American Scientific Research Journal for Engineering, Technology, and Sciences (ASRJETS)
ISSN (Print) 2313-4410, ISSN (Online) 2313-4402

http://asrjetsjournal.org/

Application of Some Finite Difference Schemes for Solving One Dimensional Diffusion Equation

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Abstract

In this paper the numerical solutions of one dimensional diffusion equation using some finite difference methods have been considered. For that purpose three examples of the diffusion equation together with different boundary conditions are examined. The finite difference methods applied on each example are (i) forward time centered space (ii) backward time centered space and (iii) Crank – Nicolson. In each case, we have studied stability of finite difference method and also obtained numerical result. The performance of each scheme is evaluated in accordance with both the accuracy of the solution and programming efforts. The implementation and behavior of the schemes have been compared and the results are illustrated pictorially. It is found in case of the test examples studied here that the Crank – Nicolson scheme gives better approximations than the two other schemes.

Keywords: Crank – Nicolson; Diffusion equation; Forward time centered space; Backward time centered space; Stability.

1. Introduction

One dimensional diffusion equation plays an important role in modeling numerous physical phenomena. The application of such diffusion equation includes a wide range of areas such as physical, biological and financial sciences. One of the most common applications is propagation of heat in the environment, where $u(x,t)$ represents the temperature of some substance at point x and time t.

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The diffusion or heat equation is applied when attempting to describe the density fluctuations in a material that undergoes diffusion [8]. In the diffusion equation there appear derivatives with respect to time and space coordinates.

Several finite difference techniques have been employed to solve these equations so as to fit their physical nature [1 – 2, 5, 7, 13, 14]. The process of solving requires specification of a suitable boundary conditions viz., (i) Dirichlet (ii) Neumann or gradient (iii) Mixed or Robin (iv) Combination of Dirichlet and Neumann. Boundary conditions are applied on the spatial coordinate at $x = 0$ and $x = L$ and initial conditions are applied on the temporal coordinate when $t = 0$. In the process of finding numerical solutions the continuous partial differential equations are replaced by their discrete approximations. In the present context the word *discrete* indicates that the numerical solution is known only at a finite number of points in the physical domain. The number of those discrete points can vary and can be fixed by the user of the numerical method. However, increment in the number of discrete points increases not only the resolution but also the accuracy of the numerical solution.

The process of discretization of a diffusion equation leads to a set of algebraic equations. These algebraic equations are evaluated so as to obtain values for the unknown quantities of the discretization. In turn, the values of unknowns provide an approximate solution to the original diffusion equation.

We now divide the xt domain into a mesh. The coordinate axes are divided into steps of uniform lengths Δx and Δt along x and t axis respectively. When horizontal and vertical lines are drawn along the step nodes the resulting image would resemble as a net or mesh. The two key parameters of the mesh are Δx and Δt. The former denotes the local distance between adjacent points in space while the latter denotes local distance between adjacent time steps. The intersection points of this mesh are called nodes. The discrete solutions are computed at the mesh nodes.

The core idea of the finite difference scheme is to replace continuous derivatives with difference formulae. Difference formulae provide discrete values of the function at nodes of the mesh. A variety of finite difference schemes are popular and widely used. Use of different combinations of mesh points in the difference formulas results in different schemes. In the limit of the mesh step spacing tending to zero i.e., as $\Delta x \to 0$ and $\Delta t \to 0$, the numerical solution obtained by any useful scheme will approach the true solution of the differential equation. However, the rate at which the numerical solution converges to the true solution varies with the scheme. In addition, there are some practically useful schemes which may fail to yield a solution for bad combinations of Δx and Δt. Hence, the selection of combinations of Δx and Δt plays an important role [3]. Further, considerable attention is required so that the physical interpretations of solutions of diffusion equation remain meaningful. That is, we have to select such a combination of Δx and Δt that provides physically meaningful approximate solution for the diffusion equation.

2. Governing Equation and Finite Difference Schemes

Here we now introduce and discuss governing equation describing one dimensional diffusion. Also we present the finite difference methods viz., forward time centered space or FTCS, backward time centered space or BTCS and Crank – Nicolson schemes.

2.1 Governing Equation

The more general diffusion equation is a partial differential equation and it describes the density fluctuations in the material undergoing diffusion. The equation can be expressed as:

$$\frac{\partial u}{\partial t} = \nabla.(D\nabla u) \tag{1}$$

Here in (1), $u \equiv u(\boldsymbol{x}, t)$ denotes the density of the diffusing material at location $\boldsymbol{x} = (x, y, z)$ and at time t. Also $D \equiv D(u(\boldsymbol{x}, t), x)$ denotes the collective diffusion coefficient for the density u at location **x.**

Now for simplicity let the diffusion coefficient be independent of both density and location i.e., D is a constant. Thus equation (1) reduces to a linear form as

$$\frac{\partial u}{\partial t} = D\nabla^2 u\,. \tag{2}$$

Equation (2) is a diffusion or heat equation and describes the distribution of material or heat in a given region over time with constant diffusion coefficient. In the present study we further simplify (2) and consider one – dimensional diffusion with constant diffusion coefficient D. This consideration simplifies (2) to give

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} \tag{3}$$

Here in (3), u is the density of the diffusing material at location x and time t. D is the diffusivity coefficient in the x – direction. We impose appropriate initial and boundary conditions on (3) in order to evaluate a numerical or approximate solution of it. Several combinations of boundary conditions are possible. We consider three distinct cases and apply them in a finite domain as follows:

Case 1: Dirichlet type of boundary conditions

$$u(x,0) = f(x) \tag{4}$$

$$u(0,t) = u_0$$

$$u(L,t) = u_L$$

Case 2: Neumann type of boundary conditions

$$u(x,0) = f(x) \tag{5}$$

$$\frac{\partial u}{\partial x}(0,t) = u_0$$

$$\frac{\partial u}{\partial x}(L,t) = u_L$$

Case 3: One end Neumann and other end Dirichlet type of boundary conditions:

$$u(x,0) = f(x) \tag{6}$$

$$\frac{\partial u}{\partial x}(0,t) = 0$$

$$u(L,t) = u_L$$

Here in (4) to (6), the quantities u_0 and u_L represent constant densities of the diffusing material respectively at $x = 0$ and $x = L$. The function $f(x)$ is an arbitrary one of its argument.

2.2 Forward Time Centered Space Explicit Scheme

The equation (3) does not always exhibit an analytical solution and even if it exhibits finding is not easy. Hence, finite difference schemes are applied for finding approximate solutions. We now approximate equation (3) by applying forward difference on time derivative and central difference on space derivative. Thus equation (3) takes the form as

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = D\left[\frac{u_{i-1}^n - 2\,u_i^n + u_{i+1}^n}{\Delta x^2}\right] + O(\Delta t) + O(\Delta x^2). \tag{7}$$

The temporal error $O(\Delta t)$ and spatial error $O(\Delta x^2)$ have different orders. Their values are very small and their influence on the solution is negligible. The big O notation expresses the rate at which the truncation error goes to zero. Hence drop the truncation error terms from equation (7) and after a rearrangement it leads to

$$u_i^{n+1} = ru_{i-1}^n + (1-2r)u_i^n + ru_{i+1}^n \tag{8}$$

In (8), we have used the notation $r = D(\Delta t/\Delta x^2)$. Furthermore, equation (8) can be expressed in terms of matrix multiplication as

$$u^{n+1} = (I + rS)\, u^n \tag{9}$$

In (9), we have used the following matrix notations

$$u^{n+1} = [u_1^{n+1}, u_2^{n+1}, \quad \ldots, u_{N-1}^{n+1}]^T$$

$$u^n = [u_1^n + ru_0^n, u_2^n, \quad \ldots, u_{N-1}^n + u_N^n]^T$$

$$I = \begin{bmatrix} 1 & 0 & 0 & \ldots & 0 \\ 0 & 1 & 0 & \ldots & 0 \\ . & . & . & \ldots & . \\ 0 & 0 & 0 & \ldots & 1 \end{bmatrix}$$

$$S = \begin{bmatrix} -2 & 1 & 0 & \ldots & 0 & 0 & 0 \\ 1 & -2 & 1 & \ldots & 0 & 0 & 0 \\ . & . & . & \ldots & . & . & . \\ 0 & 0 & 0 & \ldots & 1 & -2 & 1 \\ 0 & 0 & 0 & \ldots & 0 & 1 & -2 \end{bmatrix}. \quad (10)$$

In (9), both u^n and u^{n+1} are column vectors of dimension $N-1$. The superscript T denotes transpose of the matrix. The $N-1$ dimensional square matrices I and S respectively denote an identity and a tridiagonal matrices.

To find the stability condition of equation (8), we substitute a trial solution or a Fourier mode

$$u_i^n = \lambda^n e^{[ni\pi/p]} \quad (11)$$

to get

$$\lambda = r\left(e^{n\pi/p} + e^{-n\pi/p}\right) + 1 - 2r = 1 - 2r[1 - \cos(\pi/p)]$$

Here p is any non-zero integer. Since we must have $|\lambda| \le 1$ for non – divergence, the stability condition turns out to be $r = [D\Delta t/\Delta x^2] \le 1/2$. That is, the equation (8) is stable as long as the spatial interval Δx satisfies the condition $\Delta x \le \sqrt{2D\,\Delta t}$ for any given time interval Δt. Otherwise (8) will not be stable [13].

Further, the truncation error $T_{i,n}$ for the equation (8) can be derived and expressed as [14]

$$T_{i,n} = \left(\frac{\partial u}{\partial t} - D\frac{\partial^2 u}{\partial x^2}\right)_{i,n} + \frac{1}{2}\Delta t\left(\frac{\partial^2 u}{\partial t^2}\right)_{i,n} + \frac{1}{12}(\Delta x)^2\left(\frac{\partial^4 u}{\partial x^4}\right)_{i,n} + O((\Delta t)^2) + O((\Delta x)^4).$$

It can be observed that the truncation error $T_{i,n}$ goes to zero as both temporal and spatial intervals go to zero. That is $T_{i,n} \to 0$ as $\Delta t \to 0$ and $\Delta x \to 0$. It shows that the FTCS scheme is consistent with partial differential equation (3).

2.3 Backward Time Centered Space Implicit Scheme

To discretize equation (3), we substitute the backward difference approximation for the first partial derivative and central difference approximation for the second partial derivative,

$$\frac{u_i^n - u_i^{n-1}}{\Delta t} = D\left[\frac{u_{i-1}^n - 2\,u_i^n + u_{i+1}^n}{\Delta x^2}\right] + O(\Delta t) + O(\Delta x^2) \quad (12)$$

To present the system of equations in a simple manner let us drop the truncation error terms from (12) and rearrange the resulting equation to get

$$u_i^{n-1} = -ru_{i-1}^n + (1+2r)\;u_i^n - ru_{i+1}^n \quad (13)$$

Here in (12) and (13), we denote i is an index number taking the values $i = 1, 2, 3, \ldots, N-1$.

If the Dirichlet type of boundary condition are given i.e., values of the end points u_0^n and u_N^n are given, then (13) can be reduced into a compact form as

$$u^{n-1} = (I - rS)u^n, \tag{14}$$

Here in (14), both u^{n-1} and u^n represent $(N-1)$ dimensional column vectors. That is, $u^{n-1} = [u_1^{n-1}, u_2^{n-1}, \ldots, u_{N-1}^{n-1}]^T$ and $u^n = [(u_1^n - ru_0^n), u_2^n, \ldots, u_{N-2}^n, (u_{N-1}^n - u_N^n)]^T$

Now up on substitution of the Fourier mode (11) in (13) yields $1/\lambda = -re^{-(n\pi/p)} + (1+2r) - re^{(n\pi/p)}$ or equivalently $\lambda = \{1 + 2r[1 - \cos(\pi/p)]\}^{-1}$ and thus $|\lambda| \leq 1$. This indicates that the BTCS scheme is unconditionally stable. Further, the advantage of this scheme is it removes the stability limitation associated with the diffusion operator. The disadvantage is that the problem becomes more expensive to solve numerically [3].

The truncation error $T_{i,n}$ for the BTCS solution of the diffusion equation is [14]

$$T_{i,n} = \left(\frac{\partial u}{\partial t} - D\frac{\partial^2 u}{\partial x^2}\right)_{i,n} + \frac{1}{2}\Delta t\left(\frac{\partial^2 u}{\partial t^2}\right)_{i,n} - \frac{1}{12}(\Delta x)^2\left(\frac{\partial^4 u}{\partial x^4}\right)_{i,n} + O((\Delta t)^2) + O((\Delta x)^4).$$

It can be observed that the truncation error $T_{i,n}$ goes to zero as both temporal and spatial intervals go to zero. That is $T_{i,n} \to 0$ as $\Delta t \to 0$ and $\Delta x \to 0$. It shows that the BTCS scheme is consistent with partial differential equation (3).

2.4 Crank – Nicolson Scheme

As we have already seen both the FTCS and BTCS schemes have temporal truncation errors of order $O(\Delta t)$. However, the Crank – Nicolson scheme has the error of order $O(\Delta t^2)$. Also the Crank – Nicolson scheme is not significantly more difficult to implement than the BTCS schemes. Further, the Crank – Nicolson scheme has significant advantages whenever the time – accurate solutions play an important role. The Crank – Nicolson scheme, like BTCS, is also implicit and unconditionally stable.

The Crank – Nicolson scheme approximates equation (3) using central differences of time intervals. The spatial derivatives are estimated by the average of their values at time steps n and $n+1$ as

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{D}{2}\left(\frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{(\Delta x)^2} + \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}\right) + O((\Delta t)^2) + O((\Delta x)^2) \tag{15}$$

The Crank – Nicolson scheme has a truncation error of temporal order $O(\Delta t^2)$ and spatial order $O(\Delta x^2)$. Drop the truncation error terms from (15) and rearranging the terms so that values of u at time n are on the left and values of u at time $n+1$ are on the right gives

$$ru_{i-1}^{n} + (2-2r)u_i^n + ru_{i+1}^n = -ru_{i-1}^{n+1} + (2+2r)u_i^{n+1} - ru_{i+1}^{n+1} \qquad (16)$$

The left hand side of (16) contains three known values and the right hand contains three unknowns. This scheme generates a set of $(N-1)$ linear equation and those have to be solved at each time level. Applying (16) for all the internal mesh points at $i = 1,2,3,\dots,N-1$ and using the boundary conditions $x = 0$ and $x = L$ we obtain a tridiagonal set of linear algebraic equations. These equations have to be solved at each time level.

The compact form of such tridiagonal set of linear algebraic equations can be written as

$$u^{n+1} = (2I - rS)^{-1}(2I + rS)u^n \qquad (17)$$

The system of equations (17) can be solved very efficiently. Also its unconditional stability can be shown by substituting (11) into (16). Thus,

$$2\lambda\left(1 + r\left(1 - \cos\left(\frac{\pi}{p}\right)\right)\right) = 2\left(1 - r\left(1 - \cos\left(\frac{\pi}{p}\right)\right)\right),$$

$$\lambda = \frac{1 - r\left(1 - \cos\left(\frac{\pi}{p}\right)\right)}{1 + r\left(1 - \cos\left(\frac{\pi}{p}\right)\right)}$$

$$|\lambda| \le 1$$

The truncation error $T_{i,n}$ for the Crank – Nicolson solution of the diffusion equation is [14]

$$T_{i,n} = \left(\frac{\partial u}{\partial t} - D\frac{\partial^2 u}{\partial x^2}\right)_{i,n} + \frac{\Delta t}{2}\frac{\partial}{\partial t}\left(\frac{\partial u}{\partial t} - D\frac{\partial^2 u}{\partial x^2}\right)_{i,n} + \frac{(\Delta t)^2}{6}\left(\frac{\partial^3 u}{\partial t^3}\right)_{i,n} - \frac{1}{12}(\Delta x)^2\left(\frac{\partial^4 u}{\partial x^4}\right)_{i,n} + O((\Delta t)^3) + O((\Delta x)^3).$$

It can be observed that the truncation error $T_{i,n}$ goes to zero as both temporal and spatial intervals go to zero. That is $T_{i,n} \to 0$ as $\Delta t \to 0$ and $\Delta x \to 0$. It shows that the Crank – Nicolson scheme is consistent with partial differential equation (3).

3. Numerical Results

Consider the special case of the diffusion equation (3) with $D = 1$ to obtain

$$\partial u/\partial t = \partial^2 u/\partial x^2 \qquad (18)$$

The numerical solutions of (18) together with appropriate initial and boundary conditions are drawn using finite difference schemes (i) FTCS (ii) BTCS and (iii) Crank – Nicolson. The details are given in what follows from Sections 3.1 to 3.3. In our computations 0.1 and 0.125 are assigned to the spatial interval Δx and the values 0.4 and 0.625 for parameter r are used.

3.1 Problem 1

In this problem, consider (18) together with the following initial and boundary conditions

$$u(x,0) = \sin(\pi x), \quad 0 < x < 1, \tag{19}$$

$$u(0,t) = u(1,t) = 0, \quad t \geq 0. \tag{20}$$

However the analytical solution of (18) with the initial boundary value problem (19) and (20) can be easily found using the method of separation of variables as

$$u(x,t) = e^{-\pi^2 t}\sin(\pi x). \tag{21}$$

The numerical solutions and errors of (18) together with (19) and (20) are illustrated in the following plots.

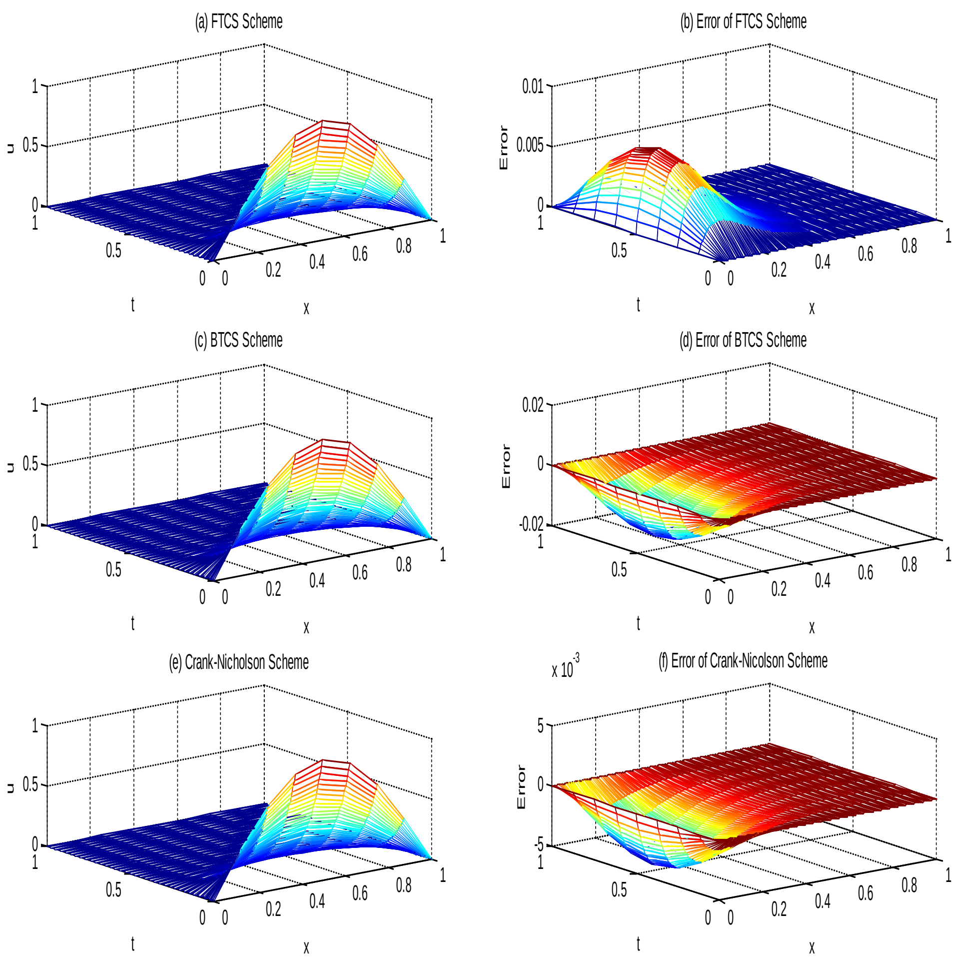

Figure 1: Numerical solutions and errors of (18) together with (19) and (20) obtained using the three different schemes when $r = 0.4$ and $\Delta x = 0.125$.

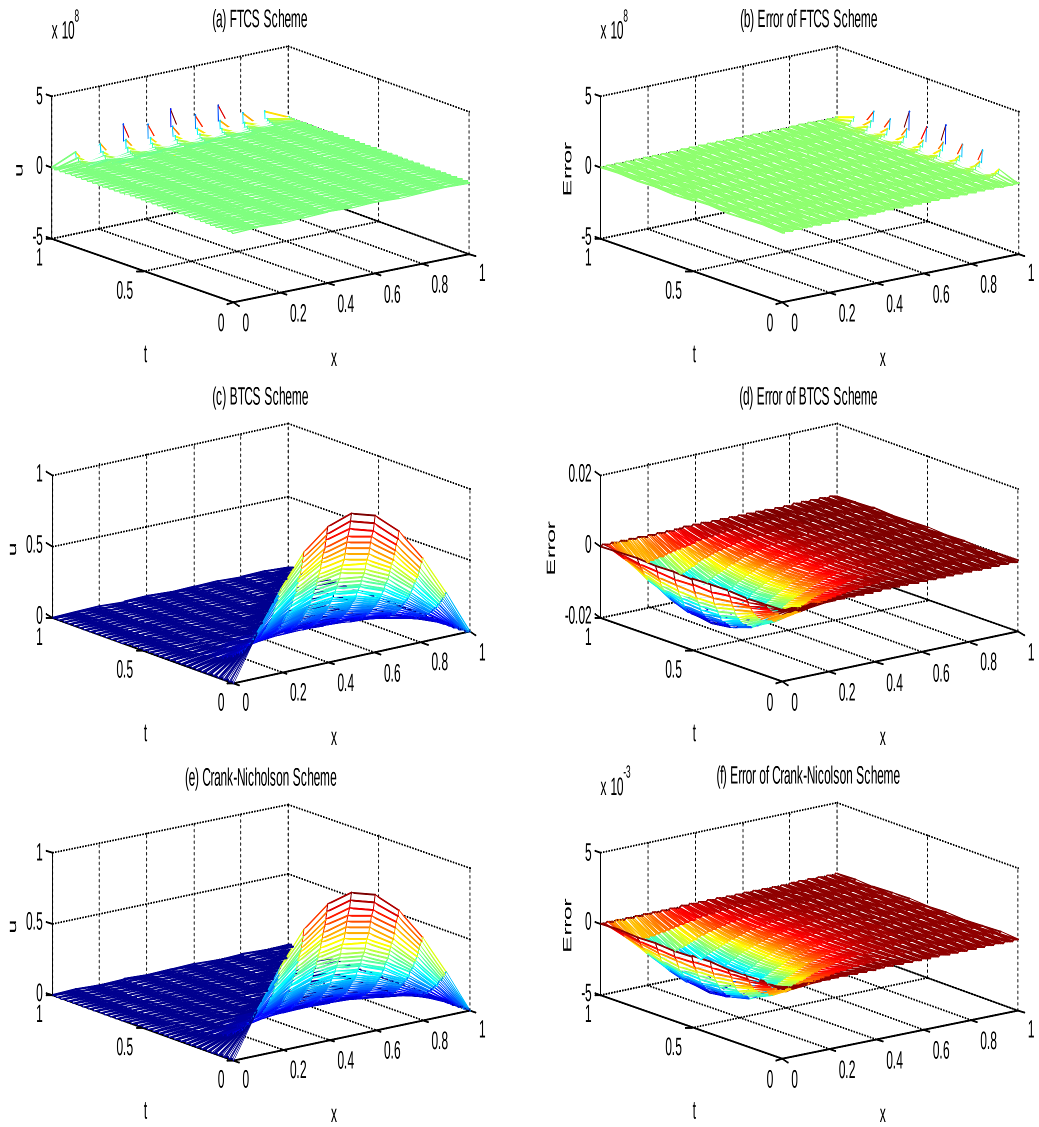

Figure 2: Numerical solutions and errors of (18) together with (19) and (20) obtained using the three different schemes when $r = 0.625$ and $\Delta x = 0.1$.

3.2 Problem 2

In this problem, consider (18) together with the following initial and boundary conditions

$$u(x, 0) = \cos(\pi x), \quad 0 \leq x \leq 1, \tag{22}$$

$$\frac{\partial u}{\partial x}(0, t) = \frac{\partial u}{\partial x}(1, t) = 0, \quad 0 < t \leq 1. \tag{23}$$

However, the analytical solution of (18) with the initial boundary value problem (22) and (23) can be easily found using the method of separation of variables as

$$u(x,t) = e^{-\pi^2 t}\cos(\pi x). \tag{24}$$

The numerical solutions and errors of (18) together with (22) and (23) are illustrated in the following plots:

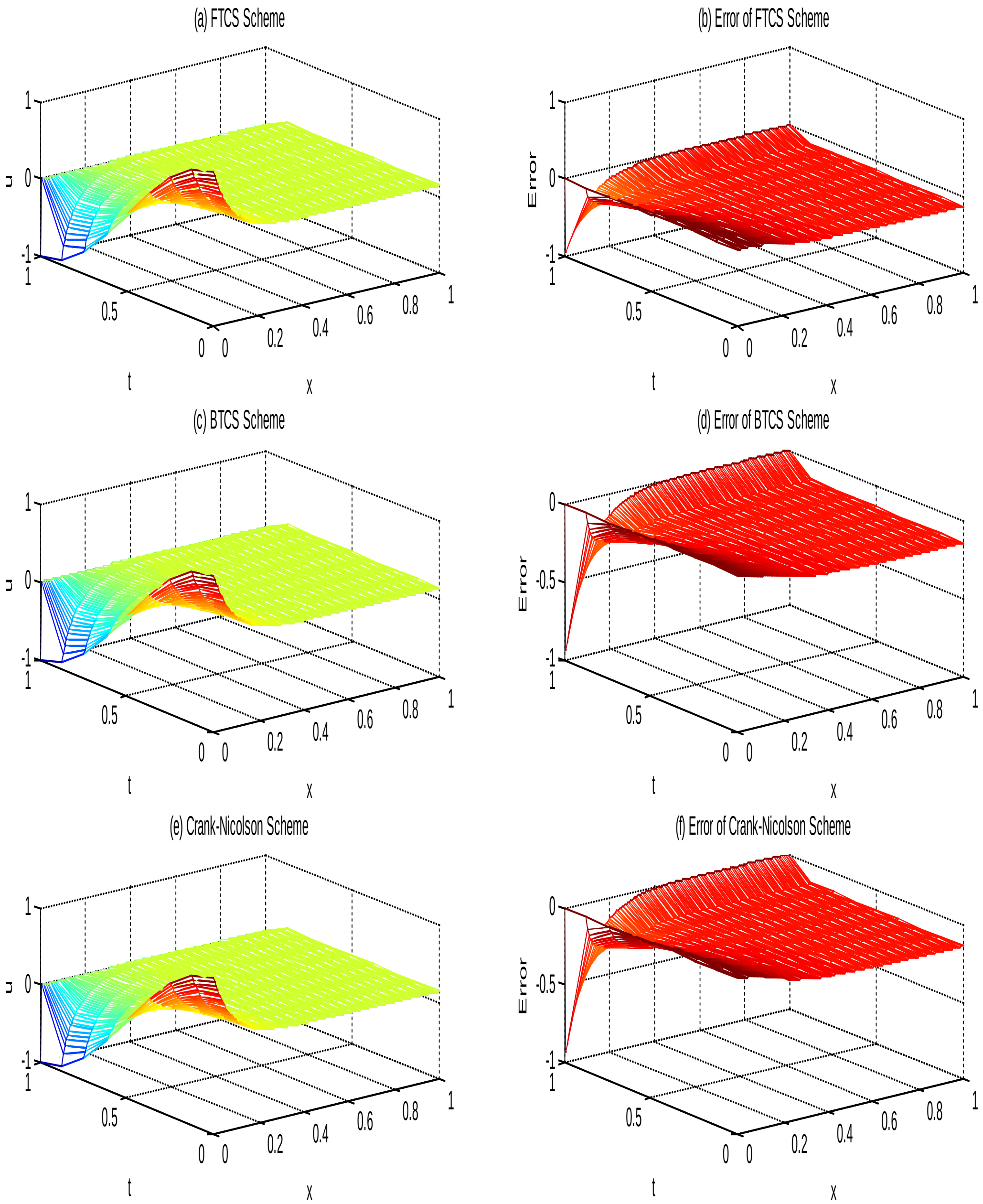

Figure 3: Numerical solutions and errors of (18) together with (22) and (23) obtained using the three different schemes when $r = 0.4$ and $\Delta x = 0.125$.

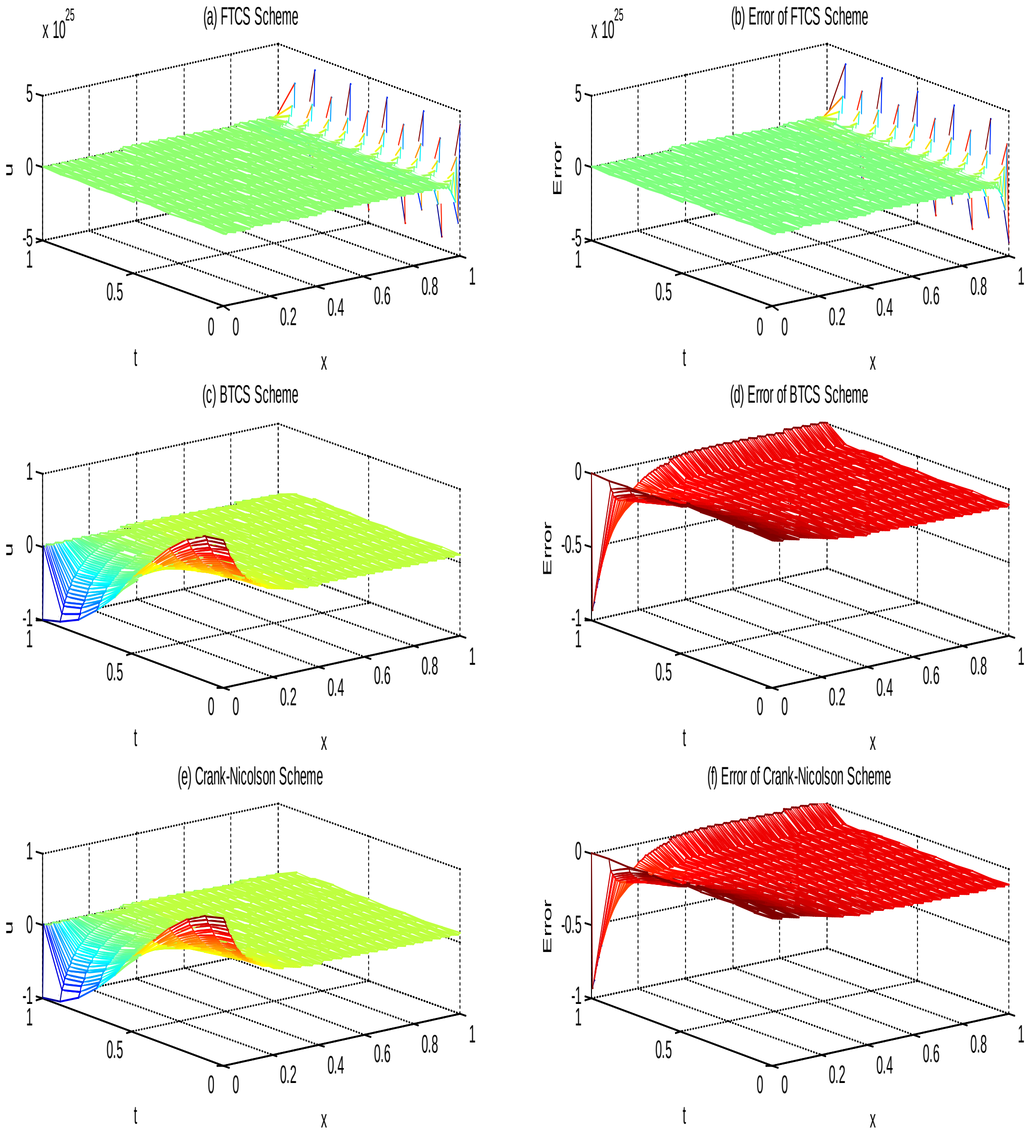

Figure 4: Numerical solutions and errors of (18) together with (22) and (23) obtained using the three different schemes when $r = 0.625$ and $\Delta x = 0.1$.

3.3 Problem 3

In this problem, consider (18) together with the following initial and boundary conditions

$$u(x,0) = \cos(x), \quad 0 < x < 1 \tag{25}$$

$$\frac{\partial u}{\partial x}(0,t) = u\left(\frac{\pi}{2},t\right) = 0, \quad t \geq 0. \tag{26}$$

However the analytical solution of (18) with the initial boundary value problem (25) and (26) can be easily found using the method of separation of variables as

$$u(x,t) = e^{-t}\cos(x). \tag{27}$$

The numerical solutions and errors of (18) together with (25) and (26) are illustrated in the following plots:

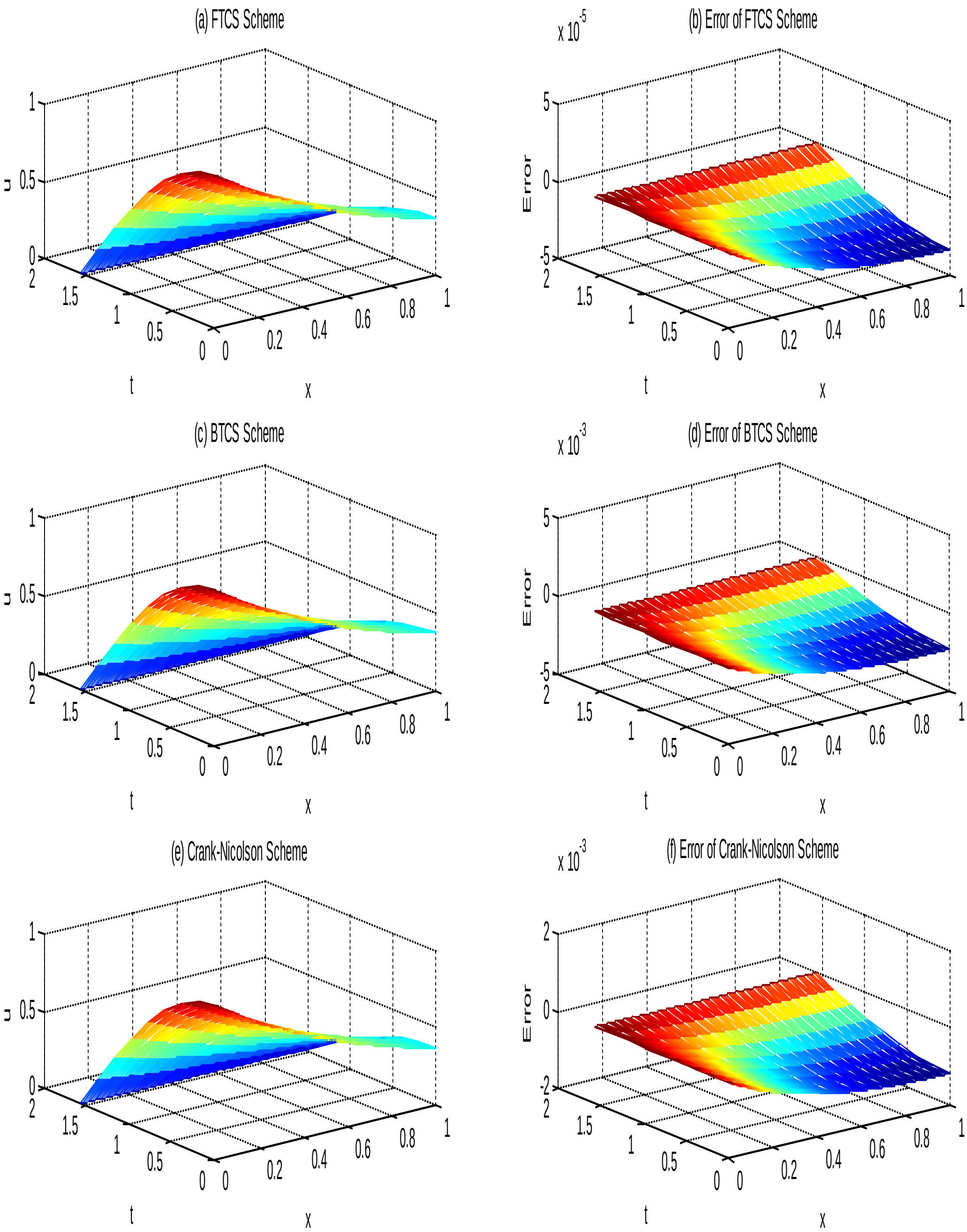

Figure 5: Numerical solutions and errors of (18) together with (25) and (26) obtained using the three different schemes when $r = 0.4$ and $\Delta x = 0.125$.

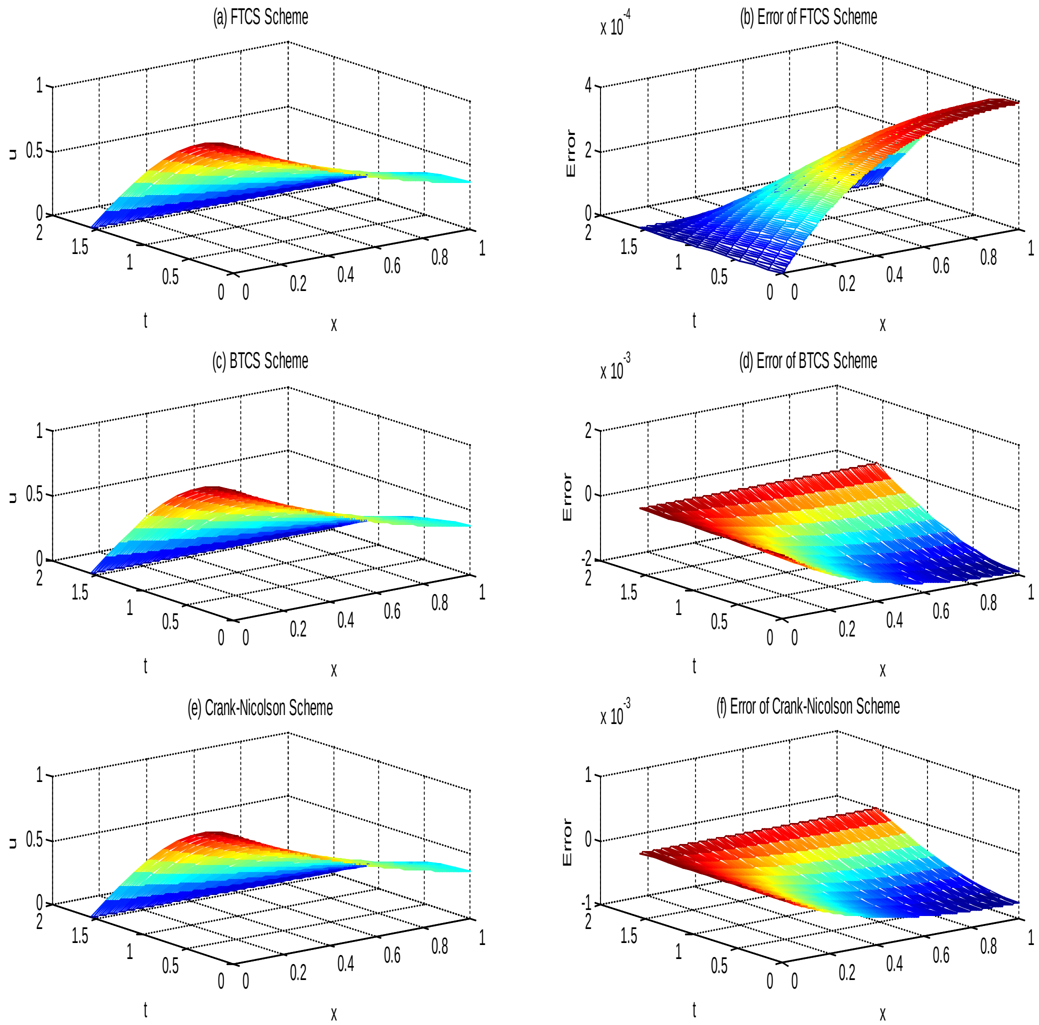

Figure 6: Numerical solutions and errors of (18) together with (25) and (26) obtained using the three different schemes when $r = 0.625$ and $\Delta x = 0.1$

Performance of the three finite difference schemes can be evaluated up on comparing some factors viz. (i) stability of numerical schemes and (ii) error. Stability criteria and numerical solutions show that the three schemes work well and each produces reasonable results in case of all test examples. The numerical results are obtained using Matlab programming and the outcomes are illustrated in Figures 1 – 6.

The selection of spatial interval $\Delta x = 0.125$ and the time step $\Delta t = 0.00625$, leads to $r = D\,[\Delta t/(\Delta x)^2] = 0.4 < 1/2$. The stability analysis FTCS scheme guarantees that if $r \leq 1/2$ then the condition is stable. This stability criterion is well supported by the solutions provided by all the three schemes in case of all problems. The same fact has observed in Figures 1, 3 and 5.

But if we decrease the spatial interval to $\Delta x = 0.1$ for better resolution and considering the same time step $\Delta t = 0.00625$, leads to $r = D\,[\Delta t/(\Delta x)^2] = 0.625 > 1/2$. The stability analysis of FTCS scheme predicts that if $r > 1/2$ then the condition is unstable. Hence, the FTCS scheme provides unstable solution and as a result the error blows up as shown in Figures 2a – 2b and 4a – 4b. However, the BTCS and Crank – Nicolson schemes work quite well and provide stable solutions as shown in Figures 2c – 2f and 4c – 4f.

With the same spatial interval $\Delta x = 0.1$ and time step $\Delta t = 0.00625$, all the three schemes including FTCS produce stable solutions. Despite of the fact that $r = 0.625$ doesn't strictly satisfy the stability condition $r \leq 1/2$ as shown in Figures 6a – 6f. This implies that the stability of the FTCS scheme is not a necessary condition, but only sufficient one. Besides, if it converges then the accuracy of FTCS may be better than that of BTCS scheme, but generally not better than that of the Crank – Nicolson scheme. The observations regarding stability of the solutions made from the figures are summarized in a tabular form as below:

Table 1: Stability of the solutions of one dimensional diffusion equation

Problems	**Finite Difference Schemes**	**Stability condition for $r \leq 0.5$**	**Stability condition for $r > 0.5$**
Problem 1	FTCS	Stable (Fig. 1a)	Unstable (Fig. 2a)
	BTCS	Stable (Fig. 1c)	Stable (Fig. 2c)
	CN	Stable (Fig. 1e)	Stable (Fig. 2e)
Problem 2	FTCS	Stable (Fig. 3a)	Unstable (Fig. 4a)
	BTCS	Stable (Fig. 3c)	Stable (Fig. 4c)
	CN	Stable (Fig. 3e)	Stable (Fig. 4e)
Problem 3	FTCS	Stable (Fig. 5a)	Stable (Fig. 6a)
	BTCS	Stable (Fig. 5c)	Stable (Fig. 6c)
	CN	Stable (Fig. 5e)	Stable (Fig. 6e)

4. Conclusions

In this study, we have discussed application of numerical schemes on one dimensional diffusion equation. It is observed from numerical computation that all the three schemes worked well according to the stability criteria and each scheme produced reasonable approximation for the density variable $u(x,t)$. The three schemes are compared based on the results of the three test problems. The comparison indicates that the approximate solution provided by Crank – Nicolson scheme is better than the other two schemes. Hence, Crank – Nicolson scheme is recommended for solving one – dimensional equation for a better approximation.

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