COLLEGE OF NATURAL AND COMPUTATIONAL SCIENCE
DEPARTMENT OF MATHEMATICS

ON SOME FINITE DIFFERENCE SCHEMES FOR THE SOLUTION OF SCHRÖDINGER EQUATION

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Abstract

The Schrödinger equation is a fundamental equation in quantum mechanics that describes the behavior of quantum systems. This thesis presents the comparison of four different finite difference schemes used for finding the solution of schrödinger equations. The schemes are: forward in time central in space(FTCS), backward in time central in space(BTCS), DuFort-Frankel, and Crank-Nicolson(CN) schemes. Knowing fully that the efficiency of a numerical schemes depends solely on their stability. Therefore, the schemes were compared based on their stability using Von Neumann method. The forward in time central in space scheme offers simplicity and computational efficiency, while backward in time central in space, Crank-Nicolson, and DuFort-Frankel scheme exhibits unconditional stability. To illustrate the performance of these schemes, we present numerical results and comparisons for representative Schrödinger equation problems. Overall, this study provides a comprehensive examination of finite difference schemes for numerical solution of the Schrödinger equation, considering the added perspective of Von Neumann stability analysis. Further, this study contributes to the understanding and comparison of finite difference schemes for solving the Schrödinger equation, providing valuable insights for researchers and practitioners in the field of quantum mechanics and computational physics.

Key words: Forward in time central in space, backward in time central in space, Crank-Nicolson, finite difference schemes.

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CHAPTER 1

INTRODUCTION

1.1 Background of the study

Partial differential equations arise in the study of many branches of applied mathematics, e.g., in fluid dynamics, heat transfer, boundary layer flow, elasticity, quantum mechanics, and electromagnetic theory. Only a few of these equations can be solved by analytical methods which are also complicated by requiring use of advanced mathematical techniques. The Schrödinger equation is a non linear partial differential equation that governs the wave function of a quantum –mechanical system Griffiths (2004). The time-independent Schrödinger equation is one of the basic equations in quantum mechanics.Plenty of methods have been developed for the solution of the one-dimensional time-independent Schrödinger equation. In the literature this problem has been treated by means of discretization of both variables Δx and Δt. It is a key result in quantum mechanics, and its discovery was a significant landmark in the development of the subject. The equation is named after Erwin Schrodinger, who postulated the equation in 1925, and published it in Schrödinger (1926), forming the basis for the work that resulted in his Nobel prize in physics in 1933 . The nonlinear Schrödinger (NLS) equation in its many versions is one of the most important models of mathematical physics with several applications to different fields such as nonlinear optic Agrawal (2001), models of protein dynamics Fordy (1990), plasma physics Stenflo & Yu (1997), self-focussing in laser pulses Sulem & Sulem (2007) and many other fields. The study of the particle-like behavior of non-linear fields, originally developed by Einstein to systematically derive the equations of motion for a particle in an external field, took a new turn with the discovery of solation solutions (Dodd et a1 1982). Soliton-type properties have since been found in a great variety of non-linear physical systems such as Korteveg-de Vries (Kdv), sine-Gordon, non-linear Schrodinger (NLS), etc. Conceptually, the Schrödinger equation is the quantum counterpart of Newton's second law in classical mechanics. Given a set of known initial conditions, Newton's second law makes a mathematical prediction as to what path a given physical system will take over time. The Schrödinger equation gives the evolution over time of a wave function, the quantum-mechanical characterization of an isolated physical system. The equation can be derived from the fact that the time-evolution operator must be unitary, and must therefore be generated by the exponential of a self-adjoint operator, which is the quantum Hamiltonian.

Introductory courses on physics or chemistry typically introduce the Schrödinger equation in a way that can be appreciated knowing only the concepts and notations of basic calculus, particularly derivatives with respect to space and time.
To find the corresponding exact solution of these types of PDEs is very difficult due to the nonlinear term, therefore uses of numerical techniques always remain an alternative for the solution. In this thesis, we take the well-known nonlinear one-dimensional time dependent Schrodinger equation (NLSE) Doha & Van Gorder (2014); Taleei & Dehghan (2014).

Solving the time dependent Schrödinger equation with arbitrary potential function is of fundamental importance in quantum dynamics calculations Hajj (1985); Ixaru (1997) and has received considerable attention because of its usefulness as a model that describes several important physical and chemical phenomena of recent interest.

1.2 Statement of the problem

The partial differential equations have an important applications in many physical situations, engineering and applied science. Schrödinger equations are one of the most common type of partial differential equations used to model many real life problems. However, due to the importance of Schrödinger equations in various application fields, the numerical approximation of such equations has been growing more and more; because it is more difficult or sometimes impossible to solve analytically. In general, the imaginary term involved in Schrödinger equations make it more difficult. For this reason, searching suitable numerical method for solving Schrödinger equations is still under development. The wide applications of Schrödinger equations in many real life phenomena and the ongoing research in this area motivate us to consider some finite difference schemes for solving Schrödinger equations. In this thesis, we consider Crank-Nicolson scheme, FTCS scheme, BTCS scheme and DuFort-Frankel scheme to solve Schrödinger equation and compare their results.

1.3 Research Question

The study would guided by the following research questions:

1. How can we solve Schrödinger equation by using Crank Nicolson, FTCS, BTCS, and DuFort-Frankel schemes and compare their results?
2. How to compare numerical solution of some finite differences schemes with each other and with exact solution?
3. How can we demonstrate the efficiency of the formulated numerical schemes by solving some test problems?

1.4 Objective of the Study

The general objective of this study is to find numerical solution of Schrödinger equation using some finite difference schemes.

1.4.1 Specific objectives of the study

The study also explored the following specific objectives

1. To solve Schrödinger equation by using Crank Nicolson, FTCS, BTCS, and DuFort-Frankel schemes and compare their results.
2. To compare numerical solution of some finite difference schemes with each other and with exact solution.
3. To demonstrate the efficiency of the formulated numerical schemes by solving some test problems.

1.5 Significance of the Study

1. Optical soliton solutions for the Schrödinger equation are conveyed by using the well known finite difference methods.
2. It will help by providing basic research skill to researcher.
3. It will help other researchers in this particular field of study in the future as a reference.

1.6 Delimitation of the Study

Linear partial differential equations has a wide branches in science and technology. Solving partial differential equation is also very wide. However, this study is limited on the solution of linear partial differential equation namely the numerical solution of Schrödinger equation.

1.7 Organization of the study

This study is organized into six chapters. Chapter 1 is the introduction, which outlines the background of the study. Chapter 2 is a review of the related literature. Chapter 3 outlines the design of the study and the methodology that is used in carrying out the study. Chapter 4 is introduction about some finite difference schemes and formulates the forward in time central in space(FTCS), backward in time central in space(BTCS), DuFort-Frankel and Crank-Nicolson(CN) schemes with Von-Neumann for stablity of each scheme for solving Schrödinger equations. Chapter 5 is the result and discussion of the findings based on the study objectives, and chapter 6 is conclusion and suggestions for further research. At the end, references and all necessary appendices documents are attached.

CHAPTER 2

LITERATURE REVIEW

Schrödinger equation is a fundamental equation in quantum mechanics. It also arise in underwater acoustics, where the Helmholtz equation for the acoustics pressure is transformed into an equation of the same form by applying the so called “parabolic approximation" Tappert (2005). Boyd & Ablowitz (2010), presents a fourth-order accurate finite difference schemes specifically designed for solving the time-dependent schrödinger equation. They propose a uniform grid and utilize high-order accurate central difference approximations for the spatial derivatives. Through numerical experiments and comparisons with other methods, they demonstrate the accuracy and efficiency of their scheme. They addresses higher-order schemes offer the advantage of achieving greater accuracy with reduced computational cost of utilizing fewer grid points. And also they discuss the treatment of boundary conditions and the solution of the resulting linear system, providing insights into the implementation aspects of the proposed scheme.Further their work is needed to explore alternative numerical approaches, such as adaptive mesh refinement and spectral methods, which my offer additional benefits in terms of accuracy and efficiency.

Solving Schrödinger’s equation is the primary task of chemists in the field of quantum chemistry. However, exact solutions for Schrödinger’s equation are available only for a small number of simple systems. Finite element method is a powerful and established method used to approximate the solution of the partial differential equation. A finite element method with B-splines defines a new weighting approximate method and possesses computational advantages of B-splines and finite elements. Spline functions have been applied to develop numerical methods for the solution of nonlinear differential equations Krowiak (2006); Saka & Dağ (2007). The analytical solution of the NLS equation is solved by using the inverse scattering method by Shabat & Zakharov (1972). Zakharov & Manakov (1974) proved that the NLS equation is completely integrable. Several schemes was used by Taha (1991) to study the analytical and numerical solutions of the linear and nonlinear one dimensional Schrödinger equations that includes finite element approaches and various implicit and explicit finite difference schemes. Bialecki & Fairweather (2001) Many researchers have worked on the solution of the partial differential equations by using collocation finite element method based on splines.

Spline-based numerical methods have been proposed by many researchers to obtain the numerical solution of nonlinear evolutionary problems. Mittal & Arora (2010) obtained the numerical solutions of the extended Fisher–Kolmogorov equation using the quintic B-spline collocation method. Saka & Dağ (2008) presented the Galerkin finite element method based on quartic B-spline functions to obtain the numerical solution of the regularized long-wave (RLW) equation. Akson & Sariahmet (2022), apply the finite difference scheme to a Schrödinger which contains a momentum operator. A priori estimate for the solution of difference scheme is obtained and proved that the difference scheme is unconditionally stable. Microscopic dynamics for non-relativistic quantum systems are described by the Schrödinger equation Feynman & Styer (2010). To apply the Schrödinger equation for a specified problem, one needs to solve a differential equation with a boundary condition and to determine eigenvalues and eigenfunctions of that problem. Dehghan & Taleei (2010) the solution for the non-linear Schrödinger equation can be expressed first, the bright soliton solutions, in which the solutions and its spatial derivatives vanish at$|x| = \infty$, Second L-periodic solutions defined by

$$\varphi\left(x+L,T\right)=\varphi\left(x,t\right),-\infty<x<\infty,\ t>0 \tag{2.1}$$

A hypothesis about the soliton solution interval must be made. For it is impossible to compute the solution on the whole real line. Iqbal A & Md. Ismail (2019) Proposed quantic B-Spline Galerkin finite element method to find the numerical solution of nonlinear Schrodinger (NLS) equation:

$$iu_{t=}-u_{xx-}\alpha|u|^{2}u \tag{2.2}$$

$$iu_{t=}-u_{xx-}\alpha|u|^{2}u=0,x\in\left[a,b\right],i=\sqrt{-1},u\left(x,0\right)=f(x) \tag{2.3}$$

$$u\left(a,t\right)=u\left(b,t\right)=u_{x}(a,t)=u_{x}(b,t)=u_{xx}(a,t)=u_{xx}(b,t) \tag{2.4}$$

Let

$$u\left(x,t\right)=r\left(x,t\right)+is\left(x,t\right) \tag{2.5}$$

where, $r\left(x,t\right)$ and $s(x,t)$ are real functions. where, $\alpha > 0$, and allows for bright soliton solutions. Substituting Equation 2.5 into Equation 2.2, we obtain the coupled partial differential equations

$$s_t - r_{xx} = \alpha\left(r^2 + s^2\right)r \tag{2.6}$$

$$r_t + s_{xx} = -\alpha\left(r^2 + s^2\right)s \tag{2.7}$$

My objective is to solve the following Schrödinger equation by using some finite difference scheme. Mathematically, the non-linear Schrodinger equation is given by:

$$i\hbar\frac{\partial u(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 u\left(x,t\right) + V\left(x,t\right)u(x,t) \tag{2.8}$$

Where $i = \sqrt{-1}$ represents the imaginary part, $\hbar$ is Planck's constant having unit in joule second, m is the mass of the particle, $u(x,t)$ is the wave function define over space and time , ∇^2 is the Laplacian Operator, and $V(x,t)$ is the potential energy influencing the particle.

CHAPTER 3

RESEARCH METHODOLOGY

3.1 Study area and period

Our study area is held at Wolkite University, under the department of mathematics in 2023.

3.2 Study design

The study design is a numerical and documentary review-design. This study will design to solve Schrödinger equation by some finite difference schemes.

3.3 Source of Information

The relevant sources of information for this study are published articles, journals and related studies from internet. Relevant Journals and books Consulted to gather information about schrödinger equation.

3.4 Mathematical procedures

This section outlined the method that would be used to succeed the general and specific objectives of the study, and materials used in the study. The experimental result is obtained by writting MATLAB code for the developed numerical method. Hence, in order to achieve the stated objectives, the study followed the following procedures,

1. Describing the problem,
2. Apply finite difference scheme to schrödinger equation,
3. Some test problem are solved and the obtained result from finite difference

schemes is compared to each other and with the exact solution in order to verify the efficiency of the present methods.

4. At the end, the obtained numerical results presented in forms of graphs for the developed numerical schemes.

CHAPTER 4

DESCRIPTION OF THE METHOD

4.1 Introduction

There are many numerical techniques available for solving Schrödinger equation. There are various types of finite difference schemes that can be employed for solving the Schrödinger equation, including explicit, implicit, and semi-implicit methods. These schemes differ in their treatment of the time-dependent and spatial derivatives and can have different levels of accuracy, stability, and computational efficiency. For time-dependent problems, finite difference schemes approximate the time derivative using either explicit or implicit methods.

Explicit schemes, such as the forward Euler method or the Runge-Kutta methods, compute the future values of the wave function based on the current values and the time derivative. Implicit schemes, such as backward Euler or Crank-Nicolson, involve solving a system of equations to obtain the future values and provide better stability properties. The Von Neumann approach to the stability is based on the discrete Fourier series of a numerical scheme. The criterion takes its name from the scientist who first developed and used it. Since it applies easily, it is the most widely used tool for the stability analysis of finite-difference methods D'acuntoi (n.d.).

Numerical method is a method of obtaining an approximate solution to a partial differential equations whose solution cannot be obtain analytically.There are different types of numerical methods but for the purpose of this work, we shall consider the explicit (FTCS), the implicit (BTCS), Crank-Nicolson and DuFort-Frankel schemes.The efficiency of the numerical schemes depends solely on their Stability. Lot of researchers have worked on finite difference methods for Schrodinger equations among them Khan (2022), Solved by finite difference method called Crank–Nicolson Method. Arora &

Mittal (2019) numerical simulation of nonlinear schrödinger equation of one and two dimensions by hybrid scheme using trigonometric cubic B-spline basis with differential quadrature. The numerical treatment is an alternative approach to get the required solution. The non-dimensionalized form of Equation 2.8 can be written as

$$i\frac{\partial u}{\partial t} + \eta\frac{\partial^2 u}{\partial x^2} + \alpha|u|^2 u + \beta f(x,t) = 0 \tag{4.1}$$

Under initial conditions

$$u(x,0) = \phi(x), \ \forall x \in [a,b] \tag{4.2}$$

and the boundary conditions

$$u(a,t) = g_0(t), \quad u(b,t) = g_1(t), \ \forall t \in [0,T] \tag{4.3}$$

where the solution domain $D := (a \times b) \times (0,T]$, and the parameter $i = \sqrt{-1}, \eta, \alpha$ are constant numbers. The complex-valued function $u(x,t)$ depends on x as well as on t and $\phi(x)$ is prescribed smooth function which represents the initial state. The constant coefficients $\eta \neq 0$, α and β may be positive or negative.

Further, if $\alpha = 0$, then Equation 2.8 becomes:

$$i\frac{\partial u}{\partial t} + \eta\frac{\partial^2 u}{\partial x^2} + \beta f(x,t) = 0 \tag{4.4}$$

Also, if $\eta = -1$, then Equation 4.4 becomes

$$i\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} + \beta f(x,t) = 0 \tag{4.5}$$

If $\beta = 0$, then Equation 4.5 becomes

$$i\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0 \tag{4.6}$$

Since the main objective of this thesis is to solve the Schrödinger equation by using Crank-Nicolson, explicit (FTCS), implicit(BTCS) and Dufort-Frankel schemes.

We begin our discussion of finite difference schemes by defining a grid of points (x,t) in the plane. Let h and k be positive numbers; then the grid will be the points $(x_j, t_n) = (jh, nk)$ for arbitrary integers j and n. For the function u defined on the grid we write u_j^n for the value of u at the grid point (x_j, t_n) when u is defined for continuously varying (x,t). The set of points (x_j, t_n) for a fixed value of n is called grid level n. We are interested in grids with small values of h and k as $h = \Delta x, k = \Delta t$.

For derivative of the scheme, we have used the following derivative:

$$\frac{\partial u_j^n}{\partial t} = \frac{u_j^{n+1} - u_j^n}{\Delta t} + O(\Delta t) \tag{4.7}$$

$$\frac{\partial u_j^n}{\partial t} = \frac{u_j^n - u_j^{n-1}}{\Delta t} + O(\Delta t) \tag{4.8}$$

$$\frac{\partial u_j^n}{\partial t} = \frac{u_j^{n+1} - u_j^{n-1}}{2\Delta t} + O(\Delta t^2) \tag{4.9}$$

$$\frac{\partial^2 u_j^n}{\partial x^2} = \frac{u_{j-1}^n - 2u_j^n + u_{j+1}^n}{(\Delta x)^2} + O(\Delta x)^2 \tag{4.10}$$

By taking the average of $\frac{\partial^2 u}{\partial x^2}$ at n^{th} time level and $(n+1)^{st}$ time level, that is

$$\frac{\partial^2 u_j^n}{\partial x^2} = \frac{u_{j-1}^n - 2u_j^n + u_{j+1}^n}{(\Delta x)^2} + O(\Delta x)^2 \tag{4.11}$$

$$\frac{\partial^2 u_j^{n+1}}{\partial x^2} = \frac{u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}}{(\Delta x)^2} + O(\Delta x)^2 \tag{4.12}$$

The average of these two different schemes Equation 4.11 and Equation 4.12 is

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{j-1}^n - 2u_j^n + u_{j+1}^n + u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}}{2(\Delta x)^2} \tag{4.13}$$

$$\frac{\partial u_j^{n+\frac{1}{2}}}{\partial t} = \frac{u_j^{n+1} - u_j^n}{\Delta t} \tag{4.14}$$

4.2 Crank-Nicolson Scheme

The Crank-Nicolson scheme is obtained by substituting Equation 4.13 and Equation 4.14 into Equation 4.6

$$i\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{u_{j-1}^n - 2u_j^n + u_{j+1}^n + u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}}{2(\Delta x)^2} \tag{4.15}$$

Rearranging Equation 4.15 such that at $(j+1)^{st}$ level in one side, we have

$$-ru_{j-1}^{n+1} + (i+2r)u_j^{n+1} - ru_{j+1}^{n+1} = ru_{j-1}^n + (i-2r)u_j^n + ru_{j+1}^n \tag{4.16}$$

where $r = \frac{\Delta t}{2(\Delta x)^2}$ and, $i = \sqrt{-1}$.
Equation 4.16 is called Crank-Nicolson Method. The local truncation error of the

implicit scheme has its principal part as

$$\left(\frac{1}{24}k^2\frac{\partial^3 u_j^{n+\frac{1}{2}}}{\partial t^3} - \frac{1}{12}h^2\frac{\partial^4 u}{\partial x^4}\right)_{j,n}$$

Therefore, its truncation error is $O(k^2) + O(h^2)$.

4.2.1 Stability Condition Using Von Neumann Method

Von Neumann stability method is the most widely used procedure for determining the stability of finite difference approximation (Lapidus Leon). The Schrödinger equation $iu_t = u_{xx}$ is a linear PDE equation and its stability can be analyzed using the Von Neumann stability analysis. To apply the Von Neumann stability analysis, we considered the discretized form of the equation using the implicit finite difference scheme:

$$-ru_{j-1}^{n+1} + (i+2r)u_j^{n+1} - ru_{j+1}^{n+1} = ru_{j-1}^{n} + (i-2r)u_j^{n} + ru_{j+1}^{n} \tag{4.17}$$

where u_j^n represents the numerical approximation of u at spatial point j and time step n, and $r = \dfrac{\Delta t}{2(\Delta x)^2}$ is the numerical parameter. Equation 4.17 in error form is written as

$$-re_{j-1}^{n+1} + (1+2r)e_j^{n+1} - re_{j+1}^{n+1} = re_{j-1}^{n} + (1-2r)e_j^{n} + re_{j+1}^{n} \tag{4.18}$$

Let's assume a solution of the form:

$$u_j^n = e^{i(kj\Delta x - \omega n\Delta t)} \tag{4.19}$$

Substituting Equation 4.19 into the finite difference scheme, we get

$$\begin{aligned} &-re^{i(k(j-1)\Delta x - \omega(n+1)\Delta t)} + (1+2r)e^{i(kj\Delta x - \omega(n+1)\Delta t)} - re^{i(k(j-1)\Delta x - \omega(n+1)\Delta t)} \\ &\qquad = re^{i(k(j-1)\Delta x - \omega n\Delta t)} + (1-2r)e^{i(kj\Delta x - \omega n\Delta t)} + re^{i(k(j+1)\Delta x - \omega n\Delta t)} \end{aligned} \tag{4.20}$$

Dividing both sides of Equation 4.20 by $e^{i(kj\Delta x - \omega n\Delta t)}$ and further simplification :

$$-re^{-ik\Delta x - i\omega\Delta t} + (1+2r)^{-i\omega\Delta t} - re^{ik\Delta x - i\omega\Delta t} = re^{-ik\Delta x} + (1-2r) + re^{ik\Delta x} \tag{4.21}$$

By using Euler method
$e^{-ik\Delta x} = \cos(k\Delta x) - i\sin(k\Delta x)$ and $e^{ik\Delta x} = \cos(k\Delta x) + i\sin(k\Delta x)$

$$-re^{-i\omega\Delta t}(2\cos(k\Delta x)) + (1+2r)e^{-i\omega\Delta t} = 2r\cos(k\Delta x) + (1-2r) \tag{4.22}$$

By taking a common term $e^{-i\omega\Delta t}$ we will arrive at:

$$e^{-i\omega\Delta t}(-2r\cos(k\Delta x)+1+2r) = 2r\cos(k\Delta x)+1-2r \tag{4.23}$$

Let $\xi = e^{-i\omega\Delta t}$

$$\xi(-2r\cos(k\Delta x)+1+2r) = 2r\cos(k\Delta x)+1-2r \tag{4.24}$$

Dividing both sides of Equation 4.24 by $-2r\cos(k\Delta x)+1+2r$ we will get:

$$\xi = \frac{2r\cos(k\Delta x)+2r-1}{-2r\cos(k\Delta x)+2r+1} \tag{4.25}$$

$$\xi = \frac{2r(\cos(k\Delta x)-1)+1}{-2r(\cos(k\Delta x)-1)+1} \leq 1 \tag{4.26}$$

$$|\xi| = \left|\frac{1-2r(1-\cos(k\Delta x))}{1+2r(1-\cos(k\Delta x))}\right| \leq 1. \tag{4.27}$$

The crank-Nicolson scheme is unconditionally stable.

4.3 Forward in time central in space scheme (FTCS)

The explicit scheme is derived from Equation 4.6 by replacing the first order derivative by Equation 4.7 and Equation 4.10 . The derivation is shown below:

$$i\frac{u_j^{n+1}-u_j^n}{\Delta t} = \frac{u_{j-1}^n-2u_j^n+u_{j+1}^n}{(\Delta x)^2} \tag{4.28}$$

$$iu_j^{n+1} = iu_j^n + \frac{\Delta t}{(\Delta x)^2}(u_{j-1}^n-2u_j^n+u_{j+1}^n) \tag{4.29}$$

Let $r = \dfrac{\Delta t}{(\Delta x)^2}$. Then, Equation 4.29 becomes

$$iu_j^{n+1} = ru_{j-1}^n + (i-2r)u_j^n + ru_{j+1}^n \tag{4.30}$$

The local truncation error of the explicit scheme has its principal part as

$$\left(\frac{1}{2}k\frac{\partial^2 u}{\partial t^2} - \frac{1}{12}h^2\frac{\partial^4 u}{\partial x^4}\right)_{j,n}.$$

Therefore, its truncation error is $O(k)+O(h^2)$.

4.3.1 Stability Condition Using Von Neumann Method

Von Newman stability method is the most widely used procedure for determining the stability of finite difference approximation (Lapidus Leon). The Schrödinger equation $iu_t = u_{xx}$ is a linear PDE equation and its stability can be analyzed using the Von Neumann stability analysis. To apply the Von Neumann stability analysis, we consider the discretized form of the equation using the explicit finite difference scheme:

$$iu_j^{n+1} = ru_{j-1}^n + (i - 2r)u_j^n + ru_{j+1}^n \tag{4.31}$$

where u_j^n represents the numerical approximation of u at spatial point j and time step n, and $r = \dfrac{\Delta t}{(\Delta x)^2}$ is the numerical parameter. Equation 4.31 in error form is written as

$$e_j^{n+1} = re_{j-1}^n + (1 - 2r)e_j^n + re_{j+1}^n \tag{4.32}$$

Let's assume a solution of the form:

$$u_j^n = e^{i(kj\Delta x - \omega n\Delta t)} \tag{4.33}$$

Substituting this equation into the finite difference scheme, we get

$$e^{i(kj\Delta x - \omega(n+1)\Delta t)} = e^{i(k(j-1)\Delta x - \omega n\Delta t)} + r(1 - 2r)e^{i(kj\Delta x - \omega n\Delta t} + re^{i(k(j+1)\Delta x) - \omega n\Delta t)} \tag{4.34}$$

Let $\xi = e^{-i\omega\Delta t}$, dividing through by $e^{i(kj\Delta x - \omega n\Delta t)}$ we obtain :

$$\xi = re^{-ik\Delta x} + (1 - 2r) + re^{ik\Delta x} \tag{4.35}$$

simplifying further:

$$\xi = 2r(\cos(k\Delta x)) + 1 - 2r \tag{4.36}$$

$$\xi = 1 + 2r(\cos(k\Delta x) - 1) \tag{4.37}$$

To ensure stability, we require the magnitude of the amplification factor $|\xi|$ to be less than or equal to 1. Therefore, we have:

$$|\xi| = |1 + 2r(\cos(k\Delta x) - 1)| \leq 1 \tag{4.38}$$

This inequality provides a stability condition for the explicit finite difference scheme applied to the schrödinger equation. By analyzing this condition, we can determine the allowable range of r (Δt and Δx) to maintain stability in the numerical scheme. In practice, the stability condition for the explicit finite difference method applied to the Schrödinger equation requires that the time step Δt and spatial step Δx be chosen such that r is within certain limits to prevent instability, such as unbounded growth or oscillations, in the numerical solution. The specific values for Δt and Δx depend on the problem setup and the desired level of accuracy. Thus, the forward in time central in space is conditionally stable.

4.4 Backward in time central in space scheme (BTCS)

The backward in time central in space scheme is derived from Equation 4.6 by replacing the first order derivative by backward difference in time and central difference in space respectively. The derivation is shown below:

$$i\frac{u_j^n - u_j^{n-1}}{\Delta t} = \frac{u_{j-1}^n - 2u_j^n + u_{j+1}^n}{(\Delta x)^2} \tag{4.39}$$

Replacing n by $n+1$, Equation 4.39 becomes

$$i\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{u_{j+1}^{n+1} - u_j^{n+1} + u_{j-2}^{n+1}}{(\Delta x)^2} \tag{4.40}$$

where, $r = \dfrac{\Delta t}{(\Delta x)^2}$, we have

$$-iu_j^n = ru_{j-1}^{n+1} - (i+2r)u_j^{n+1} + ru_{j+1}^{n+1} \tag{4.41}$$

Equation 4.41 is implicit approximation. The equation leads a tridiagonal system. The local truncation error of the forward in time central in space scheme has it principal part as

$$\left(\frac{1}{2}k\frac{\partial^2 u}{\partial t^2} - \frac{1}{12}h^2\frac{\partial^4 u}{\partial x^4}\right)_{j,n}$$

Therefore, its truncation error is $O(k) + O(h^2)$.

4.4.1 Stability Condition Using Von Neumann Method

To apply Von Neumann stability analysis for the finite difference of the form backward in time central in space, we considered the discretized form of the equation:

$$-u_j^n = ru_{j-1}^{n+1} - (1+2r)u_j^{n+1} + ru_{j+1}^{n+1} \tag{4.42}$$

Let's assume a solution of the form

$$u_j^n = e^{i(kj\Delta x - \omega n\Delta t)} \tag{4.43}$$

Substituting this solution into the finite difference scheme, we get:

$$\begin{aligned}-e^{i(kj\Delta x-\omega n\Delta t)} = re^{ik(j-1)\Delta x-\omega(n+1)\Delta t} - (1+2r)e^{i(kj\Delta x)-i\omega(n+1)\Delta t} \\ +re^{i(kj+1)\Delta x-\omega(n+1)\Delta t}\end{aligned} \tag{4.44}$$

Dividing through Equation 4.44 by $e^{i(kj\Delta x-\omega n\Delta t)}$, we obtain:

$$-1 = re^{-ik\Delta x-i\omega\Delta t} - (1+2r)e^{-i\omega\Delta t} + re^{ik\Delta x-i\omega\Delta t} \tag{4.45}$$

Let $\xi = e^{-i\omega\Delta t}$ and simplifying further:

$$-1 = \xi(2r\cos(k\Delta x) - (1+2r)) \tag{4.46}$$

$$\xi = \frac{-1}{2r(\cos(k\Delta x)) - 2r - 1} \leq 1. \tag{4.47}$$

Therefore,

$$|\xi| = \left|\frac{1}{1-2r(\cos(k\Delta x)-1)}\right| \leq 1. \tag{4.48}$$

For all $r > 0$, and k it is observed that $0 < \xi \leq 1$. Showing that the scheme is unconditionally stable.

4.5 Dufort-Frankel Scheme

The derivation of the Dufort-Frankel approximation is simply by replacing the first and second order derivatives in Equation 4.6 by central difference in time and space, resulting to the following:

$$i\frac{u_j^{n+1} - u_j^{n-1}}{2\Delta t} = \frac{u_{j-1}^n - 2u_j^n + u_{j+1}^n}{(\Delta x)^2} \tag{4.49}$$

Also u_j^n on the R.H.S is replaced with time average of previous and current time values that is $(n-1)$ and $(n+1)$ to get :

$$i\frac{u_j^{n+1} - u_j^{n-1}}{2\Delta t} = \frac{1}{(\Delta x)^2}[u_{j-1}^n - 2(\frac{u_j^{n-1} + u_j^{n+1}}{2}) + u_{j+1}^n] \tag{4.50}$$

Which can be written as

$$iu_j^{n+1} - iu_j^{n-1} = \frac{2\Delta t}{(\Delta x)^2}(u_{j-1}^n - u_j^{n-1} - u_j^{n+1} + u_{j+1}^n) \tag{4.51}$$

Which further gives

$$iu_j^{n+1} + 2ru_j^{n+1} = iu_j^{n-1} - 2ru_j^{n-1} + 2ru_{j-1}^n + 2ru_{j+1}^n \tag{4.52}$$

where, $r = \frac{\Delta t}{(\Delta x)^2}$ Equation 4.52 can be written as

$$(i + 2r)u_j^{n+1} = (i - 2r)u_j^{n-1} + 2r(u_{j-1}^n + u_{j+1}^n) \tag{4.53}$$

Equation 4.53 is called the Dufort-Frankel finite difference approximation. It can also be rewritten more explicitly as:

$$u_j^{n+1} = \frac{i - 2r}{i + 2r}u_j^{n-1} + \frac{2r}{i + 2r}(u_{j-1}^n + u_{j+1}^n) \tag{4.54}$$

The local truncation error of the Dufort-Frankel scheme has its principal part as

$$\left(\frac{-h^2}{24}\frac{\partial^4 u}{\partial x^4} + \frac{k^2}{6}\frac{\partial^3 u}{\partial t^3} + \frac{h^2}{k^2}\frac{\partial^2 u}{\partial x^2}\right)_{j,n}$$

with its local truncation error as $O\left(h^2 + k^2 + \frac{h^2}{k^2}\right)$

4.5.1 Stability Condition Using Von Neumann Method

The stability of the Dufort-Frankel scheme can be analyzed using the Von Neumann stability analysis. The scheme can be written as:

$$(1 + 2r)u_j^{n+1} = (1 - 2r)u_j^n + 2r(u_{j-1}^n + u_{j+1}^n) \tag{4.55}$$

To perform the Von Neumann stability analysis, we assume a solution of the form :

$$u_j^n = e^{i(kj\Delta x - \omega n\Delta t)} \tag{4.56}$$

Substituting this solution into the finite difference scheme, we get:

$$(1+2r)e^{i(kj\Delta x - \omega(n+1)\Delta t)} = (1-2r)e^{i(kj\Delta x - \omega n\Delta t)} + 2r(e^{i((k(j-1)\Delta x - \omega n\Delta t)} + e^{i(k(j+1)\Delta x - \omega n\Delta t)}) \tag{4.57}$$

Dividing Equation 4.57 through by $e^{i(kj\Delta x-\omega n\Delta t)}$, we obtain:
$(1+2r)e^{-i\omega\Delta t)} = (1-2r)e^{i\omega\Delta t} + 2r(e^{-ik\Delta x} + e^{ik\Delta x})$
Let $\xi = e^{-i\omega\Delta t}$

$$(1+2r)\xi = (1-2r)\xi^{-1} + 2r(e^{-ik\Delta x} + e^{ik\Delta x}) \tag{4.58}$$

Simplifying, Equation 4.57 we get

$$(1+2r)\xi = (1-2r)\xi^{-1} + 2r(2\cos(k\Delta x)) \tag{4.59}$$

solving further

$$\xi^2(1+2r) = (1-2r) + 2r\xi(2\cos(k\Delta x)) \tag{4.60}$$

By using quadratic factor for amplification factor:

$$(1+2r)\xi^2 - 4r\cos(k\Delta x)\xi + 2r - 1 = 0 \tag{4.61}$$

Whose roots are

$$\xi = \frac{2r\cos(k\Delta x) \pm \sqrt{1-4r^2\sin^2(k\Delta x)}}{1+2r} \tag{4.62}$$

We discuss now two different cases with respect to the discriminant:

1. If $1-4r^2\sin^2(k\Delta x) \leq 0$, then Equation 4.62 yields,

$$\xi = \frac{2r\cos(k\Delta x) \pm \sqrt{4r^2\sin^2(k\Delta x) - 1}}{1+2r} \tag{4.63}$$

   Hence,

$$|\xi|^2 = \frac{4r^2-1}{4r^2+4r+1} < 1 \tag{4.64}$$

2. If $1-4r\sin^2(k\Delta x) \geq 0$, then it is easy to realize that $-1-2r \leq 2r\cos(k\Delta x) \pm \sqrt{1-4r^2\sin(k\Delta x)} \leq 1+2r$, which is equivalent to $|\xi| \leq 1$. Considering the term in square root for the following $r \leq \frac{1}{2}, r \geq \frac{1}{2}, |2r\sin(k\Delta x)| \leq 1$ and $|2r\sin(k\Delta x)| \geq 1$. Consequently, the DuFort-Frankel method is unconditionally stable by using Von Neumann stability analysis Omowo Babajide Johnson (2023).

CHAPTER 5

RESULT AND DISCUSSION

5.1 Introduction

In this section, we have compared four different finite difference schemes with exact value as well as with each other. The absolute error of each scheme is shown in tables.

Example 5.1 *Consider the initial and boundary value problem*

$$i\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0, x \in [-2, 2],$$

$$u(x, 0) = \sin(x),$$

$$u(-2, t) = e^{it} \sin(-2),$$

$$u(2, t) = e^{it} \sin(2).$$

The analytic solution is $u(x, t) = e^{it} \sin(x)$.

Table 5.1: Error at different values of M for BTCS, CN and DuFort-Frankel for $h = 4/M, \Delta t = 0.1$.

M	DuFort-Frankel		BTCS		Crank-Nicolson	
	$E_\infty(\Re(u))$	$E_\infty(\Im(u))$	$E_\infty(\Re(u))$	$E_\infty(\Im(u))$	$E_\infty(\Re(u))$	$E_\infty(\Im(u))$
5	4.6563e-03	4.7108e-03	2.7382e-03	5.7730e-03	8.3730e-04	4.8173e-03
10	4.9937e-03	1.1592e-03	4.0961e-03	2.8156e-03	4.0945e-04	1.3420e-03
20	4.9937e-03	1.6623e-04	4.4803e-03	2.2427e-03	1.3637e-04	4.1564e-04
40	4.9937e-03	8.3242e-05	4.5800e-03	2.0997e-03	5.9750e-05	1.6773e-04
80	4.9948e-03	1.4572e-04	4.6052e-03	2.0658e-03	3.7667e-05	1.0543e-04
160	4.9958e-03	1.6135e-04	4.46118e-03	2.0597e-03	3.2141e-05	8.9674e-05
320	4.9958e-03	1.6528e-04	4.6142e-03	2.0574e-03	3.0749e-05	8.5732e-05

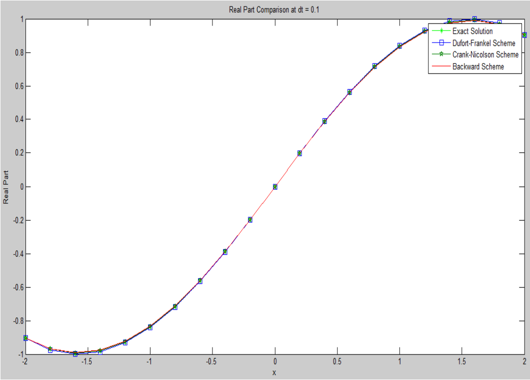

Figure 5.1: Real part comparsion of exact, DuFort-Frankel, BTCS and CN at M=20.

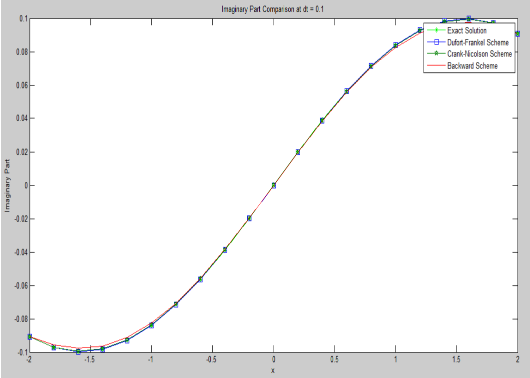

Figure 5.2: Imaginary part comparsion of exact, DuFort-Frankel, BTCS and CN at M=20.

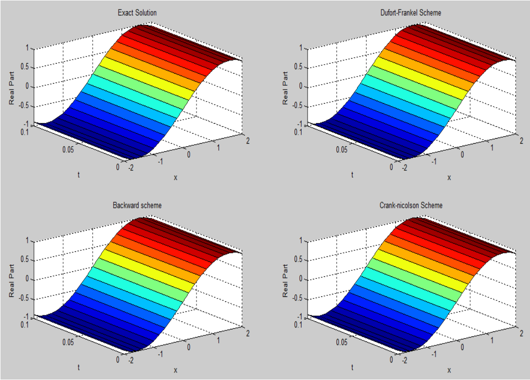

Figure 5.3: Surface comparsion of exact, DuFort-Frankel, BTCS and CN real part at M=20.

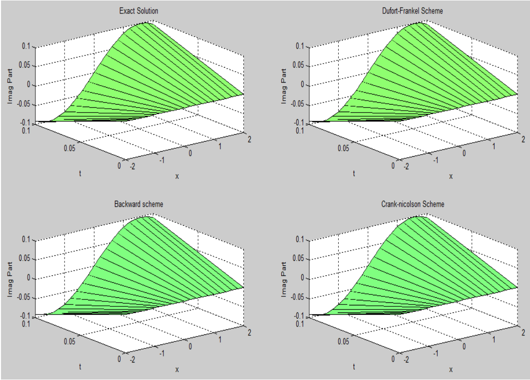

Figure 5.4: Surface comparsion of exact, DuFort-Frankel, BTCS and CN imaginary part at M=20.

Table 5.2: Error at different value of M for forward in time central in space (FTCS) at $h = 4/M, \Delta t = 0.0025$.

M	Forward in time central in space	
	$E_\infty(\Re(u))$	$E_\infty(\Im(u))$
5	9.3200e-04	1.0043e-02
10	5.5050e-04	4.7671e-03
15	3.1708e-04	5.8109e-04
20	2.4260e-04	3.3827e-04
25	2.0089e-04	2.1838e-04
30	1.9801e-04	1.7336e-04
35	6.9530e-04	7.4726e-04
40	3.8024e-02	2.6947e-02

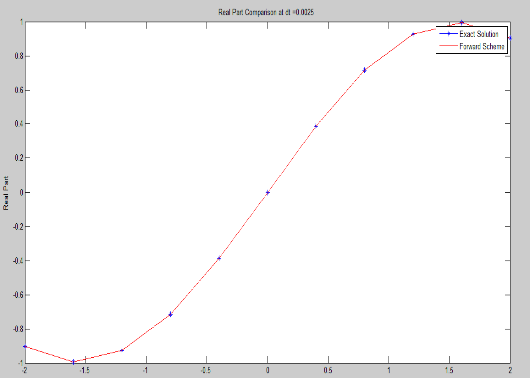

Figure 5.5: Comparsion of exact and FTCS real part at M=10.

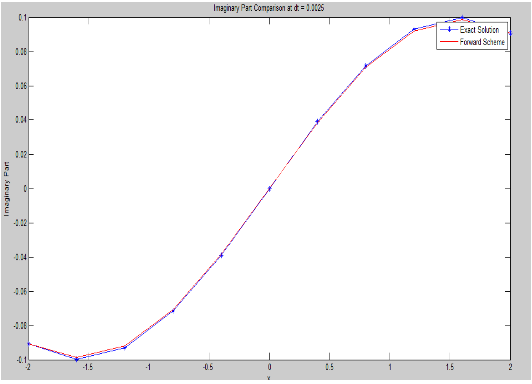

Figure 5.6: Comparsion of exact and FTCS imaginary part at M=10.

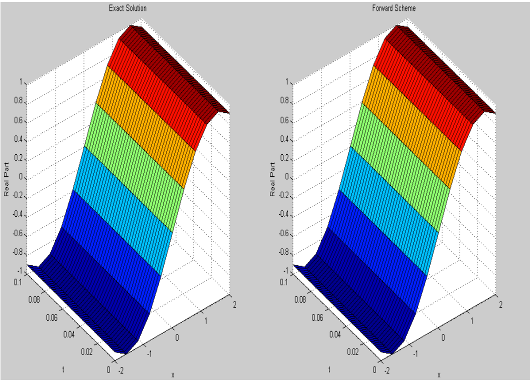

Figure 5.7: Surface comparsion real part of exact and FTCS at M=10.

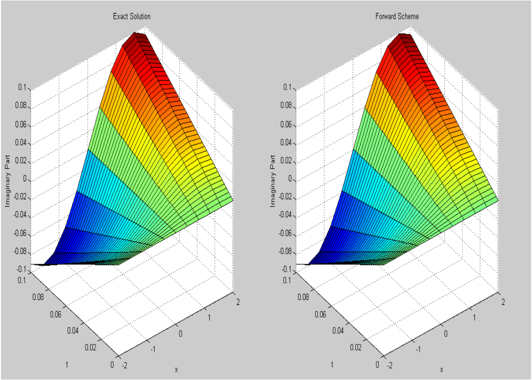

Figure 5.8: Surface comparsion imaginary part of exact and FTCS at M=10.

Example 5.2 *Consider the initial and boundary value problem*

$$i\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, x \in [-\pi, \pi]$$

$$u(x, 0) = \cos(x),$$

$$u(-\pi, t) = e^{it}\cos(-\pi),$$

$$u(\pi, t) = e^{it}\cos(\pi).$$

Table 5.3: Error at different values of M where, DuFort-Frankel, BTCS and CN $h = 2\pi/M, \Delta t = 0.1$.

M	DuFort-Frankel		BTCS		Crank-Nicolson	
	$E_\infty(\Re(u))$	$E_\infty(\Im(u))$	$E_\infty(\Re(u))$	$E_\infty(\Im(u))$	$E_\infty(\Re(u))$	$E_\infty(\Im(u))$
5	4.0417e-03	9.9666e-03	2.1067e-03	1.0452e-02	9.4728e-04	1.0090e-02
10	4.9958e-03	3.0803e-03	4.2799e-03	3.9833e-03	6.4349e-04	3.3064e-03
20	4.9958e-03	6.5318e-04	4.7520e-03	2.3523e-03	3.1054e-04	8.9645e-04
40	4.9958e-03	4.8723e-03	4.8723e-03	2.1832e-03	1.0746e-04	2.8669e-04
80	4.9958e-03	1.1519e-04	4.9025e-03	2.1340e-03	5.1208e-05	1.3379e-04
160	4.9958e-03	1.5373e-04	4.9101e-03	2.1167e-03	3.7165e-05	9.5539e-05
320	4.9958e-03	1.6337e-04	4.9119e-03	2.1126e-03	3.3488e-05	8.5974e-05

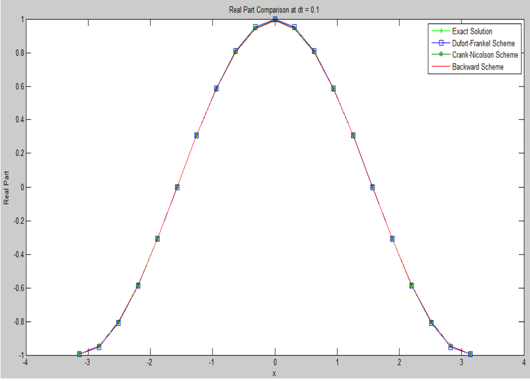

Figure 5.9: Real part comparsion of exact, DuFort-Frankel, BTCS and CN at M=20

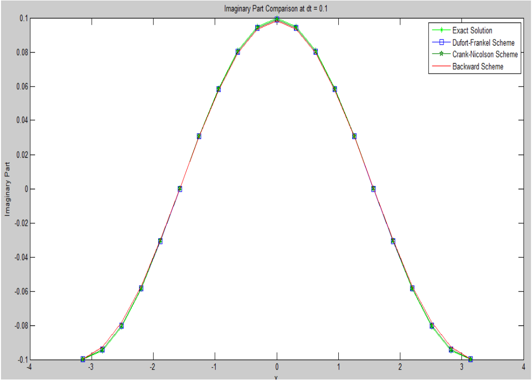

Figure 5.10: Imaginary part comparsion of exact, DuFort-Frankel, BTCS and CN at M=20

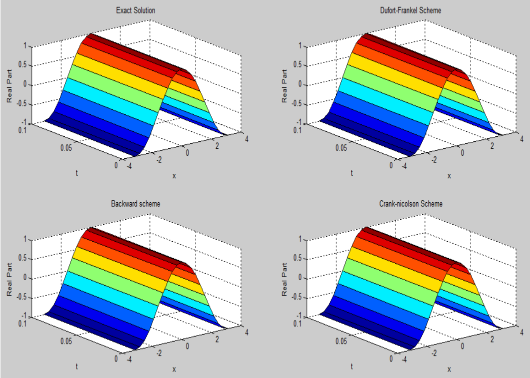

Figure 5.11: surface comparsion real part of exact,DuFort,BTCS and CN at M=20

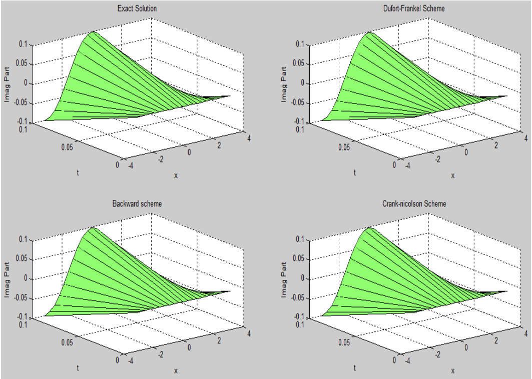

Figure 5.12: surface comparsion imaginary part of exact,DuFort,BTCS and CN at M=20

Table 5.4: Error at different value of M for forward in time central in space at $h = 2\pi/M, \Delta t = 0.0025$.

M	Forward in time central in space	
	$E_\infty(\Re(u))$	$E_\infty(\Im(u))$
5	1.0221e-03	1.0043e-02
10	7.3676e-04	3.2201e-03
15	5.8053e-04	1.4034e-03
20	4.3338e-04	8.0373e-04
25	2.9530e-04	5.0655e-04
30	2.5636e-04	3.5105e-04
35	2.0745e-04	2.5374e-04
40	1.9178e-04	1.9223e-04

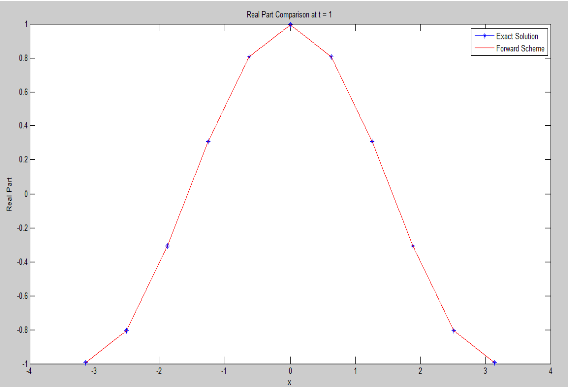

Figure 5.13: Real part of FTCS at M=10

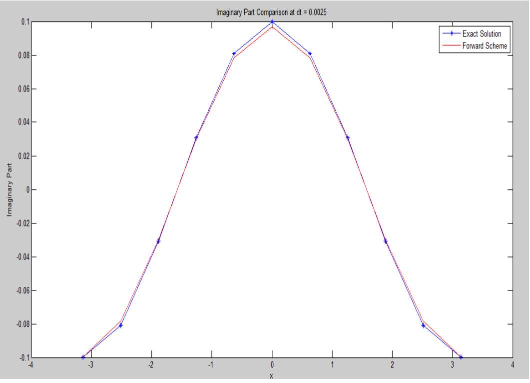

Figure 5.14: Imaginary part of FTCS at M=10

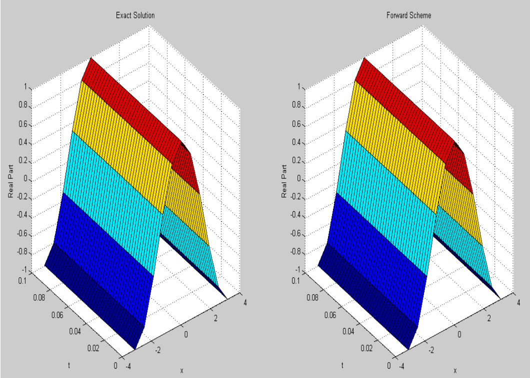

Figure 5.15: 3D of exact and FTCS Real part at M=10

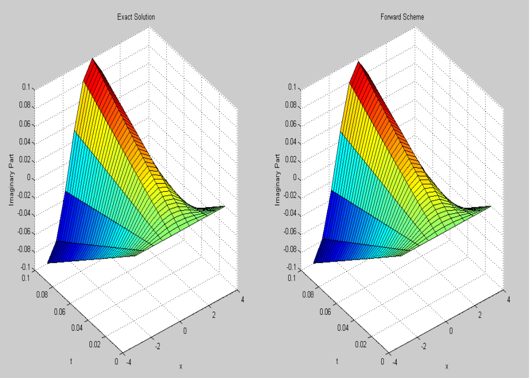

Figure 5.16: 3D of exact and FTCS imaginary part at M=10

Table 5.5: Error at different values of M forward in time central in space(FTCS) and DuFort-Frankel schemes $h = 2\pi/M, \Delta t = 0.1$.

M	FTCS		DuFort-Frankel	
	$E_\infty(\Re(u))$	$E_\infty(\Im(u))$	$E_\infty(\Re(u))$	$E_\infty(\Im(u))$
5	4.0417e-03	9.9666e-03	4.0417e-03	9.9666e-03
10	4.9958e-03	3.0803e-03	4.9958e-03	3.0803e-03
20	4.9958e-03	6.5318e-04	4.9958e-03	6.5318e-04
40	4.9958e-03	3.8864e-05	4.9958e-03	3.8864e-05
80	4.9958e-03	1.1519e-04	4.9958e-03	1.1519e-04
160	4.9958e-03	1.5373e-04	4.9958e-03	1.5373e-04
320	4.9958e-03	1.6337e-04	4.9958e-03	1.6337e-04

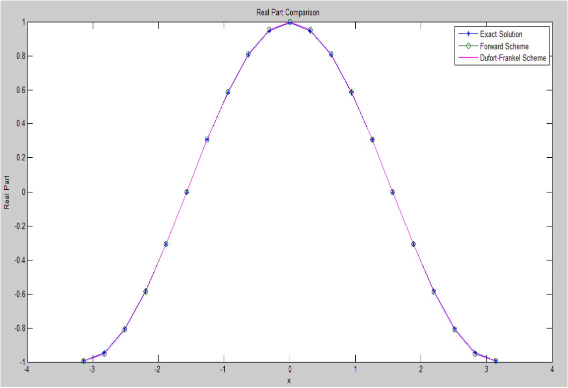

Figure 5.17: Real part of exact, FTCS and DuFort-Frankel at M=20

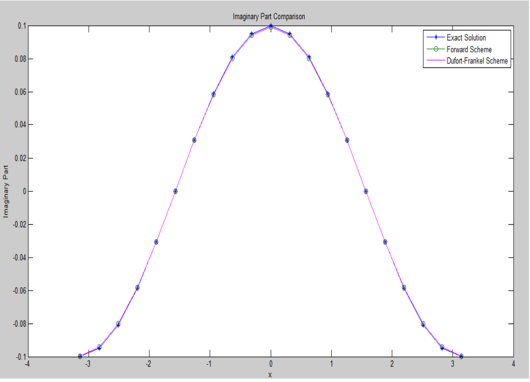

Figure 5.18: Imaginary part of exact, FTCS and DuFort-Frankel at M=10

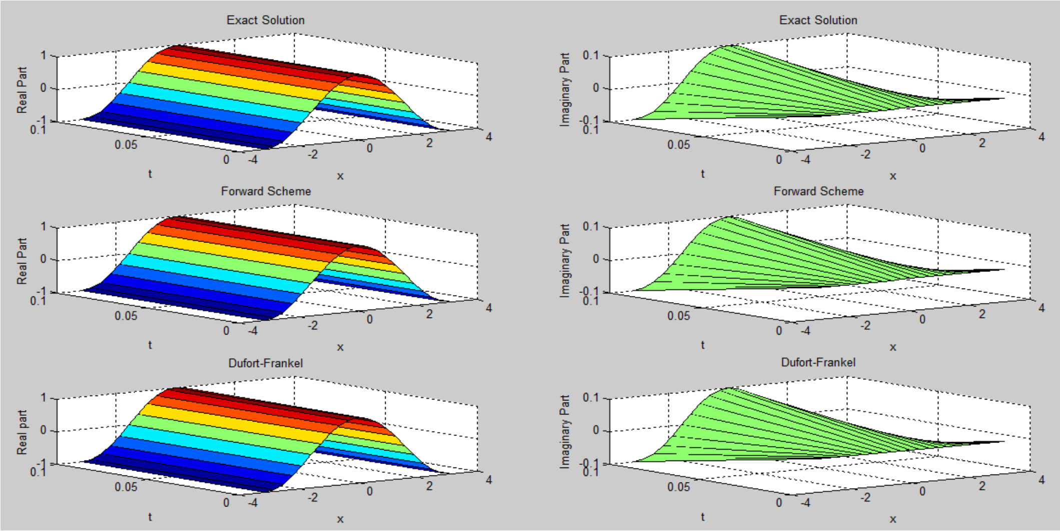

Figure 5.19: surface real part and imaginary part comparsion of exact, FTCS and DuFort-Frankel at M=20 .

From the above tables and graphs, we can draw some conclusions:

1. Comparing the absolute error of each scheme and the plots of real and imaginary parts of the exact solution with the numerical approximations using different schemes, we can see that the exact solution and the numerical solutions generally follow similar patterns. This indicates the numerical schemes are capable of capturing the behavior of the exact solution. By considering the absolute error of each scheme it shows small variation from each other in real part.

2. The forward in time central in space scheme(FTCS) show some oscillations and deviations from the exact solution, especially in the regions where the solution changes rapidly.These scheme is known to introduce numerical diffusion and dispersion, which can lead to inaccuracies and smearing of sharp features.

3. The backward in time central in space scheme, the Crank-Nicolson scheme(CN) and DuFort schemes exhibit better accuracy compared to the forward scheme.They provide smoother and more accurate approximations of the exact solution.The Crank-Nicolson scheme in particular,is known for its second order accuracy and ability to mitigate numerical diffusion and dispersion.

4. The real and imaginary part comparisons show that all the numerical schemes deviate from the exact solution to some extent. However, the backward in time central in space scheme, Crank-Nicolson scheme and DuFort-Frankel scheme generally yield closer approximations to the exact solution compard to the forward in time central in space schemes.

Based on these observations, we can conclude that backward in time central in space scheme, Crank-Nicolson and DuFort-Frankel scheme are more accurate and reliable for approximating the given Schrödinger equation compared to forward in time central in space. However, the choice of scheme depends on the specific requirements of the problem, such as computational efficiency and stability considerations.

CHAPTER 6

CONCLUSION AND RECOMMENDATION

6.1 Conclusion

From the absolute error of the methods, it is observed clearly that the implicit schemes (BTCS and CN) are efficient and fast in implementation than the other two schemes. The BTCS, Crank-Nicolson and DuFort-Frankel schemes as seen by using Von Neumann stability method are unconditionally stable, while the forward in time central in space(FTCS) scheme is conditionally stable.This can be seen in examples stated above where the three schemes perform better than the FTCS scheme, and also the implicit schemes. That means, backward in time central in space and Crank-Nicolson schemes perform better than the explicit schemes.

6.2 Recommendation

In this thesis, we considered some finite difference scheme to solve one-dimensional Schrödinger equations. The obtained result reveals that some finite differences numerical schemes stated in this paper are well suited for solving one-dimensional Schrödinger equations. Depending on this report we recommend the researchers for further study.

- Modify the present schemes for solving higher-dimensional Schrödinger equation.

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