0^1 = 100°C,\ f_5^1 = 25°C \right\}$$

For all the interior nodes, setting $n = 0,1,2$ and $i = 1,2,3,4$ in (9), (12) and (16) gives the following results shown in the Table 1 Above.

The exact solution to the above problem is given by:

$$f(x,t) = 100 - 1500x + \sum_{m=1}^{\infty} \left\{ \frac{10(-1)^m - 160}{m\pi} \right\} \exp\left((-1.4129 \times 10^{-5})(20m\pi)^2 t\right) \sin(20m\pi x) \quad (33)$$

We shall present in the Tables 2 and 3 above respectively, the results obtained at interior nodes $n = 2$ and $i = 1,2,3,4$ only in the context of exact solution by substituting the values of x and t gives the temperature inside the rod at a particular location and time and the error generated from the methods respectively.

The above results were obtained using MATLAB codes.

The temperature distribution along the length of the rod at different times for explicit, implicit and Crank Nicolson methods is plotted in Figures 4, 5 and 6 respectively.

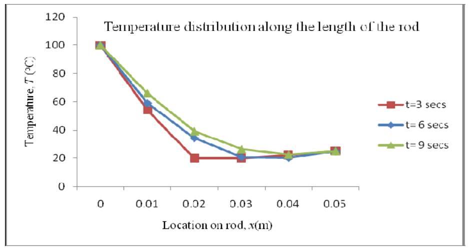

Figure 4 Temperature Distributions in Rod from Explicit Method

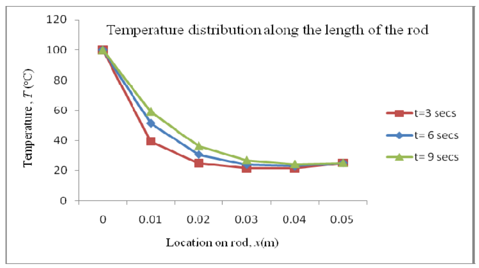

Figure 5 Temperature Distributions in Rod from Implicit Method

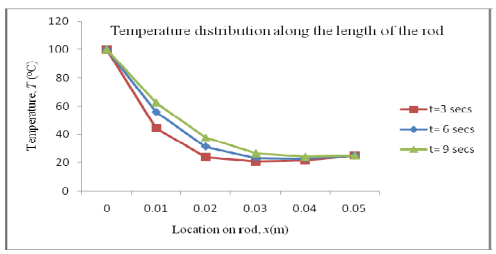

Figure 6 Temperature Distribution in Rod from Crank Nicolson Method

DISCUSSION OF THE RESULTS

From Tables 1 and 2, it is clear that among the numerical methods used to solve partial differential equations, Crank Nicolson method provides better accuracy compared to the explicit method and implicit method. Also from Table 3, the error generated from Crank Nicolson method is smaller than that of its counterparts.

CONCLUSION

The finite difference methods have become a very popular for solving initial-boundary value problems in partial differential equations. Each of the finite difference methods considered has its own advantages and disadvantages. Explicit method is very easy to calculate, simply stead ahead but has low accuracy; must use "small" δt . Implicit method is unconditionally stable but it is computational cost especially for 2D and 3D spatially. Crank Nicolson method is robust, unconditionally stable, has higher order of accuracy up to $O((\delta x)^2, (\delta t)^2)$ and converges faster than explicit and implicit finite difference methods but the main problem of Crank Nicolson method is that it starts to oscillate when the coefficient of the second derivative (the *diffusion term*) is very small or when the coefficient of the first derivative (the *convection term*) is large (or both).

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