NUMERICAL SOLUTIONS FOR TWO DIMENSIONAL TIME-FRACTIONAL DIFFERENTIAL SUB-DIFFUSION EQUATION

by

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LIST OF ABBREVIATIONS

FPDE	Fractional partial differential equation
PDE	Partial differential equation
FDM	Finite difference method
1D	One dimensions
2D	two dimensions
C-N	Crank-Nicolson
CPDEs	classical partial differential equations
IFD	implicit finite difference
TFSDE	Time fractional sub-diffusion equation
TFMSDE	Time fractional modified sub-diffusion equation
MSDE	modified sub-diffusion equation
MIDS	Modified implicit difference scheme
RSP-HGSGF	Rayleigh-Stokes problem for a heated generalized second grade fluid

PENYELESAIAN BERANGKA BAGI PERSAMAAN PEMBEZAAN PECAHAN MASA SUB-RESAPAN DUA DIMENSI

ABSTRAK

Dalam beberapa dekad kebelakangan ini, persamaan pembezaan pecahan (persamaan pembezaan yang melibatkan peringkat rambang) telah menjana kepopularitian dalam bidang sains dan kejuruteraan. Ini kerana persamaan sedemikian dapat memodelkan dengan baik permasalahan khususnya dalam bidang mekanik bendalir, fizik, sains biologi, kimia, hidrologi dan kewangan kerana ia boleh mewakili sistem dengan memori dengan baik. Walau bagaimanapun, kebanyakan persamaan pembezaan pecahan tidak dapat diselesaikan dengan teknik analitikal tepat. Dengan itu, anggaran kaedah analitikal dan berangka diperlukan dalam menyelesaikan persamaan pembezaan pecahan ini. Objektif utama tesis ini adalah untuk membangunkan, menganalisis dan menggunakan kaedah berangka berdasarkan kaedah beza terhingga untuk menyelesaikan persamaan pembezaan separa pecahan masa dua dimensi. Kaedah beza terhingga seperti beza terhingga tersirat, beza terhingga jelas dan kaedah Crank-Nicolson bagi penyelesaian persamaan pembezaan pecahan masa sub-resapan tak homogen dua dimensi dibangunkan. Di samping itu, kaedah padat tersirat, kaedah padat yang jelas dan kaedah padat Crank-Nicolson bagi persamaan pembezaan pecahan masa sub-resapan juga disiasat. Skema beza tersirat juga diubahsuai dan digunakan untuk persamaan pembezaan pecahan masa sub-resapan ganjil melibatkan dua kali pembezaan pecahan masa dan masalah Rayleigh-Stokes bagi pemanasan cecair gred kedua dalam pembezaan pecahan. Selanjutnya, untuk membuktikan keberkesanan bagi cadangan skema tersirat yang diubahsuai tersebut, teknik ini akan diaplikasi pada persamaan diubahsuai pecahan sub-resapan ganjil peringkat pembolehubah dan masalah Rayleigh-Stokes bagi pemanasan cecair gred kedua dalam pembezaan pecahan peringkat pembolehubah. Kestabilan dan penumpuan bagi skema-skema yang dicadangkan akan dianalisis melalui kaedah kestabilan von-Neumann. Eksperimen berangka dijalankan dan keputusan eksperimen ini menunjukkan skema-skema yang dicadangkan itu menunjukkan prestasi yang sangat baik.

NUMERICAL SOLUTIONS FOR TWO DIMENSIONAL TIME-FRACTIONAL DIFFERENTIAL SUB-DIFFUSION EQUATION

ABSTRACT

In the past several decades, fractional differential equations (differential equation involving arbitrary order derivatives) have acquired much popularity in the area of science and engineering. This is because such equations can better model certain problems of fluid mechanics, physics, biological science, chemistry, hydrology and finance, amongst others, due to the fact that it can better represent system with memory. However, most fractional differential equations cannot be solved by exact analytical techniques. Thus, approximate analytical and numerical methods are required in the solution of such fractional differential equations. The main objectives of this thesis is to develop, analyze and apply numerical methods based on the finite difference approximations for solving the two-dimensional time fractional partial differential equation. Finite difference methods such as implicit finite difference, explicit finite difference and Crank-Nicolson methods for the solution of two-dimensional time fractional inhomogeneous sub-diffusion equation are constructed. In addition, compact implicit, compact explicit and compact Crank-Nicolson methods for time fractional sub-diffusion equation are also investigated. An implicit difference scheme is also modified and applied to modified fractional anomalous sub-diffusion equation involving two times fractional derivatives and Rayleigh-Stokes problem for a heated generalized second grade fluid with fractional derivative. Further, to establish the effectiveness of the proposed modified implicit scheme, the scheme is applied to modified fractional variable order anomalous sub-diffusion equation and Rayleigh-Stokes problem for a heated generalized second grade fluid with variable order fractional derivative. The stability and convergence of the proposed numerical schemes are analyzed by the von-Neumann stability method. Numerical experiments are conducted, which shows that the finite difference schemes are easy to implement and the results indicate good performance of the proposed schemes.

CHAPTER 1

INTRODUCTION

Real life phenomena are modelled in different ways depending on the phenomena at hand. Some of these phenomena can be modelled by partial differential equations and some by ordinary differential equations. Recently fractional partial differential equation have been developed from classical partial differential equation by replacing the fractional derivative of order α (in the Riemann-Liouville or Caputo sense) to model phenomena which are not adequately modelled by partial differential equations (Zhuang and Liu, 2007). The focus of this thesis is the study of numerical methods to find the solution of fractional differential equations.

The concept of fractional calculus is as old as classical calculus (integer order integrals and derivatives). According to Miller and Ross (1993), at the end of seventeenth century the discussion between L'Hôspital and Leibniz was believed to be the first discussion about fractional calculus. Many famous mathematicians worked on this and made contributions, a list of mathematicians includes Laplace, Fourier, Abel, Liouville, Riemann, Günwald, Letnikov, Heaviside, Levy, Riesz and Erdelyi (Yang, 2010). More recent attention in this field started in 1968 when it was realized that the use of fractional order integrals and derivatives plays an important role in the solution of certain chemical problems. These chemical problems relate to Fick's law of diffusion. Since then there have been many interesting applications of non integer order integrals and derivative operators and rapid theoretical development.

Many researchers have written books on fractional calculus and applications. These include Oldham and Spanier (1974), Samko et al. (1993), and Miller and Ross (1993). The most famous book in the field of fractional calculus is Podlubny (1999) which explain the fundamental theory of fractional calculus, applications and their solution. The book of Zaslavsky (2005), Kilbas et al. (2006), Sabatier et al. (2007), and numerical techniques for fractional ordinary differential and FPDEs have been discussed in Li and Zeng (2015).

Fractional differential equations provide a powerful tool for the description of memory and hereditary properties of different substances (Khan and Faraz, 2011). There has been increased research studies conducted on fractional differential equations over the last two decades or so with the tempo rising over the last few years. A cursory examination of relevant databases can easily verify this. For example in 2015 there were 1090 publications in scopus, 1216 in 2016, 1516 in 2017, and 1639 in 2018.

One particular fractional differential equation which has attracted much interest due to numerous important applications is the fractional diffusion equations (FDE). It has the form

$$ {}_0D_t^{\alpha}u(x,t) = \Delta u(x,t), \tag{1.1} $$

where D represent the differential operator, 0 and t are intervals of integration, Δ is the Laplace operator and α is positive real number. If $\alpha > 1$, we have anomalous super diffusion or super diffusion for short. This is the case when the diffusion is enhanced due to active transport process (Caspi et al., 2000). If $0 < \alpha < 1$, then we have anomalous sub-diffusion or sub-diffusion for short. This is the case when we have crowded system situation or increasing in the concentration of particles (Weiss et al., 2004). If $\alpha = 1$, then the classical diffusion is obtained (Henry and Wearne, 2000;

Mainardi and Pagnini, 2007);

$$
{}_0D_t u(x,t) = \Delta u(x,t). \tag{1.2}
$$

The advantage of the FDE is that it can better represent super diffusion and sub-diffusion than the classical diffusion equation.

For instance, in hydrology the trapping interval times of contaminants in groundwater and in biology, the diffusion of proteins across the cell membranes can be explained by sub-diffusion behaviour more accurately than the classical diffusion. A super-diffusive process is a process in which the mean-squared displacement grows faster than in normal-diffusion (Klafter and Sokolov, 2005). During a continuous time random walk process, the range of jumps and the duration between two consecutive jumps are assumed by different probability density functions which leads to different fractional models such as fractional heat, kinetic, advection-dispersion, Fokker-Plank, Riesz kinetic models (Angulo et al., 2000; Povstenko, 2014; Zaslavsky, 2002; Ciesielski and Leszczynski, 2005; Liu et al., 2004). Some researchers have explained that derivatives and integrals of fractional order are more appropriate for modelling the memory and hereditary properties of different materials and process by anomalous diffusion (Yang, 2010). Fractional derivative have been applied to many problems in physics (Barkai et al., 2000), finance (Sabatelli et al., 2002), materials (Diethelm and Freed, 1999) and control theory (Podlubny, 1999).

Fractional differential equations are not easy to solve by analytical methods and thus numerical techniques are often used. Amongst numerical approximation techniques, finite difference methods are established and are often used due to its simplicity and ease of implementation (Mattheij et al., 2005).

1.1 Motivation

Fractional differential equations (FDEs) are derived from classical differential equations and can, in certain situations, describe physical phenomena more accurately than the integer order counterparts (Gong et al., 2015). Many problems in different fields of science related to time or space or space-time fractional derivatives can be modelled by fractional differential equations (FDEs). The significant problem that is considered in this thesis is the solution of FPDEs. The shape of area of integration, the complicated boundary or initial conditions of differential equations and the nonlinear terms often make analytical solutions of FPDEs difficult or impossible. Thus, we should have a large number of numerical methods available to deal with various FPDEs describing various situations. Further, the methods should be reasonably straight forward and effective. This gives one motivation to develop more numerical methods to solve FDEs. Specifically, in solving the time-fractional sub-diffusion, modified sub-diffusion and Rayleigh-Stokes (constant and variable-order) problems. Furthermore, most problems that have been considered are one dimensional, and there are relatively few studies about numerical methods suitable for two dimensional problems. Herein lies another motivation. The final motivation is the fact that the existing numerical methods do not often make use of the Grunwald-Letnikov formula and the discretized Riemann-Liouville fractional formula. The advantage of these formulaes is that they are simple to apply numerically as compared to the more frequently used Caputo formula.

The purpose of this research then is to develop effective finite difference methods (FDMs), compact finite difference methods (CFDMs) and modified implicit difference method (MIDM) to obtain reasonably accurate approximate solutions of 2D FDEs.

This research will be beneficial in the mathematical modeling of various phenomena that can be modeled by 2D fractional differential equations.

1.2 Research Objectives

The objectives of this research are as follows:

1. To develop implicit, explicit and Crank-Nicolson numerical methods for the solution of the 2D time-fractional sub-diffusion equations.
2. To develop compact formulation for the above methods to solve the 2D time-fractional sub-diffusion equations.
3. To modify an implicit numerical scheme and apply on the 2D time-fractional modified sub-diffusion equation (TFMSDE) and Rayleigh-Stokes problem for a heated generalized second grade fluid (RSP-HGSGF) with fractional derivative, and compare the results with previous studies.
4. To apply the modified implicit difference scheme on the 2D fractional variable order modified sub-diffusion equation (MSDE) and fractional variable order RSP-HGSGF, and compare the results with previous studies.
5. To investigate the stability and convergence of the methods discussed above.

1.3 Methodology

The methodology used in this study are as follows:

1. Discretize the 2D FDE by Riemann-Liouville derivative fractional formula and Grünwald-Letnikov fractional formula.
2. The finite difference approximations will be carried out for 2D TFSDE, TFMSDE, RSP-HGSGF with fractional derivative, variable order TFMSDE and variable order

fractional RSP-HGSGF.

3. Investigate the stability and convergence of the methods using von-Neumann (Fourier) analysis.

4. Conduct and discuss numerical experiments by using the PC with 2.93 GHz Core 2 Duo, 2 Gb of RAM, Window 7 Professional and Maple 15 software, for the proposed schemes.

1.4 Organization of the Thesis

Description of the chapters contained in this thesis are as follows:

Chapter 2 contains the basic concepts and background of fractional calculus with definitions and properties. The review of literature of numerical methods for the solution of TFSDE, TFMSDE and RSP-HGSGF with fractional derivative are also part of this chapter. Chapter 3 contains some discussion of fundamental numerical methods for solving TFSDE, such as implicit, explicit and Crank-Nicolson methods, as well as stability and convergence analysis. Numerical results are also included in this chapter. Chapter 4 discusses the solution of TFSDE by using compact numerical methods such as: compact implicit, compact explicit and compact Crank-Nicolson methods. It also contains analysis and numerical experiments. Chapter 5 contains the solution of TFMSDE and RSP-HGSGF by modified difference scheme (MIDS). In Chapter 6, we extend MIDS to variable order fractional MSDE and RSP-HGSGF. Analysis and numerical experiments are also included in the same chapter. Chapter 7 presents the conclusion and discusses some related future work.

CHAPTER 2

BASIC CONCEPTS AND LITERATURE REVIEW

2.1 Introduction

In this chapter, we discuss preliminary concepts and give a detailed background of fractional derivatives. Fractional (partial and ordinary) differential equations (FDE) are used as tools to describe real life phenomena in nature and their solution are of importance in science and engineering. Here, we also review existing numerical methods for 2D-TFSDE, TFMSDE and RSP-HGSGF with fractional derivative.

2.2 Classifications of Partial Differential Equations

Partial differential equations can be defined as rate of change of dependent variable (usually denoted u) with respect to two or more independent variables (usually denoted by $x, y, z, \ldots t$) is known as PDE. The highest derivative in the equation is called order of the equation.

Consider the generalized form of PDE for two variables, x, y (Smith, 1985),

$$Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu = G. \tag{2.1}$$

The above equation will be linear if A, B, C, D, E, F and G are constants or functions of independent variables x, y. If A, B, C, D, E, F are function of u then equation (2.1) will be nonlinear. The type of second order PDE (2.1) can be determined by the discriminant formula as

$$Discriminant = B^2 - 4AC. \tag{2.2}$$

The classification of PDEs can be written as (Lynch, 2004),

if, $B^2 - 4AC < 0$, elliptic; for example, Poisson equation $u_{xx} + u_{yy} = G$,

if, $B^2 - 4AC = 0$, parabolic; for example, diffusion equation $u_t - u_{xx} = 0$,

if, $B^2 - 4AC > 0$, hyperbolic; for example, Wave equation $u_{tt} - u_{xx} = 0$.

2.3 Fractional Calculus

Fractional calculus is a powerful tool for modeling complex system. The concept of fractional order derivative is the main idea of fractional calculus. Many researchers have defined fractional order integrals and derivatives by different ways.

2.3.1 Fractional Integrals

In the literature, a fractional order, $\gamma > 0$ integral is denoted by the notations ${}_aD_t^{-\gamma}$ or ${}_aI_t^{\gamma}$ and for variable order, replace γ by $\gamma(x,y,t)$. Here, a and t are the intervals (limits) of the integral operator from a to t and these are generally called the terminals of the fractional integral (Podlubny, 1999). In the literature, there are many definitions of fractional order integration as follows:

2.3.1(a) Definition of Fractional Integral

There are many types of fractional integrals such as Hadamard, Weyl, Chen, local fractional Yang Cossar etc (Oliveira and Machado, 2014). But one of the important ones is Riemann-Liouville fractional integral, because it can be easily converted into discretized form.

The left side of Riemann-Liouville integral can be written as (Yang, 2010);

$$_{a^+}D_t^{-\gamma}f(t) = {_aI_t^{\gamma}}f(t) = \frac{1}{\Gamma(\gamma)}\int_a^t \frac{f(\xi)}{(t-\xi)^{1-\gamma}}d\xi, \ \text{t} \geq a. \tag{2.3}$$

The right side of Riemann-Liouville integral is;

$$_{a^-}D_x^{-\gamma}f(t) = \frac{1}{\Gamma(\gamma)}\int_t^x \frac{f(\xi)}{(\xi-t)^{1-\gamma}}d\xi, \ \text{x} \leq t. \tag{2.4}$$

The equations (2.3) and (2.4) will become the variable order fractional integral by using $\gamma(x,t)$ in place of γ. Some properties of Riemann-Liouville integral are as follows; (Diethelm, 2010)

$$I^0 f(t) = f(t),$$

$$I^\alpha I^\beta f(t) = I^{\alpha+\beta} f(t),$$

$$I^\alpha I^\beta f(t) = I^\beta I^\alpha f(t),$$

$$I^\alpha t^\gamma = \frac{\Gamma(\gamma+1)}{\Gamma(\alpha+\gamma+1)} t^{\alpha+\beta}.$$

2.3.2 Fractional Derivatives

The non-integer order derivative describes the derivative of fractional order. There are many notations in the literature represent the fractional order derivatives, such as

$$D_{aJ}^{\gamma}f(t) = (D_{aJ}^{\gamma}f)(t) =_a D_t^{\gamma}f(t) =_a I_t^{-\gamma}f(t) = \frac{\partial^\gamma}{\partial t^\gamma}f(t) \ . \tag{2.5}$$

Equation (2.5) shows notations used for fractional derivatives operator, the mostly used notation is $_aD_t^{\gamma}$. Here a and t are the limits of integration. For left and right sided fractional derivatives, some authors are using ${}_{a^+}D_t^{\gamma}$, ${}_{a^-}D_t^{\gamma}$ or ${}_{+}D_t^{\gamma}$, ${}_{-}D_t^{\gamma}$ respectively. In this thesis, we are using the notation ${}_aD_t^{\gamma}f(t)$ for fractional order derivatives.

2.3.2(a) Definitions of Fractional Derivatives

The generalized form of the left side of Riemann-Liouville fractional derivative is written as; (Heymans and Podlubny, 2006; Meerschaert and Tadjeran, 2006)

$$ {}^{RL}_{a^+}D_t^{\gamma}f(t) = \frac{1}{\Gamma(n-\gamma)}\left(\frac{d^n}{dt^n}\right)\int_a^t f(\eta)(t-\eta)^{n-\gamma-1}d\eta, \quad t \geq a. \tag{2.6} $$

The right side of Riemann-Liouville fractional derivative is;

$$ {}^{RL}_{t}D_{c^-}^{\gamma}f(t) = \frac{(-1)^n}{\Gamma(n-\gamma)}\left(\frac{d^n}{dt^n}\right)\int_t^c f(\eta)(\eta-t)^{n-\gamma-1}d\eta, \quad t \leq c. \tag{2.7} $$

The left side of Grünwald-Letnikov derivative (Meerschaert and Tadjeran, 2006) is;

$$ {}^{GL}D_+^{\gamma}f(t) = lim_{n_+\to\infty}\frac{1}{\tau^{\gamma}}\sum_{k=0}^{n_+} g_k f(t-k\tau). \tag{2.8} $$

The right side of Grünwald-Letnikov derivative is;

$$ {}^{GL}D_-^{\gamma}f(t) = lim_{n_-\to\infty}\frac{1}{\tau^{\gamma}}\sum_{k=0}^{n_-} g_k f(t+k\tau), \tag{2.9} $$

where n_-, n_+ are positive integers, and the coefficient function g_k can be defined by $g_0 = 1$, $g_k = (1-\frac{\alpha+1}{k})g_{k-1}$.

The left side of Caputo fractional derivative is (Yang et al., 2015)

$$ {}_{a^+}^{c}D_t^{\gamma} f(t) = \frac{1}{\Gamma(n-\gamma)} \int_a^t (t-\eta)^{n-\gamma-1} \frac{d^n}{d\eta^n} f(\eta) d\eta, \quad t \geq a. \tag{2.10} $$

The right side of Caputo fractional derivative is

$$ {}_t^{c}D_{b^-}^{\gamma} f(t) = \frac{(-1)^n}{\Gamma(n-\gamma)} \int_t^c (\eta - t)^{n-\gamma-1} \frac{d^n}{d\eta^n} f(\eta) d\eta, \quad t \leq a. \tag{2.11} $$

Properties of Caputo fractional derivative are as follows;

$$ {}_0D_t^{\alpha} t^{\gamma} = \frac{\Gamma(\gamma+1)}{\Gamma(\alpha-\gamma+1)} t^{\gamma-\alpha}, $$
$$ J^{\alpha} D_t^{\alpha} f(t) = f(t) - \sum_{m=0}^{n-1} \frac{f^{(k)}(0)}{k!} t^m, \quad x > 0. $$

Marchaud derivative is given by (Yang et al., 2015);

$$ {}_{-\infty}D_t^{\gamma} f(t) = \frac{\gamma}{\Gamma(1-\gamma)} \int_{-\infty}^t (f(t) - f(\eta))(t-\eta)^{-(\gamma+1)} d\eta. \tag{2.12} $$

The Liouville fractional derivative is obtained as (Oliveira and Machado, 2014);

$$ D^{\gamma} f(t) = \frac{1}{\Gamma(1-\gamma)} \frac{d}{dx} \int_{-\infty}^t f(\eta)(t-\eta)^{-\gamma} d\eta, \quad -\infty < x < +\infty. \tag{2.13} $$

The Riesz fractional derivative is (Yang, 2010);

$$ D_t^{\gamma} f(t) = -\frac{1}{2cos(\frac{\gamma\pi}{2})} \frac{1}{\Gamma(\gamma)} \frac{d^k}{dt^k} \Big(\int_{-\infty}^t (t-\eta)^{k-\gamma-1} f(\eta) d\eta + \int_t^{\infty} (\eta - t)^{k-\gamma-1} f(\eta) d\eta \Big). \tag{2.14} $$

The fractional modified Riemann-Liouville derivative is (Jumarie, 2006);

$$D_t^{\gamma} f(t) = \frac{1}{\Gamma(1-\gamma)} \frac{d}{dt} \int_0^t (t-\eta)^{-\gamma} (f(\eta) - f(0) d\eta. \qquad (2.15)$$

Some properties of fractional modified Riemann-Liouville derivative are as follows (Jumarie, 2006, 2009):.

$$D_t^{\gamma} c = 0,\ \gamma > 0,\ c = constant,$$

$$D_t^{\alpha} t^{\gamma} = \frac{\Gamma(\alpha+1)}{\Gamma(\beta-\alpha+1)} t^{\beta-\alpha},\ \alpha > 0,\ \gamma > 0,$$

$$D_t^{\alpha}[cf(t)] = cD_t^{\alpha} f(t),\ \alpha > 0,\ c = constant,$$

$$\int_0^t t^{\gamma} (dt)^{\beta} = \frac{\Gamma(\gamma+1)\Gamma(\beta+1)}{\Gamma(\gamma+\beta+1)} t^{\gamma+\beta},\ 0 < \gamma \leq 1,$$

$$\frac{1}{\Gamma(\alpha)} \int_0^t (t-\xi)^{\alpha-1} f(\xi) d\xi = \frac{1}{\Gamma(\alpha+1)} \int_0^t f(\xi)(d\xi)^{\alpha},\ \alpha > 0.$$

2.3.2(b) Relationship of Fractional Derivatives

In the literature, there are many definitions of fractional derivatives, but three of them are more important. The three fractional derivatives are Riemann-Liouville, Caputo and Grünwald-Letnikov. This is due to the definitions of the fractional derivatives itself that can be converted easily into discretized form for the numerical methods; (see for instance, Zhuang and Liu (2006); Chen et al. (2013); Al-Shibani and Ismail (2015)).

The relation between Caputo and Riemann-Liouville fractional derivative can be derived as (Lin and Jiang, 2011; Hackbusch, 2012);

$$^{RL}D_t^{1-\gamma} f(x,y,t) = {}^{c}D_t^{1-\gamma} f(x,y,t) + \frac{f(x,y,0)}{\Gamma(\gamma) t^{1-\gamma}}, \qquad (2.16)$$

where c means Caputo fractional derivative and RL means Riemann-Liouville.

The two fractional derivatives in equations (2.6) and (2.10) are equivalent if and only if the initial condition $f(x,y,0)$ is zero.

The time-fractional Grünwald-Letnikov formula is defined by (Zhai et al., 2014).

$$D_t^{\gamma} f(x,y,t) = \frac{f(x,y,0)t^{-\alpha}}{\Gamma(1-\gamma)} + \frac{1}{\Gamma(1-\gamma)} \int_0^t (t-\eta)^{-\gamma} \frac{d}{d\eta} f(x,y,\eta) d\eta, \tag{2.17}$$

The Caputo and Grünwald-Letnikov fractional derivative are equivalent if the initial conditions are $f(x,y,0) = 0$. From the definitions in equations (2.16) and (2.17), it is clear that all three fractional derivatives are equivalent if the initial conditions are zero.

2.4 Finite Difference Method

The FDMs are numerical methods which are efficient and universally applicable for solving differential equations. Numerical methods compute the approximate solution and the main idea of finite difference methods is to replace the derivatives in the differential equation by finite difference approximations. Solving the resulting algebraic equations will result in the approximate solutions of the original differential equation.

Let the approximate solution of the continuous function $u(x,y,t)$ at the grid point $u(x_i,y_j,t_k)$ be denoted by $u_{i,j}^k$. Taylor series play a great role to formulate and derive the approximation for the derivatives. The Taylor series expansion approximating the derivatives at the grid point (x_i,y_j,t_k) with respect to x are is as follows:

$$u_{i+1,j}^{k} = u_{i,j}^{k} + \frac{(\Delta x)}{1!} u_x(x,y,t)\Big|_{i,j}^{k} + \frac{(\Delta x)^2}{2!} u_{xx}(x,y,t)\Big|_{i,j}^{k} + \frac{(\Delta x)^3}{3!} u_{xxx}(x,y,t)\Big|_{i,j}^{k} + \ldots. \tag{2.18}$$

and

$$u_{i-1,j}^{k} = u_{i,j}^{k} - \frac{(\Delta x)}{1!} u_x(x,y,t)\Big|_{i,j}^{k} + \frac{(\Delta x)^2}{2!} u_{xx}(x,y,t)\Big|_{i,j}^{k} - \frac{(\Delta x)^3}{3!} u_{xxx}(x,y,t)\Big|_{i,j}^{k} + \ldots \tag{2.19}$$

In equation (2.18), Δx is a space step size assumed to be sufficiently small. By neglecting the fourth and higher terms, we can write (Atkinson and Han, 2005)

$$u_x(x,y,t)\Big|_{i,j}^{k} = \frac{u_{i+1,j}^{k} - u_{i,j}^{k}}{(\Delta x)} - \frac{(\Delta x)}{2!} u_{xx}(x,y,t)\Big|_{i,j}^{k} - \frac{(\Delta x)^2}{3!} u_{xxx}(x,y,t)\Big|_{i,j}^{k} + \ldots, \tag{2.20}$$

$$= \frac{u_{i+1,j}^{k} - u_{i,j}^{k}}{(\Delta x)} + O(\Delta x). \tag{2.21}$$

Similarly from equation (2.19), we can get

$$\begin{aligned} u_x(x,y,t)\Big|_{i,j}^{k} &= \frac{u_{i,j}^{k} - u_{i-1,j}^{k}}{(\Delta x)} - \frac{(\Delta x)}{2!} u_{xx}(x,y,t)\Big|_{i,j}^{k} - \frac{(\Delta x)^2}{3!} u_{xxx}(x,y,t)\Big|_{i,j}^{k} \ldots, \\ &= \frac{u_{i+1,j}^{k} - u_{i,j}^{k}}{(\Delta x)} + O(\Delta x). \end{aligned} \tag{2.22}$$

Now by subtracting (2.19) from (2.18), we get

$$\begin{aligned} u_x(x,y,t)\Big|_{i,j}^{k} &= \frac{u_{i+1,j}^{k} - u_{i-1,j}^{k}}{2(\Delta x)^2} - \frac{(\Delta x)^2}{3!} u_{xxx}(x,y,t)\Big|_{i,j}^{k} - \frac{(\Delta x)^4}{5!} u_{xxxxx}(x,y,t)\Big|_{i,j}^{k} \ldots, \\ &= \frac{u_{i+1,j}^{k} - u_{i-1,j}^{k}}{2(\Delta x)} + O(\Delta x)^2. \end{aligned} \tag{2.23}$$

The truncated terms, $O(\Delta x)$ are known as truncation error or discretization error because finite numbers of discrete terms are used to approximate the derivative of continuous function. The error is inversely proportional to the number of space step size,

$O(\Delta x)$. The error can be minimized but it is unavoidable. Dropping $O(\Delta x)$ from the equations (2.21), (2.22) and (2.23), we get the approximate discretized form as

$$u_x(x,y,t)\Big|_{i,j}^{k} \approx \frac{u_{i+1,j}^{k} - u_{i,j}^{k}}{(\Delta x)}, \tag{2.24}$$

$$u_x(x,y,t)\Big|_{i,j}^{k} \approx \frac{u_{i,j}^{k} - u_{i-1,j}^{k}}{(\Delta x)}, \tag{2.25}$$

and the central difference approximation for the first order derivative,

$$u_x(x,y,t)\Big|_{i,j}^{k} \approx \frac{u_{i+1,j}^{k} - u_{i-1,j}^{k}}{2(\Delta x)}. \tag{2.26}$$

The equations (2.24), (2.25) and (2.26) represent forward difference, backward difference and central difference approximations respectively, for the first order derivative. The central difference approximation is more accurate because the truncation errors have a higher order. Now, to approximate the second order derivative, by adding equations (2.18) and (2.19), the central difference approximation is obtained:

$$\begin{aligned} u_{xx}(x,y,t)\Big|_{i,j}^{k} &= \frac{u_{i+1,j}^{k} - 2u_{i,j}^{k} + u_{i-1,j}^{k}}{(\Delta x)^2} + \frac{2(\Delta x)^2}{4!} u_{xxxx}(x,y,t)\Big|_{i,j}^{k} + \ldots \\ &= \frac{u_{i+1,j}^{k} - 2u_{i,j}^{k} + u_{i-1,j}^{k}}{(\Delta x)^2} + O(\Delta x^2). \end{aligned} \tag{2.27}$$

Similarly, the following difference formulas for the first order derivative with respect to y; $u_y(x,y,t)\Big|_{i,j}^{k}$ can be obtained:

Forward difference formula ;

$$u_y(x,y,t)\Big|_{i,j}^{k} \approx \frac{u_{i,j+1}^{k} - u_{i,j}^{k}}{(\Delta y)}, \tag{2.28}$$

Backward difference formula ;

$$u_y(x,y,t)\Big|_{i,j}^{k} \approx \frac{u_{i,j}^{k} - u_{i,j-1}^{k}}{(\Delta y)}, \tag{2.29}$$

Central difference formula ;

$$u_y(x,y,t)\Big|_{i,j}^{k} \approx \frac{u_{i,j+1}^{k} - u_{i,j-1}^{k}}{2(\Delta y)}, \tag{2.30}$$

Central difference formula for the second order derivative ;

$$u_{yy}(x,y,t)\Big|_{i,j}^{k} = \frac{u_{i,j+1}^{k} - 2u_{i,j}^{k} + u_{i,j-1}^{k}}{(\Delta y)^2} + O(\Delta y)^2. \tag{2.31}$$

2.5 Truncation Error and Consistency

The truncation error, $T_{i,j}^{n}$ is the value by which the exact solution of the PDEs is not able to satisfy the approximate equation. Here, n refers to time level. Let $F_{i,j}^{n}(U) = 0$ represents approximate equation of the PDE at mesh point (i, j, n), with the exact solution U. If U is replaced by u, the value of $F_{i,j}^{n}(u)$ is called the local truncation error $T_{i,j}^{n}$.

If the local truncation error, $T_{i,j}^{n}$ approaches zero as the sizes of the mesh point $(\Delta x, \Delta y, \Delta t)$ approaches zero, the approximate equation is said to be consistent (Smith, 1985).

2.6 Convergence

A scheme is said to be convergent if the difference between the numerical solution at a fixed point in the domain of interest tends to zero uniformly as the space and the time discretizations tends to zero.

Suppose $u(x,y,t)$ denote the exact solution of a PDE and $u_{i,j}^n$ is the computed approximate solution of PDE constructed by finite difference scheme (FDS). The constructed scheme is said to be convergent if an approximate solution, $u_{i,j}^n$ tends to $u(x,y,t)$ as the steps size $\Delta x, \Delta y$ and Δt approaches zero (Fletcher, 1988). The difference between the approximate solution $u_{i,j}^n$ and the exact solution $U(x,y,t)$ is known as the solution error, which is represented by $e_{i,j}^n$ as in the following:

$$e_{i,j}^n = U(x,y,t) - u_{i,j}^n.$$

2.7 Stability

A numerical scheme is said to be stable if the error solution (the difference between exact and approximate solution) remains bounded as the number of steps tends to infinity. According to Lax Equivalence theorem, consistency and stability are both necessary and sufficient for convergence (Irudayaraj and Jun, 2008). Proving that the numerical solution is convergent will not only validate that the discrete form of the equations represents a faithful representation of the continuum ones, but also the solution will be bounded at all times (Rezzolla, 2011). There are many methods to find the stability, but the mostly used for investigating the stability are the von-Neumann method and matrix method due to their easy implementation. In the thesis we will be analyzing the stability by von Neumann method (Fourier series analysis) for the TFSDE, TFMSDE, RSP-HGSGF with fractional derivative, variable order TFMSDE and fractional variable order RSP-FGSGF.

2.8 Von Neumann Method

Von Neumann method for stability analysis was introduced by John von Neumann in the mid-twentieth century (Olver, 2008). It is not easy to find the stability directly from the definition. Thus, an easy way is to use tools from the Fourier series to find the stability of the finite difference schemes.

2.9 Literature Review

This literature review is organized based on the types of equation. First, the two-dimensional TFSDE will be considered. Secondly, the literature studied is related to the fractional order (fixed and variable order) TFMSDE and finally the RSP-HGSGF with fractional (fixed and variable order) derivative. Sufficient information regarding the FDM used for solving equations presented in the thesis will be briefly explained in the upcoming sub-topics.

2.9.1 Finite Difference Methods for Solving Time Fractional sub-Diffusion Equation (TFSDE)

The PDEs involving the fractional differential operators in space and/or time are seen to be a general form of the classical partial differential equations. Various finite difference schemes such as explicit, implicit and Crank-Nicolson have been developed to solve two-dimensional TFSDE (Langlands and Henry, 2005).

Recently, a lot of interest has been shown in solving the 2D TFSDE given in the form of;

$$ {}_0D_t^{\alpha} u(x,y,t) = Au_{xx}(x,y,t) + Bu_{yy}(x,y,t) + f(x,y,t), \tag{2.32} $$

with the following initial and boundary conditions

$$u(x,y,0) = g(x,y),$$

$$u(0,y,t) = g_1(y,t),\ u(1,y,t) = g_2(y,t),$$

$$u(x,0,t) = g_3(x,t),\ u(x,1,t) = g_4(x,t), \tag{2.33}$$

where $0 < \alpha < 1$ is the order of the time fractional derivative.

Zhuang and Liu (2007) solved equation (2.32) by an implicit difference method and used the Caputo definition to approximate the time derivative of fractional order. The stability and convergence were analyzed by mathematical induction and it was proved that the implicit difference scheme was unconditionally stable and convergent. Chen et al. (2010) developed the implicit and explicit difference scheme for the solutions of the 2D-TFSDEs. They used the link between the Riemann-Liouville and Grünwald-Letnikov fractional derivatives for Riemann-Liouville derivative. For the second order space derivatives, they used the central difference approximations. The Fourier series method was used for the stability and convergence analysis. Further more, they discussed the solvability and the multivariate extrapolation method was used to improve the accuracy of the method. Chen et al. (2012) developed the same schemes (the implicit and explicit) for the solution of the 2D variable-order TFSDE. The stability, convergence and solvability are discussed by using Fourier analysis method. They proved that the implicit difference scheme is unconditionally stable whereas the explicit difference scheme was conditionally stable. Zhang and Sun (2011) constructed two new alternating direction implicit schemes based on L_1 approximation and backward Euler method by adding two small different terms. These two schemes are different from the general alternating direction implicit schemes used for the solution of TFSDE. The solvability, unconditional stability and H^1 norm convergence were proved for the proposed schemes. Cui (2012) studied the compact finite difference scheme with the operator splitting technique to solve TFSDE. They discretized the time fractional derivative by the Grünwald-Letnikov definition and the second order space derivatives by the compact difference scheme to obtain fully discrete implicit scheme. The method was found to be unconditionally stable by Fourier method. Later, Cui (2013) constructed the compact alternating direction implicit schemes for TFSDE. Therein replace the Caputo derivative have approximated by L_1 approximation and the second order space derivative approximated by compact difference approximation. The stability was analyzed by Fourier method and convergence was proved by energy method. Using the earlier approaches of Zhang and Sun (2011), Wang (2013) considered the 2D TFSDE. The Caputo derivatives has been used for the time-fractional derivatives. Furthermore, they discussed the explicit error estimation for the two methods in the discrete maximum norm. They showed that the two methods had a similar order as their truncation errors with respect to the discrete maximum norm. Gong et al. (2014) then proposed the parallel algorithm for 2D TFSDE with implicit difference method. The solution of the method is discussed and the numerical results proved that the parallel algorithm converges more efficiently to the exact solution. Gao et al. (2015) followed the approach of Nasir et al. (2013) for 1D and 2D TFSDE utilizing the finite difference method based on superconvergence at some fixed points of the fractional derivative. Furthermore, first order Grünwald Letnikov formula has been used for the time fractional derivative and obtained the effective numerical schemes. The second order and fourth order compact schemes are constructed for the second order space derivative. The unconditional stability and convergence of the schemes was investigated by discrete energy method. Wang and Wang (2016b) developed modified compact alternating direction implicit method to solve 2D TFSDE with time fractional Riemann-Liouville derivative of order $(1-\alpha)$, where α lies between 0 and 1. The Riemann-Liouville fractional derivative was discretized by L_1 approximation and the second order space derivatives are discretized by fourth order compact difference method. The unconditional stability, solvability and convergence are analyzed of the proposed scheme and they upgraded temporal accuracy by using Richardson extrapolation algorithm. Zhai and Feng (2016) studied three compact alternating direction implicit methods based on superconvergence approximation for the solution of 2D TFSDE. The two schemes were unconditionally stable with second order of accuracy in time and fourth order of accuracy in space by the Fourier analysis method. The numerical examples proved the theoretical results and also made comparison among the proposed methods. Chen and Li (2016) suggested a novel compact alternating direction implicit method for the solution of two space direction TFSDE and TFMSDE with linear forcing term. They constructed the scheme based on modified L_1 approximation in time and compact difference approximation for second order space derivatives. The stability and convergence have been discussed and the numerical examples have shown that the proposed scheme is more feasible and accurate.

2.9.2 Finite Difference Methods for Solving Time Fractional Modified sub-Diffusion Equation (TFMSDE)

The fractional modified sub-diffusion equation has been proposed to describe the procedure that became less anomalous as the time progresses by the addition of secondary time derivative of fractional order acting on linear second order diffusion operator (Chechkin et al., 2003; Sokolov et al., 2004; Sokolov and Klafter, 2005);

$$u_t(x,y,t) = ({}_0D_t^{1-\alpha} + {}_0D_t^{1-\beta})\Big(Au_{xx}(x,y,t) + Bu_{yy}(x,y,t)\Big) + f(x,y,t), \qquad (2.34)$$

where α, β laying between 0 and 1. For variable order, it depends on independent variables as $(\alpha(x,y,t), \beta(x,y,t))$, A and B are the positive constants. The quantity u represents the concentration or probability density function for the particles suspended in the liquid on a bounded domain. Many researchers have solved TFMSDE by different numerical methods.

Langlands (2006) solved the modified equation (2.34) on an infinite domain in the form of an infinite series of Fox functions. Most fractional differential equation cannot be solved by an analytical method, thus many authors, such as Liu et al. (2009) has constructed a new implicit difference method, which provided feasible and effective tools for the solution of TFMSDE. The stability and convergence were analyzed by a new energy method. Then Zhang et al. (2012) presented finite difference and finite element methods for the solution of TFMSDE. Firstly, they analyze the time semi-discrete scheme and then for the full discrete scheme. The time fractional derivative is discretized by L_1 approximation and finite element method for the second order space derivative. They investigated that the semi-discrete and fully discrete schemes are unconditionally stable and convergent. In their conclusion, they discussed the numerical examples to demonstrate the effectiveness of schemes. Abbaszadeh and Mohebbi (2013) then proposed the compact difference scheme for the solution of 2D-TFMSDE with nonlinear source term. The high order compact difference scheme has an advantage of higher accuracy. By Fourier analysis, the proposed scheme is unconditionally stable and convergent and produce high accuracy solutions. Chen (2013) developed implicit difference scheme for 2D variable order TFMSDE. By Fourier series analysis, they investigated the stability, convergence and solvability of the proposed method together with the temporal accuracy of the method. Wang and Wang (2016a) developed a compact locally one-dimensional (LOD) finite difference method for the solution of 2D TFMSDE with time fractional Riemann-Liouville derivatives. They investigated the unconditional stability and convergence, and also increased the temporal accuracy by Richardson extrapolation algorithm. The numerical results demonstrated the effectiveness of the compact LOD method and the extrapolation algorithm. Dehghan et al. (2016) introduced an efficient numerical method for the 1D and 2D TFMSDE. The introduced method is based on finite difference method for time and Legendre spectral element method for space to obtain a semi-discrete and fully discrete approximation, respectively. The time discrete method is unconditionally stable and convergent.

2.9.3 Finite Difference Methods for Solving Rayleigh-Stokes Problem for a Heated Generalized Second Grade Fluid (RSP-HGSGF) with Fractional Derivative

The RSP-HGSGF with fractional and variable order fractional derivative has received much attention due to their numerous practical application such as Tan and Masuoka (2005a), Tan and Masuoka (2005b), and Wu (2009). Chen et al. (2008) have considered the implicit and explicit difference methods for RSP-HGSGF with fractional derivative. The stability and convergence are discussed using the new method of Fourier analysis. The solvability of the implicit difference method is also discussed. Finally, the theoretical results is tested by numerical examples. Later, Chen et al. (2013) developed the same theoretical analysis for 2D variable order RSP-HGSGF and proved that the numerical results are in agreement with the theoretical analysis. Mohebbi et al. (2013) constructed the comparison of two numerical methods, high order scheme and radial basis functions meshless method for the solution of 2D-RSP-HGSGF with fractional derivative. In the high order difference scheme, the space derivative is discretized with fourth order compact scheme and Riemann-Liouville fractional derivative is discretized by Grünwald-Letnikov formula. The radial basis functions method have taken the integration for both sides of the equation to discretize the time fractional derivative and for the space derivative using Kansa's method. The stability and convergence have been investigated for high order scheme using Fourier method and for radial basis functions, energy method is applied. Bazhlekova et al. (2015) have studied the analysis in semi-discrete and fully discrete formulation. A space semi-discrete Galerkin scheme using continuous piecewise linear finite elements, and optimal with respect to initial data regularity error estimates for the finite element approximations are derived.

2.10 Summary

In this chapter, the classification of partial differential equation, definitions of fractional integrals and derivatives are discussed. The properties and relationships of some fractional derivatives were also studied. This is followed by an explanation on the finite difference method with stability and convergence. Finally, the literature on finite difference method for solving 2D TFSDE, TFMSDE and RSP-HGSGF with fractional (constant and variable order) derivative are reviewed. In the next chapter, studies on the finite difference methods and their theoretical analysis will be discussed and explained on some examples.