The Numerical and Approximate Analytical Solution of Parabolic Partial Differential Equations with Nonlocal Boundary Conditions

by

Seyed Mohammad Ghoreishi

Thesis Submitted in fulfilment of the requirements for the Degree of (Doctor of Philosophy)

December 2011

ACKNOWLEDGMENTS

I would like to express my sincere gratitude to my supervisor, Professor Ahmad Izani Md. Ismail. Through his many roles as an supervisor, a mentor, he has had a tremendous influence on both professional and personal development. Without his guidance and encouragement, this thesis would not have been possible. Most importantly, he has dedicated precious time and energy to provide countless contributions is shaping in this thesis. I am very grateful for his support and patience throughout my Ph.D work. Actually, it is my honor to become one of his students.
I am also very grateful to my co-supervisor Professor Abdur Rashid for many useful discussion, good advise, deep insight and infinite patience that made this thesis possible.
I am grateful to my wife Farzaneh and my daughter Kimia for her patience and my mother for her affection. Without them this work would never have come into existence.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

ODEs	Ordinary differential equations
PDEs	Partial differential equations
FDM	Finite difference method
FTCS	Forward time central space
BTCS	Backward time central space
NFTCS	New explicit finite difference method
NECF	New explicit Crandall formula
CPU	Central process unit
Δ	Laplace operator
∇u	Gradient of u
ADM	Adomian decomposition method
SADM	Standard Adomian decomposition method
MADM	Modified Adomian decomposition method
VIM	Variational iteration method
MVIM	Modified variational iteration method
λ	Lagrange multiplier
HPM	Homotopy perturbation method
MHPM	Modified homotopy perturbation method
HAM	Homotopy analysis method
MHAM	Modified homotopy analysis method
OHAM	Optimal homotopy asymptotic method

$\rho(\mathbf{A})$	Spectral radius of matrix $\mathbf{A}$
μ_k	Eigenvalue of tradiagonal matrix
τ	Truncation error
$U - u$	Discretization error
$\lambda(x, \xi)$	Lagrange multiplier (VIM)
p	Embedding parameter (HPM)
u_i^n	Approximation of $u(x, t)$ at (ih, jk)
$\hbar$	Convergence-control parameter (HAM)
$\mathcal{H}(x, t)$	Auxiliary function (HAM)
$\mathcal{L}$	Linear operator (HAM)
A_n	Adomian polynomials
$R_\hbar$	Invalid region of convergence (HAM)
$\Delta_{\hbar,m}$	Residual error at mth-order approximation (HAM)
R	Set of real numbers
$\mathcal{R}$	Auxiliary function (HAM)

Penyelesaian Berangka dan Hampiran Analisis untuk Persamaan Pembezaan Separa dengan Syarat Sempadan Tak Setempat

ABSTRAK

Banyak masalah saintifik dan kejuruteraan boleh dimodel oleh persamaan pembezaan separa parabolik dengan syarat sempadan tak setempat. Contoh masalah seperti ini boleh didapati dalam bidang penyebaran kimia, keanjalan haba, proses konduksi haba, dinamik reaktor nuklear, masalah songsang, teori kawalan dan sebagainya. Sepanjang dua dekad yang lalu, pembangunan teknik berangka dan teknik hampiran analisis untuk menyelesaikan persamaan-persamaan ini telah menjadi bidang penyelidikan penting kerana keperluan untuk lebih memahami fenomena asas fizikal. Terdapat keperluan untuk membangunkan teknik baru yang lebih tepat dan perkara ini adalah tumpuan tesis ini. Dalam tesis ini, kami mencadangkan kaedah baru beza terhingga baru dan mengkaji kaedah analisis hampiran untuk menyelesaikan persamaan pembezaan separa parabolik linear dan tak homogen dengan syarat sempadan tak setempat. Kami memperkenalkan kacdah beza terhingga tak tersirat yang baru dan kaedah rumus Crandall (3,3) yang baru serta membincangkan keputusan berangka yang diperoleh. Di samping itu, kami juga telah mengkaji beberapa kaedah analisis hampiran iaitu kaedah penguraian Adomian, kaedah lelaran perubahan, kaedah pengusikan homotopi, kaedah analisis homotopy, Kaedah homotopi optimum asimptot dan telah menggunakan pendekatan piawai dan diubahsuai untuk menyelesaikan persamaan pembezaan separa parabolik linear dan tak homogen dengan syarat sempadan tak setempat. Adalah diketahui kaedah analisis hampiran menyelesaikan persamaan pembezaan dengan menggunakan syarat awal sahaja. Oleh itu, kami juga mencadangkan pengubahsuaian baru kaedah penguraian Adomian untuk menyelesaikan persamaan pembezaan parabolik linear dan tak homogen dengan syarat sempadan tak setempat dengan menggunakan syarat tak setempat. Kami telah menunjukkan bahawa kaedah beza terhingga yang dibangunkan dan kaedah hampiran analisis yang dipertimbangkan mampu menyelesaikan persamaan pembezaan separa parabolik linear dan tak homogen dengan syarat sempadan setempat dengan jitu.

The Numerical and Approximate Analytical Solution of Parabolic Partial Differential Equations with Nonlocal Boundary Conditions

ABSTRACT

Many scientific and engineering problems can be modeled by parabolic partial differential equations with nonlocal boundary conditions. Examples of such problems can be found in chemical diffusion, thermoelasticity, heat conduction processes, nuclear reactor dynamics, inverse problems, control theory and so forth. In the last two decades, the development of numerical and approximate analytical techniques to solve these equations has been an important area of research due to the need to better understand the underlying physical phenomena. There is a need to develop new and more accurate techniques and this is the area of focus of this thesis. In this thesis, we propose new finite difference methods and study approximate analytical methods for solving linear and nonhomogeneous parabolic partial differential equations with nonlocal boundary conditions. We have introduced a new explicit finite difference method and a new (3,3) Crandall- formula method and have discussed the obtained results. In addition, we have also studied several approximate analytical methods- Adomian Decomposition Method, Variation Iterative Method, Homotopy Perturbation Method, Homotopy Analysis Method, Optimal Homotopy Asymptotic Method and have applied the standard approach and modifications to solve linear and nonhomogeneous parabolic partial differential equations with nonlocal boundary conditions. It is known that the approximate analytical methods solve differential equations by using the initial condition only. Thus, we also proposed a new modification of Adomian Decomposition Method to solve linear and nonhomogeneous parabolic partial differential equations with nonlocal boundary conditions by using nonlocal boundary conditions. We also show that the finite difference methods developed and approximate analytical methods

considered are capable of accurately solving linear and nonhomogeneous parabolic partial differential equations with nonlocal boundary conditions.

CHAPTER 1
INTRODUCTION

1.1 Introduction

Many problems in science and engineering require the solution of partial differential equations where the independent variables are space and time coordinates. To fully understand the underlying physical problems, a relationship between the independent and dependent variables need to be established and this effectively means the equations must be "solved". In general, the complexity of these equations and the auxiliary conditions are such that analytical solution methods (yielding exact analytical solutions) cannot be used and numerical or approximate analytical techniques are required. The focus of this thesis is the study of numerical and approximate analytical techniques for the solution of parabolic partial differential equation with nonlocal boundary conditions. In this chapter, we give an introduction to our study.

1.2 Partial Differential Equation

Partial differential equations are a type of differential equation, i.e, a relation involving an unknown function (or functions) of several independent variables and their partial derivatives with respect to those variables. Partial differential equations appear frequently in all areas of physics and engineering. In recent years, we have seen a dramatic increase in the use of these equations in areas such biology, chemistry, chemical engineering, computer science (partially in relation to image processing and graphics) and economics. In this section, we introduce the general form of the these equations. The general form of partial differential equations are

$$\sum_{i,j=1}^{n+1} a_{i,j}\frac{\partial^2 u}{\partial x_i \partial x_j} - q(x_1, x_2, ..., x_n, x_{n+1}, u, \frac{\partial u}{\partial x_1}, ..., \frac{\partial u}{\partial x_n}, \frac{\partial u}{\partial x_{n+1}}) = 0, \tag{1.1}$$

where $q(.) \in R$ [206]. We assume that $t = x_{n+1}$ if the equations involve the variable t. $a_{i,j}$ may depend on $x_1, x_2, ..., x_n, x_{n+1}, u, \dfrac{\partial u}{\partial x_1}, ..., , \dfrac{\partial u}{\partial x_n}, \dfrac{\partial u}{\partial x_{n+1}}$. It is often assumed that $a_{i,j} = a_{j,i}$ and thus the matrix $\mathbf{A} = [a_{i,j}]$ is a symmetric matrix. If all eigenvalues of $\mathbf{A}$ have the same sign, then the equations are called elliptic PDEs. If at least one eigenvalue is zero, then the equations are parabolic PDEs. If n of the eigenvalues have the same sign, and the remaining one has opposite sign, then the equations are called hyperbolic PDEs.

Equations in the form of (1.1) can be very complicated. It is difficult to deal with equations which have many variables. Also, if the coefficients $a_{i,j}$ are complicated functions, then the equations are usually difficult to solve. Many PDEs in real applications contain fewer variables, or even have constant coefficients, such as Laplace's equation, Poisson's equation, and the heat equation. Typical second order PDEs are [206]

$$a_1 \frac{\partial^2 u}{\partial x_1^2} + a_2 \frac{\partial^2 u}{\partial x_2^2} + \cdots + a_n \frac{\partial^2 u}{\partial x_n^2} - q = 0, \tag{1.2}$$

$$a_1 \frac{\partial^2 u}{\partial x_1^2} + a_2 \frac{\partial^2 u}{\partial x_2^2} + \cdots + a_n \frac{\partial^2 u}{\partial x_n^2} - q - \frac{\partial u}{\partial t} = 0, \tag{1.3}$$

$$a_1 \frac{\partial^2 u}{\partial x_1^2} + a_2 \frac{\partial^2 u}{\partial x_2^2} + \cdots + a_n \frac{\partial^2 u}{\partial x_n^2} - q - \frac{\partial^2 u}{\partial t^2} = 0, \tag{1.4}$$

where in (1.2), $q = q\left(x_1, x_2, ..., x_n, u, \dfrac{\partial u}{\partial x_1}, ..., \dfrac{\partial u}{\partial x_n}\right)$, and in (1.3) and (1.4), $q = q\left(x_1, x_2, ..., x_n, u, t, \dfrac{\partial u}{\partial x_1}, ..., \dfrac{\partial u}{\partial x_n}\right)$. The equation (1.2) are elliptic PDEs, the equation (1.3) are parabolic PDEs, and the equations (1.4) are hyperbolic PDEs. $a_1, a_2, ..., a_n$ are nonnegative constants. For elliptic PDEs of the form (1.2), at least two of a_i, $i = 1, 2, ..., n$ cannot be zero. For the parabolic and hyperbolic equations defined in (1.3) and (1.4), at least one of a_i, $i = 1, 2, ..., n$ cannot be zero. The equations discussed in the present thesis are parabolic PDEs, which are used to describe phenomena that are time-dependent.

For introducing a new class of finite difference method and approximate analytical methods for parabolic PDEs in this thesis, we consider equations which have variable coefficients. Also, the equations considered in this thesis only contain one dependent variable with two independent variables $u(x,t)$, and the equations are linear.

The general form of parabolic PDEs can be written as [207]

$$\frac{\partial u}{\partial t} = \Delta u - q(X,t,u,\nabla u), \qquad X \in \Omega \subset R^n, \;\; t \in [t_0,t_1] \subset R, \tag{1.5}$$

where $u(x,t) \in R$, Δ is Laplace's operator of u with respect to X, ∇u is the gradient of u with respect to X, $q(X,t,u,\nabla u) \in R$; i.e,

$$\Delta = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}, \qquad \nabla = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots, \frac{\partial}{\partial x_n}\right)^*, \tag{1.6}$$

where $*$ denotes transpose, ∇u is a vector and $\Delta = \nabla.\nabla$.

According to [207], equation (1.5) is called semi-linear parabolic equation. If

$$q(X,t,u,\nabla u) = b(X,t)^* \nabla u + c(X,t)u + f(X,t), \tag{1.7}$$

where $b(X,t) \in R^n$, $c(X,t)$, $f(X,t) \in R$, then equation (1.5) is called a linear parabolic PDE. Thus we can write a linear parabolic PDE as [205]

$$\frac{\partial u}{\partial t} = \Delta u - b(X,t)^* \nabla u - c(X,t)u - f(X,t). \tag{1.8}$$

In the two dimensional case, this becomes

$$\frac{\partial u}{\partial t} = \Delta u - b_1(x,y,t)\frac{\partial u}{\partial x} - b_2(x,y,t)\frac{\partial u}{\partial y} - c(x,y,t)u - f(x,y,t), \tag{1.9}$$

where $b_1, b_2 \in R$.

The general form of the second order nonlinear parabolic PDEs are [204]

$$\frac{\partial u}{\partial t} = F(t, X, u, \nabla u, \nabla^2 u), \qquad D_T = (0, T) \times \Omega, \tag{1.10}$$

where

$$\begin{aligned} &F \in C[\overline{D_T} \times R \times R^n \times R^{n^2}, R], \\ &\nabla u = (u_{x_1}, u_{x_2}, \ldots, u_{x_n}), \\ &\nabla^2 u = (u_{x_1 x_1}, u_{x_1 x_2}, \ldots, u_{x_n x_n}), \end{aligned}$$

and Ω is a bounded domain in R^n and $X = (x_1, x_2, \ldots, x_n)$.

1.3 Parabolic Partial Differential Equations

According to [200], parabolic partial differential equations are one of the most challenging areas in the field of partial differential equations. The variety of methods and applications is growing more and more in this field of research. Several new problems that arise in applications in natural sciences and engineering cannot be addressed by existing mathematical and numerical methods. At the same time, these problems turn out to require the development of new mathematical techniques. Parabolic PDE, arise from a variety of diffusion phenomena which appear widely in nature. They are suggested as mathematical models of physical problems in many fields, such as filtration, phase transition, biochemistry and dynamics of biological groups. In many cases, these equations possess degeneracy or singularity. The appearance of degeneracy or singularity makes the study more involved and challenging. Many new ideas and methods have been developed to overcome the special difficulties caused by the degeneracy and singularity, which enrich the theory of partial differential equations [200].

In this thesis, we are interested in solving linear second-order parabolic partial differential equations (PDEs) in one space dimension. A typical example of such a problem is given by the heat equation. Various phenomena in the engineering, science and other branches of mathematical sciences require the solution of a parabolic partial differential equation which include integral terms which appear in the boundary conditions. In this case, the boundary conditions is called nonlocal boundary conditions. Let us define a spatial differential operator Δ by

$$\Delta \equiv A(x,t)\frac{\partial^2}{\partial x^2} + B(x,t)\frac{\partial}{\partial x} + C(x,t),$$

where A, B and C are given functions.

The problem we want to solve is described by parabolic PDE of the form

$$\frac{\partial u}{\partial t} = \Delta u + D(x,t), \qquad 0 < x < 1, \;\; 0 < t \le T, \tag{1.11}$$

subject to the initial condition

$$u(x,0) = f(x), \tag{1.12}$$

and the boundary conditions

$$\mathcal{B} \equiv \{u(0,t) = \beta_0(t) + g_0(t), u(1,t) = \beta_1(t) + g_1(t)\}, \tag{1.13}$$

where D, f, β_0 and β_1 are given functions, and u is the unknown function to be determined or approximated. We study the parabolic PDE problem with nonlocal boundary conditions in (1.13) where the functions of $\beta_0(t)$ and $\beta_1(t)$ are defined as

$$\beta_0(t) = \int_0^1 \phi(x,t)u(x,t)dx,$$

$$\beta_1(t) = \int_0^1 \psi(x,t)u(x,t)dx,$$

and where $\phi(x,t)$ and $\psi(x,t)$ are known functions.

Parabolic partial differential equations with nonlocal boundary conditions are also classified as homogeneous and nonhomogeneous. In general, a PDE of any order is called homogeneous if every term of PDE contains the dependent variable $u(x,t)$ or one of its derivatives, otherwise, it is called nonhomogeneous PDE. Thus the equation (1.11) is homogeneous if $D(x,t) = 0$ else is called nonhomogeneous.

1.4 Motivation

Non-local mathematical models play an important role in physical phenomena. For example, the diffusion equation with non-local boundary conditions can be used to model various physical phenomena in the context of thermoelasticity, control theory, heat conduction process and population dynamics. Recently, there has been growing interest in developing computational methods for the numerical and approximate analytical solution solution of these equations [18, 53, 54, 55, 166, 188, 189, 208]. Most of the studies and papers that deal with problems of this type are concentrated to one-dimensional equations [53, 54, 188, 189, 208]. The presence of the integral term in boundary conditions can greatly complicate the application of standard numerical schemes such as finite difference schemes, finite element schemes and etc. Therefore it is important to be able to convert nonlocal boundary condition to a more suitable form. The use of approximations in these equations are not without their difficulties. The accuracy of the approximation must be compatible with that of the discretization of the differential equation. As it has been introduced in section 1.3, the nonlocal boundary conditions cannot be solved because the integrals in boundary conditions include an unknown function $u(x,t)$. Thus there is no suitable method to obtain the exact solution.

Our purpose in this research is to study techniques to obtain accurate approximate solutions for parabolic PDE with nonlocal boundary conditions. We are motivated by the observation that the methods proposed in the literature are quite abundant and there is a need to consolidate and conduct a comparative study. According to [53, 188], the development of numerical techniques for the solution of the parabolic partial differential equation with nonlocal boundary conditions is an important research topic in many branches of science and engineering. Various researchers have proposed modifications to approximate analytical methods. It is important that the effectiveness to these various modifications be studied and compared. One of the new approximate analytical methods which has recently been introduced is the Optimal Homotopy Asymptotic Method (OHAM). This method has yet to be extensively applied in solving various ordinary and partial differential equations.

1.5 Objective

The objective of this study is

1. To conduct a comparative study of existing finite difference and approximate analytical methods for linear and nonhomogeneous parabolic partial differential equation with nonlocal boundary conditions.

2. To develop a new and accurate finite difference method and to apply to linear nonhomogeneous parabolic partial differential equation with nonlocal boundary condition. To investigate the accuracy of the new finite difference method.

3. To apply modified approximate analytical techniques to linear nonhomogeneous parabolic partial differential equation with nonlocal boundary condition. To investigate the accuracy of the modified methods.

4. To apply a new approximate analytical method called the Optimal Homotopy Asymptotic Method (OHAM) to nonhomogeneous parabolic partial differential equation with nonlocal boundary conditions. To investigate the accuracy

of OHAM.

5. To apply a new modification of Adomian Decomposition Method (MADM) to nonhomogeneous parabolic partial differential equations with nonlocal boundary conditions by using boundary conditions. We also aim to investigate the accuracy of this MADM.

1.6 Methodology

The methodology of this study is

1. Detailed literature survey on linear and nonlinear finite difference and approximate analytical methods of solution. Method which will be studied are chosen.

2. A comparative study of finite difference methods will be conducted via numerical experiments using Mathematica. A new method will be developed and it's performance in relation to other methods gauged. Test problem with known solutions will be used. The theoretical properties of the new method will be established using standard analysis techniques.

3. A comparative study of approximate methods will be conducted via computational experiments using Mathematica. Modification of approximate analytical methods will be made and the performance of the modification assessed. Test problem with known solutions will be used.

4. An in-depth study of a new approximate analytical method (OHAM) will be made and it will then be applied to linear and nonhomogeneous parabolic partial differential equation with nonlocal boundary conditions. Computational experiments will be conducted using Mathematica.

5. A new modification of ADM (MADM) will be made and applied to nonhomogeneous parabolic partial differential equations with nonlocal boundary conditions by using boundary conditions. Computational experiments will be conducted using Mathematica.

1.7 Thesis outline

An outline of the remainder of this thesis is as follows

Chapter 2 provides a review of basic concepts, basic methods and theory. In this chapter, we discuss the basic concepts and issues related to the solution of parabolic partial differential equations with nonlocal boundary conditions. At the end of this chapter, we have given a literature review on the uniqueness and global existence of the solution of semi-linear and nonlinear parabolic equations with nonlocal boundary conditions.

In chapter 3, we review the numerical and approximate analytical methods which has been introduced by many authors and researchers. We divide the discussion into two cases

1. Finite difference methods

2. Approximate analytical methods

In chapter 4, we apply the finite difference methods, for example, BTCS, FTCS, Crank-Nicolson, Dufort-Frankel and (3,3) explicit Crandal formula method to numerically solve linear and nonhomogeneous parabolic equation with nonlocal boundary conditions.

Chapter 5 is devoted to approximate analytical methods and we will conduct a comparative study. These methods include Adomian Decomposition Method (ADM), Variational Iteration Method (VIM), Homotopy Perturbation Method (HPM) and Homotopy analysis Method (HAM). We use these methods for solving linear and homogeneous parabolic partial differential equation with nonlocal boundary conditions.

The new explicit method and new (3,3) explicit Crandal formula is introduced and developed in chapter 6. The feasibility and accuracy of the new method was tested on two examples used by many previous researchers. At the end of this chapter, the theoretical properties of the method that we have developed will be investigated.

Chapter 7 has been devoted to apply the modification of approximate analytical methods for numerical solving linear and nonhomogeneous parabolic equation with nonlocal boundary conditions. In this chapter, we will show that the these methods are very powerful and capable to solve parabolic PDEs. We also conduct a comparative study.

Chapter 8 is dedicated to study and develop a new method which is called Optimal Homotopy Asymptotic Method (OHAM) to be used for solving linear and nonhomogeneous parabolic equations with nonlocal boundary conditions. To illustrate of the capability and accuracy of the OHAM, it was tested on three examples which have been solved in chapters 6 and 7. The obtained results show that this method is very accurate in solving parabolic partial differential equation with nonlocal boundary condition.

Chapter 9 is devoted to introduce and apply a new modification of ADM (MADM) to find approximate solution of parabolic partial differential equations with nonlocal boundary conditions. This method solves the equations by using boundary conditions. To illustrate the capability and accuracy of the MADM proposed in this chapter, it will be tested on four examples which have been solved in chapter 6 and 7. By considering the obtained results, it can be concluded that the MADM is very accurate in finding approximate solution of parabolic partial differential equations with nonlocal boundary conditions.

Finally, in chapter 10 we give the conclusion of our study and discuss the possibilities for further work in this area.

CHAPTER 2
BASIC METHODS, CONCEPTS, THEORY

2.1 Introduction

In this chapter, we introduce some basic methods, concepts and theory which play an important role in the numerical and approximate analytical solution of partial differential equations. In addition, we also describe two examples of applications of parabolic partial differential equation with nonlocal boundary conditions.

2.2 Parabolic Equations

Parabolic partial differential equations that arise in scientific and engineering problems are often of the form [67]

$$u_t = Lu, \tag{2.1}$$

where Lu is a second-order elliptic partial differential operator which may be linear or nonlinear. We assume U to be an open, bounded subset of R^n, and set $U_t = U \times (0, T]$ for some fixed time $T > 0$. We consider the initial boundary value problem [67]

$$\begin{aligned} &u_t + Lu = f, \qquad U_t, \\ &u = 0, \qquad \partial U \times [0, T], \\ &u = g, \qquad U \times t = 0, \end{aligned} \tag{2.2}$$

where $f : U_t \longrightarrow R$ and $g : U \longrightarrow R$ are given, and $u : \overline{U_t} \longrightarrow R$ is the unknown, $u = u(x, t)$. The letter L denotes for each time t a second-order partial differential operator, having either divergence form [67]

$$Lu = -\sum_{i,j=1}^{n} (a_{i,j}(x, t)u_{x_i})_{x_j} + \sum_{i=1}^{n} b_i(x, t)u_{x_i} + c(x, t)u, \tag{2.3}$$

or else the non-divergence form

$$Lu = -\sum_{i,j=1}^{n} a_{i,j}(x,t)u_{x_i x_j} + \sum_{i=1}^{n} b_i(x,t)u_{x_i} + c(x,t)u. \tag{2.4}$$

For given coefficient $a_{i,j}$, b_i and c, the partial differential operator $\dfrac{\partial}{\partial t} + L$ is said to be (uniformly) parabolic if there exists a constant $\theta > 0$ such that [67]

$$\sum_{i,j=1}^{n} a_{i,j}(x,t)\xi_i\xi_j \geq \theta|\xi|^2, \tag{2.5}$$

for all $(x,t) \in U_t$, $\xi \in R^n$. It should be noted that for each fixed time $0 \leq t \leq T$ the operator L is a uniformly elliptic operator in the spatial variable x. An example is $a_{i,j} = \delta_{i,j}$, $b_i = c = f = 0$, in which case $L = -\Delta$ and the partial differential equation $\dfrac{\partial u}{\partial t} + Lu$ becomes the heat equation. The solutions of the general second-order parabolic partial differential equation are similar in many ways to solutions of the heat equation . General second-order parabolic equations describe in physical applications the time-evolution of the density of some quantity u, say a chemical concentration , within the region U. In [67], it was noted that for equilibrium setting, the second-order $\sum_{i,j=1}^{n} a_{i,j}(x,t)u_{x_i x_j}$ describes diffusion, the first-order term $\sum_{i=1}^{n} b_i(x,t)u_{x_i}$describes transport, and the zeroth-order term cu describes creation or depletion.

2.3 Finite Difference Approximation

The Finite Difference Method (FDM) is a method of approximating the derivatives of a function in terms of the known values of the function itself. When these approximations are introduced into a PDE, and the derivatives are evaluated on a set of points (usually called grid points), an approximate solution of the PDE at the point of the grid can be found. Formally, the domain of solution of the given partial differential equation is first subdivided by a net with a finite number of mesh points. The derivative at each point is then replaced by finite difference approximation which results in an algebraic equation (or system of such equations) which are more easily solved that the original PDE.

Let us first consider $u(x,t)$, in which u is a continuous function of the two independent variables x and t. The x and t is discretized into a set of points such that

$$u(x_i, t_n) = u(ih, nk) = u_i^n,$$

where the spacing in the x direction is h an in the t direction k. Taylor series expansions play a very important rule in the formulation and classification of finite difference schemes. It is necessary that we use Taylor series expansions for the approximation of derivatives. Thus we can have

$$u_{i+1}^n = u_i^n + h(u_x)_i^n + \frac{h^2}{2}(u_{xx})_i^n + \frac{h^3}{6}(u_{xxx})_i^n + \frac{h^4}{24}(u_{xxxx})_i^n + \cdots .$$

If h is sufficiently small, the 4^{th} and higher terms are much smaller than the 3^{rd} terms. Then, we can write

$$u_{i+1}^n = u_i^n + h(u_x)_i^n + O(h^2). \tag{2.6}$$

The notation $O(h^2)$ means that the absolute value of the sum of the truncation error is at most a constant multiplier of h^2. Dividing (2.6) by h and rearranging the terms produce the following

$$\left.\frac{\partial u}{\partial x}\right|_{x=x_i, t=t_n} = (u_x)_i^n = \frac{u_{i+1}^n - u_i^n}{h} + O(h).$$

The term $\dfrac{u_{i+1}^n - u_i^n}{h}$ is called the forward-difference approximation for $\dfrac{\partial u}{\partial x}$ at the point (x_i, t_n), and it is first order accurate or $O(h)$ accurate.

We can use the same procedure and obtain backward and central-difference approximation for the partial derivative $\dfrac{\partial u}{\partial x}$ as follows

$$(u_x)_i^n = \frac{u_i^n - u_{i-1}^n}{h} + O(h), \qquad \text{Backward-difference}$$

$$(u_x)_i^n = \frac{u_{i+1}^n - u_{i-1}^n}{2h} + O(h^2). \qquad \text{Central-difference}$$

For the second order derivative, we can obtain

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{x=x_i, t=t_n} = (u_{xx})_i^n = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{h^2} + O(h^2).$$

The term $\dfrac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{h^2}$ is called the central-difference approximation to $\dfrac{\partial^2 u}{\partial x^2}$ at (x_i, t_n) and it is second-order accurate.

2.4 Finite Difference Methods for Parabolic Equation

In this section, we describe the Forward Time Central Space (FTCS) scheme, Backward Time Central Space (BTCS) scheme and Crank-Nicolson scheme.

2.4.1 Explicit Method (FTCS)

Consider the dimensionless initial boundary value problem in one space variable [15, 181, 187]

$$\begin{aligned}
&u_t = u_{xx} + q(x,t), && 0 \le x \le 1, \quad t \ge 0,\\
&u(x,0) = f(x), && 0 < x < 1,\\
&u(0,t) = g_1(t), && t > 0,\\
&u(1,t) = g_2(t), && t > 0.
\end{aligned} \tag{2.7}$$

The exact solution to equation (2.7), denoted by $u(x,t)$, is assumed to exist and to have four continuous derivatives with respect to x and two continuous derivatives with respect to t that is, $u \in C^{4,2}$. Let $M \geq 1$ be a given integer and define the grid spacing in the x-direction by $h = \frac{1}{M}$. The grid points in the x-direction are given by $x_i = ih$ for $i = 0, 1, ..., M$. Similarly, define $t_n = nk$ for integer $n \geq 0$, where k denotes the time step. Finally, let u_i^n denote an approximation of $u(x_i, t_n)$. We use forward-difference for u_t and central-difference for u_{xx} evaluated at (x_i, t_n) in (2.7). Thus we can obtain [15, 181, 187]

$$\frac{u_i^{n+1} - u_i^n}{k} = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{h^2} + q_i^n. \tag{2.8}$$

By using the boundary conditions of (2.7), we put

$$u_0^n = g_1(nk), \qquad u_M^n = g_2(nk),$$

for all $n \geq 0$. The scheme is initialized by

$$u_i^0 = f(ih), \qquad i = 1, 2, ..., M-1.$$

Let $s = \frac{k}{h^2}$, then the scheme can be written in a more convenient form [15, 181, 187]

$$u_i^{n+1} = su_{i-1}^n + (1-2s)u_i^n + su_{i+1}^n + kq_i^n, \tag{2.9}$$

where $i = 1, 2, ..., M-1$ and $n = 0, 1, ..., N-1$. When the scheme is written in this form, it should be observed that the values on the time level t_{n+1} are computed using only the values on the previous time level (in this case t_n). Thus the FTCS scheme is an explicit method. The scheme is first order accurate in time ($O(h)$ accurate) and second order accurate in space ($O(h^2)$). Numerical schemes can be unstable in that the accumulated rounding errors become unbounded and overwhelm the solution. Stable explicit methods are usually conditionally stable in that there is a maximum time-step which is allowed. If the time-step is exceeded, the scheme becomes unstable.

2.4.2 Implicit Method (BTCS)

In equation (2.7), if we were to use backward-difference for u_t and central-difference for u_{xx} evaluated at (x_i, t_{n+1}) then we can obtain

$$\frac{u_i^{n+1} - u_i^n}{k} = \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{h^2} + q_i^n, \tag{2.10}$$

for $i = 1, 2, ..., M-1$. The boundary conditions gives

$$u_0^n = g_1(nk), \qquad u_M^n = g_2(nk),$$

for all $n \geq 0$ and the initial condition gives

$$u_i^0 = f(ih), \qquad i = 1, 2, ..., M-1.$$

Thus the following recursive formula is obtained

$$(I + kA)U^{n+1} = U^n, \tag{2.11}$$

where I is identity matrix and A is as

$$A = \frac{1}{h^2}\begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{pmatrix}_{M \times M},$$

We observe that it is not possible to solve (2.11) directly even if we know all values on the right hand side (i.e. the lower time level). In order to compute numerical solution based on this scheme, we have to solve a linear system of the form (2.11) which is non-singular such that U^{n+1} is uniquely determined by U^n. This is an example of an implicit scheme. Implicit schemes are thus not as straightforward to solve as explicit schemes and they require more computations. However stable implicit schemes have the advantage of being unconditionally stable. This means there is no maximum allowable time-step. A large time-step may be useful in many computations. The BTCS scheme is first order accurate in time and second order accurate in space.

2.4.3 Crank-Nicolson Method

In this method, we seek to satisfy the partial differential equation at the midpoint $(ih, (n+\frac{1}{2})k)$. The derivative $\dfrac{\partial^2 u}{\partial x^2}$ is replaced by the mean of its central-difference approximations at the nth and $(n+1)$th time level. The derivative $\dfrac{\partial u}{\partial t}$ at the midpoint is approximated by the use of central-difference. In other words, the finite differences approximate the equation [15, 181]

$$(u_t)_{i,n+\frac{1}{2}} = (u_{xx})_{i,n+\frac{1}{2}} + q_i^n,$$

giving

$$-su_{i-1}^{n+1} + (2+2s)u_i^{n+1} - su_{i+1}^{n+1} = su_{i-1}^{n} + (2-2s)u_i^{n} + su_{i+1}^{n} + 2kq_i^n, \quad (2.12)$$

where $i = 1, 2, \ldots, M-1$, $n = 0, 1, \ldots, N-1$ and $s = \dfrac{k}{h^2}$. (2.12) cannot be solved directly even if all values at the lower time level are known. Thus, the Crank-Nicolson scheme is also an implicit scheme. We will show that the Crank-Nicolson method is unconditionally stable. Further it is second order accurate in both time and space. The structure of the matrix associated with equation (2.12) is such that it is tridiagonal and thus the more economical Thomas algorithm (rather than the Gauss-Elimination method) can be used to solve the system.

2.5 Stability

There are two methods normally used to evaluated the stability of numerical schemes.

2.5.1 Matrix Method

Assume that the vector of solution values $U^{n+1} = [u_1^{n+1}, u_2^{j+1}, \ldots, u_M^{n+1}]$ of the finite difference equations at $(n+1)$th time-level is related to the vector of solution values the nth time level by the equation [181]

$$U^{n+1} = \mathbf{A}U^n + b^n, \tag{2.13}$$

where b_n is a column vector of unknown boundary values and zeroes, and matrix $\mathbf{A}$ an $(N-1)\times(N-1)$ matrix of known elements. For a computation to be stable (in the sense described in section 2.4.1) a norm of matrix $\mathbf{A}$ compatible with a norm of u must satisfy

$$\| \mathbf{A} \| \leq 1,$$

when the solution of the PDE does not increase as t increases, or

$$\| \mathbf{A} \| \leq 1 + O(k),$$

when the solution of PDE increase as t increases.

In an actual computation, the time-step k and space-step h are normally kept constant as the solution is propagated forward time-level by time-level from $t = 0$ to $t_n = nk$, and in many textbooks and papers stability is defined in terms of the bounded-ness of this numerical solution as $n \longrightarrow \infty$, k fixed. In this process, the order $N - 1$ of matrix $\mathbf{A}$ remains constant, unlike $\mathbf{A}$ associated with Lax and Richtmyer's definition. The matrix method of analysis then shows that the equations are stable if the largest of the moduli of the eigenvalues of matrix $\mathbf{A}$, i.e. spectral radius $\rho(\mathbf{A})$ of $\mathbf{A}$, satisfy [181]

$$\rho(\mathbf{A}) \leq 1,$$

when the solution of the differential equation does not increase with increasing t. It is to be noted that the matrix method can be only applied to linear Initial Value Problems (IVPs) with constant coefficients.

2.5.2 Fourier Method

Assume we are concerned with the stability of a linear two time-level difference equation in $u(x,t)$ in the interval $0 \leq t \leq T = nk$, with T finite. The Fourier series expresses the initial value at the mesh points along $t = 0$ in term of finite fourier series. Then consider the growth of a function that reduces to this series for $t = 0$ by a "variables separable" method identical to that commonly used for solving partial differential equation. To explain further, we change our usual notation u_i^n to $u(ph, qk) = u_p^q$. In terms of this notation [181]

$$A_n e^{\frac{in\pi}{l}x} = A_n e^{i\beta_n ph},$$

where $\beta_n = \dfrac{n\pi}{Mh}$, $Mh = l$ and A_n are constant. The initial values at $t = 0$ are displayed by $u(ph, 0) = u_p^0$ for $p = 0, 1, ..., M$. Then the $M + 1$ equations

$$u_p^0 = \sum_{n=0}^{M} A_n e^{i\beta_n ph}, \qquad p = 0, 1, \ldots, M,$$

are sufficient to determine the $n + 1$ unknown $A_0, ..., A_M$ uniquely showing that the initial mesh values can be expressed in this complex exponential form. To investigate the propagation of this term as t increases, put

$$u_p^q = e^{i\beta x} e^{\alpha t} = e^{i\beta ph} e^{\alpha qk} = e^{i\beta ph} \xi^q,$$

where $\xi = e^{\alpha k}$ and α, in general, is a complex constant. ξ is called the amplification factor. The finite-difference equation will be stable if u_p^q remains bounded for all $q \leq J$ as $h \to 0$ and $k \to 0$, and for all values of β needed to satisfy the initial condition. If the exact solution of the difference equation does not increase exponentially with time, then a necessary and sufficient condition for stability is that

$$-1 \leq \xi \leq 1.$$

If u_p^q does increase with t, then the necessary and sufficient condition for stability is

$$|\xi| \leq 1 + Kh = 1 + O(k),$$

where the positive number K is independent of h, k and β.

2.5.3 Stability Condition for the FTCS, BTCS and Crank-Nicolson Method

This section is devoted to stability of FTCS, BTCS and Crank-Nicolson using the matrix method.

Stability of the FTCS :

The FTCS scheme for equation (2.7) can be written as [181]

$$u_i^{n+1} = su_{i-1}^n + (1-2s)u_i^n + su_{i+1}^n + kq_i^n, \tag{2.14}$$

for $i = 1, 2, ..., M-1$. It can be expressed in the following matrix form

$$\begin{pmatrix} u_1^{n+1} \\ u_2^{n+1} \\ \vdots \\ \vdots \\ u_{M-1}^{n+1} \end{pmatrix} = \begin{pmatrix} 1-2s & s & & & \\ s & 1-2s & s & & \\ & \ddots & \ddots & \ddots & \\ & & s & 1-2s & s \\ & & & s & 1-2s \end{pmatrix} + \begin{pmatrix} su_0^n + kq_1^n \\ kq_2^n \\ \vdots \\ kq_{M-2}^n \\ su_M^n + kq_{M-1}^n \end{pmatrix},$$

i.e.

$$U^{n+1} = \mathbf{A}U^n + b, \tag{2.15}$$

where

$$\mathbf{A} = \begin{pmatrix} 1-2s & s & & & \\ s & 1-2s & s & & \\ & \ddots & \ddots & \ddots & \\ & & s & 1-2s & s \\ & & & s & 1-2s \end{pmatrix}, \qquad b = \begin{pmatrix} su_0^n + kq_1^n \\ kq_2^n \\ \vdots \\ kq_{M-2}^n \\ su_M^n + kq_{M-1}^n \end{pmatrix},$$

where $n = 0, 1, \ldots, N-1$ and $s = \dfrac{h}{k^2}$. Now, we can write the matrix $\mathbf{A}$ as

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & & & \\ 0 & 1 & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & 1 & 0 \\ & & & 0 & 1 \end{pmatrix} + s \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix} = I_{M-1} + sT_{M-1},$$

where I_{M-1} is the unite matrix of order $(M-1)$ and T_{M-1} an $(M-1)\times(M-1)$ tridiagonal matrix. It can be shown the eigenvalues of T_{m-1} are

$$\lambda_k = -4\sin^2\frac{k\pi}{2M}, \qquad k = 1, 2, \ldots, M-1.$$

Hence the eigenvalues of $\mathbf{A}$ are $\mu_k = 1 - 4s\sin^2\dfrac{k\pi}{2M}$. Therefore the equations will be stable when

$$\| A \|_2 = \max|1 - 4s\sin^2\frac{k\pi}{2M}| \leq 1,$$

i.e.,

$$-1 \leq 1 - 4s\sin^2\frac{k\pi}{2M} \leq 1, \qquad k = 1, 2, \ldots, M-1.$$

The left hand inequality gives

$$0 < s \leq \frac{1}{2}\sin^2\frac{k\pi}{2M}.$$

Hence

$$0 < s \leq \frac{1}{2}.$$

Stability of the BTCS :

The BTCS scheme for equation (2.7) can be written as [181]

$$-su_{i-1}^{n+1} + (1+2s)u_i^{n+1} - su_{i-1}^{n+1} = u_i^n + kq_i^n, \tag{2.16}$$

for $i = 1, 2, ..., M-1$. In matrix form, for known boundary values, these give

$$\begin{pmatrix} 1+2s & -s & & & \\ -s & 1+2s & -s & & \\ & \ddots & \ddots & \ddots & \\ & & -s & 1+2s & -s \\ & & & -s & 1+2s \end{pmatrix} \begin{pmatrix} u_1^{n+1} \\ u_2^{n+1} \\ \vdots \\ u_{M-2}^{n+1} \\ u_{M-1}^{n+1} \end{pmatrix} =$$

$$\begin{pmatrix} u_1^n \\ u_2^n \\ \vdots \\ u_{M-2}^n \\ u_{M-1}^n \end{pmatrix} + \begin{pmatrix} su_0^n + kq_1^n \\ kq_2^n \\ \vdots \\ kq_{M-2}^n \\ su_M^n + kq_{M-1}^n \end{pmatrix},$$

where $n = 0, 1, \ldots, N-1$ and $s = \dfrac{h}{k^2}$. This can be written as

$$(I_{M-1} + sT'_{M-1})\mathbf{U}^{n+1} = \mathbf{U}^n + b,$$

from which it follows that matrix $\mathbf{A}$ of equation (2.16) is

$$\mathbf{A} = (I_{M-1} + sT'_{M-1})^{-1},$$

where I_{M-1} is the unite matrix of order $(M-1)$ and T'_{M-1} an $(M-1)\times(M-1)$