August 2017

Exponential Integrator Methods for Nonlinear Fractional Reaction-diffusion Models

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A Dissertation Submitted in

Partial Fulfillment of the

Requirements for the Degree of

Doctor of Philosophy

in Mathematics

at

The University of Wisconsin–Milwaukee

August 2017

ABSTRACT

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The University of Wisconsin-Milwaukee, 2017
Under the Supervision of Bruce Wade

Nonlocality and spatial heterogeneity of many practical systems have made fractional differential equations very useful tools in Science and Engineering. However, solving these type of models is computationally demanding. In this work, we propose an exponential integrator method for nonlinear fractional reaction-diffusion equations. This scheme is based on using a real distinct poles discretization for the underlying matrix exponentials. Due to these real distinct poles, the algorithm could be easily implemented in parallel to take advantage of multiple processors for increased computational efficiency. The method is established to be second-order convergent; and proven to be robust for problems involving non-smooth/mismatched initial and boundary conditions and steep solution gradients. We examine the stability of the scheme through its amplification factor and plot the boundaries of the stability regions comparative to other second-order FETD schemes. This numerical scheme combined with fractional centered differencing is used for simulating many important nonlinear fractional models in applications. We demonstrate the superiority of our method over competing second order FETD schemes, BDF2 scheme, and IMEX schemes. Our experiments show that the proposed scheme is computationally more efficient (in terms of cpu time). Furthermore, we investigate the trade-off between using fractional centered differencing and matrix transfer technique in discretization of Riesz fractional derivatives.

The generalized Mittag-Leffler function and its inverse is very useful in solving fractional differential equations and structural derivatives, respectively. However, their computational complexities have made them difficult to deal with numerically. We propose a real distinct pole rational approximation of the generalized Mittag-Leffler function. Under some mild conditions, this approximation is proven and empirically shown to be L-Acceptable. Due to the complete monotonicity property of the Mittag-Leffler function, we derive a rational approximation for the inverse generalized Mittag-Leffler function. These approximations are especially useful in developing efficient and accurate numerical schemes for partial differential equations of fractional order. Several applications are presented such as complementary error function, solution of fractional differential equations, and the ultraslow diffusion model using the structural derivative. Furthermore, we present a preliminary result of the application of the M-L RDP approximation to develop a generalized exponetial integrator scheme for time-fractional nonlinear reaction-diffusion equation.

To my parents, who gave all they had to ensured that I received the best education possible; my beautiful wife (Bose), whose support throughout the program is inestimable and my wonderful daughters (Esther and Priscilla), they are part of the success.

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ACKNOWLEDGMENTS

I express my sincere gratitude to God almighty for His unfailing love, peace, wisdom, and strength to bring this PhD to fruition. I deeply appreciate my advisor, Dr. Bruce Wade, for consistently believing in my problem-solving ability and offering clear directives for advancing this work. My PhD committee members Dr. Dexuan Xie, Dr. Kevin McLeod, Dr. Istvan Lauko and Dr. Lei Wang are acknowledged for their support and for their time spent to review my dissertation. Your suggestions are useful and valuable. I also want to thank Dr. Abdul Khaliq of Middle Tennessee State University (MTSU) and Dr. Kkaled Furati of King Fahd University of Petroleum and Minerals (KFUPM) for their advice related to fractional calculus. In addition, I appreciate the support of Dr. E.O. Asante-Asamani (Drake University). My fellow graduate students in Mathematics department are also appreciated for their great support and inspirations. Finally, I am very grateful to the Department of Mathematical Sciences, UWM for fully funding me for the entire duration of my graduate studies.

Chapter 1

Introduction and Preliminaries

1.1 Background

For many centuries, the concept of calculus has been indispensable in the field of mathematical sciences. Various applications could be found in physical sciences (astronomy, physics, chemistry, and the Earth sciences), biology, actuarial science, computer science, statistics, engineering, business, economics, demography, medicine and in many other fields wherever a problem can be mathematically modeled and an optimal solution is desired. There have been many studies on this concept following the modern development started in 17th-century by Isaac Newton and Gottfried Wilhelm Leibniz in Europe. In 1695, among many correspondences between L'Hopital and Leibniz, the question that gave birth to the concept of non-integer (fractional) calculus was asked: What would be the $\frac{1}{2}$-th order derivative of a function? Leibniz then responded, saying, "An apparent paradox, from which one day useful consequences will be drawn."

In recent time, the use of fractional (non-integer) order derivatives has become popular due to its non-locality property which is an intrinsic property of many complex systems. Various applications are in modeling of different phenomena such as nanotechnology, control theory of dynamical systems, viscoelasticity, anomalous transport and anomalous diffusion, financial modeling, random walk, and biological modeling see [16, 32, 78, 87, 95, 98, 101, 109, 129]. More detailed work on physical and engineering processes with more applications of fractional calculus can be found in [62, 78, 103, 107, 109]. Furthermore, sub-diffusion (fractional in time) and super-diffusion (fractional in space) have been observed and the effect of the fractional orders have been seen in the solution profiles in many models, see [20, 93, 94]. The following two major applications are highlighted, see [109] for detailed discussion of many more applications. The definitions of the fractional integrals and derivatives used in this section will be given in Chapter Two.

Fractional Calculus Applications in Viscoelasticity

It is well known that for solids, stress is proportional to the zeroth derivative of strain while it is proportional to the first derivative of the strain for fluids. G.W. Scott Blair in [122] proposed that for "intermediate" materials, stress is proportional to the "intermediate" derivative (non-integer order) of the strain given as:

$$\sigma(t) = E D_t^{\alpha} \varepsilon(t), \tag{1.1}$$

where $0 < \alpha < 1$ and E are material-dependent constants and D_t^{α} is the so-called fractional derivative. About the same time, A.N. Gerasimov in [50] proposed a similar equation for the generalization of basic law of deformation using the so-called Caputo fractional derivative, ${}_{-\infty}D_t^{\alpha}$, given as:

$$\sigma(t) = \kappa \, {}_{-\infty}D_t^{\alpha} \varepsilon(t), \tag{1.2}$$

where $0 < \alpha < 1$ and κ is a generalized viscosity. Furthermore, A.N. Gerasimov studied the movement of a viscous fluid between surfaces described by using two problems which led to the following equations:

$$\rho(t)\frac{\partial^2 y}{\partial t^2} = \kappa\, {}_{-\infty}D_t^{\alpha}\left(\frac{\partial^2 y}{\partial x^2}\right), \tag{1.3}$$

$$\rho(t)x^3\frac{\partial^2 y}{\partial t^2} = \kappa\frac{\partial}{\partial x}\left[x^3\frac{\partial}{\partial x}\left({}_{-\infty}D_t^{\alpha} y\right)\right], \tag{1.4}$$

where $y = y(x,t)$. The solutions to Equations (1.3)-(1.4) are based on the assumption that both the unknown function and given functions are equal to zero for $t < 0$. It is known that Gerasimov was the first to formulate and solve fractional-order partial differential models for particular applied problems.

Another way of formulating fractional-order models of viscoelasticity is by using power-law stress relaxation in real materials. In [90], P.G. Nutting was the first to give the formulation as:

$$\varepsilon = a t^{\alpha}\sigma^{\beta}, \tag{1.5}$$

where a, α, β are the model parameters. Therefore, for $\beta = 1$ and taking $c_0 = \frac{1}{a}$, we have the following power-law relationship between stress and strain:

$$\sigma(t) = c_0\varepsilon t^{-\alpha}, \tag{1.6}$$

where ε is constant and

$$\varepsilon(t) = \frac{\sigma}{c_0}t^{\alpha}, \tag{1.7}$$

where σ is constant.

In [100], T.F. Nonnemnacher showed that the functions $\varepsilon(t)$ and $\sigma(t)$ satisfied the fractional differential equations given as:

$$D_t^{\alpha}\sigma(t) = \frac{\Gamma(1-\alpha)t^{-\alpha}}{\Gamma(1-2\alpha)}\sigma(t), \tag{1.8}$$

$$D_t^{\alpha}\varepsilon(t) = \Gamma(1+\alpha)t^{-\alpha}\varepsilon(t). \tag{1.9}$$

This established relationship that exist between power-law representation of viscoelastic behaviour and fractional calculus.

Fractional Calculus and Abel's Integral Equation

There have been extensive studies of Abel's integral equation and its applications by many researchers in many fields, see [54, 109] for a detailed discussion. The equation is given as:

$$\frac{1}{\Gamma(\alpha)}\int_0^t \frac{\varphi(s)}{(t-s)^{1-\alpha}}ds = g(t), \quad t>0, \tag{1.10}$$

where $0<\alpha<1$. The solution to this equation is given by the formula

$$\frac{1}{\Gamma(1-\alpha)}\frac{d}{dt}\int_0^t \frac{g(s)}{(t-s)^{1-\alpha}}ds = \varphi(t), \quad t>0. \tag{1.11}$$

Equations (1.10) and (1.11) can be written in form of fractional differential equations respectively as:

$$ {}_0D_t^{-\alpha}\varphi(t) = g(t), \qquad t>0, \tag{1.12}$$

$$ {}_0D_t^{\alpha}g(t) = \varphi(t), \qquad t>0. \tag{1.13}$$

Abel's integral equation became very popular and of great interest to many researchers due to the ability to reduce many integral equations or mathematical models to Abel's integral equation. This possibility is very important for obtaining solutions to those equations. Among many of such equations that can be reduced to Abel's integral equation and their corresponding solutions in terms of fractional differential equations are summarized in Table 1.1; see the detailed work on the derivation in [109].

A centered issue in the early biological and biochemical evolution is dealing with the mechanisms underlying spatial pattern formation. It is not enough to study genetics in order to understand the interaction between the physical and chemical properties of embryonic material

Integral Equations	Transformed Abel's Integral Equations	Corresponding Solutions
$\int_0^\infty \frac{\varphi(\sqrt{s^2+y^2})}{\sqrt{s^2+y^2}} ds = \frac{g(y)}{2y}$	$\int_0^t (t-\tau)^{-\frac{1}{2}} \phi(\tau) d\tau = g\left(\frac{1}{\sqrt{t}}\right)$, where: $t = \frac{1}{y^2}$, $\phi(r) = t^{-\frac{3}{2}} \sqrt{r} \varphi\left(\frac{1}{\sqrt{r}}\right)$	$\varphi\left(\frac{1}{\sqrt{t}}\right) = \frac{t}{\sqrt{\pi}} D_t^{\frac{1}{2}} g\left(\frac{1}{\sqrt{t}}\right)$
$\int_0^{\frac{\pi}{2}} \varphi(r\cos\omega) \sin^{2\beta+1}\omega d\omega = g(r)$	$\int_0^t (t-\tau)^{\beta} \phi(\tau) d\tau = f(t)$, where: $t = r^2$, $\tau = r^2\cos^2\omega$, $\phi(\tau) = \frac{\varphi(\sqrt{\tau})}{\sqrt{\tau}}$, $f(t) = 2t^{\beta-\frac{1}{2}} g(\sqrt{t})$	$\phi(t) = \frac{1}{\Gamma(\beta+1)} D_t^{\beta} f(t)$
$\int_0^y \frac{1}{(y^2-x^2)^\beta} \varphi(x) dx = g(y)$	$\int_0^t \frac{1}{(t-\tau)^\beta} \phi(\tau) d\tau = 2g(\sqrt{t})$, where: $t = y^2$, $\tau = x^2$, $\phi(\tau) = \frac{\varphi(\sqrt{\tau})}{\sqrt{\tau}}$	$\phi(t) = \frac{2}{\Gamma(1-\beta)} D_t^{1-\beta} g(\sqrt{t})$
$\int_\theta^{\frac{\pi}{2}} \frac{\rho(\varphi)}{(\cos\theta-\cos\varphi)^\beta} d\varphi = G(\theta)$	$\int_0^t \frac{1}{(t-\tau)^\beta} \phi(\tau) d\tau = g(t)$, where: $t = \cos\theta$, $\tau = \cos\varphi$, $\phi(\tau) = \frac{\rho(\arccos\tau)}{\sqrt{1-\tau^2}}$, $g(t) = F(\arccos t)$	$\rho(\arccos t) = \frac{\sqrt{1-t^2}}{\Gamma(1-\beta)} D_t^{1-\beta} g(t)$

Table 1.1: Connection between fractional calculus and Abel's integral equation, see [109]

to produce the complex spatio-temporal signalling cues that eventually determine the fate of the cell, see [30]. Generally, the mechanisms of cell motility and/or the generation of chemical prepatterns are modeled using ideas of biological pattern formation, see [30]. In [51], several models for pattern formation are proposed to explain the regenerative properties of hydra which have been experimentally observed in various transplantations. Invoking the intrinsic properties of fractional calculus is therefore apparent in biological and biochemical systems due to these complexities.

Due to the non-local properties of the fractional calculus, there are many computational challenges associated with solving fractional differential equations. The common numerical approach for solving these brand of problems is to use the method-of-lines to reduce the fractional differential equation (FPDE) to an ordinary differential equation (ODE) and then search for an efficient scheme to solve the resulting ODE. Some numerical methods have been proposed in the literature, such as finite difference, finite element or finite volume discretisation of the fractional operator, combined with a semi-implicit Euler formulation for the time evolution of the solution. In particular for space fractional equations, methods like Krylov methods, fast numerical integration in conjunction with effective preconditioners and Fourier spectral methods have been introduced in [20, 21, 143], see also [13, 28, 147, 149].

In [58], Hairer & Wanner defined 'stiff equation' as a problem for which explicit methods do not work well. Many effective implicit methods have been proposed to integrate stiff equations such as Runge-Kutta, Rosenbrock and Backward difference schemes. The computational cost of these methods, however, is very high and may be impractical for certain applications. Some other methods are also proposed to cut down on the computational cost associated with integrating stiff problems such as linearly implicit methods, semi-implicit methods, projection methods, see [3, 26, 49, 76, 132, 132]. The IMEX schemes, the class of implicit-explicit methods, are introduced and have gained popularity in integrating stiff problems, see [65]. The effectiveness of these schemes is in the fact that the non-stiff part of the problem is integrated explicitly while the stiff part is handled implicitly. This is a way to offset any stability constraints while computational speed is gained. However, these schemes have been shown to have some instabilities in the case where both the diffusion and reaction terms are stiff, and could lead to spurious oscillation for the case of nonsmooth/mismatched initial/boundary conditions.

To fill in this gap related to maintaining stability even in the presence nonsmooth and stiff problems, time integration schemes are introduced. Fractional Exponential Time Differencing (FETD) schemes are among the schemes introduced to achieve this aim, see [29, 77, 92]. These schemes make use of a single step representation of the evolutionary dynamics with an appropriate technique in the discretization of the resulting matrix exponentials. This has attracted many researchers in this field due to the fact that these schemes treat the linear part of the model exactly through the exponential solution operator, and the semi-implicitly treat the reaction terms. Over the years, there have been various versions of ETD schemes which use different approximations to the integral of the non-linear reaction term [36, 64, 77]. In [81], Kleefeld et al. proposed an ETD where a Padé-(1,1) rational approximation for the matrix exponential is used. This is called the ETD Crank-Nicolson Scheme. Nonsmooth initial and boundary conditions generate spurious oscillations and can be handled well (damping out spurious oscillations) by an L-stable scheme. This is a major setback for ETD Crank-Nicolson Scheme.

An L-acceptable scheme was then porposed in a follow-up paper by Yousuf *et. al* in [146] to address this problem. In this scheme, a Padé-(0,2) rational approximation was used instead of the Padé-(1,1) rational approximation due to the fact that the former is L-acceptable. Again, the partial fraction decomposition of this approximation (Padé-(0,2)) used in deriving the scheme has complex poles and requires complex arithmetic in all applications. This is a potential drag to the speed of the the evolution process, depending on the matrices. We remark that these notable issues with these existing schemes become worse when dealing with fractional order derivative due to the full matrix involved.

In this thesis, we introduce a Fractional Exponential Time Differencing Scheme (FETD-RDP) for nonlinear fractional reaction-diffusion equations (one-dimensional, two-dimensional and systems of two-dimensional problems). In the case of integer order derivatives, this scheme was first introduced in [8, 9], called the ETD-RDP scheme, for reaction-diffusion problems. This scheme utilizes a non-Padé rational approximation with real and distinct poles for approximating the underlying matrix exponentials. The scheme is second-order and L-acceptable, which help to damps out spurious oscillations. Furthermore, complex arithmetic is completely avoided and parallel implementation is possible to speed up computation. We compare the performance of the scheme to well known time integrator schemes. New real distinct poles rational function approximations of the generalized Mittag-Leffler function and its inverse are introduced. Under some mild conditions, this approximation is proven to be L-acceptable. Many applications are explored from the complementary error function to the ultraslow diffusion model.

The thesis is organized as follows: In the remainder of this Chapter, a survey of some standard time discretization schemes is provided. These are very useful ingredients for motivation and the work that follows. This introductory and preliminaries chapter is closed by a brief introduction to Padé rational functions for comparison purposes. In Chapter Two, we give a survey of important definitions of fractional calculus and provide detailed proofs of some of the results of or related to fractional calculus. Theoretical results on the existence and uniqueness of solutions to fractional differential models are presented in Chapter Three. Some of the earlier theoretical results of this thesis on the existence and uniqueness of solutions to inverse problem involving fractional derivatives are included in this Chapter. Spatial discretization methods for fractional derivatives are presented in Chapter Four. Here we introduce fractional centered finite differences, the so-called matrix transfer technique and short memory principle. Detailed proofs of many of the important results related to the fractional centered finite difference are also provided. The FETD-RDP scheme is proposed in Chapter Five for fractional order differential equations. Analysis of its absolute stability region, some results on the error estimate and convergence result are included in this Chapter. The performance and second-order convergence of the proposed scheme to very interesting well known stiff problems are presented in Chapter Six. Many of these systems of two-dimensional models involving nonsmooth or mismatched initial/boundary conditions have applications in biochemical and biological pattern formations. We further show empirically in this Chapter that there is a trade off in using matrix transfer techniques compared to fractional centered finite difference. New real distinct poles rational function approximations of the generalized Mittag-Leffler function and its inverse are introduced in Chapter Seven. Under some mild conditions, this approximation is proven to be L-acceptable. We present several applications of this approximations to complementary error function, the ultraslow diffusion model etc. We close this Chapter by presenting a preliminary result of the application of the M-L RDP approximation to develop a generalized exponetial integrator scheme for time-fractional nonlinear reaction-diffusion equation. Finally, Chapter Eight highlights some recommendations and possible future directions.

1.2 A Survey of Some Time Discretization Schemes

Linear Multistep Schemes

The general form of linear multistep methods is given as:

$$\sum_{j=0}^{q} a_j w_{n+j} = k \sum_{j=0}^{q} b_j \mathcal{H}\left(t_{n+j}, w_{n+j}\right), \quad n = 0, 1, 2, \cdots,$$

with $\mathcal{H} : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$. For the case of a fractional reaction-diffusion equation, we do have $\mathcal{H}(t,u) = -Au + f(t,u)$ with differential matrix A and nonlinear reaction term f.

These methods make use of multiple approximations from previous time levels to compute the current solution. The scheme is implicit except when $b_q = 0$. The fact that in a linear multi-step method, one needs to solve just one nonlinear system is a major advantage. However, the requirement for q starting values can lead to loss of accuracy or stability if not computed at very small time steps. The method has order p, for a sufficiently smooth $\mathscr{H}$, if, see [65, Pg. 172],

$$\begin{aligned} \sum_{j=0}^{q} a_j &= 0 \\ \sum_{j=0}^{q} a_j j^i &= i \sum_{j=0}^{q} b_j j^{i-1}, \qquad i = 1, 2, 3, \cdots p. \end{aligned}$$

A very popular multistep method, particularly for stiff problems, is the backward difference formula (BDF) introduced by Curtis & Hirchschfelder [31]. It requires

$$b_q = 1, \quad b_j = 0, \quad 0 \le j \le q-1$$

and a_j chosen conveniently to attain an optimal order of accuracy.

Second Order Backward Difference Scheme (BDF2)

A general non-autonomous formulation of an initial value problem for a system of ordinary differential equations is considered, see [9, 31, 58],

$$u_t = \mathscr{H}(t, u), \quad t > 0, \quad u(0) = u_0 \tag{1.14}$$

with $\mathscr{H} : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$ and $u_0 \in \mathbb{R}^m$. In [31], the second order backward difference scheme (BDF2) as a multistep method for stiff problems is introduced as follows:

$$u_{n+2} = \frac{4}{3} u_{n+1} - \frac{1}{3} u_n + \frac{2k}{3} \mathscr{H}(t_{n+2}, u_{n+2}), \tag{1.15}$$

with some one-step starting scheme. Newton's method is requred at each step for this scheme. In this work, FETD-RDP's performance is compared to the second order backward difference scheme (BDF2). The reader should see Hairer & Wanner [58] for a more comprehensive discussion of multistep methods.

Implicit-Explicit (IMEX) Schemes

IMEX methods are introduced to effectively handle time integration of problems comprising very stiff and mildly or non-stiff parts, see [58, 65]. These methods compete very well with the existing schemes. Advection-diffusion equations fit very well into this category with the advective parts being non-stiff and the diffusion part stiff. Also, some advection-diffusion reaction equations with mild or non-stiff reactions are also suitable. Here we consider separating the ODE system (1.14) into the form

$$u_t = \mathscr{H}_1(t, u(t)) + \mathscr{H}_2(t, u(t)) \tag{1.16}$$

where $\mathscr{H}_1(t, u(t))$ and $\mathscr{H}_2(t, u(t))$ represent the non-stiff component and the stiff components, respectively. This separation allows the use of implicit schemes to handle the stiff component and explicit methods to speed up computations of non-stiff parts.

The following are two second order IMEX schemes we consider for the purpose of comparison.

1. IMEX-BDF2

$$\begin{aligned}\frac{3}{2}u_{n+1} = {} & 2k\mathscr{H}_1(t_n, u_n) - k\mathscr{H}_1(t_{n-1}, u_{n-1}) + \omega k\mathscr{H}_2(t_{n+1}, u_{n+1}) + 2(1-\omega)k\mathscr{H}_2(t_n, u_n) \\ & - (1-\omega)k\mathscr{H}_2(t_{n-1}, u_{n-1}) + 2u_n - \frac{1}{2}u_{n-1},\end{aligned}$$

where $\omega \geq 0$. This method is derived from a combination of the explicit and implicit two-step BDF schemes. Here, $\omega = 1$ is used for our comparison as recommended in [65].

2. IMEX-Adams2

$$\begin{aligned}u_{n+1} = {} & \frac{3}{2}k\mathscr{H}_2(t_n, u_n) - \omega k\mathscr{H}_2(t_{n+1}, u_{n+1}) + \left(\frac{3}{2} - 2\omega\right)k\mathscr{H}_2(t_n, u_n) \\ & + \left(\omega - \frac{1}{2}\right)k\mathscr{H}_2(t_{n-1}, u_{n-1}) + u_n.\end{aligned}$$

This method uses the explicit and implicit two-step Adam's methods. Our choice of $\omega = \frac{9}{16}$ is motivated by the fact that the scheme with this parameter is known to provide maximum damping [10].

Readers are also directed to [9, 58] for details of these methods.

1.3 Padé Rational Approximation

Padé approximation, dated 1892, [106], are rational functions which, for a given degree of the numerator and the denominator, have highest order of approximation of the exponential function. Padé schemes are designed to approximate the exponential function, e^z, for complex number z with high order of accuracy, see also [7, 37].

Theorem 1.3.1. *[58, Thm 3.12] The (k,j)-Padé approximation to e^z is given by*

$$R_{k,j}(z) = \frac{P_{k,j}(z)}{Q_{k,j}(z)}$$

where

$$P_{k,j}(z) = 1 + \frac{k}{j+k}z + \frac{k(k-1)}{(j+k)(j+k-1)}\frac{z^2}{2!} + \cdots + \frac{k(k-1)\cdots 1}{(j+k)\cdots(j+1)}\frac{z^k}{k!}$$

$$Q_{k,j}(z) = 1 - \frac{j}{k+j}z + \frac{j(j-1)}{(k+j)(k+j-1)}\frac{z^2}{2!} - \cdots + \frac{(-1)^j j(j-1)\cdots 1}{(k+j)\cdots(k+1)}\frac{z^j}{j!}$$

with error

$$e^z - R_{k,j}(z) = (-1)^j \frac{j!k!}{(j+k)!(j+k+1)!} z^{j+k+1} + \mathcal{O}(z^{j+k+2})$$

Definition 1.3.2. We say that the rational approximation $R(z)$ is A-acceptable if $|R(z)| < 1$ for every $z \in \mathbb{C}$ such that $R(z) < 0$, and it is A_0-acceptable if $|R(z)| < 1$ for every real and negative z. If in addition to A-acceptability, $|R(z)| \to 0$ as $Re(z) \to \infty$, we say that $R(z)$ is L-acceptable.

Theorem 1.3.3. *[19] If $k = j$ the $R_{k,j}(z)$ is A-acceptable.*

Theorem 1.3.4. *[130] If $j \geq k$ then $R_{k,j}(z)$ is A_0-acceptable.*

Theorem 1.3.5. *[37] If $j \geq k+1$ or $j = s+2$, then $R_{k,j}(z)$ is L-acceptable.*

The existing Exponential Time Differencing, FETD-Padé schemes which use rational functions to approximate the matrix exponential use Padé approximations. Particularly, the following Padé rational functions are used to develop FETD-Padé schemes:

$$\begin{aligned}
\text{Padé}(0,1): &\qquad e^z \approx \tfrac{1}{1-z}, \\
\text{Padé}(1,1): &\qquad e^z \approx \tfrac{1+\frac{1}{2}}{1-\frac{1}{2}z}, \\
\text{Padé}(0,2): &\qquad e^z \approx \tfrac{1}{1-z+\frac{z^2}{2!}},
\end{aligned}$$

Some other well known Padé approximations are summarized in Table A1.

Chapter 2

Fractional Calculus

In this Chapter, we give some definitions of fractional calculus and discuss many of the important results of or related to fractional calculus.

2.1 Riemann-Liouville Fractional Integral and Derivatives

The Riemann-Liouville fractional integral and derivative form the basis for many other proposed definitions of fractional derivatives.

Definition 2.1.1. The gamma function, Γ, is defined as

$$\Gamma(\alpha) = \int_0^\infty y^{\alpha-1} e^{-y} dy, \qquad \alpha > 0. \tag{2.1}$$

Using integration by parts, we obtain the relation

$$\Gamma(\alpha+1) = \alpha\Gamma(\alpha). \tag{2.2}$$

Note that this is a generalization of the factorial function: when $\alpha = n$, n any positive integer, we have the relation

$$\Gamma(n) = (n-1)!. \tag{2.3}$$

Definition 2.1.2. The Beta function, also called the Euler integral of the first kind, is defined as

$$B(\alpha,\beta) = \int_0^1 y^{\alpha-1}(1-y)^{\beta-1}dy, \quad Re(\alpha) > 0,\ Re(\beta) > 0. \tag{2.4}$$

By appropriate change of variables, the following is the relationship that exists between the Gamma function and the Beta function.

$$B(\alpha,\beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}. \tag{2.5}$$

In 1850, the idea of Cauchy formula for repeated integration was generalized to arbitrary order using Gamma function Γ as

Definition 2.1.3. (Riemann-Liouville Integral, [43, 109]). Let $w \in L^1[a,b]$, where $-\infty \le a < x < b \le -\infty$, be a real valued locally integrable function. The left-sided and right-sided Riemann-Liouville (R-L) fractional integrals of order α of the function w are given, respectively, as

$${}_aI_x^{\alpha}w(x) = \frac{1}{\Gamma(\alpha)}\int_a^x (x-s)^{\alpha-1}w(s)\,ds, \qquad x > a, \qquad \alpha > 0, \tag{2.6}$$

and

$${}_xI_b^{\alpha}w(x) = \frac{1}{\Gamma(\alpha)}\int_x^b (s-x)^{\alpha-1}w(s)\,ds, \qquad x > a, \qquad \alpha > 0. \tag{2.7}$$

Notice that (R-L) fractional integral could be written as a convolution of two functions:

$${}_aI_x^{\alpha}w(x) = (w * J_\alpha)(x),$$

where $J_\alpha(x) = x^{\alpha-1}/\Gamma(\alpha)$. For $\alpha = 0$, we set ${}_aI_x^0 := I$, the identity operator.

Lemma 2.1.4. *Let $w \in L^1[a,b]$ and $\alpha > 0$. Then the integral ${}_aI_x^{\alpha}w(x)$ exists for almost every $x \in [a,b]$ and the function ${}_aI_x^{\alpha}w$ belongs $L^1[a,b]$.*

Proof. Define the following functions:

$$\Phi_1(s) = \begin{cases} s^{\alpha-1} & 0 < s \le b-a \\ 0 & \text{otherwise,} \end{cases} \qquad \text{and} \qquad \Phi_2(s) = \begin{cases} w(s) & a \le s \le b \\ 0 & \text{otherwise.} \end{cases}$$

By construction, it is clear that $\Phi_1, \Phi_2 \in L^1(\mathbb{R})$. We also have

$$\int_{-\infty}^{\infty} \Phi_1(x-s)\Phi_2(s)ds = \int_{-\infty}^{a} \Phi_1(x-s)\Phi_2(s)ds + \int_{a}^{x} \Phi_1(x-s)\Phi_2(s)ds + \int_{x}^{\infty} \Phi_1(x-s)\Phi_2(s)ds.$$

Since $\Phi_2(s) = 0$ for $s < a$, then

$$\int_{-\infty}^{a} \Phi_1(x-s)\Phi_2(s)ds = 0.$$

Also, we have that

$$\Phi_1(x-s) = \begin{cases} (x-s)^{\alpha-1} & a-(b-x) \le s < x \\ 0 & \text{otherwise,} \end{cases}$$

Hence,

$$\int_{x}^{\infty} \Phi_1(x-s)\Phi_2(s)ds = 0 \qquad \text{and} \qquad \int_{a}^{x} \Phi_1(x-s)\Phi_2(s)ds = \int_{a}^{x} (x-s)^{\alpha-1} w(s)ds.$$

Therefore,

$$\begin{aligned} {}_aI_x^{\alpha} w(x) &= \frac{1}{\Gamma(\alpha)} \int_{a}^{x} (x-s)^{\alpha-1} w(s)ds \\ &= \frac{1}{\Gamma(\alpha)} \int_{-\infty}^{\infty} \Phi_1(x-s)\Phi_2(s)ds \\ &= \frac{1}{\Gamma(\alpha)} (\Phi_1 * \Phi_2)(x). \end{aligned}$$

Since $\Phi_1, \Phi_2 \in L^1(\mathbb{R})$, then $(\Phi_1 * \Phi_2)(x)$ exists for almost every $x \in \mathbb{R}$ and $\Phi_1 * \Phi_2 \in L^1(\mathbb{R})$. Hence, the integral ${}_aI_x^{\alpha} w(x)$ exists for almost every $x \in [a,b]$ and the function ${}_aI_x^{\alpha} w$ belongs $L^1[a,b]$.

□

Definition 2.1.5. (Riemann-Liouville Derivative, [43, 109]). Let $w \in L^1[a,b]$, where $-\infty \leq a < x < b \leq -\infty$, and $(w * J_{m-\alpha}) \in W^{m,1}[a,b]$, $m = \lceil \alpha \rceil$, $\alpha > 0$. The left-sided and right-sided Riemann-Liouville (R-L) fractional derivatives of order α, of the function w are given, respectively, as

$$ {}_aD_x^\alpha w(x) = \frac{d^m}{dx^m} {}_aI_x^{m-\alpha} w(x) = \frac{1}{\Gamma(m-\alpha)} \frac{d^m}{dx^m} \int_a^x (x-s)^{m-\alpha-1} w(s)\, ds, \quad x > a, \tag{2.8} $$

and

$$ {}_xD_b^\alpha w(x) = (-1)^m \frac{d^m}{dx^m} {}_xI_b^{m-\alpha} w(x) = \frac{(-1)^m}{\Gamma(m-\alpha)} \frac{d^m}{dx^m} \int_x^b (s-x)^{m-\alpha-1} w(s)\, ds, \quad x > a, \tag{2.9} $$

where $\lceil \cdot \rceil$ is the ceiling function and the space $W^{m,1}$ is defined as

$$ W^{m,1}[a,b] = \left\{ w \in L^1[a,b] : \quad \frac{d^m}{dx^m} w \in L^1[a,b] \right\}. \tag{2.10} $$

Lemma 2.1.6. *Let $w \in L^1(a,b)$, $\alpha \geq 0$, and $\beta \geq 0$. Then we have the following*

$$ {}_aI_x^\alpha \, {}_aI_x^\beta w(x) = {}_a I_x^{\alpha+\beta} w(x), \tag{2.11} $$

for x almost everywhere $(a.e)$ on $[a,b]$.

Proof. By Lemma (2.1.4), the two integral exists for almost every $x \in [a,b]$ and by Fubini's Theorem, we have the following estimate

$$ \begin{aligned} {}_aI_x^\alpha \, {}_aI_x^\beta w(x) &= \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x (x-s)^{\alpha-1} \int_a^s (s-\tau)^{\beta-1} w(\tau) d\tau ds \\ &= \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x \int_\tau^x (x-s)^{\alpha-1} (s-\tau)^{\beta-1} w(\tau) ds d\tau \\ &= \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x w(\tau) \int_\tau^x (x-s)^{\alpha-1} (s-\tau)^{\beta-1} ds d\tau \end{aligned} \tag{2.12} $$

Change of variable $s = \tau + t(x-\tau)$ gives

$$\begin{aligned} {}_aI_x^\alpha {}_aI_x^\beta w(x) &= \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x w(\tau) \int_0^1 [(x-\tau)(1-t)]^{\alpha-1} (x-\tau)^\beta t^{\beta-1} dt d\tau \\ &= \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x w(\tau)(x-\tau)^{\alpha+\beta-1} \left(\int_0^1 t^{\beta-1}(1-t)^{\alpha-1} dt \right) d\tau. \end{aligned}$$

By the definition of Beta function and using the identity (2.5), we then obtain

$$\begin{aligned} {}_aI_x^\alpha {}_aI_x^\beta w(x) &= \frac{B(\alpha,\beta)}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x (x-\tau)^{\alpha+\beta-1} w(\tau) d\tau \\ &= \frac{1}{\Gamma(\alpha+\beta)} \int_a^x (x-\tau)^{\alpha+\beta-1} w(\tau) d\tau \\ &= {}_aI_x^{\alpha+\beta} w(x), \end{aligned} \tag{2.13}$$

for x almost everywhere $(a.e)$ on $[a,b]$. □

Lemma 2.1.7. *Let $w \in L^1(a,b)$, and $\alpha > 0$. Then*

$$ {}_aD_x^\alpha {}_aI_x^\alpha w(x) = w(x), \tag{2.14}$$

for x $(a.e)$ on $[a,b]$. If furthermore there exists a function $g \in L^1[a,b]$ such that $w = {}_aI_x^\alpha g$ then

$$ {}_aI_x^\alpha {}_aD_x^\alpha w(x) = w(x), \tag{2.15}$$

almost everywhere.

Proof. Let $m = \lceil \alpha \rceil$. By the definition of R-L fractional derivative and the semigroup property of R-L fractional integral (Lemma (2.1.6)) and the left inverse of the integer order differential operator, we have

$$ {}_aD_x^\alpha {}_aI_x^\alpha w(x) = \frac{d^m}{dx^m} {}_aI_x^{m-\alpha} {}_aI_x^\alpha w(x) = \frac{d^m}{dx^m} {}_aI_x^m w(x) = w(x).$$

To prove the second part, we use (4.23) and the fact that ${}_aI_x^\alpha g \in L^1[a,b]$ to get

$$ {}_aI_x^\alpha\,{}_aD_x^\alpha w(x) = {}_aI_x^\alpha\left({}_aD_x^\alpha\,{}_aI_x^\alpha g\right)(x) = \left({}_aI_x^\alpha\,{}_aD_x^\alpha\right){}_aI_x^\alpha g(x) = {}_aI_x^\alpha g(x) = w(x). $$

□

Lemma 2.1.8. *Let $x > a$ and $\beta > -1$. Then*

$$ {}_aI_x^\alpha (x-a)^\beta = \frac{\Gamma(\beta+1)}{\Gamma(\beta+\alpha+1)}(x-a)^{\beta+\alpha}, \quad \alpha > 0, \tag{2.16} $$

$$ {}_aD_x^\alpha (x-a)^{\alpha-1} = 0, \quad 0 < \alpha < 1. \tag{2.17} $$

Proof. By definition and the change of variable $\tau = a + s(x-a)$, we have

$$ \begin{aligned} {}_aI_x^\alpha (x-a)^\beta &= \frac{1}{\Gamma(\alpha)}\int_a^x (x-\tau)^{\alpha-1}(\tau-a)^\beta d\tau \\ &= \frac{1}{\Gamma(\alpha)}(x-a)^{\alpha+\beta}\int_0^1 s^{(\beta+1)-1}(1-s)^{\alpha-1}ds \\ &= \frac{\Gamma(\beta+1)}{\Gamma(\beta+\alpha+1)}(x-a)^{\beta+\alpha}. \end{aligned} $$

This establishes the first part. The second part also follows by definition.

$$ {}_aD_x^\alpha (x-a)^{\alpha-1} = \frac{d}{dx}\left({}_aI_x^{1-\alpha}(x-a)^{\alpha-1}\right) = \frac{d}{dx}(\Gamma(\alpha)) = 0. $$

□

2.2 Caputo Fractional Derivative

In 1967, M. Caputo introduced another definition of fractional derivative. We denote by $AC^n[a,b]$, $n \in \mathbb{N}$, the space of real-valued functions $w(x)$ which have continuous derivatives up to order $n-1$ on $[a,b]$ such that $w^{(n-1)}(x)$ belong to the space of absolutely continuous functions

$AC[a,b]$. That is

$$AC^n[a,b] = \left\{ w : [a,b] \to \mathbb{R} : \quad \frac{d^{n-1}}{dx^{n-1}} w \in AC[a,b] \right\}. \tag{2.18}$$

Definition 2.2.1. Let $\alpha > 0$, $m = \lceil \alpha \rceil$, and $w \in AC^m[a,b]$. The left-sided and right-sided Caputo fractional derivatives of order α of the function w are given, respectively, as

$${}_a^c D_x^\alpha w(x) = {}_a I_x^{m-\alpha} \frac{d^m}{dx^m} w(x) = \frac{1}{\Gamma(m-\alpha)} \int_a^x (x-s)^{m-\alpha-1} w^{(m)}(s)\, ds, \quad x > a, \tag{2.19}$$

and

$${}_x^c D_b^\alpha w(x) = (-1)^m {}_x I_b^{m-\alpha} \frac{d^m}{dx^m} w(x) = \frac{(-1)^m}{\Gamma(m-\alpha)} \int_x^b (s-x)^{m-\alpha-1} w^{(m)}(s)\, ds, \quad x > a. \tag{2.20}$$

Despite the fact that the Caupto and the Riemann-Liouville fractional derivatives have different definitions, there are connections between the two given in the following Theorem:

Lemma 2.2.2. *Let $\alpha \in \mathbb{R}^+ - \mathbb{N}$, $m = [\alpha]$, and $w \in AC^m[a,b]$. Then the left-sided and right-sided R-L fractional derivatives of order α of w exist almost everywhere and can be written as*

$${}_a D_x^\alpha w(x) = {}_a^c D_x^\alpha w(x) + \sum_{j=1}^{m-1} \frac{w^{(j)}(a)}{\Gamma(j-\alpha+1)} (x-a)^{j-\alpha}, \tag{2.21}$$

and

$${}_x D_b^\alpha w(x) = {}_x^c D_b^\alpha w(x) + \sum_{j=1}^{m-1} \frac{w^{(j)}(b)}{\Gamma(j-\alpha+1)} (b-x)^{j-\alpha}. \tag{2.22}$$

Proof. Applying repeatedly integration by parts to the Riemann-Liouville fractional derivative, we obtain

$$\begin{aligned} {}_a D_x^\alpha w(x) &= \sum_{j=1}^{m-1} \frac{w^{(j)}(a)}{\Gamma(j-\alpha+1)} (x-a)^{j-\alpha} + \frac{1}{\Gamma(m-\alpha)} \int_a^x (x-s)^{m-\alpha-1} w^{(m)}(s)\, ds, \quad x > a, \\ &= \sum_{j=1}^{m-1} \frac{w^{(j)}(a)}{\Gamma(j-\alpha+1)} (x-a)^{j-\alpha} + {}_a^c D_x^\alpha w(x). \end{aligned}$$

Similarly, the result holds for the right-sided case. □

An immediate consequence of this Lemma is given as proposition below.

Proposition 2.2.3. *Let $\alpha \in \mathbb{R}^+ - \mathbb{N}$, $m = [\alpha]$, and $w \in AC^m[a,b]$. Then*

$$ {}_a^cD_x^\alpha w(x) = {}_aD_x^\alpha w(x), \qquad \textit{if} \quad w(a) = w'(a) = \cdots = w^{(m-1)}(a) = 0, \tag{2.23}$$

$$ {}_x^cD_b^\alpha w(x) = {}_xD_b^\alpha w(x), \qquad \textit{if} \quad w(b) = w'(b) = \cdots = w^{(m-1)}(b) = 0. \tag{2.24}$$

One major difference between Riemann-Liouville and Caputo fractional derivatives is the fact that

$$ {}_0^cD_x^\alpha 1 = 0, \qquad \text{while} \qquad {}_0D_x^\alpha 1 = \frac{x^{-\alpha}}{\Gamma(1-\alpha)} \neq 0, \quad \alpha \geq 0,\, x > 0. $$

2.3 Hilfer Fractional Derivative

R. Hilfer in a series of works (see [62] and the references therein), considered a generalized fractional operator, called the two-parameter fractional derivative, to study some applications of fractional calculus. This generalized operator possesses special cases coinciding with the R-L and the Caputo fractional derivatives.

Definition 2.3.1. Let $0 < \alpha < 1$, $0 \leq \beta \leq 1$, $w \in L^1[a,b]$, $-\infty \leq a < x < b \leq -\infty$, and $(w * J_{(1-\alpha)(1-\beta)}) \in AC^1[a,b]$. Then the Hilfer fractional derivative is defined as

$$ {}_aD_x^{\alpha,\beta} w(x) = \left({}_aI_x^{\beta(1-\alpha)} \frac{d}{dx} \left({}_aI_x^{(1-\alpha)(1-\beta)} w \right) \right)(x). \tag{2.25}$$

Note that the Riemann-Liouville fractional derivative D_t^α and the Caputo fractional derivative ${}^cD_t^\alpha := I_t^{1-\alpha} D$ are special cases of the two-parameter fractional derivative $D_t^{\alpha,\gamma}$ for $\beta = 0$ and $\beta = 1$, respectively. Thus, $D_t^{\alpha,\gamma}$ is considered as an interpolant between D_t^α and ${}^cD_t^\alpha$.

2.4 Grünwald-Letnikov Fractional Derivative

An alternative definition of fractional derivative was introduced by A.K. Grünwald and A.V. Letnikov between 1867 and 1868. This is a direct extension of the integer-order derivative to the non-integer case. Grünwald-Letnikov fractional derivative definition will allow us later on to construct numerical methods for differential equations of fractional order, using either the R-L or Caputo fractional derivatives. We start with a formal definition.

Definition 2.4.1. The Grünwald-Letnikov fractional derivative of a function w is defined as:

$$ {}_{a}^{GL}D_x^{\alpha} w(x) = \lim_{h \to 0^+} \frac{1}{h^{\alpha}} \sum_{j=0}^{\left[\frac{x-a}{h}\right]} (-1)^j \binom{\alpha}{j} w(x - jh), \qquad \alpha > 0, \tag{2.26} $$

where

$$ \binom{\alpha}{j} = \frac{\Gamma(\alpha+1)}{j!\,\Gamma(\alpha - j + 1)}. $$

This definition is particularly useful for developing numerical schemes for solving fractional differential equations. The next Lemma is important in gaining an insight into the connection among the Grünwald-Letnikov derivative, the R-L fractional derivative and Caputo fractional derivative.

Lemma 2.4.2. *[102] Let $w \in C^m[a,b]$, $\alpha \geq 0$, and $m = \lceil \alpha \rceil$. Then*

$$ {}_{a}^{GL}D_x^{\alpha} w(x) = \sum_{j=1}^{m-1} \frac{w^{(j)}(a)}{\Gamma(j - \alpha + 1)} (x-a)^{j-\alpha} + \frac{1}{\Gamma(m-\alpha)} \int_a^x (x-s)^{m-\alpha-1} w^{(m)}(s)\, ds. \tag{2.27} $$

Lemma (2.2.2) and Lemma (2.4.2) provide the link among the Grünwald-Letnikov fractional derivative, Riemann-Liouville fractional derivative and Caputo fractional derivative for a sufficiently smooth function. Hence, when it comes to numerical implementation of the Riemann-Liouville and Caputo fractional derivatives, one could adopt the definition of the Grünwald-Letnikov fractional derivative.

We adopt the following notations for convenience.

$$ {}_0^{GL}D_x^\alpha = {}^{GL}D_x^\alpha, \qquad {}_0^{c}D_x^\alpha = {}^{c}D_x^\alpha, \qquad \text{and} \qquad {}_0D_x^\alpha = D_x^\alpha. $$

The Laplace and The Fourier Transforms

Introduction of the Laplace transform and the Fourier transform to fractional derivative is very important in the study of fractional differential equations.

Definition 2.4.3. For a $w \in L^1(\mathbb{R})$, we define the Fourier transform and the inverse Fourier transform respectively as:

$$ \mathscr{F}w = (\mathscr{F}w)(\xi) = \mathscr{F}\{w(t);\xi\} = \hat{w}(\xi) = \int_{-\infty}^{\infty} e^{ix\xi} w(x)dx, \tag{2.28} $$

$$ \left(\mathscr{F}^{-1}\hat{w}\right)(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\xi x}\hat{w}(\xi)d\xi. \tag{2.29} $$

Definition 2.4.4. The Laplace transform of a function $w(x)$, denoted as $W(s)$, is define as

$$ W(s) = \mathscr{L}\{w(x);s\} = \int_0^\infty e^{-sx} w(x)dx, \tag{2.30} $$

where $Re(s) > 0$, provided the right-hand side exists.

The following are the formulas for the Laplace transforms of the Riemann-Liouville and Caputo fractional derivatives, respectively, for $m-1 < \alpha \le m$, see [109]

$$ \mathscr{L}\{D^\alpha w(x);s\} = s^\alpha W(s) - \sum_{j=0}^{m-1} s^j D^{\alpha-j-1} w(x)|_{x=0}, \tag{2.31} $$

and

$$ \mathscr{L}\{{}^cD^\alpha w(x);s\} = s^\alpha W(s) - \sum_{j=0}^{m-1} s^{\alpha-j-1} w^{(j)}(x). \tag{2.32} $$

We point out here that these formulas, (2.31) and (2.32), are the reason for using integral type initial condition when dealing with the Riemann-Liouville differential equation while the classical initial condition is used when dealing with the Caputo differential equation. This is a major reason why many researchers use the Caputo fractional derivative.

2.5 Fractional Laplacian/Riesz Fractional Derivative

Another alternative definition is given to fractional derivatives which is commonly used in the literature, called the Riesz fractional derivative. The link between fractional Laplacian and Riesz fractional derivative has been established using Fourier analysis.

According to Samko *et al.* in [119], a fractional power of the Laplace operator is defined as follows:

$$-(-\Delta)^{\alpha/2} w(x) = -\mathscr{F}^{-1}|x|^{\alpha}\mathscr{F} w(x), \tag{2.33}$$

where $\mathscr{F}$ and $\mathscr{F}^{-1}$ are the Fourier transform and inverse Fourier transform, respectively.

Definition 2.5.1. The Riesz fractional derivative of function w with order $m-1<\alpha\le m$, $m\ge 1$ is defined as [153]

$$\frac{\partial^{\alpha}}{\partial|x|^{\alpha}} w(x) = -\frac{c_{\alpha}}{\Gamma(m-\alpha)}\frac{d^m}{dx^m}\int_{-\infty}^{+\infty}|x-\xi|^{m-\alpha-1}w(\xi)d\xi, \tag{2.34}$$

where

$$c_{\alpha} = \frac{1}{2\cos\left(\frac{\alpha\pi}{2}\right)}, \qquad \alpha\neq 1.$$

Lemma 2.5.2. *For a function $w(x)$ defined on the infinite domain $-\infty<x<\infty$, the following equality holds:*

$$-(-\Delta)^{\alpha/2} w(x) = -c_{\alpha}\left[{}_{-\infty}D_x^{\alpha} w(x) + {}_x D_{+\infty}^{\alpha} w(x)\right] = \frac{\partial^{\alpha}}{\partial|x|^{\alpha}} w(x), \tag{2.35}$$

where ${}_{-\infty}D_x^{\alpha} w(x)$ and ${}_x D_{+\infty}^{\alpha} w(x)$ are the left-sided and right-sided the Riemann-Liouville frac-

tional derivatives given as:

$$
{}_{-\infty}D_x^{\alpha} w(x) = \frac{1}{\Gamma(m-\alpha)} \frac{\partial^m}{\partial x^m} \int_{-\infty}^{x} \frac{w(\xi)}{(x-\xi)^{\alpha+1-m}} d\xi, \tag{2.36}
$$

and

$$
{}_{x}D_{+\infty}^{\alpha} w(x) = \frac{1}{\Gamma(m-\alpha)} \frac{\partial^m}{\partial x^m} \int_{x}^{+\infty} \frac{w(\xi)}{(\xi-x)^{\alpha+1-m}} d\xi. \tag{2.37}
$$

Before proving the above Lemma 2.5.2, we recall the following:

1. The Laplace transform of a power function:

$$
\mathscr{L}\{y^r\} = \int_0^{\infty} e^{-sy} y^r dy = \frac{\Gamma(r+1)}{s^{r+1}}, \qquad r > -1, \quad s > 0. \tag{2.38}
$$

2. Euler's reflection formula:

$$
\Gamma(\nu)\Gamma(1-\nu) = \frac{\pi}{\sin(\pi\nu)}, \qquad \nu \notin \mathbb{Z}. \tag{2.39}
$$

3.

$$
i^{\nu-1} + (-i)^{\nu-1} = i\left(e^{-\frac{i\pi\nu}{2}} - e^{\frac{i\pi\nu}{2}}\right) = 2\sin\left(\frac{\pi\nu}{2}\right). \tag{2.40}
$$

We also prove the following:

(a)

$$
I_1 = i\int_{-\infty}^{\infty} e^{i\xi(\mu-x)} \frac{|\xi|^{\nu}}{\xi} d\xi = \frac{sign(x-\mu)\pi}{\cos\left(\frac{\pi\nu}{2}\right)|x-\mu|^{\nu}\Gamma(1-\nu)}, \qquad 0 < \nu < 1. \tag{2.41}
$$

(b)

$$
I_2 = \int_{-\infty}^{\infty} e^{i\xi(\mu-x)} |\xi|^{\nu-2} d\xi = \frac{-\pi}{\cos\left(\frac{\pi\nu}{2}\right)|x-\mu|^{\nu-1}\Gamma(2-\nu)}, \qquad 1 < \nu < 2. \tag{2.42}
$$

Proof. (a) Let $0 < \nu < 1$. Using (2.38), (2.39) and (2.40), we obtain

$$\begin{aligned}
I_1 &= i\left[-\int_0^\infty e^{i\xi(x-\mu)}\xi^{\nu-1}d\xi + \int_0^\infty e^{i\xi(\mu-x)}\xi^{\nu-1}d\xi\right] \\
&= i\left[-\frac{\Gamma(\nu)}{[i(\mu-x)]^\nu} + \frac{\Gamma(\nu)}{[i(x-\mu)]^\nu}\right] \\
&= \frac{sign(x-\mu)\Gamma(\nu)\Gamma(1-\nu)}{|x-\mu|^\nu\Gamma(1-\nu)}\left[i^{\nu-1} + (-i)^{\nu-1}\right] \\
&= \frac{sign(x-\mu)\pi}{\cos\left(\frac{\pi\nu}{2}\right)|x-\mu|^\nu\Gamma(1-\nu)}.
\end{aligned}$$

(b) Similarly, for $1 < \nu < 2$, we have

$$\begin{aligned}
I_2 &= \left[\int_0^\infty e^{i\xi(x-\mu)}\xi^{\nu-2}d\xi + \int_0^\infty e^{i\xi(\mu-x)}\xi^{\nu-2}d\xi\right] \\
&= \frac{\Gamma(\nu-1)}{[i(\mu-x)]^{\nu-1}} + \frac{\Gamma(\nu-1)}{[i(x-\mu)]^{\nu-1}} \\
&= \frac{\Gamma(\nu-1)\Gamma(2-\nu)}{|x-\mu|^{\nu-1}\Gamma(2-\nu)}\left[i^{\nu-1} + (-i)^{\nu-1}\right] \\
&= \frac{-\pi}{\cos\left(\frac{\pi\nu}{2}\right)|x-\mu|^{\nu-1}\Gamma(2-\nu)}.
\end{aligned}$$

□

We are ready now to prove Lemma (2.5.2).

Proof. **Case 1:** $0 < \alpha < 1$

By definition, we have

$$-(-\Delta)^{\alpha/2}w(x) = -\frac{1}{2\pi}\int_{-\infty}^\infty e^{-ix\xi}|\xi|^\alpha\int_{-\infty}^\infty e^{i\xi\mu}w(\mu)d\mu d\xi.$$

Applying integration by parts on the inner integral in the right-hand side and assuming that w

vanishes at $x = \pm\infty$ to get

$$
\begin{aligned}
-(-\Delta)^{\alpha/2} w(x) &= -\frac{1}{2\pi}\int_{-\infty}^{\infty} w'(\mu)\left[i\int_{-\infty}^{\infty} e^{i\xi(\mu-x)}\frac{|\xi|^{\alpha}}{\xi}d\xi\right]d\mu \\
&= -\frac{1}{2\pi}\int_{-\infty}^{\infty} w'(\mu)\left[\frac{sign(x-\mu)\pi}{\cos\left(\frac{\pi\alpha}{2}\right)|x-\mu|^{\alpha}\Gamma(1-\alpha)}\right]d\mu \\
&= -\frac{1}{2\cos\left(\frac{\pi\alpha}{2}\right)}\left[\frac{1}{\Gamma(1-\alpha)}\int_{-\infty}^{x}\frac{w'(\mu)}{(x-\mu)^{\alpha}}d\mu - \frac{1}{\Gamma(1-\alpha)}\int_{x}^{\infty}\frac{w'(\mu)}{(\mu-x)^{\alpha}}d\mu\right].
\end{aligned}
$$

From Lemma (2.4.2) for $0 < \alpha < 1$, the Grünwald-Letnikov fractional derivative in $[a, x]$ is given by

$$ {}_{a}^{GL}D_x^{\alpha} w(x) = \frac{w(a)(x-a)^{-\alpha}}{\Gamma(1-\alpha)} + \frac{1}{\Gamma(1-\alpha)}\int_{a}^{x}\frac{w'(\mu)}{(x-\mu)^{\alpha}}d\mu. $$

Therefore, if $w(x)$ tends to zero as $a \to -\infty$ and $w(x)$ tends to zero as $b \to -\infty$, then we have the following

$$ {}_{-\infty}^{GL}D_x^{\alpha} w(x) = \frac{1}{\Gamma(1-\alpha)}\int_{-\infty}^{x}\frac{w'(\mu)}{(x-\mu)^{\alpha}}d\mu, $$

and

$$ {}_{x}^{GL}D_{\infty}^{\alpha} w(x) = -\frac{1}{\Gamma(1-\alpha)}\int_{x}^{\infty}\frac{w'(\mu)}{(\mu-x)^{\alpha}}d\mu. $$

So, if w is continuous and w' is integrable for $x \geq a$, the Riemann-Liouville fractional derivative exists and coincides with the Grünwald-Letnikov fractional derivative for every $0 < \alpha < 1$. Hence we have for $0 < \alpha < 1$,

$$ -(-\Delta)^{\alpha/2} w(x) = -c_{\alpha}\left[{}_{-\infty}D_x^{\alpha} w(x) + {}_{x}D_{+\infty}^{\alpha} w(x)\right] = \frac{\partial^{\alpha}}{\partial|x|^{\alpha}} w(x), $$

where

$$ {}_{-\infty}D_x^{\alpha} w(x) = \frac{1}{\Gamma(1-\alpha)}\frac{\partial}{\partial x}\int_{-\infty}^{x}\frac{w(\mu)}{(x-\mu)^{\alpha}}d\mu, $$

and

$$ {}_{x}D_{+\infty}^{\alpha} w(x) = \frac{1}{\Gamma(1-\alpha)}\frac{\partial}{\partial x}\int_{x}^{+\infty}\frac{w(\mu)}{(\mu-x)^{\alpha}}d\mu. $$

Case 2: $1 < \alpha < 2$

In a similar way, we assume that w and w'' vanish at $x = \pm\infty$ and applying integration by parts twice to get

$$
\begin{aligned}
-(-\Delta)^{\alpha/2} w(x) &= -\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ix\xi}|\xi|^{\alpha}\left[-\xi^{-2}\int_{-\infty}^{\infty} e^{i\xi\mu} w''(\mu)\,d\mu\right]d\xi \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} w''(\mu)\left[\int_{-\infty}^{\infty} e^{i\xi(\mu-x)}|\xi|^{\alpha-2}d\xi\right]d\mu \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} w''(\mu)\left[\frac{-\pi}{\cos\left(\frac{\pi\alpha}{2}\right)|x-\mu|^{\alpha-1}\Gamma(2-\alpha)}\right]d\mu \\
&= -\frac{1}{2\cos\left(\frac{\pi\alpha}{2}\right)}\left[\frac{1}{\Gamma(2-\alpha)}\int_{-\infty}^{x}\frac{w''(\mu)}{(x-\mu)^{\alpha-1}}d\mu + \frac{1}{\Gamma(2-\alpha)}\int_{x}^{\infty}\frac{w''(\mu)}{(\mu-x)^{\alpha-1}}d\mu\right].
\end{aligned}
$$

Again from Lemma (2.4.2) for $1 < \alpha < 2$, the Grünwald-Letnikov fractional derivative in $[a, x]$ is given by

$$
{}_{a}^{GL}D_{x}^{\alpha} w(x) = \frac{w(a)(x-a)^{-\alpha}}{\Gamma(1-\alpha)} + \frac{w'(a)(x-a)^{1-\alpha}}{\Gamma(1-\alpha)} + \frac{1}{\Gamma(2-\alpha)}\int_{a}^{x}\frac{w''(\mu)}{(x-\mu)^{\alpha}}d\mu.
$$

Therefore, if $w(x)$ and $w'(x)$ tend to zero as $a \to -\infty$ and $w(x)$ and $w'(x)$ tend to zero as $b \to -\infty$, then we have the following respectively

$$
{}_{-\infty}^{GL}D_{x}^{\alpha} w(x) = \frac{1}{\Gamma(2-\alpha)}\int_{-\infty}^{x}\frac{w''(\mu)}{(x-\mu)^{\alpha}}d\mu,
$$

and

$$
{}_{x}^{GL}D_{\infty}^{\alpha} w(x) = -\frac{1}{\Gamma(2-\alpha)}\int_{x}^{\infty}\frac{w''(\mu)}{(\mu-x)^{\alpha}}d\mu.
$$

So, if w and w' is continuous and w'' is integrable for $x \geq a$, the Riemann-Liouville fractional derivative exists and coincides with the Grünwald-Letnikov fractional derivative for every $1 < \alpha < 2$. Hence we have for $1 < \alpha < 2$,

$$
-(-\Delta)^{\alpha/2} w(x) = -c_{\alpha}\left[{}_{-\infty}D_{x}^{\alpha} w(x) + {}_{x}D_{+\infty}^{\alpha} w(x)\right] = \frac{\partial^{\alpha}}{\partial|x|^{\alpha}} w(x),
$$

where

$$
{}_{-\infty}D_x^{\alpha} w(x) = \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_{-\infty}^{x} \frac{w(\mu)}{(x-\mu)^{\alpha-1}} d\mu,
$$

and

$$
{}_{x}D_{+\infty}^{\alpha} w(x) = \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_{x}^{+\infty} \frac{w(\mu)}{(\mu-x)^{\alpha-1}} d\mu.
$$

Repeating this process, if $m = \lceil \alpha \rceil$, then

$$
-(-\Delta)^{\alpha/2} w(x) = -c_{\alpha} \left[{}_{-\infty}D_x^{\alpha} w(x) + {}_{x} D_{+\infty}^{\alpha} w(x) \right] = \frac{\partial^{\alpha}}{\partial |x|^{\alpha}} w(x),
$$

where

$$
{}_{-\infty}D_x^{\alpha} w(x) = \frac{1}{\Gamma(m-\alpha)} \frac{\partial^m}{\partial x^m} \int_{-\infty}^{x} \frac{w(\mu)}{(x-\mu)^{\alpha+1-m}} d\mu,
$$

and

$$
{}_{x}D_{+\infty}^{\alpha} w(x) = \frac{1}{\Gamma(m-\alpha)} \frac{\partial^m}{\partial x^m} \int_{x}^{+\infty} \frac{w(\mu)}{(\mu-x)^{\alpha+1-m}} d\mu.
$$

□

Lemma 2.5.2 still holds if the function w is given in a finite interval $[0, L]$ by imposing homogeneous conditions.

2.6 Generalized Mittag-Leffler Functions

The fundamental role of the Mittag-Leffler function in the theory of fractional calculus remains extremely important. No wonder it is called, "the Queen function of the fractional calculus." In this section, we will give some useful definitions and important results of this function. The Prabhakar generalized Mittag-Leffler function [112] is defined as

$$
E_{\alpha,\beta}^{\rho}(w) = \sum_{k=0}^{\infty} \frac{\Gamma(\rho+k)}{\Gamma(\rho)\Gamma(\alpha k+\beta)} \frac{w^k}{k!}, \qquad w, \beta, \rho \in \mathbb{C}, \quad \operatorname{Re}\alpha > 0. \tag{2.43}
$$

Some special cases of this function are the Mittag-Leffler function in one parameter $E_\alpha(w) = E^1_{\alpha,1}(w)$, and in two parameters $E_{\alpha,\beta}(w) = E^1_{\alpha,\beta}(w)$.

The function $E^\rho_{\alpha,\beta}$ is an entire function [112] and therefore bounded in any finite interval. In addition, for $w, \beta, \lambda \in \mathbb{C}$ and $\operatorname{Re} \alpha > 0$, this function satisfies the following recurrence relations [59, 78]:

$$\lambda w^\alpha \, E_{\alpha,\alpha+\beta}(\lambda w^\alpha) = E_{\alpha,\beta}(\lambda w^\alpha) - \frac{1}{\Gamma(\beta)}, \tag{2.44}$$

and

$$\alpha E^2_{\alpha,\beta}(\lambda w^\alpha) = (1+\alpha-\beta)\, E_{\alpha,\beta}(\lambda w^\alpha) + E_{\alpha,\beta-1}(\lambda w^\alpha). \tag{2.45}$$

Combining the relations (2.44) and (2.45) yields the recurrence relation:

$$\alpha\lambda w^\alpha \, E^2_{\alpha,\beta}(\lambda w^\alpha) = (1+\alpha-\beta)\, E_{\alpha,\beta-\alpha}(\lambda w^\alpha) + E_{\alpha,\beta-\alpha-1}(\lambda w^\alpha), \tag{2.46}$$

for $w, \beta, \lambda \in \mathbb{C}$ and $\operatorname{Re} \alpha > 0$.

On the real line, we have the following upper bounds.

Lemma 2.6.1. *Let $0 < \alpha < 2$, $\beta \in \mathbb{R}$, and $\rho = 1, 2$. Then, there is a constant $M = M(\alpha, \beta) > 0$ such that*

$$\lambda^\rho t^{\alpha\rho} \left| E^\rho_{\alpha,\beta}(-\lambda t^\alpha) \right| \le M, \qquad t \ge 0, \quad \lambda \ge 0. \tag{2.47}$$

Proof. When $\rho = 1$, the result is a special case of Theorem 1.6 in [109]. When $\rho = 2$, the bound follows from (2.46).

The function $E^\rho_{\alpha,\beta}$ possesses the following positivity and monotonicity properties [55].

Lemma 2.6.2. *Let $0 < \alpha \le 1$, $\lambda > 0$, and $\rho > 0$. Then the functions $E^\rho_{\alpha,\beta}(-\lambda t^\alpha)$, $\alpha\rho \le \beta$, and $t^{\gamma-1} E^\rho_{\alpha,\gamma}(-\lambda t^\alpha)$, $\alpha\rho \le \gamma \le 1$, are positive monotonically decreasing functions of $t > 0$.*

Lemma 2.6.2 and the recurrence relation (2.44) imply the following corollary.

Corollary 2.6.3. *Let $0 < \alpha \le 1$, $2\alpha \le \beta$, and $\lambda > 0$. Then $t^\alpha E_{\alpha,\beta}(-\lambda t^\alpha)$ is a monotonically increasing function of $t > 0$.*

Proof. Since $\beta-\alpha \geq \alpha$, then by Lemma 2.6.2, $E_{\alpha,\beta-\alpha}(-\lambda t^{\alpha})$ is a monotonically decreasing function of $t>0$. Let $0<s<t$, then from (2.44) we have

$$\begin{aligned} \lambda s^{\alpha} E_{\alpha,\beta}(-\lambda s^{\alpha}) &= 1/\Gamma(\beta-\alpha) - E_{\alpha,\beta-\alpha}(-\lambda s^{\alpha}) \\ &< 1/\Gamma(\beta-\alpha) - E_{\alpha,\beta-\alpha}(-\lambda t^{\alpha}) = \lambda t^{\alpha} E_{\alpha,\beta}(-\lambda t^{\alpha}). \end{aligned}$$

We conclude this section by recalling two Laplace transform formulas.

$$\mathscr{L}\left\{t^{\beta-1}E^{\rho}_{\alpha,\beta}(\lambda t^{\alpha})\right\} = \frac{s^{\alpha\rho-\beta}}{(s^{\alpha}-\lambda)^{\rho}}, \quad |\lambda s^{-\alpha}|<1, \tag{2.48}$$

where $\alpha,\beta,\lambda,\rho \in \mathbb{C}$, Re $\alpha>0$, Re $\beta>0$, and Re $\rho>0$. See for example (1.9.13) in [78] and (11.8) in [59]. From [62], we have the formula

$$\mathscr{L}\left\{D^{\alpha,\gamma} w(t)\right\} = s^{\alpha}\mathscr{L}\{w\} - s^{\alpha-\gamma} I^{1-\gamma} w(0). \tag{2.49}$$

Chapter 3

A Survey of Existence and Uniqueness Results for Fractional Differential Models

The tremendous impact fractional calculus has had in many fields of applications has drawn attentions of many researchers to its study. However, the fractional derivative operator is a quasi-differential operator with nonlocal and weak singularity properties. Therefore, some of the useful tools for theoretical studies such as the semigroup properties, the commutative law, and many others are not satisfied by this operator. It is therefore very important to study analytic properties of solutions of fractional differential equations. In this section, we give survey of the existence and uniqueness of solutions of differential equation of fractional type both direct and inverse version. This is done by highlighting key results and Theorems in most cases. Further detail may be found in the reference.

Many researchers depend heavily on the properties of the Fourier and Laplace transforms to verify properties of classical solutions for fractional differential equations. Another way to study the theoretical analysis of solutions to fractional differential equations is by studying the corresponding variational problem (weak elliptic problem) in suitable functional spaces and their corresponding norms. In this case, the existence and uniqueness results of weak solutions are obtained by using the existing theory of elliptic problems such as Lax-Milgram theorem.

Furthermore, there has been extensive study on the existence and uniqueness of solutions to the fractional differential equations using fixed point theory approach. The following are the commonly used Theorems to achieve the desirable results (existence and uniqueness of solutions of fractional differential equations): (i) the Banach and Schauder fixed point theorems, (ii) the Leggett-Williams fixed point theorem on a convex cone, (iii) the contraction mapping principle and the Krasnoselskii fixed point theorems, (iv) the Arzelá-Ascoli compact theorem and many more, see [2, 15, 23, 24, 113–115, 150, 151], see also [1, 38, 57, 60, 71, 134].

3.1 Direct Problems

Experts in this field have done various studies on the existence and uniqueness of solutions to time-space fractional differential equations both linear and nonlinear for direct problems. We focus attention on a few results and refer the readers to the cited works and the references therein.

3.1.1 Space Fractional Models

Consider a Cauchy problem of the form

$$w_t - \epsilon \Delta w_t + (-\Delta)^\alpha w = w^{\theta+1}, \qquad x \in \mathbb{R}^n,\ t > 0, \tag{3.1}$$

subject to initial condition

$$w(x,0) = w_0(x), \qquad x \in \mathbb{R}. \tag{3.2}$$

This is called a pseudo-parabolic equation when $\alpha = 1$ and $\epsilon > 0$.

Existence of solutions to Equations (3.1)-(3.2) together with time-decay rates for small-amplitude solutions has been study by L. Jin et al in [72] for $\alpha > 0$. They proved the following Theorems:

Theorem 3.1.1. *Let $\alpha \geq 1$, $s > \frac{n}{2}$, $\theta > \frac{4\alpha}{n}$, and $\theta \in \mathbb{Z}$. Assume that $w_0 \in H^s(\mathbb{R}^n) \cap L^1(\mathbb{R}^n)$ and let $E_0 = ||w_0||_{H^s} + ||w_0||_{L^2}$. Then there exists a small positive constant δ_0 such that for $E_0 \leq \delta_0$,* (3.1)-(3.2) *has a solution satisfying*

$$\left\|(-\Delta)^{\frac{l}{2}} w(t)\right\|_{L^2} \leq cE_0(1+t)^{-\frac{n}{4\alpha}-\frac{1}{2\alpha}}, \qquad \forall\, 0 \leq l \leq s. \tag{3.3}$$

Theorem 3.1.2. *Assume that* $0<\alpha<1$, $\theta > \frac{4\alpha}{n}$, $\theta \in \mathbb{Z}$ *and* $\left[\frac{s}{2\bar{\alpha}}\right] \geq \frac{n}{2\alpha} + \frac{3}{2}\bar{\alpha}$*. Let* $E_0 = ||w_0||_{H^s} + ||w_0||_{L^2}$ *for* $w_0 \in H^s(\mathbb{R}^n) \cap L^1(\mathbb{R}^n)$*. Then there exists a small positive constant* δ_0 *such that for* $E_0 \leq \delta_0$, (3.1)-(3.2) *has a solution satisfying*

$$\left\|(-\Delta)^{\frac{l}{2}} w(t)\right\|_{L^2} \leq cE_0(1+t)^{-\frac{n}{4\alpha}-\frac{1}{2\alpha}}, \qquad \textit{for} \quad 0 \leq l \leq N_0,. \tag{3.4}$$

with

$$\bar{\alpha} = 1-\alpha, \quad N_0 = \alpha \min\left\{s - \frac{n}{2\alpha}\bar{\alpha}, \quad \left(\left[\frac{s}{2\bar{\alpha}}\right]-1\right)\bar{\alpha} - \frac{n}{2\alpha}\bar{\alpha}+2\right\}.$$

The following have been used in the estimate:

$$\langle f,g\rangle_{H^s} = \int_{\mathbb{R}^n} \hat{f}(\xi)\overline{\hat{g}(\xi)}(1+|\xi|^2)^s d\xi, \tag{3.5}$$

with norm

$$||f||^2_{H^s} = \int_{\mathbb{R}^n} (1+|\xi|^2)^s |\hat{f}(\xi)|^2 d\xi, \tag{3.6}$$

where $\hat{f}$ is the Fourier transform of f on $\mathbb{R}^n$ and $H^s(\mathbb{R}^n)$ denotes the general Sobolev space with $H^0(\mathbb{R}^n) = L^2(\mathbb{R}^n)$.

The Duhamel principle is used to transform (3.1)-(3.2) into an integral equation to make the analysis easier to handle. Also, time-weighted energy method was introduced in their paper to overcome the weakly dissipative property of the equations. Readers are directed to full detail results of this problem in [72].

3.1.2 Time-Space Fractional Models

Here, we consider the time-space fractional nonlinear super-diffusion equation with homogeneous Dirichlet boundary condition of the form:

$$ {}^{c}D_t^{\alpha} w + \frac{\partial}{\partial x} f(w) = \epsilon\left(-(-\Delta)^{\frac{\beta}{2}}\right) w, \qquad \text{in} \quad \Omega_T, \tag{3.7}$$

subject to initial condition

$$ w(0,x) = \psi_1(x) \qquad \text{and} \qquad w_t(0,x) = \psi_2(x), \qquad x \in \Omega, \tag{3.8}$$

where $1 < \alpha < 2$, $1 < \beta \le 2$, $\epsilon > 0$, $\Omega_T = [0,T] \times \Omega$, Ω is bounded region with smooth boundary in $\mathbb{R}^n$, $n \ge 1$. $\psi_1, \psi_2 \in H_0^1(\Omega)$ are given real-valued smooth functions and $w \in H^1(\Omega)$ is a smooth unknown function. The nonlinear term f is also assumed to be Lipschitz continuous on a bounded domain Ω. In [115], the following function spaces are defined together with their corresponding norms.

Let the closures of $C_0^{\infty}(E)$ with respect to the norms $||w||_{{}^{\sigma}H_0^{\nu}}$ and $||w||_{{}^{r}H_0^{\nu}}$ be ${}^{\sigma}H_0^{\nu}(E)$ and ${}^{r}H_0^{\nu}(E)$, respectively, for a constant $\nu > 0$ and

$$ ||w||_{{}^{\sigma}H_0^{\nu}} := \left[||w||_{L^2}^2 + |w|_{{}^{\sigma}H_0^{\nu}}^2 \right]^{\frac{1}{2}}, \qquad \text{where} \quad |w|_{{}^{\sigma}H_0^{\nu}}^2 := ||D_t^{\alpha} w||_{L^2}^2, \tag{3.9}$$

and similarly,

$$ ||w||_{{}^{r}H_0^{\nu}} := \left[||w||_{L^2}^2 + |w|_{{}^{r}H_0^{\nu}}^2 \right]^{\frac{1}{2}}, \qquad \text{where} \quad |w|_{{}^{r}H_0^{\nu}}^2 := ||D_t^{\alpha} w||_{L^2}^2. \tag{3.10}$$

Also, the norm in the usual Sobolev space, $H_0^{\nu}(E)$, is defined as follows:

$$ ||w||_{H_0^{\nu}} := \left[||w||_{L^2}^2 + |w|_{H_0^{\nu}}^2 \right]^{\frac{1}{2}}, \qquad \text{where} \quad |w|_{H_0^{\nu}}^2 := \left[\frac{\langle D_t^{\alpha} w,{}_t D^{\alpha} w \rangle_{L^2}}{\cos(\pi\nu)} \right]. \tag{3.11}$$

M. Qiu et al in [115] established the existence and uniqueness of weak solutions for a class of fractional super-diffusion equations (3.7)-(3.8) in an appropriate function space, $\mathscr{B}$, a closed, bounded, convex subspace (subset) of the standard Banach space $C\left(H_0^1(\Omega);[0,T]\right)$. The idea of the proof is again based on transforming (3.7)-(3.8) into integral form, then formulating a variational problem in the appropriate function space, then applying the Schauder fixed point theorem and the Arzelá-Ascoli compactness theorem to obtain the existence and uniqueness of the weak solution.

3.2 Inverse Problems

In this section, we present some of our results on inverse problem involving two-parameter fractional derivatives, see [42]. This is an inverse problem, in the sense that the source term function is unknown, and by imposing extra conditions on the data, the problem is well-posed.

Consider determining the solution u and the space-dependent source f for the following two-parameter fractional diffusion equation (FDE):

$$\begin{aligned}
&D_t^{\alpha,\gamma} u(x,t) - u_{xx}(x,t) = f(x), \quad x \in (0,1), \quad t \in (0,T), \quad 0 < \alpha \le \gamma \le 1,\\
&u(x,T_m) = z(x), \quad u(x,T) = h(x), \quad x \in [0,1], \qquad 0 < T_m < T, \qquad\qquad (3.12)\\
&u(1,t) = 0, \quad u_x(0,t) = u_x(1,t), \qquad t \in (0,T],
\end{aligned}$$

where z and h are square integrable functions. The operator $D_t^{\alpha,\gamma}$ is the generalized Hilfer fractional derivative.

A similar inverse source problem to (3.12) has been considered by Kirane *et al.* [79] but with the Caputo derivative for which the initial condition is the traditional local condition. Furati *et al.* [41] constructed a series representation of u and f for problem (3.12), but subject to an integral-type initial condition instead, using a bi-orthogonal system. Unlike in [41], in the current problem, the value of the solution at some time $t = T_m$ is used rather than the value of the fractional integral of the solution $I^{1-\gamma}u(x,t)$ at $t = 0$, which may neither be measurable nor have a physical meaning. As a result, the construction of the series representation of u and f is not a straightforward extension of the one in [41]. This is mainly due to the complexity in ensuring the solvability of the arising linear systems and in achieving the necessary lower and upper bounds for showing the convergence of the constructed series.

Inverse source problems for a one-parameter FDE with Caputo derivative have been investigated by many researchers under various initial, boundary and over determination conditions. For a space-dependent source f, Zhang and Xu [152] used Duhamel's principle and an extra boundary condition to uniquely determine f. Kirane and Malik [79] studied first a one-dimensional problem with non-local non-self-adjoint boundary conditions and subject to initial and final conditions. The results were extended to the two-dimensional problem by Kirane *et al.* [80]. Özkum *et al.* [105] used the Adomian decomposition method to construct the source term for a linear FDE with a variable coefficient in the half plane. In a bounded interval, Wang *et al.* [135] reconstructed a source for an ill posed time-FDE by the Tikhonov regularization method. A numerical method for reproducing kernel Hilbert space to solve an inverse source problem for a two-dimensional problem is proposed by Wang *et al.* [136]. Wei and Wang [138] proposed a modified version of quasi-boundary value method to determine the source term in a bounded domain from a noisy final data. The analytic Fredholm theorem and some operator properties are used by Tatar and Ulusoy [127] to prove the well-posedness of a one-dimensional inverse source problem for a space-time FDE. Feng and Karimov [40] used eigenfunctions to analyze an inverse source problem for a fractional mixed parabolic hyperbolic equation. They formulated the problem as an optimization problem and then used a semismooth Newton algorithm to solve it. Gülkaç [56] applied the Homotopy Perturbation Method to find the source term allowing space dependent diffusivity. For a three-dimensional inverse source problem, we refer the reader to the work by Sakamoto and Yamamoto [117] and by Ruan *et al.* [116]. In relation to the above, for the case of time-dependent source term f, see [5,70,117,137,140,142].

In all the previous works cited above, the problems considered involve the Caputo derivative together with the classical initial conditions. In our work, we consider a two parameter fractional derivative, of which the Caputo and Riemann-Liouville derivatives are special cases. As a result, we need to consider the possibility of having a nonlocal initial condition, which in general may not have a clear physical meaning or a direct way of measuring. We show that these nonlocal initial conditions can be replaced by a local observation.

In later sections, we deal with a 2×2 linear system with a coefficient matrix of the form

$$A_{\alpha,\gamma,\mu}(\lambda, s, t) := \begin{bmatrix} t^{\alpha} E_{\alpha,\mu}(-\lambda t^{\alpha}) & t^{\gamma-1} E_{\alpha,\gamma}(-\lambda t^{\alpha}) \\ s^{\alpha} E_{\alpha,\mu}(-\lambda s^{\alpha}) & s^{\gamma-1} E_{\alpha,\gamma}(-\lambda s^{\alpha}) \end{bmatrix}. \tag{3.13}$$

In the next lemma, we show that the determinant of this matrix, denoted by $|\dots|$, has a positive lower bound, and consequently the matrix is non-singular. This property plays a crucial role for obtaining the coefficients of the series representation of u and f. Also, it provides the necessary bounds for showing the convergence of these series.

Lemma 3.2.1. *Let* $0 < \alpha \le \gamma \le 1$, $\mu \ge 2\alpha$, *and* $0 < s < t$. *Then, there is a constant* $A > 0$, *independent of* λ, *such that*

$$|A_{\alpha,\gamma,\mu}(\lambda, s, t)| > \frac{A}{\lambda^2}, \qquad \lambda > 0. \tag{3.14}$$

Proof. By Lemma 2.6.2 and Corollary 2.6.3, from (3.13), the determinant of the matrix is

$$\begin{aligned} &\left|A_{\alpha,\mu,\gamma}(\lambda, s, t)\right| = \\ &\quad t^{\alpha} E_{\alpha,\mu}(-\lambda t^{\alpha})\, s^{\gamma-1} E_{\alpha,\gamma}(-\lambda s^{\alpha}) - t^{\gamma-1} E_{\alpha,\gamma}(-\lambda t^{\alpha})\, s^{\alpha} E_{\alpha,\mu}(-\lambda s^{\alpha}) > 0. \end{aligned}$$

In addition, from (2.44) we have

$$\begin{aligned} \lim_{\lambda\to\infty} \lambda^2 |A_{\alpha,\gamma,\mu}(\lambda, s, t)| &= \frac{1}{\Gamma(\mu-\alpha)} \frac{s^{\gamma-1-\alpha}}{\Gamma(\gamma-\alpha)} - \frac{t^{\gamma-1-\alpha}}{\Gamma(\gamma-\alpha)} \frac{1}{\Gamma(\mu-\alpha)}. \\ &= \frac{s^{\gamma-1-\alpha} - t^{\gamma-1-\alpha}}{\Gamma(\gamma-\alpha)\,\Gamma(\mu-\alpha)} > 0. \end{aligned}$$

Therefore, $\lambda^2 |A_{\alpha,\gamma,\mu}(\lambda, s, t)|$, as a function of λ, is bounded below by a positive constant.

By combining Lemmas 2.6.1 and 3.2.1 we obtain the following estimate.

Corollary 3.2.2. *Let* $0 < \alpha \le \gamma \le 1$, $\mu \ge 2\alpha$, *and* $0 < s < t$. *Then, there is a constant* $B > 0$, *independent of* λ, *such that*

$$\left[A^{-1}_{\alpha,\gamma,\mu}(\lambda, s, t)\right]_{ij} < B\lambda, \qquad \lambda > 0. \tag{3.15}$$

Series Representations

Following [41, 79], the boundary conditions in (3.12) suggest the bi-orthogonal pair of bases $\Phi = \{\varphi_0, \varphi_{1,n}, \varphi_{2,n}\}_{n=1}^{\infty}$ and $\Psi = \{\psi_0, \psi_{1,n}, \psi_{2,n}\}_{n=1}^{\infty}$ for the space $L^2(0,1)$ where,

$$\varphi_{1,0}(x) = 2(1-x), \quad \varphi_{1,n}(x) = 4(1-x)\cos\lambda_n x, \quad \varphi_{2,n}(x) = 4\sin\lambda_n x, \tag{3.16}$$

with $\lambda_n = 2\pi n$, and

$$\psi_{1,0}(x) = 1, \qquad \psi_{1,n}(x) = \cos\lambda_n x, \qquad \psi_{2,n}(x) = x\sin\lambda_n x. \tag{3.17}$$

Although the sequences Φ and Ψ are not orthogonal, it is proven in [68] that they both are Riesz bases. We seek series representations of the solution u and the source term f in the form

$$u(x,t) = u_{1,0}(t)\,\varphi_{1,0}(x) + \sum_{k=1}^{2}\sum_{n=1}^{\infty} u_{k,n}(t)\,\varphi_{k,n}(x), \tag{3.18}$$

$$f(x) = f_{1,0}\,\varphi_{1,0}(x) + \sum_{k=1}^{2}\sum_{n=1}^{\infty} f_{k,n}\,\varphi_{k,n}(x). \tag{3.19}$$

Substituting (3.18) and (3.19) into (3.12) yields the following system of fractional differential equations:

$$D^{\alpha,\gamma} u_{1,n}(t) + \lambda_n^2 u_{1,n}(t) = f_{1,n}, \qquad n \ge 0, \tag{3.20}$$

$$D^{\alpha,\gamma} u_{2,n}(t) + \lambda_n^2 u_{2,n}(t) - 2\lambda_n u_{1,n}(t) = f_{2,n}, \qquad n \ge 1, \tag{3.21}$$

where $\lambda_0 := 0$.

We solve (3.20) and (3.21) via Laplace transform. For convenience, we introduce the following notations:

$$c_{1,0} = I^{1-\gamma} u_{1,0}(0) \quad \text{and} \quad c_{k,n} = I^{1-\gamma} u_{k,n}(0), \quad k = 1,2, \quad n \geq 1.$$

By applying the Laplace transform (2.49) to (3.20), we obtain

$$U_{1,n}(s) = f_{1,n} \frac{1}{s(s^\alpha + \lambda_n^2)} + c_{1,n} \frac{s^{\alpha-\gamma}}{s^\alpha + \lambda_n^2}. \tag{3.22}$$

Similarly, by applying the Laplace transform to (3.21) and then substituting (3.22), we obtain

$$\begin{aligned} U_{2,n}(s) &= \frac{f_{2,n}}{s(s^\alpha + \lambda_n^2)} + \frac{c_{2,n}\, s^{\alpha-\gamma}}{s^\alpha + \lambda_n^2} + \frac{2\lambda_n}{s^\alpha + \lambda_n^2} U_{1,n}(s) \\ &= \frac{f_{2,n}}{s(s^\alpha + \lambda_n^2)} + \frac{c_{2,n}\, s^{\alpha-\gamma}}{s^\alpha + \lambda_n^2} + 2\lambda_n \left[f_{1,n} \frac{1}{s(s^\alpha + \lambda_n^2)^2} + c_{1,n} \frac{s^{\alpha-\gamma}}{(s^\alpha + \lambda_n^2)^2} \right]. \end{aligned}$$

Hence, from formula (2.48) we have

$$u_{1,n}(t) = f_{1,n}\, t^\alpha E_{\alpha,\alpha+1}(-\lambda_n^2 t^\alpha) + c_{1,n}\, t^{\gamma-1} E_{\alpha,\gamma}(-\lambda_n^2 t^\alpha), \qquad n \geq 0, \tag{3.23}$$

and

$$u_{2,n}(t) = f_{2,n}\, t^\alpha E_{\alpha,\alpha+1}(-\lambda_n^2 t^\alpha) + c_{2,n}\, t^{\gamma-1} E_{\alpha,\gamma}(-\lambda_n^2 t^\alpha) + d_n(t), \quad n \geq 1, \tag{3.24}$$

where

$$d_n(t) = 2\lambda_n \left[f_{1,n}\, t^{2\alpha} E^2_{\alpha,2\alpha+1}(-\lambda_n^2 t^\alpha) + c_{1,n}\, t^{\alpha+\gamma-1} E^2_{\alpha,\alpha+\gamma}(-\lambda_n^2 t^\alpha) \right]. \tag{3.25}$$

Next, we determine the unknowns $\{c_{1,0}, c_{k,n}\}$ and $\{f_{1,0}, f_{k,n}\}$. From the two time conditions in (3.12) we have

$$u_{1,0}(T_m) = z_{1,0}, \quad u_{k,n}(T_m) = z_{k,n}, \quad u_{1,0}(T) = h_{1,0}, \quad u_{k,n}(T) = h_{k,n}, \tag{3.26}$$

for $n \geq 1$ with $k = 1, 2$, where $\{z_{1,0}, z_{k,n}\}$ and $\{h_{1,0}, h_{k,n}\}$ denote the Fourier coefficients of the series representations of z and h in terms of the basis (3.16), respectively. That is,

$$z_{1,0} = \langle z, \psi_{1,0} \rangle, \qquad z_{k,n} = \langle z, \psi_{k,n} \rangle, \qquad h_{1,0} = \langle h, \psi_{1,0} \rangle, \qquad h_{k,n} = \langle h, \psi_{k,n} \rangle,$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product in $L^2(0,1)$.

Using (3.26) in (3.23), we obtain the linear system

$$A_n \begin{bmatrix} f_{1,n} \\ c_{1,n} \end{bmatrix} = \begin{bmatrix} h_{1,n} \\ z_{1,n} \end{bmatrix}, \qquad n \geq 0, \tag{3.27}$$

where,

$$A_n = A_{\alpha,\gamma,1+\alpha}(\lambda_n^2, T_m, T) = \begin{bmatrix} T^{\alpha} E_{\alpha,\alpha+1}(-\lambda_n^2 T^{\alpha}) & T^{\gamma-1} E_{\alpha,\gamma}(-\lambda_n^2 T^{\alpha}) \\ T_m^{\alpha} E_{\alpha,\alpha+1}(-\lambda_n^2 T_m^{\alpha}) & T_m^{\gamma-1} E_{\alpha,\gamma}(-\lambda_n^2 T_m^{\alpha}) \end{bmatrix}. \tag{3.28}$$

By Lemma 3.2.1, the linear system (3.27) is uniquely solvable and

$$\begin{bmatrix} f_{1,n} \\ c_{1,n} \end{bmatrix} = A_n^{-1} \begin{bmatrix} h_{1,n} \\ z_{1,n} \end{bmatrix}, \qquad n \geq 0. \tag{3.29}$$

In a similar fashion, by using (3.26) in (3.24), we observe

$$\begin{bmatrix} f_{2,n} \\ c_{2,n} \end{bmatrix} = A_n^{-1} \begin{bmatrix} h_{2,n} - d_n(T) \\ z_{2,n} - d_n(T_m) \end{bmatrix}, \qquad n \geq 1. \tag{3.30}$$

To determine the coefficients in the series representations (3.18) and (3.19), we first perform the calculations in (3.29) and (3.30) and then substitute in the formulas (3.23) and (3.24). Therefore, the construction of the series representation of u and f is now completed.

Existence and Uniqueness Result for Inverse Problem

In this section, under some regularity assumptions on the given data functions h and z in problem (3.12), we show that the series representations of the solution u in (3.18) and of the source f in (3.19) satisfy certain smoothness properties. These smoothness properties will allow us to show the existence and uniqueness of such u and f, and also to show that u form a classical solution of (3.12).

Theorem 3.2.3. *Let h, $z \in C^4[0,1]$ be such that*

$$z'(0) = z'(1), \quad z(1) = z''(1) = 0, \quad h'(0) = h'(1), \quad h(1) = h''(1) = 0. \tag{3.31}$$

Let u and f be as determined in the previous section. Then $u(.,t) \in C^2[0,1]$, $D^{\alpha,\gamma} u(x,.) \in C(0,T]$, and $f \in C[0,1]$. In addition, u and f form the unique classical solution and source of (3.12), *respectively.*

Proof. Let $\Omega = (0,T] \times [0,1]$ and $\Omega_\epsilon = [\epsilon, T] \times [0,1] \subset \Omega$. We show that the series corresponding to u, u_x, u_{xx}, $D^{\alpha,\gamma} u$ are uniformly convergent and represent continuous functions on Ω_ϵ, for any $\epsilon > 0$. Also we show that the series representation of f is uniformly convergent in $[0,1]$. This is shown by bounding all these series by over-harmonic series then applying Weierstrass M-test. Throughout this proof, $L = L(\alpha,\gamma)$ is some positive (generic) constant.

Through repeated integration by parts, the assumptions in (3.31) yield

$$\langle z, \psi_{1,n} \rangle = \frac{1}{\lambda_n^4} \left\{ z'''(0) - z'''(1) + \langle z^{(4)}, \psi_{1,n} \rangle \right\},$$

and

$$\langle z, \psi_{2,n} \rangle = \frac{1}{\lambda_n^4} \int_0^1 \left[4z'''(x) + x z^{(4)}(x) \right] \sin \lambda_n x \, dx.$$

The same expressions hold for the function h. Thus, there is a constant $L > 0$ such that

$$\left| z_{k,n} \right| \le L/\lambda_n^4, \qquad \left| h_{k,n} \right| \le L/\lambda_n^4, \qquad n \ge 1, \quad k = 1,2. \tag{3.32}$$

Using these bounds and (3.15), it follows from (3.29) that

$$|c_{1,n}| \leq L/\lambda_n^2, \qquad |f_{1,n}| \leq L/\lambda_n^2, \qquad n \geq 1. \tag{3.33}$$

Consequently, from (3.25) and (2.47) we have $|d_n(T)|, |d_n(T_m)| \leq L/\lambda_n^5$, $n \geq 1$. Therefore, it follows from (3.30) that

$$|c_{2,n}| \leq L/\lambda_n^2, \qquad |f_{2,n}| \leq L/\lambda_n^2, \qquad n \geq 1. \tag{3.34}$$

Using the bounds (3.32), (3.33), (3.34) and (2.47), the formulas (3.23) and (3.24) imply that

$$t^{1-\gamma+\alpha}|u_{k,n}(t)| \leq L\lambda_n^4, \qquad n \geq 1, \quad k = 1,2, \quad t \in (0,T]. \tag{3.35}$$

Furthermore, by inserting this bound in the (3.20)-(3.21), we have

$$t^{1-\gamma+\alpha}\,|D^{\alpha,\gamma}u_{k,n}(t)| \leq L/\lambda_n^2, \qquad n \geq 1, \quad k = 1,2, \quad t \in (0,T]. \tag{3.36}$$

When $n = 0$, it is obvious from (3.23) that the first term $u_{1,0}(t)\phi_{1,0}(x)$ of the series (3.18) is continuous on Ω and has a continuous t fractional derivative on Ω. In addition, it has continuous first and second derivatives with respect to x on Ω.

Therefore, the series in (3.18) is uniformly convergent in Ω_ϵ. Furthermore, the series obtained through term-by-term fractional differentiation with respect to t, and through term-by-term first and second differentiation with respect to x are all uniformly convergent in Ω_ϵ. Hence, being represented by uniformly convergent series of continuous functions on Ω_ϵ, the functions $u, D^{\alpha,\gamma}u$, u_x, and u_{xx} are all continuous on Ω. Similarly, f is continuous on $[0,1]$.

The next step is to show that $u(x,t)$ satisfies the intermediate and final conditions. From (3.26), the series representation (3.18) at $t = T_m$ yields

$$u(x,t)|_{t=T_m} = 2z_{1,0}(1-x) + \sum_{n=1}^{\infty} 4(1-x)z_{1,n}\cos(\lambda_n x) + \sum_{n=1}^{\infty} 4z_{2,n}\sin(\lambda_n x) = z(x),$$

for $x \in [0,1]$. Similarly, we have $u(x,T) = h(x)$, $x \in [0,1]$. Therefore, u form a classical solution.

Finally, the uniqueness follows by observing that when $z = h = 0$ in (3.12), then from (3.29) and (3.30), all the coefficients c_{kn} and f_{kn} are zero. As a result, from (3.23) and (3.24), all the coefficients in the series representations of u and f are identically zero.

Analytical and Computational Examples

To complement the achieved results, an analytical and a numerical example are presented.

Example 1 (Linear source and source-free diffusion)

Consider the problem (3.12) with

$$z(x) = 2(1-x), \quad \text{and} \quad h(x) = 2c(1-x), \quad c > 0.$$

Then clearly, z and h satisfy the hypothesis of Theorem 3.2.3, and

$$z_{1,0} = 1, \quad h_{1,0} = c, \qquad z_{k,n} = h_{k,n} = 0, \qquad n \geq 1, \quad k = 1,2.$$

Thus, it follows from (3.29) and (3.25) that

$$c_{1,n} = f_{1,n} = d_n = 0, \qquad n \geq 1,$$

which imply that

$$c_{2,n} = f_{2,n} = 0, \qquad n \geq 1.$$

Accordingly, from (3.20) and (3.21), for $t \in (0,T]$,

$$u_{k,n}(t) = 0, \qquad n \geq 1, \quad k = 1,2.$$

Thus, from (3.18) and (3.19), the series representations of f and u reduce to

$$f(x) = 2f_{1,0}(1-x),$$

and

$$u(x,t) = 2u_{1,0}(t)(1-x) = 2\left[\frac{f_{1,0}}{\Gamma(\alpha+1)}\, t^{\alpha} + \frac{c_{1,0}}{\Gamma(\gamma)}\, t^{\gamma-1}\right](1-x).$$

Next, from (3.29), to determine $f_{1,0}$ and $c_{1,0}$ we calculate A_0^{-1}. From (3.28),

$$A_0 = \begin{bmatrix} T^{\alpha}E_{\alpha,\alpha+1}(0) & T^{\gamma-1}E_{\alpha,\gamma}(0) \\ T_m^{\alpha}E_{\alpha,\alpha+1}(0) & T_m^{\gamma-1}E_{\alpha,\gamma}(0) \end{bmatrix} = \begin{bmatrix} T^{\alpha}/\Gamma(\alpha+1) & T^{\gamma-1}/\Gamma(\gamma) \\ T_m^{\alpha}/\Gamma(\alpha+1) & T_m^{\gamma-1}/\Gamma(\gamma) \end{bmatrix}.$$

Thus,

$$A_0^{-1} = \frac{1}{T_m^{\gamma-1}T^{\alpha} - T^{\gamma-1}T_m^{\alpha}} \begin{bmatrix} \Gamma(\alpha+1)\, T_m^{\gamma-1} & -\Gamma(\alpha+1)\, T^{\gamma-1} \\ -\Gamma(\gamma)\, T_m^{\alpha} & \Gamma(\gamma)\, T^{\alpha} \end{bmatrix}.$$

Therefore,

$$\begin{aligned} \begin{bmatrix} f_{1,0} \\ c_{1,0} \end{bmatrix} &= A_0^{-1} \begin{bmatrix} h_{1,0} \\ z_{1,0} \end{bmatrix} = A_0^{-1} \begin{bmatrix} c \\ 1 \end{bmatrix} \\ &= \frac{1}{T_m^{\gamma-1}T^{\alpha} - T^{\gamma-1}T_m^{\alpha}} \begin{bmatrix} \Gamma(\alpha+1)(cT_m^{\gamma-1} - T^{\gamma-1}) \\ \Gamma(\gamma)(T^{\alpha} - cT_m^{\alpha}) \end{bmatrix}. \end{aligned}$$

Notice that, when $c = (T_m/T)^{1-\gamma}$, then $f(x) = 0$ and thus problem (3.12) is source-free. On the other hand, when $c = (T/T_m)^{\alpha}$, then the problem corresponds to the homogeneous initial condition, $u(x,0) = 0$.

Example 2

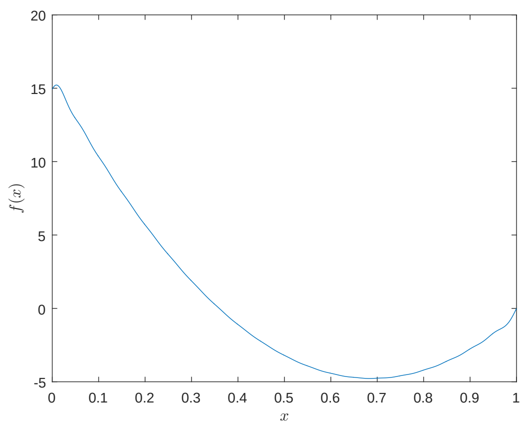
Consider the problem (3.12) with

$$z(x) = \frac{1}{10}\left[1-(2x-1)^3\right] \quad \text{and} \quad h(x) = -3x^2(x^2+2)+8x^3+1.$$

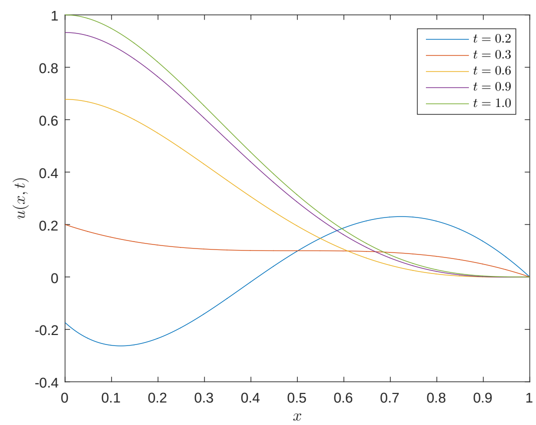
Then, by direct calculations, we can verify that z and h satisfy the hypothesis of Theorem 3.2.3.

We solve the system of equations in (3.29) and (3.30) to find the Fourier series coefficients and then substitute in the series representations of u and f in (3.18) and (3.19). We evaluated u and f by truncating the series in (3.18) and (3.19) after 20 terms.

The graph of u at different times and the graph of f are shown in Figure 3.1 for $T = 1$, $T_m = 0.3$, and $\alpha = \gamma = 0.5$. The graph of u at $t = 0.2$ represents the solution prior to the measurement at $T_m = 0.3$.



(a)



(b)

Figure 3.1: The solution and source term for Example 2.

3.3 Conclusion

An inverse two-parameter fractional diffusion problem subject to nonlocal non-self-adjoint boundary conditions and two local time-distinct datum is studied. A series representation of the solution and the space-dependent source term is obtained using a bi-orthogonal pair of bases. The asymptotic behavior and estimates of the generalized Mittag-Leffler function were used to justify the solvability of the delicate 2×2 linear systems for the Fourier coefficients of the source term and of the fractional integral of the solution at $t = 0$. Under certain regularity and compatibility assumptions on the given data, the existence and uniqueness of the constructed solution and source term in the classical sense are obtained.

This work should be a first step towards studying the well-posedness of our inverse model problem under weaker regularity and compatibility assumptions on the given data. In addition, our results will call for the extension to the two-dimensional two-parameter fractional diffusion problem. These will be topics of future research.

Chapter 4

Spatial Discretization Methods for Fractional Derivatives

In this section, we introduce the fractional centered differencing and the matrix transfer approaches for the discretization of the Riesz fractional derivative.

4.1 Fractional Centered Difference Method

Definition 4.1.1. [104] Let $\alpha > -1$. The fractional centered difference is defined as

$$\Delta_h^\alpha w(x) = \sum_{j=-\infty}^{\infty} \frac{(-1)^j \Gamma(\alpha+1)}{\Gamma\left(\frac{\alpha}{2} - j + 1\right)\Gamma\left(\frac{\alpha}{2} + j + 1\right)} w(x - jh). \tag{4.1}$$

It has been shown in [104] that

$$\lim_{h \longrightarrow 0} \frac{\Delta_h^\alpha w(x)}{h^\alpha} = \lim_{h \longrightarrow 0} \frac{1}{h^\alpha} \sum_{j=-\infty}^{\infty} \frac{(-1)^j \Gamma(\alpha+1)}{\Gamma\left(\frac{\alpha}{2} - j + 1\right)\Gamma\left(\frac{\alpha}{2} + j + 1\right)} w(x - jh), \tag{4.2}$$

represents the Riesz fractional derivative defined in (2.34) when $1 < \alpha \le 2$.

Lemma 4.1.2. *Let the coefficients of the centered finite difference approximation given in* (4.2) *be* *denoted as:*

$$g_j = \frac{(-1)^j \Gamma(\alpha+1)}{\Gamma\left(\frac{\alpha}{2}-j+1\right)\Gamma\left(\frac{\alpha}{2}+j+1\right)}, \quad j = 0, \mp 1, \mp 2, \cdots, \quad \alpha > -1. \tag{4.3}$$

Then we have the following:

1. $g_0 \geq 0$;
2. $g_{-j} = g_j \leq 0, \quad \textit{for} \quad |j| \geq 1$;
3. $g_{j+1} = \left(1 - \frac{\alpha+1}{\frac{\alpha}{2}+j+1}\right) g_j$.

Proof. Clearly, by the definition of the Gamma function $\Gamma(z) > 0$ for $\alpha > 0$, we have

$$g_0 = \frac{\Gamma(\alpha+1)}{\Gamma\left(\frac{\alpha}{2}+1\right)^2} > 0.$$

For all $|j| \geq 1$, we also have

$$g_{-j} = \frac{(-1)^{-j}\Gamma(\alpha+1)}{\Gamma\left(\frac{\alpha}{2}+j+1\right)\Gamma\left(\frac{\alpha}{2}-j+1\right)} = \frac{(-1)^j\Gamma(\alpha+1)}{\Gamma\left(\frac{\alpha}{2}-j+1\right)\Gamma\left(\frac{\alpha}{2}+j+1\right)} = g_j.$$

i.e $g_j = g_{-j}$.

Using the Gamma function relation in (2.2) and the $(j+1)$-th coefficient, we obtain the following recursive relation

$$\begin{aligned} g_{j+1} &= \frac{(-1)^{j+1}\Gamma(\alpha+1)}{\Gamma\left(\frac{\alpha}{2}-j\right)\Gamma\left(\frac{\alpha}{2}+j+2\right)} \\ &= \frac{(j-\frac{\alpha}{2})(-1)^j\Gamma(\alpha+1)}{(\frac{\alpha}{2}+j+1)\Gamma\left(\frac{\alpha}{2}-j+1\right)\Gamma\left(\frac{\alpha}{2}+j+1\right)} \\ &= \left(1 - \frac{\alpha+1}{\frac{\alpha}{2}+j+1}\right) g_j. \end{aligned}$$

i.e

$$g_{j+1} = \left(1 - \frac{\alpha+1}{\frac{\alpha}{2}+j+1}\right) g_j \leq 0, \qquad j = \mp 1, \mp 2, \cdots.$$

□

Lemma 4.1.3. *Let the coefficients of the centered finite difference approximation be given as g_k for $\alpha > -1$. Then*

$$g_j = \mathcal{O}\left(j^{-\alpha-1}\right), \qquad |j| \to +\infty. \tag{4.4}$$

This Lemma 4.1.3 guarantee that the series in (4.1) converges absolutely for a bounded function $w \in L^1(\mathbb{R})$.

Proof. Using the Gamma function identity

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin(\pi z)}, \qquad z \in \mathbb{C}, \tag{4.5}$$

we can write

$$\frac{\Gamma(\alpha+1)}{\Gamma(\beta+1)\Gamma(\alpha-\beta+1)} = \frac{\sin\left((\beta-\alpha)\pi\right)}{\pi} \frac{\Gamma(\alpha+1)\Gamma(\beta-\alpha)}{\Gamma(\beta+1)}. \tag{4.6}$$

Setting $\beta = \alpha/2 - k$ in (4.6) and using the well known Wendy's Theorem in [119] given as

$$\frac{\Gamma(z+a)}{\Gamma(z+b)} = z^{a-b}\left(1 + \sum_{k=1}^{N} \frac{c_k}{z^k} + \mathcal{O}\left(z^{-N-1}\right)\right), \qquad |z| \to \infty, \tag{4.7}$$

(4.4) is obtained. $\square$

Theorem 4.1.4. *Suppose $w \in C^5(\mathbb{R})$ and all derivatives up to order five belong to $L^1(\mathbb{R})$ and let*

$$\Delta_h^\alpha w(x) = \sum_{j=-\infty}^{\infty} \frac{(-1)^j \Gamma(\alpha+1)}{\Gamma\left(\frac{\alpha}{2} - j + 1\right)\Gamma\left(\frac{\alpha}{2} + j + 1\right)} w(x - jh), \tag{4.8}$$

be the fractional centered difference. Then

$$-\frac{\Delta_h^\alpha w(x)}{h^\alpha} = \frac{\partial^\alpha w(x)}{\partial |x|^\alpha} + O(h^2), \qquad h \longrightarrow 0, \tag{4.9}$$

where $\frac{\partial^\alpha}{\partial |x|^\alpha}$ is the Riesz fractional derivative with $1 < \alpha \le 2$.

Proof. We first recall that from [104], the generator function for the coefficient of the approximation (4.2) for $z \in \mathbb{R}$ is given as

$$\left|2\sin\left(\frac{z}{2}\right)\right| = \sum_{j=-\infty}^{\infty} \frac{(-1)^j \Gamma(\alpha+1)}{\Gamma\left(\frac{\alpha}{2}-j+1\right)\Gamma\left(\frac{\alpha}{2}+j+1\right)} e^{ijz}.$$

Applying the Fourier transform to both sides of Equation (4.8), since $\Delta_h^\alpha w \in L^1(\mathbb{R})$, $\xi \in \mathbb{R}$, to get

$$\mathscr{F}\left\{\Delta_h^\alpha w(x)\right\} = \sum_{j=-\infty}^{\infty} \frac{(-1)^j \Gamma(\alpha+1)}{\Gamma\left(\frac{\alpha}{2}-j+1\right)\Gamma\left(\frac{\alpha}{2}+j+1\right)} e^{ijh\xi}\,\hat{w}(\xi) = \left|2\sin\left(\frac{\xi h}{2}\right)\right|^\alpha \hat{w}(\xi). \qquad (4.10)$$

Define

$$\hat{\varphi}(\xi,h) := |\xi|^\alpha \left(\frac{\left|2\sin\left(\frac{\xi h}{2}\right)\right|^\alpha}{|\xi h|^\alpha} - 1\right)\hat{w}(\xi). \qquad (4.11)$$

Setting $y = \xi h$, we have

$$\begin{aligned}
\frac{\left|2\sin\left(\frac{y}{2}\right)\right|^\alpha}{|y|^\alpha} &= \left|\frac{2}{y}\right|^\alpha \left|\frac{y}{2} - \left(\frac{y}{2}\right)^3\frac{1}{3!} + \cdots\right|^\alpha \\
&= \left|1 - \left(\frac{y}{2}\right)^2\frac{1}{3!} + \cdots\right|^\alpha \\
&\leq \left(1 + \left|\left(\frac{y}{2}\right)^2\frac{1}{3!} + \cdots\right|\right)^\alpha \\
&= 1 + \alpha\left|\left(\frac{y}{2}\right)^2\frac{1}{3!} + \cdots\right| + \frac{\alpha(\alpha-1)}{2}\left|\left(\frac{y}{2}\right)^2\frac{1}{3!} + \cdots\right|^2 + \cdots \\
&\leq 1 + \alpha\left|\frac{y}{2}\right|^2\left|\frac{1}{3!} + C_0 y^2\right| + C_1|y|^4 \\
&\leq 1 + C_2 y^2, \qquad (4.12)
\end{aligned}$$

for some constant $C_2 > 0$, independent of y. Hence, we have

$$\frac{\left|2\sin\left(\frac{y}{2}\right)\right|^\alpha}{|y|^\alpha} = 1 + \mathscr{O}(y^2), \quad \text{for small } y.$$

Using the fact that $w \in C^5(\mathbb{R})$ and all derivatives up to order five belong to $L^1(\mathbb{R})$, there exists a positive constant C_3 such that

$$|\hat{w}(\xi)| \leq C_3(1+|\xi|)^{-5}. \qquad (4.13)$$

Combining (4.12) and (4.13) in (4.11), we then get

$$\begin{aligned}
|\hat{\varphi}(\xi,h)| &= |\xi|^\alpha \left| \frac{\left|2\sin\left(\frac{y}{2}\right)\right|^\alpha}{|y|^\alpha} - 1 \right| |\hat{w}(\xi)| \\
&\leq |\xi|^\alpha C_2 |\xi h|^2 C_3 (1+|\xi|)^{-5} \\
&\leq C_4 h^2 (1+|\xi|)^{\alpha+2} (1+|\xi|)^{-5} \\
&= C_4 h^2 (1+|\xi|)^{\alpha-3}, \qquad (4.14)
\end{aligned}$$

where $C_4 = C_2 C_3$ is a constant independent of ξ. This means that for $1 < \alpha \leq 2$, the inverse Fourier transform of the function $\hat{\varphi}$ which can be estimated as follows

$$\begin{aligned}
|\varphi(x,h)| &= \frac{1}{2\pi} \left| \int_{-\infty}^{\infty} e^{-i\xi x} \hat{\varphi}(\xi,h)\, d\xi \right| \\
&\leq \frac{1}{2\pi} \int_{-\infty}^{\infty} \left|\hat{\varphi}(\xi,h)\right| d\xi \\
&\leq \frac{1}{2\pi} \int_{-\infty}^{\infty} C_4 h^2 (1+|\xi|)^{\alpha-3} d\xi \\
&= Ch^2, \qquad (4.15)
\end{aligned}$$

where $C = \frac{C_4}{\pi(2-\alpha)}$.

Observe that using (4.10) and (4.11), we can write

$$-h^{-\alpha} \mathscr{F}\left\{\Delta_h^\alpha w(x)\right\} = |\xi|^\alpha \hat{w}(\xi) + \hat{\varphi}(\xi,h). \qquad (4.16)$$

Taking the inverse Fourier transform of (4.16), we obtain

$$-h^{-\alpha} \Delta_h^\alpha w(x) = \frac{\partial^\alpha w(x)}{\partial |x|^\alpha} + \varphi(x,h). \qquad (4.17)$$

Hence by the estimate in (4.15), we obtain

$$-h^{-\alpha} \Delta_h^\alpha w(x) = \frac{\partial^\alpha w(x)}{\partial |x|^\alpha} + \mathscr{O}(h^2). \qquad (4.18)$$

$\square$

If we define function w^* as

$$w^*(x) = \begin{cases} w(x) & x \in [a, b] \\ 0 & otherwise, \end{cases} \tag{4.19}$$

such that $w^* \in C^5(\mathbb{R})$ and all derivatives up to order five belong to $L^1(\mathbb{R})$, then direct consequence of Theorem 4.1.4 results into the following:

$$\frac{\partial^\alpha w(x)}{\partial |x|^\alpha} = -\frac{1}{h^\alpha} \sum_{j=-\left[\frac{b-x}{h}\right]}^{\left[\frac{x-a}{h}\right]} g_j w(x - jh) + \mathscr{O}(h^2), \tag{4.20}$$

where $h = \frac{b-a}{M}$, and M is the number of partitions of the interval $[a, b]$.

Using the approach of the fractional centered difference method by Ortigueira in [104], the symmetric Riesz fractional derivative of order α on $(0, L)$ can be approximated by an $(M-1) \times (M-1)$ symmetry Toeplitz matrix $G^{(\alpha)}$. Assume that $w(x)$ is zero outside $(0, L)$, $L = Mh$. Let $x = jh$ and $w_j = w(x_j)$, $j = 1, 2, \cdots, M-1$. Then we have

$$\Delta_h^\alpha w(x_j) = \sum_{i=j-M+1}^{j-1} g_i^{(\alpha)} w_{j-i}. \tag{4.21}$$

That is

$$\Delta_h^\alpha W = G^{(\alpha)} W, \tag{4.22}$$

where

$$G^{(\alpha)} = \begin{bmatrix} g_0^{(\alpha)} & g_1^{(\alpha)} & g_2^{(\alpha)} & g_3^{(\alpha)} & \cdots & g_{M-2}^{(\alpha)} \\ g_1^{(\alpha)} & g_0^{(\alpha)} & g_1^{(\alpha)} & g_2^{(\alpha)} & \cdots & g_{M-3}^{(\alpha)} \\ g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} & g_1^{(\alpha)} & \cdots & \omega_{M-4}^{(\alpha)} \\ \ddots & \ddots & \ddots & \ddots & \cdots & \cdots \\ g_{M-3}^{(\alpha)} & \ddots & g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} & g_1^{(\alpha)} \\ g_{M-2}^{(\alpha)} & g_{M-3}^{(\alpha)} & \ddots & g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} \end{bmatrix}, \qquad W = \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_{M-3} \\ w_{M-2} \\ w_{M-1} \end{bmatrix}.$$

An alternative approach for the discretization of Riesz fractional derivative is to approximate both the left-sided and the right-sided Riemann-Liouville fractional derivative and then take the linear combination. Consider equidistant nodes $x = jh,\ j = 0, 1, \cdots, M$ with the step h in the interval $[a, b]$, where $x_0 = a$ and $x_M = b$. For a left-sided Riemann-Liouville fractional derivative, the backward fractional difference approximation for the α-th derivative at the points $x_j,\ j = 0, 1, \cdots, M$ of a function $w(x)$ defined on $[a, b]$ such that $w(x) \equiv 0$ for $x < a$ is given by

$$_aD_{x_j}^{\alpha} w(x) \approx \frac{\Delta^{\alpha} w(x_j)}{h^{\alpha}} = h^{-\alpha} \sum_{i=0}^{j} (-1)^i \binom{\alpha}{i} w_{j-i}, \qquad j = 0, 1, \cdots, M. \tag{4.23}$$

In matrix form, we can write (4.23), with $g_i^{(\alpha)} = (-1)^i \binom{\alpha}{i}$, as

$$\begin{pmatrix} h^{-\alpha}\Delta^{\alpha} w(x_0) \\ h^{-\alpha}\Delta^{\alpha} w(x_1) \\ h^{-\alpha}\Delta^{\alpha} w(x_2) \\ \vdots \\ h^{-\alpha}\Delta^{\alpha} w(x_{M-1}) \\ h^{-\alpha}\Delta^{\alpha} w(x_M) \end{pmatrix} = \frac{1}{h^{\alpha}} \begin{pmatrix} g_0^{(\alpha)} & 0 & 0 & 0 & \cdots & 0 \\ g_1^{(\alpha)} & g_0^{(\alpha)} & 0 & 0 & \cdots & 0 \\ g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \cdots & \cdots \\ g_{M-1}^{(\alpha)} & \ddots & g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} & 0 \\ g_M^{(\alpha)} & g_{M-1}^{(\alpha)} & \ddots & g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_{M-1} \\ w_M \end{pmatrix}.$$

That is, the left-sided Riemann-Liouville derivative $_{-\infty}D_x^{\alpha} v(x,\ t)$ can be approximated with an

$(M+1)\times(M+1)$ lower triangular Toeplitz matrix $L_M^{(\alpha)}$ as:

$$\left[w_0^{(\alpha)}\ \ w_1^{(\alpha)}\ \ \cdots\ \ w_{M-1}^{(\alpha)}\ \ w_M^{(\alpha)}\right]^\top = L_M^{(\alpha)}\left[w_0\ \ w_1\ \ \cdots\ \ w_{M-1}\ \ w_M\right]^\top, \tag{4.24}$$

where

$$L_M^{(\alpha)} = \frac{1}{h^\alpha}\begin{pmatrix} g_0^{(\alpha)} & 0 & 0 & 0 & \cdots & 0 \\ g_1^{(\alpha)} & g_0^{(\alpha)} & 0 & 0 & \cdots & 0 \\ g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \cdots & \cdots \\ g_{M-1}^{(\alpha)} & \ddots & g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} & 0 \\ g_M^{(\alpha)} & g_{M-1}^{(\alpha)} & \ddots & g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} \end{pmatrix}. \tag{4.25}$$

In a similar way, the right-sided Riemann-Liouville derivative ${}_xD_{+\infty}^{\alpha} v(x,\ t)$ can be approximated with an $(M+1)\times(M+1)$ upper triangular strip matrix $L_M^{(\alpha)}$, assuming $w(x)\equiv 0$ for $x>b$ as:

$$\left[w_0^{(\alpha)}\ \ w_1^{(\alpha)}\ \ \cdots\ \ v_{M-1}^{(\alpha)}\ \ v_M^{(\alpha)}\right]^\top = U_M^{(\alpha)}\left[w_0\ \ w_1\ \ \cdots\ \ w_{M-1}\ \ w_M\right]^\top, \tag{4.26}$$

where

$$U_M^{(\alpha)} = \frac{1}{h^\alpha}\begin{pmatrix} g_0^{(\alpha)} & g_1^{(\alpha)} & \ddots & \ddots & g_{M-1}^{(\alpha)} & g_M^{(\alpha)} \\ 0 & g_0^{(\alpha)} & g_1^{(\alpha)} & \ddots & \ddots & g_{M-1}^{(\alpha)} \\ 0 & 0 & g_0^{(\alpha)} & g_1^{(\alpha)} & \ddots & \ddots \\ \cdots & \cdots & \cdots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & 0 & g_0^{(\alpha)} & g_1^{(\alpha)} \\ 0 & 0 & \cdots & 0 & 0 & g_0^{(\alpha)} \end{pmatrix}. \tag{4.27}$$

These approximations of symmetric Riesz fractional derivatives have been proven to give practically the same numerical results and, in the case of numerical solution of partial fractional differential equations, lead to a well-posed matrix of the resulting algebraic system, see [104, 109].

4.2 Matrix Transfer Techniques

Since the main idea of matrix transfer techniques is transferring the fractional exponent of fractional derivative operator to the matrix obtained from discretization of the Laplacian, we first introduce the definition of fractional exponent of a matrix from the theory of matrix functions, see [61].

Definition 4.2.1. Given a generic matrix A, the fractional power of A is defined as a contour integral

$$A^{\alpha} = \frac{A}{2\pi i}\int_{\Gamma} z^{\alpha-1}(zI-A)^{-1}dz, \tag{4.28}$$

where Γ is a suitable closed contour enclosing the spectrum of A, $\sigma(A)$, in its interior.

We consider the case where the fractional exponent of matrix A is expressed in terms of a real integral. Detailed proofs can be found in [18], see also [4] which is based on a particular choice of Γ and a subsequent change of variable.

Proposition 4.2.2. *Let $A \in \mathbb{R}^{m\times m}$ be such that $\sigma(A) \subset \mathbb{C} - (-\infty, 0]$. For $0 < \alpha < 1$, the following representation holds*

$$A^{\alpha} = \frac{A\sin(\alpha\pi)}{\alpha\pi}\int_0^{\infty}(\rho^{\frac{1}{\alpha}}I + A)^{-1}d\rho. \tag{4.29}$$

In what follows in this section, spectral decomposition plays important role. We give an overview in the following definition.

Definition 4.2.3. Assume that the Laplacian $(-\Delta)$ has a complete set of orthonormal eigenfunctions and the corresponding eigenvalues, respectively φ_j and λ_j^2, on a bounded region Ω. That is,

$$(-\Delta)\varphi_j = \lambda_j^2\varphi_j, \qquad \text{in}\,\Omega.$$

In addition, we suppose that $\mathscr{B}(\varphi) = 0$ on $\partial\Omega$, the boundary of Ω, where $\mathscr{B}(\varphi)$ is one of the standard three homogeneous boundary conditions. Let

$$W_r = \left\{ w = \sum_{j=1}^{\infty} c_j \varphi_j \,\middle|\, \quad c_j = \langle w, \varphi_j \rangle, \sum_{j=1}^{\infty} |c_j|^2 |\lambda_j|^r < \infty, r = \max(\alpha, 0) \right\}. \tag{4.30}$$

Then for any $w \in W_r$, $(-\Delta)^{\frac{\alpha}{2}} w$ is defined as

$$(-\Delta)^{\frac{\alpha}{2}} w = \sum_{j=1}^{\infty} c_j \left(\lambda_j^2\right)^{\frac{\alpha}{2}} \varphi_j, \tag{4.31}$$

where $c_j \in \mathbb{R}$, for $j = 1, 2, 3, \cdots$. It can be easily seen that the operator $(-\Delta)^{\frac{\alpha}{2}}$ is both linear and self-adjoint. Also, if $w \in W_{r^*}$, where $r^* = \max(\alpha_1, \alpha_2, \alpha_1 + \alpha_2, 0)$, then

$$(-\Delta)^{\frac{\alpha_1}{2}} (-\Delta)^{\frac{\alpha_2}{2}} w = (-\Delta)^{\frac{\alpha_2}{2}} (-\Delta)^{\frac{\alpha_1}{2}} w.$$

In the matrix transfer technique [66, 67], the fractional Laplacian is approximated by the fractional power of the approximating matrix of the standard Laplacian. That is,

$$-(-\Delta)^{\frac{\alpha}{2}} \approx -\frac{1}{h^\alpha} \mathscr{T}^{\frac{\alpha}{2}}, \tag{4.32}$$

where $\mathscr{T}$ is the approximate matrix representation of the standard Laplacian, $-\Delta$, obtained using finite difference methods. Note that the matrix $\mathscr{T}$ is required to be positive definite so that its fractional power is well defined. However, this requirement is fulfilled by the underlying standard centered difference scheme. The matrix transfer technique has been demonstrated to be computationally efficient and accurate for space fractional differential equation, see [4, 143].

4.3 Short Memory Principle

The nonlocality of the fractional derivative operators is a key issue in understanding and developing efficiently numerical schemes for solving the associated differential equations. The so called memory is associated with the fact that the definition of fractional derivatives involve integral over the interval $[a, x]$. This is evident from the resulting matrix discretization.

The short memory principle has to do with ignoring the tail of the integral and then carry out the integration only over a 'smaller' part in a neighborhood of the point of interest. This principle makes sense for both time and space fractional derivatives. For problems involving space fractional derivatives, far away points presumably have less impact on the determination of the spatial derivatives, while for the problems involving time fractional derivatives, it is understood that remote events have minor effect.

Lemma 4.1.2 and Lemma 4.4 plays a very crucial role in the implementation of the short memory principle. For instance, with Lemma 4.4, the entries in the matrix $G_M^{(\alpha)}$ decay away from the main diagonal and for very large meshes, the diagonals of $G_M^{(\alpha)}$ become so indicative as we move from the main diagonal, so that the resulting matrices after applying the short memory principle, may be treated as banded matrices and can benefit from all the advantages of sparse and structured matrices. Hence, the computational cost involved with the full matrix can be greatly reduced.

When a threshold ε has been fixed for the amplitude of the smallest acceptable entries, Lemma 4.4 can be applied to exactly establish the bandwidth. In fact, for

$$j > \varepsilon^{\frac{-1}{\alpha+1}} \tag{4.33}$$

the value $|g_j|$ is smaller than ε and can be ignored.

Chapter 5

The FETD Real Distinct Poles Scheme (FETD-RDP)

Our attention is focused on the nonlinear Riesz space fractional reaction-diffusion equation with homogeneous Dirichlet boundary condition given as

$$\begin{cases} u_t + \lambda (-\Delta)^{\frac{\alpha}{2}} u = f(t, u), \text{ in } \Omega \times (0,\ T], \\ u(.,0) = u_0, \text{ in } \Omega, \end{cases} \tag{5.1}$$

where $\lambda > 0$ is the diffusion coefficient, Ω is a bounded domain in $\mathbb{R}^N$ with smooth boundary, $\partial\Omega$, $1 < \alpha \leq 2$ and $(-\Delta)^{\frac{\alpha}{2}}$ represents the Riesz fractional derivative. We assume that f is a sufficiently smooth function to ensure that the problem with the specified initial and boundary conditions possesses a unique solution.

5.1 Overview of FETD Schemes

By approximating the space fractional derivative in (5.1), we obtain the following systems of nonlinear ordinary differential equations (ODEs):

$$U_t + AU = \mathscr{F}(t, U), \tag{5.2}$$

where U is the vector containing the approximation to u, A is a matrix derived from the approximation of the space fractional derivatives, and the term $\mathscr{F}(t, U)$ approximates the nonlinear function $f(t, u)$.

Using a variation of constants formula in (5.2) on the time interval $[t_n, t_{n+1}]$, we have

$$U(t_{n+1}) = e^{-kA}U(t_n) + \int_{t_n}^{t_{n+1}} e^{-A(t_{n+1}-s)}\mathscr{F}(s, U(s))ds, \tag{5.3}$$

where $k = \Delta t$. Taking $s = t_n + \tau k$ with $t_n = nk$, $\tau \in [0,1]$ and k is the time-step, the following recurrence formula is obtained:

$$U(t_{n+1}) = e^{-kA}U(t_n) + k\int_0^1 e^{-kA(1-\tau)}\mathscr{F}(t_n + \tau k, U(t_n + \tau k))d\tau. \tag{5.4}$$

Note that the expression (5.4) is an exact solution of system (5.2), and its approximation leads to different Fractional Exponential Time Differencing (FETD) schemes. For the case of integer order derivative, see details work in [81].

FETD schemes have been very attractive due to the fact that the linear part of the Equation (5.4) can be treated separately. This is done by first discretizing the exponential operator and then employing the advantage of the one-step variation of constants integral formula to avoid iteration of the non-linearity in order to reduce computational time and preserve accuracy. A class of exponential time differencing schemes called ETD Runge-Kutta schemes was proposed in [29]. However, the efficient resolution of the matrix exponentials is a major challenge in this work and many other schemes for more general problems. Due to the possibility of splitting, many researchers have explored the idea of using particular rational approximations of the matrix exponential, see [81, 146]. Among such ETD schemes is an ETD Crank-Nicolson Scheme (ETD-CN) which utilizes a Padé-(1,1) rational approximation [58]. Although, this ETD-CN is highly efficient, it is not L-stable and therefore does not damp out spurious oscillations generated by non-smooth initial and boundary conditions. Using an L-acceptable scheme for the partial fraction decomposition of this approximation, the evolution process may be more robust.

Different discretizations of the integral part lead to various methods of different orders and properties. However, our interest is in second-order FETD schemes for which a linear approximation of the non-linear function is used,

$$\mathscr{F}(t_n+\tau k, \mathrm{U}(t_n+\tau k)) \approx \mathscr{F}(t_n, \mathrm{U}(t_n)) + \tau k\left(\frac{\mathscr{F}(t_{n+1}, \mathrm{U}(t_{n+1})) - \mathscr{F}(t_n, \mathrm{U}(t_n))}{k}\right),$$

which leads to the semi-discretized scheme given as

$$\mathrm{U}_{n+1} = e^{-Ak}\mathrm{U}_n + A^{-1}\left(I - e^{-Ak}\right)\mathscr{F}(t_n, \mathrm{U}_n) + \frac{A^{-2}}{k}\left(kA - I + e^{-Ak}\right)[\mathscr{F}(t_{n+1}, \mathrm{U}_{n+1}) - \mathscr{F}(t_n, \mathrm{U}_n)]. \tag{5.5}$$

Observe that the scheme in Equation (5.5) is fully implicit and would require Newton-type iterations to recover the approximate solution. We therefore seek a linearly implicit implementation for computational efficiency. By employing the constant approximation $\mathscr{F}(t_n+s, \mathrm{U}(t_n+s)) = \mathscr{F}(t_n, \mathrm{U}(t_n))$ in (5.4) and integrating, first order accuracy approximation is obtained as

$$U^*_{n+1} = e^{-kA}U_n + A^{-1}\left(I - e^{-kA}\right)\mathscr{F}(t_n, \mathrm{U}_n). \tag{5.6}$$

The final semi-discretized scheme is then obtained by setting $\mathscr{F}(t_{n+1}, \mathrm{U}^*_{n+1}) = \mathscr{F}(t_{n+1}, \mathrm{U}_{n+1})$ as:

$$\begin{aligned} \mathrm{U}_{n+1} &= e^{-Ak}\mathrm{U}_n + A^{-1}\left(I - e^{-Ak}\right)\mathscr{F}(t_n, \mathrm{U}_n) \\ &\quad + \frac{A^{-2}}{k}\left(kA - I + e^{-Ak}\right)[\mathscr{F}(t_{n+1}, \mathrm{U}^*_{n+1}) - \mathscr{F}(t_n, \mathrm{U}_n)] \\ \mathrm{U}^*_{n+1} &= e^{-Ak}\mathrm{U}_n + A^{-1}\left(I - e^{-Ak}\right)\mathscr{F}(t_n, \mathrm{U}_n). \end{aligned} \tag{5.7}$$

5.2 The FETD-RDP Scheme

A major problem in the ETDRK schemes proposed by Cox and Mathews in [29] is in dealing with the numerical cancellation errors inherent in evaluating coefficients such as $A^{-1}(I - e^{-kA})$, particularly when A has eigenvalues close to zero. In order to handle this issue, a contour integral approach was introduced in [73] by Kassam and Trefethen to evaluate the coefficients. However, new challenges emerged, each time the problem is changed or the spatial resolution is adjusted, due to the fact that there is a need to choose a contour in the complex plane that completely encloses all the eigenvalues of A. Another approach was introduced in [81, 96, 97, 146] which uses Padé rational functions in approximating the matrix exponentials called ETD Padé schemes. The issue with the numerical cancellation errors is avoided in these schemes. This is achieved through a series of matrix algebraic operations, performed after replacing the exponential matrix with an appropriate Padé rational function. Among existing and commonly used ETD Padé schemes are the ETD Crank Nicolson (ETD-CN) and ETD Padé(0,2) (ETD-P02). Again, the proposed ETD Padé schemes also come with their shortcomings. One of these shortcomings these schemes is the lack of damping for the ETD-CN scheme and the complex poles associated with the ETD-P02 scheme. These issues with complex poles have been known to slow down the evolution.

Employing parallel techniques in dealing with multidimensional problems is an option most researchers in this field would desire. Thus is essential to speed up the evolution. There is then a need for a good separation between the poles of the rational approximation. However, Padé schemes do not have this property. In [8], a (non-Padé) rational approximation for the discretization of the matrix exponential is introduced among various ways for discretization of the matrix exponential in (5.7) [81, 96, 97, 146]. This is splittable into simple real pole rational functions, having error constant nearly best possible [133]. It was shown [133] that the approximation

$$R(z) = \frac{1+\frac{5}{12}z}{(1-\frac{1}{3}z)(1-\frac{1}{4}z)} = \frac{9}{1-\frac{1}{3}z} - \frac{8}{1-\frac{1}{4}z} \approx e^z \tag{5.8}$$

is nearly optimal (in error constant) for second-order rational approximations. This rational approximation is called the real distinct poles (RDP) approximation.

Lemma 5.2.1. *[8, 133] Given a generic rational function of the form*

$$r(z) = \frac{1+a_1 z}{(1-b_1 z)(1-b_2 z)}, \tag{5.9}$$

such that $b_1 + b_2 + a_1 = 1$ and $b_1 + b_2 - b_1 b_2 = \frac{1}{2}$. Then $r(z)$ is a second order approximation to e^z i.e

$$r(z) - e^z = C_3 z^3 + \mathcal{O}(z^{p+2})$$

with error constant

$$C_3 = \frac{a_1}{2} - \frac{1}{6}. \tag{5.10}$$

Note that from (5.8) when compared with (5.9), $a_1 = \frac{5}{12}$, $b_1 = \frac{1}{3}$ and $b_2 = \frac{1}{4}$. Therefore, the error constant $C_3 = 0.041\bar{6}$.

Using the RDP rational function in (5.8) to approximate the matrix exponentials in (5.7), we have

$$R_{RDP}(-Ak) = \left(I - \frac{5}{12}Ak\right)\left[\left(I + \frac{1}{3}Ak\right)\left(I + \frac{1}{4}Ak\right)\right]^{-1} \approx e^{-kA}.$$

We utilize Padé-(0,1) as a locally second-order predictor of the solution in (5.7) given as

$$R_{0,1}(-Ak) = (I + Ak)^{-1}.$$

Substituting these approximations into the semi-discrete equation (5.7), we obtain

$$\begin{aligned}
\mathrm{V}_{n+1} &= R_{RDP}(-Ak)\mathrm{V}_n + A^{-1}\left(I - R_{RDP}(-Ak)\right)\mathscr{F}(t_n,\mathrm{V}_n) \\
&\quad + \frac{A^{-2}}{k}\left(kA - I + R_{RDP}(-Ak)\right)\left[\mathscr{F}(t_{n+1},\mathrm{V}^*_{n+1}) - \mathscr{F}(t_n,\mathrm{V}_n)\right] \\
\mathrm{V}^*_{n+1} &= R_{01}(-Ak)\mathrm{V}_n + A^{-1}(I - R_{01}(-Ak))\mathscr{F}(t_n,\mathrm{V}_n),
\end{aligned}$$

where $\mathrm{V}_{n+1} \approx \mathrm{U}_{n+1}$.

We obtain a fully discretized scheme after simplifying as follows:

$$\begin{aligned}
\mathrm{V}_{n+1} &= \left(I - \frac{5}{12}Ak\right)\left(I + \frac{1}{4}Ak\right)^{-1}\left(I + \frac{1}{3}Ak\right)^{-1}\mathrm{V}_n \\
&\quad + \frac{k}{2}\left(I + \frac{Ak}{4}\right)^{-1}\left(I + \frac{Ak}{3}\right)^{-1}\mathscr{F}(t_n,\mathrm{V}_n) \\
&\quad + \frac{k}{2}\left(I + \frac{1}{6}kA\right)\left(I + \frac{1}{4}kA\right)^{-1}\left(I + \frac{1}{3}kA\right)^{-1}\mathscr{F}(t_{n+1},\mathrm{V}^*_{n+1}) \\
\mathrm{V}^*_{n+1} &= (I + Ak)^{-1}\left(\mathrm{V}_n + k\mathscr{F}(t_n,\mathrm{V}_n)\right).
\end{aligned}$$

Note that we could take advantage of the following partial fraction decompositions

$$\begin{aligned}
\left(I - \frac{5}{12}Ak\right)\left(I + \frac{1}{4}Ak\right)^{-1}\left(I + \frac{1}{3}Ak\right)^{-1} &= 9\left(I + \frac{1}{3}Ak\right)^{-1} - 8\left(I + \frac{1}{4}Ak\right)^{-1} \\
\left(I + \frac{Ak}{4}\right)^{-1}\left(I + \frac{Ak}{3}\right)^{-1} &= 4\left(I + \frac{1}{3}Ak\right) - 3\left(I + \frac{1}{4}Ak\right)^{-1} \\
\left(I + \frac{Ak}{6}\right)\left(I + \frac{Ak}{4}\right)^{-1}\left(I + \frac{Ak}{3}\right)^{-1} &= 2\left(I + \frac{1}{3}Ak\right)^{-1} - \left(I + \frac{1}{4}Ak\right)^{-1}
\end{aligned}$$

to improve the computational efficiency of the scheme. Hence, using these decompositions and simplifying, we have the final efficient scheme:

$$\begin{aligned}
\mathrm{V}_{n+1} &= \left(I + \frac{1}{3}Ak\right)^{-1}\left[9\mathrm{V}_n + 2k\mathscr{F}(t_n,\mathrm{V}_n) + k\mathscr{F}(t_{n+1},\mathrm{V}^*_{n+1})\right] \\
&\quad + \left(I + \frac{1}{4}Ak\right)^{-1}\left[-8\mathrm{V}_n - \frac{3k}{2}\mathscr{F}(t_n,\mathrm{V}_n) - \frac{k}{2}\mathscr{F}(t_{n+1},\mathrm{V}^*_{n+1})\right] \qquad (5.11) \\
\mathrm{V}^*_{n+1} &= (I + Ak)^{-1}(\mathrm{V}_n + k\mathscr{F}(t_n,\mathrm{V}_n)).
\end{aligned}$$

Full details of the derivation of this scheme for integer-order reaction-diffusion equations could be found in [8]. When the matrix involved comes from the discretization of fractional derivatives, we called the scheme Fractional Exponential Time Differencing (FETD)

This final scheme is called the FETD Real Distinct Poles (FETD-RDP) Scheme. The following algorithm implements the FETD-RDP Scheme:

Algorithm 1 FETD-RDP Scheme

1: Solve for first order predictor V^*_{n+1}

$$(I + Ak)\mathrm{V}^*_{n+1} = \mathrm{V}_n + k\mathscr{F}(t_n, \mathrm{V}_n)$$

2: Solve for a_{n+1} (Processor 1)

$$\left(I + \frac{1}{3}Ak\right) a_{n+1} \quad = 9\mathrm{V}_n + 2k\mathscr{F}(t_n, \mathrm{V}_n) + k\mathscr{F}(t_{n+1}, \mathrm{V}^*_{n+1})$$

3: Solve for b_{n+1} (Processor 2)

$$\left(I + \frac{1}{4}Ak\right) b_{n+1} = -8\mathrm{V}_n - \frac{3}{2}k\mathscr{F}(t_n, \mathrm{V}_n) - \frac{k}{2}\mathscr{F}(t_{n+1}, \mathrm{V}^*_{n+1}) \tag{5.12}$$

4: Obtain approximate solution V_{n+1}

$$\mathrm{V}_{n+1} \quad = a_{n+1} + b_{n+1} \tag{5.13}$$

5.3 Stability Analysis

Theorem 5.3.1. *The modulus of the rational approximation, $R(z)$, given in* (5.8) *of e^{-z} is less than or equal to one, that is:*

$$|R(z)| = \left| \frac{9}{(1 + \frac{1}{3}z)} - \frac{8}{(1 + \frac{1}{4}z)} \right| \leq 1,$$

if the real part of z, $Re(z)$, is nonnegative. In addition, $|R(z)| \longrightarrow 0$ as $Re(z) \longrightarrow \infty$.

Proof. Let $z = a + ib,\ a,\ b \in \mathbb{R}$ and $a \geq 0$. Simplifying (5.8), we have

$$|R(z)| = \left| \frac{9}{(1+\frac{1}{3}z)} - \frac{8}{(1+\frac{1}{4}z)} \right| = \left| \frac{12-5z}{12+7z+z^2} \right|.$$

Hence, it suffices to prove that

$$|12+7z+z^2|^2 - |12-5z|^2 \geq 0. \tag{5.14}$$

For $a \geq 0$, we have

$$\begin{aligned} |12+7z+z^2|^2 - |12-5z|^2 &= (12+7z+z^2)(12+7\bar{z}+\bar{z}^2) - (12-5z)(12-5\bar{z}) \\ &= 144(z+\bar{z}) + 24z\bar{z} + 12(z^2+\bar{z}^2) + 7z\bar{z}(z+\bar{z}) + z^2\bar{z}^2 \\ &= 144(2a) + 24(a^2+b^2) + 12(2a^2-2b^2) + 7(a^2+b^2)(2a) \\ &\quad + a^4 + 2a^2b^2 + b^4 \\ &= a^4 + 14a^3 + 48a^2 + 288a + 2a(7+2a)b^2 + b^4 \geq 0. \end{aligned}$$

Clearly, using the partial fractional decomposition of $R(z)$, $|R(z)| \longrightarrow 0$ as $Re(z) \longrightarrow \infty$. This proves Theorem (5.3.1).

Remark 5.3.2.

Theorem 5.3.1 establishes the L-acceptablility of the RDP approximation given by (5.8). This is further shown empirically through Figure 5.1.

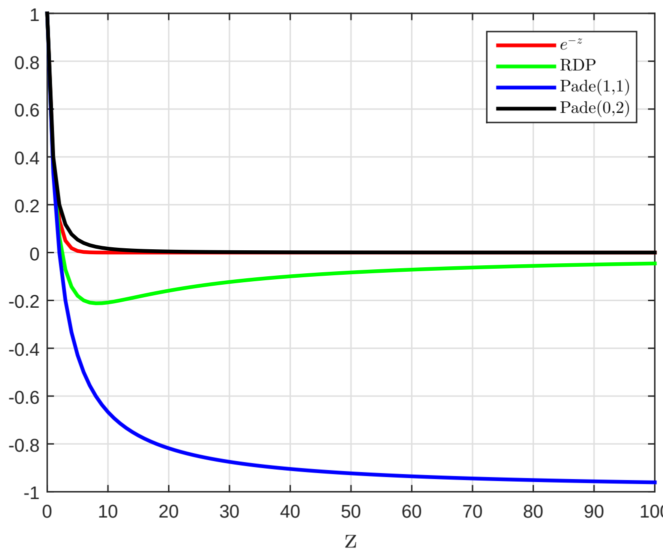


Figure 5.1: Behavior of functions e^{-z}, RDP, Pade(0,2) and Pade(1,1) for $z \in [0, 100]$.

The RDP approximation is therefore an excellent choice for solving problems with high frequency components with discontinuous boundary or initial data as well as significant advection see [8, 133] for more detail. This resolves many problems of spurious oscillations and avoids complex poles associated with Padé-(0,2) and Padé-(1,1) approximation of matrix exponentials, [58].

Stability Region

Following the same approach given in [17, 29, 36, 84], we analyze the stability of the scheme (5.11) with the plots of its absolute stability regions. Consider a nonlinear autonomous ordinary differential equation,

$$u_t + \lambda u = \mathcal{N}(u), \tag{5.15}$$

where $\mathcal{N}(u)$ is a nonlinear function. Assume that there exists a fixed point u_0 such that $\mathcal{N}(u_0) - \lambda u_0 = 0$. If u is a perturbation of u_0 and $\gamma = \mathcal{N}'(u_0)$, then linearization gives the following test equation:

$$u_t = \gamma u - \lambda u. \tag{5.16}$$

We say that the fixed point u_0 is stable if $\mathrm{Re}(\gamma-\lambda)<0$. In the context of the problem (5.1), λ corresponds to the approximation of fractional diffusion terms.

Applying the semi-discretized form of the second order ETD (5.7) to the scalar test equation (5.16) with $\lambda k = m$, we have

$$\begin{aligned} u_{n+1} &= e^{-m}u_n + k\gamma\left[\frac{(1-e^{-m})}{m}+\frac{(m-1+e^{-m})(e^{-m}-1)}{m^2}\right]u_n \\ &\quad + k^2\gamma^2\left[\frac{(m-1+e^{-m})(1-e^{-m})}{m^3}\right]u_n. \end{aligned} \tag{5.17}$$

We generate different stability boundaries on the plane (δ_r,δ_j) using the substitution $\gamma k=\delta=\delta_r+i\delta_j$. The region in the complex-λ plane where the solution u_n remains bounded as $n\to\infty$ is desired. Assume the solution is of the form, $u_n=z^n$ where $z=|z|e^{i\theta}$. Obviously, for $|z|<1$, the solution decays with n and it grows for $|z|>1$. So, the condition $|z|=1$ determines the boundary of the stability region. Therefore, to find the boundary we set $z=e^{i\theta}$, with $\theta\in[0,2\pi]$. Let

$$a=\frac{(m-1+e^{-m})(1-e^{-m})}{m^3} \qquad \text{and} \qquad b=\frac{(1-e^{-m})}{m}+\frac{(m-1+e^{-m})(e^{-m}-1)}{m^2}.$$

Then, substituting $k\gamma=\delta_r+i\delta_j$, $U_n=e^{in\theta}$ in (5.17) and dividing through by $e^{in\theta}$, we obtain:

$$e^{i\theta}=e^{-m}+(\delta_r+i\delta_j)b+(\delta_r+i\delta_j)^2a. \tag{5.18}$$

Comparing the real and imaginary part after expanding (5.18) , we get

$$\left(\delta_r^2-\delta_j^2\right)a+\delta_r b=\cos\theta-e^{-m}, \tag{5.19}$$

$$2\delta_r\delta_j a+\delta_i b=\sin\theta. \tag{5.20}$$

Solving these equations and simplifying we obtain the following system that defines our stability region:

$$A\delta_r^4 + B\delta_r^3 + C\delta_r^2 + D\delta_r - E = 0$$
$$\delta_j = \frac{\sin\theta}{2\delta_r a + b}$$

where $A = 4a^3$, $B = 8a^2 b$, $C = 5ab^2 - 4a^2(\cos\theta - e^{-m})$, $D = b^3 - 4ab(\cos\theta - e^{-m})$, $E = a\sin^2\theta + b^2(\cos\theta - e^{-m})$.

For comparison purpose with the various second order FETD schemes, we make the following substitutions to investigate the variation in stability regions

$$\text{FETD-RDP}: \quad e^{-m} \approx \frac{9}{1+\frac{1}{3}m} - \frac{8}{1+\frac{1}{4}m} \tag{5.21}$$
$$\text{FETD-CN}: \quad e^{-m} \approx \frac{\left(1-\frac{1}{2}m\right)}{\left(1+\frac{1}{2}m\right)} \tag{5.22}$$
$$\text{FETD-P02}: \quad e^{-m} \approx \frac{2}{2+2m+m^2}. \tag{5.23}$$

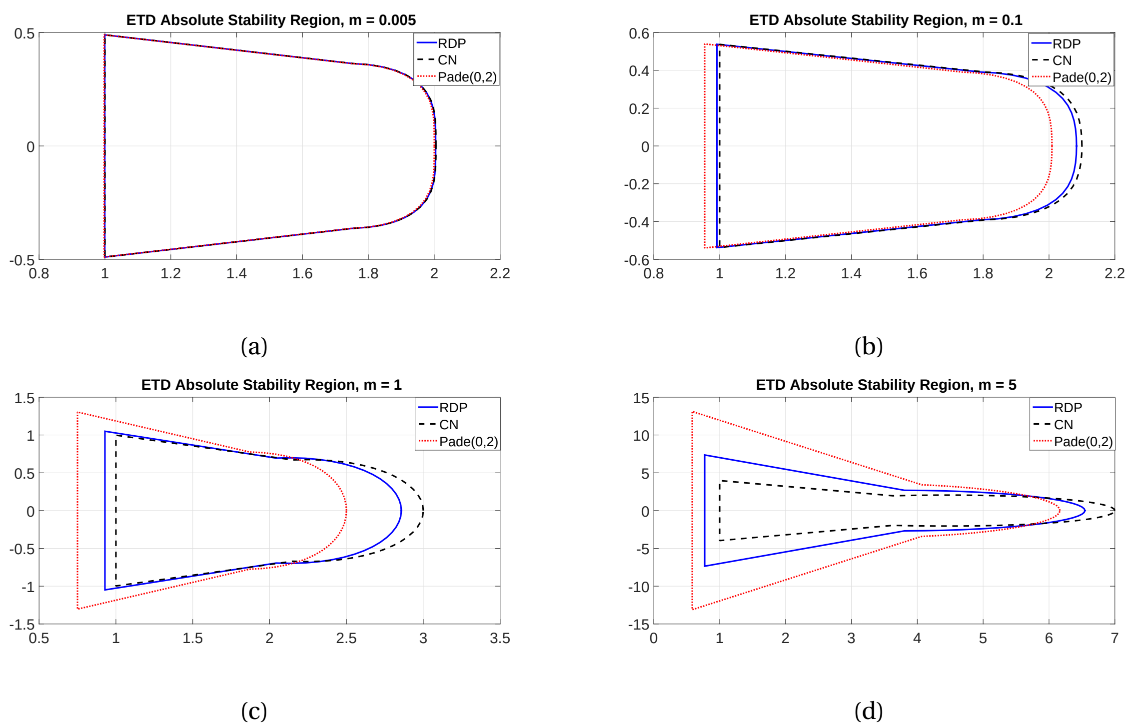


Figure 5.2: Stability regions of FETD-RDP, FETD-CN, and FETD-P02 for different values of m.

Remark 5.3.3.

1. Observe from Figure (7.1) that as we increase m, the stability regions of the schemes widen. This then allows for larger time steps while the solution still remain stable.

2. Based on this comparison, we observe that the FETD-RDP has a better stability than FETD-CN since the stability region of FETD-RDP contains larger values along the real axis,, which means we can consider larger $k = dt$ than for FETD-CN.

5.4 Error Estimates

Our interest here is to present error estimate results for ETD-RDP in the discretization of the following semilinear evolution equation.

$$\begin{aligned} \mathrm{U}_t + Au &= \mathscr{F}(\mathrm{U}(t)) \quad \text{for } t \in (0, T], \\ \mathrm{U}(0) &= \mathrm{U}_0. \end{aligned} \tag{5.24}$$

For these estimates, the following assuptions are made: (i) A is a self-adjoint positive definite operator with compact inverse in a Hilbert space H, (ii) the semilinear equation has a sufficiently smooth solution $u : [0, T] \to E = \mathscr{D}(A)$ with derivatives in E, (iii) the function $\mathscr{F} : E \to H$ is sufficiently often Fréchet differentiable and satisfies the local Lipschitz condition. Under this assumption the composition $g : [0, T] \to H$ defined by $t \to g(t) = \mathscr{F}(\mathrm{U}(t))$ is a smooth mapping. It is well known that the solution to this problem satisfies the integral equation.

$$u(t) = S(t)\mathrm{U}_0 + \int_0^t S(t-s)\mathscr{F}(\mathrm{U}(s))ds, \tag{5.25}$$

where $S(t) := e^{-At}$ is the analytic semigroup generated by A [154, Lemma 2.2.3, Theorem 2.6.2]. The recurrence relation on which these results are based is given as

$$u(t_{n+1}) = S(k)u(t_n) + k\int_0^1 S(k-sk)\mathscr{F}(u(t_n+\tau k))d\tau \tag{5.26}$$

obtained using the change of variables $t_n = nk$, $n \in \mathscr{N}^+, 0 < k \le k_0 \in \mathrm{Re}^+$, and $s = t_n + \tau k$.

Definition 5.4.1 (Local Lipschitz condition)**.** Suppose F is a nonlinear operator from a Banach space $\mathscr{B}$ into $\mathscr{B}$. F is said to satisfy the local Lipschitz condition if for any positive constant $M > 0$, there is a positive constant L_M depending on M such that when $u, v \in \mathscr{B}$, $\| u \| \le M$ and $\| v \| \le M$,

$$\| F(u) - F(v) \| \le L_M \| u - v \| .$$

Lemma 5.4.2. *[9] The time discretization scheme* (5.11) *applied to the semilinear problem* (5.24) *is accurate of order* 2*.*

Lemma 5.4.3 (Stability Estimate, [9])**.** *Let T_{j+1} and $T_{j,2}$ denote the local truncation errors at the main and predictor stages of the scheme* (5.11)*, then for k_0 sufficiently small with $0 < k \le k_0$ and for $t \in (0, T]$, there exists a constant C, depending on T, such that the error at time t_n has bound*

$$\| e_n \| \le Ck\sum_{j=0}^{n-1} \Psi_{j+1} \tag{5.27}$$

where

$$\Psi_{j+1} = C \| T_{j,2} \| + k^{-1} \| T_{j+1} \|, \quad 1 \le j \le n, nk \le T$$

Theorem 5.4.4. *[9] Under the stated assumption on $\mathscr{F}$, if we assume further that $g^{(l)}(t) \in \mathscr{D}(A^{2-l})$ for $l < 2$, and the initial data $v \in \mathscr{D}(A^3)$ then for the numerical scheme* (5.11) *applied to the semi-*

linear problem (5.24)*, the following estimate for the error bound holds, for* $t \in (0, T]$

$$\| e_n \| \leq Ck^2 \Big[(\log n + 1) \left(\| A^2 v \| + \| Av \| \right) + \bar{t} \sup_{0 \leq s \leq t_n} \| A^2 g(s) \| + \bar{t} \sup_{0 \leq s \leq t_n} \| Ag(s) \|$$
$$+ \bar{t} \sup_{0 \leq s \leq t_n} \| Ag^{(1)}(s) \| + \int_0^{t_n} \| g^{(1)}(\tau) \| \, d\tau + \int_0^{t_n} \| g^{(2)}(\tau) \| \, d\tau \Big]$$

where the constant C *depends on* T.

Chapter 6

Numerical Experiments

Using several examples, we investigate the performance and robustness of the FETD-RDP scheme for space fractional reaction-diffusion problems. In particular, we consider problems having sharp variations in solution profile and non-smooth/mismatched initial and boundary data. The accuracy of the scheme in all cases is measured using the relative error

$$E(k) = \frac{||u - \tilde{u}||_\infty}{||u||_\infty},$$

where u and $\tilde{u}$ are the reference and approximate solutions, respectively. An exact solution can be used as a reference solution if available, otherwise, an appropriate solution with a very fine grid can be used. Leveque in [88] reported this idea as a well suited approach for recovering the rate of convergence of numerical schemes, though it may not reflect the true error in using the numerical scheme. The rate of convergence is calculated using the formula [88]:

$$p \approx \frac{\log\left(\tilde{E}(k)/\tilde{E}(\frac{k}{2})\right)}{\log 2},$$

where $\tilde{E}(k)$ is the approximate relative error on the temporal resolution k.

6.1 Introduction

The description of transport dynamics in many complex systems is made possible by Kinetic equations of the diffusion, diffusion advection, and Fokker-Planck equations with partial fractional derivatives. These are governed by anomalous diffusion and non-exponential relaxation patterns [93]. In [101], a Darcy-type law is derived from a fractional Newton's law of viscosity using spatial averaging methods. With this, description of shear stress phenomena in non-homogeneous porous media is made possible. Furthermore, they studied reaction-diffusion phenomena in disordered porous media in [129] with non-Fickian diffusion effects where an effective medium equation of the concentration dynamics, using a fractional Fick's law for the particles flux was obtained. It was shown that the disordered structure of the porous medium and the scaling from mesoscale to macroscale affect the the macroscale diffusion parameter.

In this section, we consider again nonlinear Riesz space fractional reaction-diffusion equation with homogeneous Dirichlet boundary condition given as

$$\begin{cases} u_t + \lambda(-\Delta)^{\frac{\alpha}{2}} u = f(t,u), \text{ in } \Omega \times (0,\ T], \\ u(.,0) = u_0, \text{ in } \Omega, \end{cases} \tag{6.1}$$

where λ is the diffusion coefficient, Ω is bounded in $\mathbb{R}^N$, $1 < \alpha \leq 2$ and $(-\Delta)^{\frac{\alpha}{2}}$ represents the Riesz fractional derivative. We assume that f is a sufficiently smooth function to ensure that the problem with the specified initial and boundary conditions possesses a unique solution.

In [13, 14, 28], existence and uniqueness of solutions to the class of problem in (6.1) has been investigated using some assumptions on f (such as local/global Lipschitz continuity). Also, there have been many attempts to solve Equation (6.1) numerically. These include using finite difference, finite element or finite volume discretisation of the fractional operator combined with a semi-implicit Euler formulation for the time evolution of the solution. In this, a linear system of equations involving a fractional power matrix at each time stepmust be solved. Recently, many authors have directed their effort to space discretization due to the fact that the resulting matrix is full. For example, approaches such as Krylov methods, fast numerical integration in conjunction with effective preconditioners and Fourier spectral methods have been employed, see [13, 20, 21, 28, 143, 147, 149]. However, there are very few works addressing the study of time-discretization schemes for this class of multidimensional problems that can complement the huge effort already put into the spatial part.

The purpose of this section is to fill in the gap described above. Our focus is to develop a novel Fractional Exponential Time Differencing (FETD) method for non-linear Riesz space fractional nonlinear reaction-diffusion equations. The advantage of this method is that it is stable, second order convergent, and proven to be robust for problems involving non-smooth initial and boundary conditions and steep solution gradients. Using some examples, we compare our method over competing second order FETD schemes and discuss its superiority. Our experiments show that the proposed scheme is computationally more efficient (in terms of CPU time).

Model Problem with Exact Solution

To validate the second-order accuracy of the proposed FETD-RDP scheme, we consider the following Riesz space fractional reaction diffusion equation with homogeneous Dirichlet boundary conditions [149].

$$\frac{\partial u}{\partial t} = \lambda \frac{\partial^\alpha u}{\partial |x|^\alpha} + f(x,t,u), \qquad (x,t) \in (0,1) \times (0,1], \quad 1 < \alpha \leq 2, \tag{6.2}$$

subject to initial condition

$$u(x,0) = 0, \quad x \in (0,1),$$

where $\lambda > 0$ and

$$f(x,t,u) = \frac{\lambda}{4}\left\{3\left[1+(2\pi)^\alpha\right]\sin(2\pi x) - \left[1+(6\pi)^\alpha\right]\sin(6\pi x)\right\} + \alpha t^{\alpha-1}\sin^3(2\pi x) - \lambda u.$$

By this construction, the exact solution to (6.2) is given as

$$u(x,t) = t^{\alpha} \sin^3(2\pi x).$$

The numerical results are presented in Figures 6.1 and 6.2, and Table 6.1.

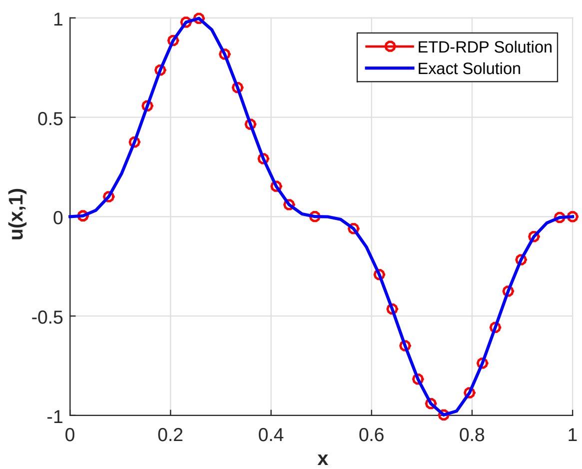
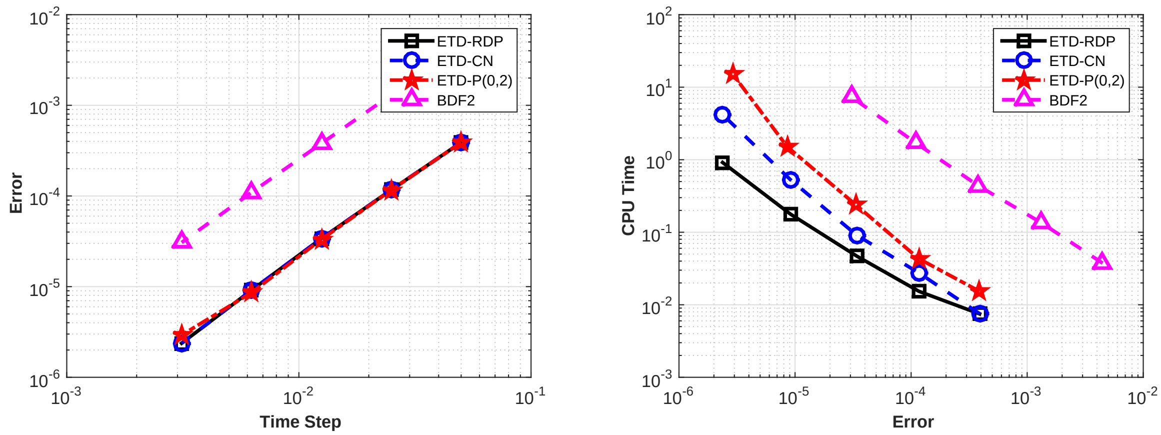


Figure 6.1: The numerical solution of 6.2 obtained via FETD-RDP scheme vs the exact solution when $\alpha = 1.8$ and $\lambda = 10^{-7}$

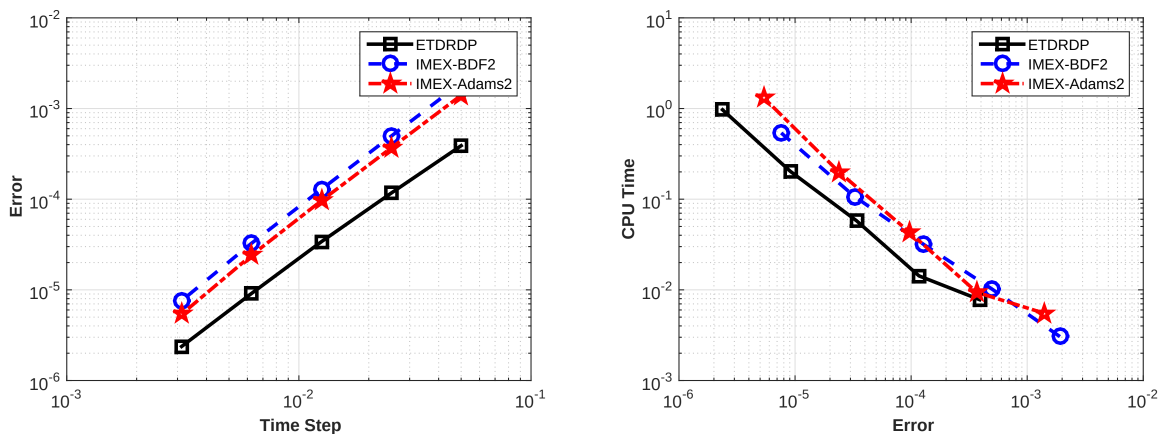
k	h	L_{∞} Error	Rate	Time (sec)
0.050000	0.050000	3.8926e-04	-	0.00147
0.025000	0.025000	1.1684e-04	1.74	0.00350
0.012500	0.012500	3.3961e-05	1.78	0.01240
0.006250	0.006250	9.1239e-06	1.90	0.05552
0.003125	0.003125	2.3743e-06	1.94	0.27502

Table 6.1: Emperical tested time rate of convergence of FETD-RDP for (6.2) with $\alpha = 1.8$ and $\mathscr{K} = 10^{-7}$



(a) Convergence (b) Efficiency

Figure 6.2: Log-log plots showing convergence and efficiency of FETD-RDP with FETD-CN and FETD-P(0,2) for the problem (6.2).



(a) Convergence (b) Efficiency

Figure 6.3: Log-log plots showing convergence and efficiency of FETD-RDP with IMEX-BDF2 and IMEX-Adams2 for the problem (6.2)

Remark 6.1.1.

1. The second-order convergence of the FETD-RDP scheme is empirically validated by the grid refinement given in Table 6.1.

2. The comparison of the FETD-RDP with other second order FETD schemes such as FETD-

Pade(0,2) and FETD-CN shows that FETD-RDP is computationally more efficient see Figure 6.2.

3. Moving out of the FETD schemes, we also compare our proposed FETD-RDP scheme with the well known BDF2 and IMEX-Schemes (IMEX-BDF2 and IMEX-Adams). As shown in Figure 6.3, in general, the FETD-RDP scheme is more robust and computationally efficient compared with the IMEX schemes.

6.2 Numerical Experiment I: Scalar Models

In this section, we discuss some numerical experiments for two-dimensional space-fractional reaction-diffusion problems. These models are of particular important in applications.

6.2.1 Space Fractional Allen-Cahn Equation

We consider the nonlinear space fractional Allen-Cahn (S-FACE) problem of the form

$$\frac{\partial u}{\partial t} = \lambda \frac{\partial^\alpha u}{\partial |x|^\alpha} + (u+x) - (u+x)^3, \qquad x \in [-1,1], \qquad t > 0, \tag{6.3}$$

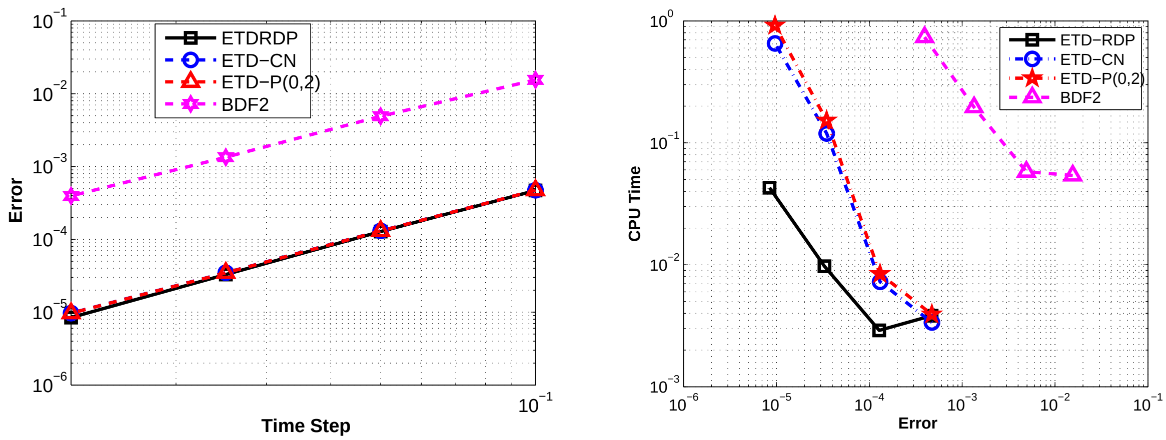
subject to initial and boundary conditions given as

$$u(x,0) = 0.47\sin(-1.5\pi x) - 0.47x,\ x \in [-1,1] \quad \text{and} \quad u(-1,t) = 0, \quad u(1,t) = 0 \quad t > 0.$$

Here, u represents the concentration of one of the species of the alloy and the parameter λ represents the diffuse interface width parameter. Note that this equation has solution regions near ± 1 that are flat and where the interface does not change for a relatively long period of time, then changes suddenly. Also, $f(u)$, the nonlinear term, is the derivative of a free energy functional $F(u)$. However, the choice $f(u) = (u+x) - (u+x)^3$ represents the bistable non-linearity for the double-well potential.

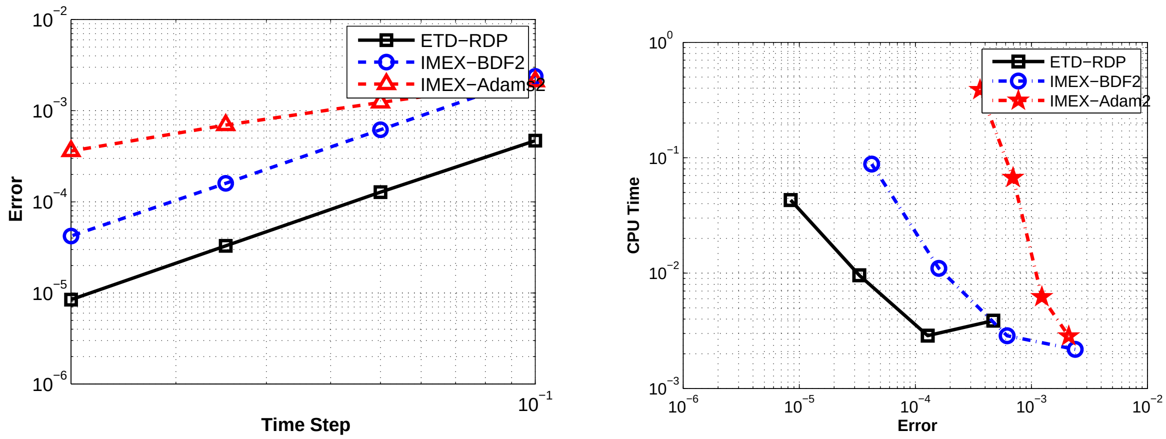
k	h	L_∞ Error	Rate	Time (sec)
0.1000	0.1000	4.6948×10^{-4}	-	0.00850
0.0500	0.0500	1.2791×10^{-4}	1.88	0.00566
0.0250	0.0250	3.2893×10^{-5}	1.96	0.02546
0.0125	0.0125	8.4377×10^{-6}	1.96	0.12003

Table 6.2: Time rate of convergence of FETD-RDP for S-FACE with $\alpha = 1.8$ and $\lambda = 10^{-5}$



(a) Convergence (b) Efficiency

Figure 6.4: Log-log plots showing convergence and efficiency of FETD-RDP with FETD-CN and FETD-P(0,2) for the S-FACE (6.3)



(a) Convergence (b) Efficiency

Figure 6.5: Log-log plots showing convergence and efficiency of FETD-RDP with IMEX-BDF2 and IMEX-Adams2 for the for S-FACE (6.3)

Remark 6.2.1.

1. The second-order accuracy of FETD-RDP is again demonstrated in Table 6.2.

2. As expected, the FETD-RDP scheme applied to S-FACE in Equation (6.3) is computationally more efficienct than FETD-CN and FETD-P(0,2) without compromising the accuracy. Furthermore, from Figure 6.28, it is interesting to observe that the FETD solutions to the space fractional Allen-Cahn equation have comparable accuracy to BDF2 with much higher computational efficiency. This is due to the necessity of iterating at each step.

3. The FETD-RDP scheme also has a very good comparison with the IMEX Schemes (IMEX-BDF2 and IMEX-Adams2) both in accuracy and computational efficiency.

6.2.2 Fractional Enzyme Kinetics

We consider the two-dimensional Riesz space fractional enzyme kinetics (S-FEK) reaction-diffusion problem with homogeneous Dirichlet boundary conditions:

$$\frac{\partial u}{\partial t} = \lambda\left(\frac{\partial^\alpha u}{\partial |x|^\alpha} + \frac{\partial^\alpha u}{\partial |y|^\alpha}\right) - \frac{u}{1+u} \quad 0 < x < 1,\ 0 < y < 1,\ t > 0, \tag{6.4}$$

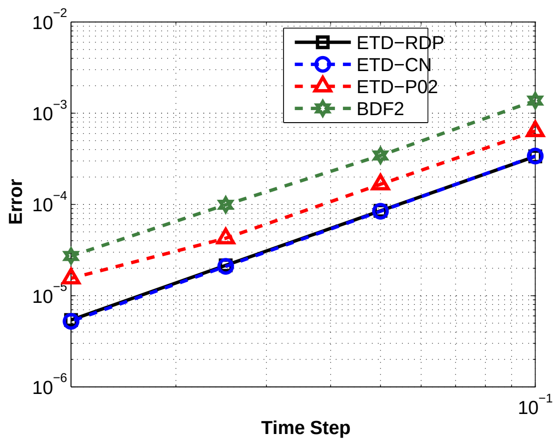
subject to initial condition

$$u(x, y, 0) = 1, \quad 0 \le x, y \le 1.$$

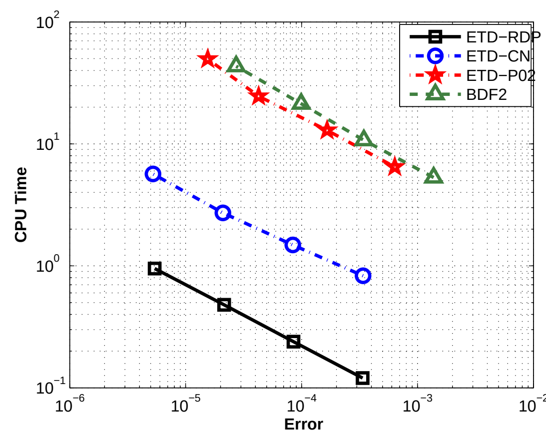
Observe that this equation is an example of a model with mismatched conditions due to the fact that the boundary and the initial condition do not match. We use the model to examine the ability of FETD-RDP to damp out spurious oscillation in two dimensional problems with non-smooth data.

k	h	L_∞ Error	Rate	Time
0.1000	0.0250	3.3610×10^{-4}	-	0.12023
0.0500	0.0250	8.5225×10^{-5}	1.98	0.23894
0.0250	0.0250	2.1502×10^{-5}	1.99	0.47916
0.0125	0.0250	5.4032×10^{-6}	1.99	0.94955

Table 6.3: Time rate of convergence of FETD-RDP for S-FEK with $\alpha = 1.6$, $\lambda = 0.01$

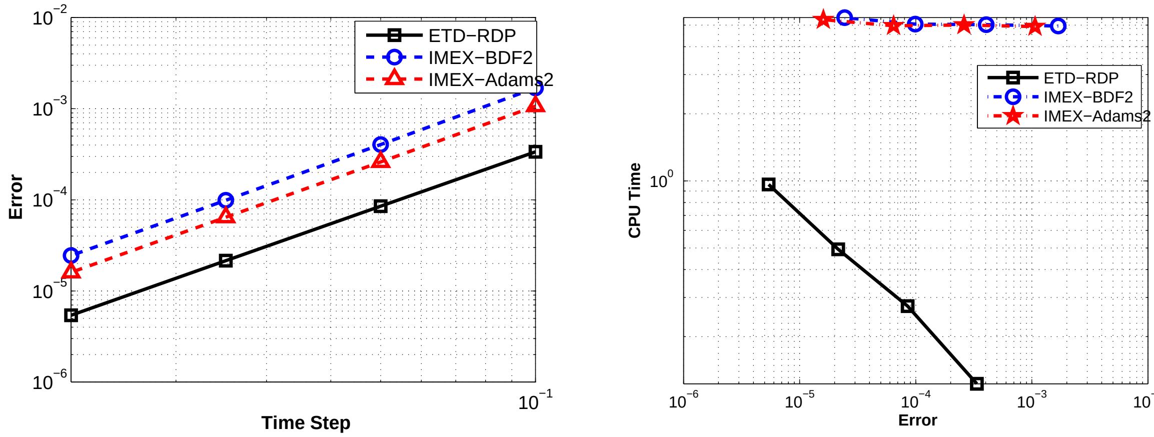


(a) Convergence



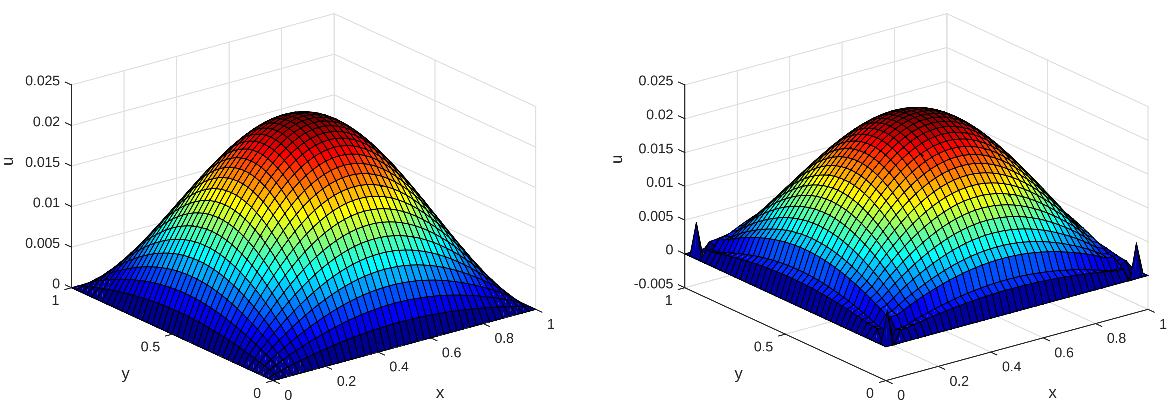
(b) Efficiency

Figure 6.6: Log-log plots showing convergence and efficiency of FETD-RDP over FETD-CN, FETD-P(0,2) and BDF2 schemes for S-FEK using $\alpha = 1.6$ and $\lambda = 0.01$



(a) Convergence (b) Efficiency

Figure 6.7: Log-log plots showing convergence and efficiency of FETD-RDP over IMEX-BDF2 and IMEX-Adams2 for the for S-FEK using $\alpha = 1.6$ and $\lambda = 0.01$



(a) FETD-RDP (b) FETD-CN

Figure 6.8: Solution of the two dimensional space fractional enzyme kinetics equation simulation for $t = 1$ using 0.01 time step, $\alpha = 1.8$ and $\lambda = 0.01$

Remark 6.2.2.

1. Again, the results presented in Table 6.3 and Figures 6.6-6.7 confirm the ability of the FETD-RDP scheme not only to solve two dimensional space fractional problems, but also fractional models with non-smooth data.

2. The FETD-RDP scheme compared to other FETD schemes (FETD-CN and FETD-P(0,2)) and IMEX schemes (IMEX-BDF2 and IMEX-Adams): Once again it is the most accurate and computationally efficient.

3. Moreover, we observe from Figure (6.8) that FETD-RDP damps spurious oscillations and is therefore the most computational efficient scheme for space fractional enzyme kinetics.

4. The accuracy of the FETD-CN solution is compromised by the spurious oscillations. However, the performance can be improved using initial smoothing steps [77]. This aspect has not been considered here.

6.3 Numerical Experiment II: System of Two-dimensional Models

Introduction

Consider a system of two-dimensional nonlinear Riesz space fractional reaction-diffusion equations with homogeneous Dirichlet boundary condition on $\partial\Omega$ given as

$$u_t + \zeta_1 \frac{\partial^\alpha u}{\partial|x|^\alpha} + \zeta_2 \frac{\partial^\alpha u}{\partial|y|^\alpha} = f_1(u,v),\ (x,y,t) \in \Omega \times (0,T] \tag{6.5}$$

$$v_t + \mathcal{K}_1 \frac{\partial^\alpha v}{\partial|x|^\alpha} + \mathcal{K}_2 \frac{\partial^\alpha v}{\partial|y|^\alpha} = f_2(u,v),\ (x,y,t) \in \Omega \times (0,T], \tag{6.6}$$

with initial conditions

$$u(x,y,0) = u_0(x,y),\ (x,y) \in \Omega \cup \partial\Omega, \tag{6.7}$$

$$v(x,y,0) = v_0(x,y),\ (x,y) \in \Omega \cup \partial\Omega. \tag{6.8}$$

where ζ_1, ζ_2, $\mathscr{K}_1$ and $\mathscr{K}_2$ are the diffusion coefficients, Ω is a bounded domain in $\mathbb{R}^2$, $1 < \alpha \leq 2$ and $\frac{\partial^\alpha}{\partial |x|^\alpha}$ represents the Riesz fractional derivative. f_1 and f_2 are assumed to be sufficiently smooth functions to ensure that the problem with the specified initial and boundary conditions possesses unique solutions.

When $\alpha = 2$, the system (6.5)-(6.6) is the classical time-dependent system of reaction-diffusion models. For many decades, this time-dependent system of reaction-diffusion equations has been used to describe the time evolution of chemical or biological species in a fluid medium. The description of transport of pollutants in the atmosphere, ground and surface water, tracking the progression of tumours, and studying pattern formation in biological species are made possible using this type of system, see [6, 27, 48, 65, 82, 128, 131, 155] for detail. Many of these phenomena have displayed anomalous processes such as sub-diffusion and super-diffusion of which the classical ($\alpha = 2$) mathematical models are not suitable. Recently, the attention of researchers has been drawn to the study of fractional (non-integer) calculus due to its ability to capture these anomalous processes. We now find systems of fractional reaction-diffusion equations in many applications, including sound wave propagation in rigid porous materials, and the memory and hereditary properties of different substances, see [39, 145]. In particular, the anomalous diffusion or dispersion effects caused by the movement of particles, which is inconsistent with the classical Brownian motion model, is modelled using space fractional derivatives, see [93]. The nonlinear Schrodinger equation with space fractional derivative in one dimension is used to model the evolution of an inviscid perfect fluid with nonlinear dynamics, see [75]. In [69], the associated fractional Laplacian represents the dispersion effect of the linearized gravity water waves equation for one dimensional surfaces.

The aim of this section is to develop a novel exponential integrator method for the system of two dimensional nonlinear space fractional reaction-diffusion equations. This method uses a real distinct poles discretization for the underlying matrix exponentials. The advantage of this method is that it is stable, second order convergent, and proven to be robust for problems involving nonsmooth/mismatched initial and boundary conditions. Our approach is exhibited by solving biological and biochemical systems of two dimensional problems: the fractional Schnakenberg, Grey-Scott, Brusselator FitzHugh-Nagumo models. We empirically show the effect of the fractional power of the underlying Laplacian operator on the pattern formations in these systems. This actually confirms the need for fractional calculus in understanding the complexities involved in these models. Furthermore, the superiority of our method over some competing second order FETD schemes, BDF2 scheme, and IMEX schemes is demonstrated. Our experiments confirm that the proposed scheme is computationally more efficient and robust for system of two dimensional fractional differential equations.

6.3.1 The Fractional Schnakenberg Model and the Turing Pattern

We consider nonlinear two dimensional space fractional Schnakenberg model (S-FSM) with homogeneous Dirichlet boundary conditions:

$$\frac{\partial u}{\partial t} = \lambda_1 \frac{\partial^\alpha u}{\partial |x|^\alpha} + \lambda_2 \frac{\partial^\alpha u}{\partial |y|^\alpha} + \gamma(a - u + u^2 v), \quad (x,y) \in (0,1)\times(0,1), \quad t>0, \tag{6.9}$$

$$\frac{\partial v}{\partial t} = d_1 \frac{\partial^\alpha v}{\partial |x|^\alpha} + d_2 \frac{\partial^\alpha v}{\partial |y|^\alpha} + \gamma(b - u^2 v), \quad (x,y) \in (0,1)\times(0,1), \quad t>0, \tag{6.10}$$

subject to initial conditions given as

$$u(x,y,0) = a + b + 10^{-3} \exp\left\{-100\left(\left(x-\frac{1}{3}\right)^2 + \left(y-\frac{1}{2}\right)^2\right)\right\},$$

and

$$v(x,y,0) = \frac{b}{(a+b)^2},\ 0 \le x, y \le 1,$$

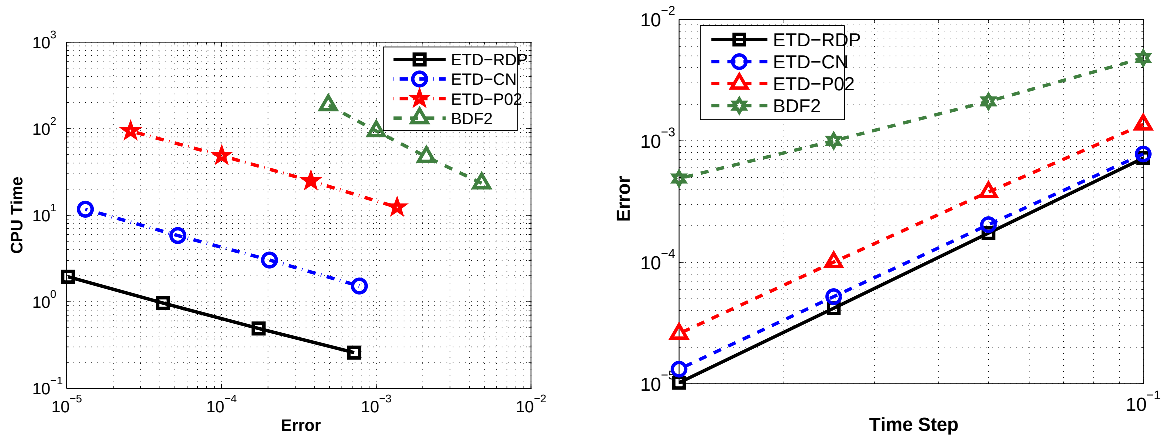
where u and v represent chemical concentrations, $\lambda_1, \lambda_2, d_1, d_2$ are the diffusion coefficients, a and b are reaction kinetic parameters, γ represents the relative strength of the reaction terms. An increase in the value of γ may result in an increase in activity of some rate-limiting. Schnakenberg system was first introduced in [120] to model autocatalytic chemical reaction which could posses oscillatory behaviours. The presence of diffusion-driven instability gives rise to the spatial pattern formation found in this model.

Comparison of FETD-RDP Scheme with other Second-order Schemes for S-FSM

We choose $a = 0.1305$, $b = 0.7695$, $\gamma = 1.5$, $\lambda_1 = \lambda_2 = 0.1$, and $d_1 = d_2 = 0.001$ for our computation, using fractional centered difference method for the spatial discretization. The proposed FETD-RDP scheme is compared to some other second-order schemes for efficiency and accuracy.

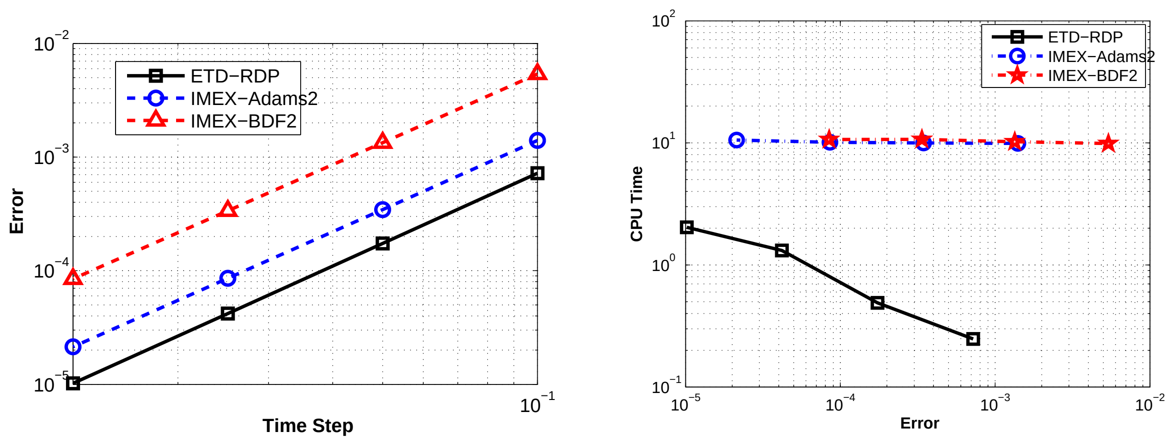
Table 6.4: Time rate of convergence of FETD-RDP for S-FSM with different values of α and $t = 1$

	k	h	L_∞ Error	Rate	Time
$\alpha = 1.3$	0.1000	0.0250	5.4656×10^{-4}	-	0.25348
	0.0500	0.0250	1.3445×10^{-4}	2.02	0.50799
	0.0250	0.0250	3.3023×10^{-5}	2.03	1.00368
	0.0125	0.0250	8.1489×10^{-6}	2.02	1.97288
$\alpha = 1.5$	0.1000	0.0250	7.2130×10^{-4}	-	0.25861
	0.0500	0.0250	1.7388×10^{-4}	2.05	0.49116
	0.0250	0.0250	4.1919×10^{-5}	2.05	0.96467
	0.0125	0.0250	1.0193×10^{-5}	2.04	1.94773
$\alpha = 1.7$	0.1000	0.0250	9.6645×10^{-4}	-	0.26776
	0.0500	0.0250	2.3029×10^{-4}	2.07	0.47287
	0.0250	0.0250	5.5694×10^{-5}	2.05	1.18154
	0.0125	0.0250	1.3863×10^{-5}	2.01	2.04230



(a) Efficiency (b) Convergence

Figure 6.9: Log-log plots showing convergence and efficiency of FETD-RDP with FETD-CN and FETD-P(0,2) for the S-FSM (6.9)-(6.10), $t = 1$ and $\alpha = 1.5$.



(a) Efficiency (b) Convergence

Figure 6.10: Log-log plots showing convergence and efficiency of FETD-RDP with IMEX-BDF2 and IMEX-Adams2 for the for S-FSM (6.9)-(6.10), $t = 1$ and $\alpha = 1.5$.

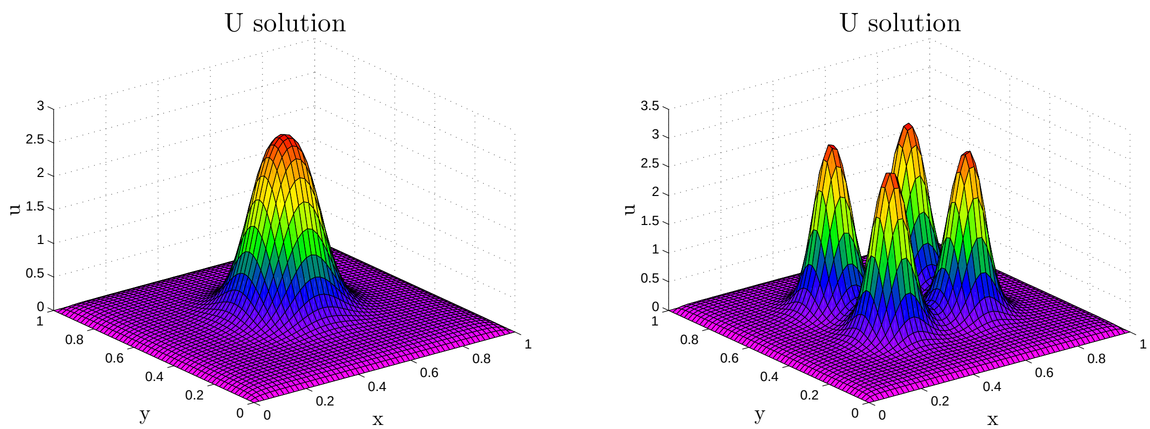
Remark 6.3.1.

1. The second-order convergence of the FETD-RDP scheme is empirically validated by the grid refinement given in Table 6.6 for different values of α.

2. The comparison of the FETD-RDP scheme with other second order FETD schemes such

as FETD-Pade(0,2) and FETD-CN shows that FETD-RDP is computationally more efficient see Figures 6.9.

3. Considering second-order non-FETD schemes, we compare our proposed the FETD-RDP scheme with the well known BDF2 and IMEX-Schemes (IMEX-BDF2 and IMEX-Adams). As shown in Figure 6.10, in general, FETD-RDP scheme is more robust and computationally efficient compared with the IMEX schemes.

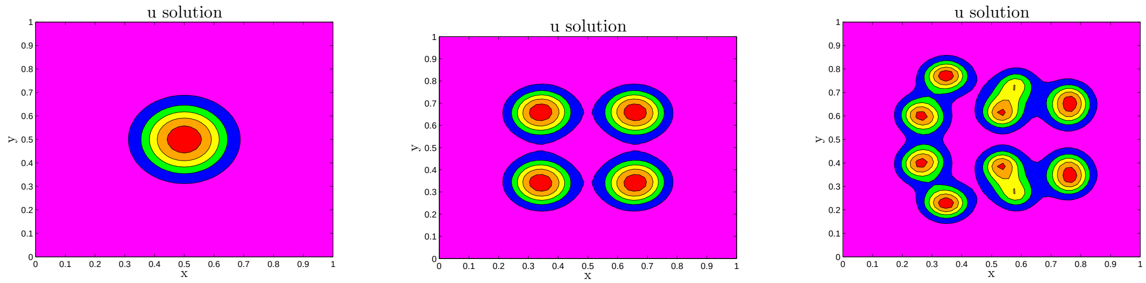


(a) $\alpha = 2.0$ (b) $\alpha = 1.8$

Figure 6.11: Solution plot of S-FSM (6.9)-(6.10) with $t = 1$ and $\gamma = 40$.

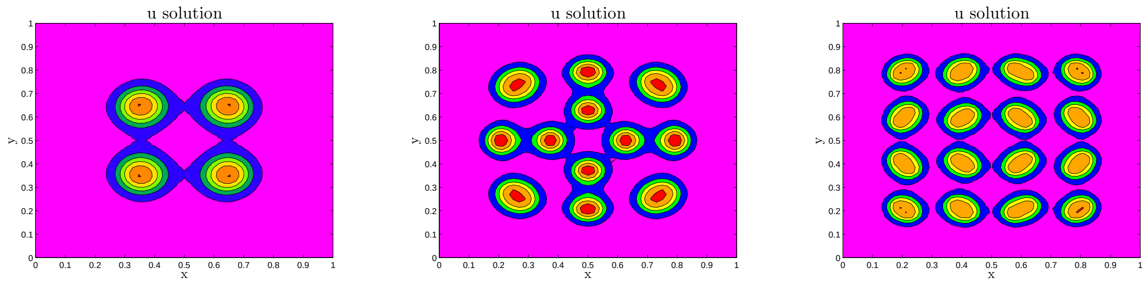
Effect of γ on the Turing pattern nature of Schnakenberg model

We examine the effect of the relative strength of the reaction terms, γ, on the solution profile and how this affect the turing pattern found in this model.



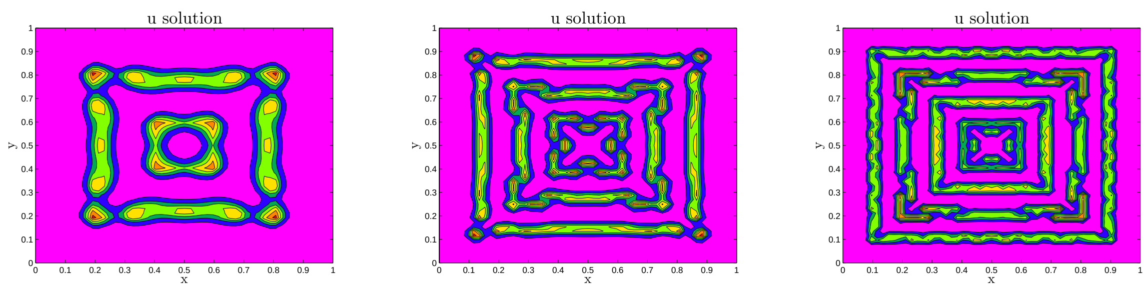
(a) $\gamma = 40$ (b) $\gamma = 80$ (c) $\gamma = 120$

Figure 6.12: Effect of γ on the solution of S-FSM (6.9)-(6.10) with $t = 1$ and $\alpha = 2.0$.



(a) $\gamma = 40$ (b) $\gamma = 80$ (c) $\gamma = 120$

Figure 6.13: Effect of γ on the solution of S-FSM (6.9)-(6.10) with $t = 1$ and $\alpha = 1.8$.



(a) $\gamma = 40$ (b) $\gamma = 80$ (c) $\gamma = 120$

Figure 6.14: Effect of γ on the solution of S-FSM (6.9)-(6.10) with $t = 1$ and $\alpha = 1.5$.

Remark 6.3.2.

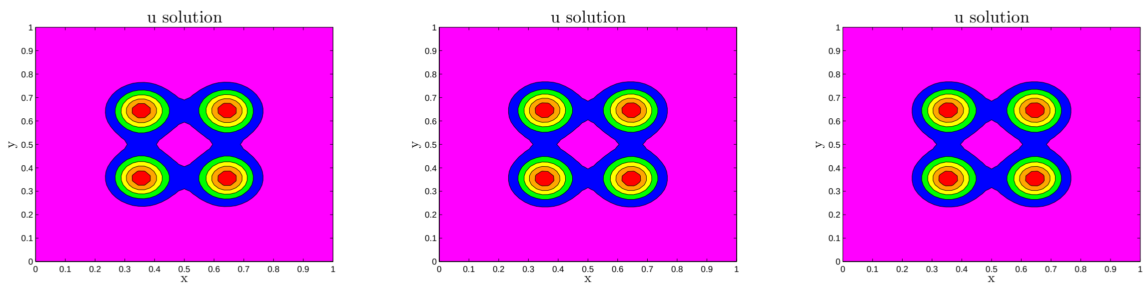
1. We observe from Figures 6.29-6.14, that a Turing pattern is exhibited for all different values of fractional order, α, and the relative strength of the reaction terms, γ.

2. The Turing patterns are different across different values of α for different values of γ. While the case of $\alpha = 2.0$ exhibits cell division nature, mitosis-like, the division found when $\alpha = 1.8$ is completely different. Furthermore, when $\alpha = 1.5$, the solution profile exhibits chain-pattern in which the divisions are in the chains.

3. Super-diffusion processes are observed even for different relative strength of the reaction terms, γ using different values of α.

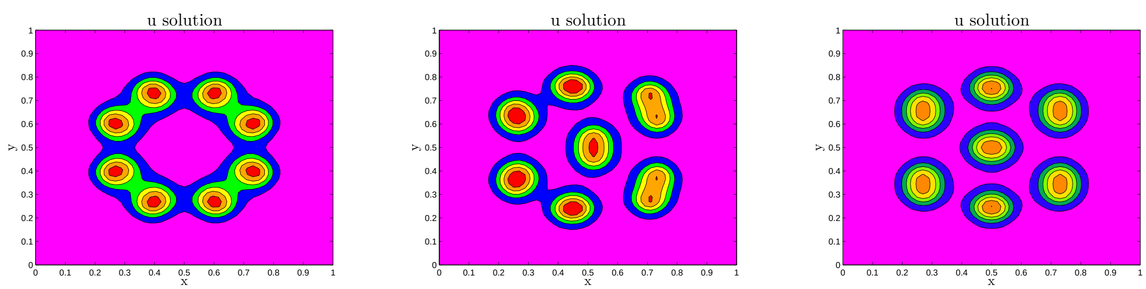
Effect of the fractional order, α, on the Turing pattern nature of Schnakenberg model

We examine the effect of the fractional order, α, on the solution profile and how this affects the Turing pattern found in this model.



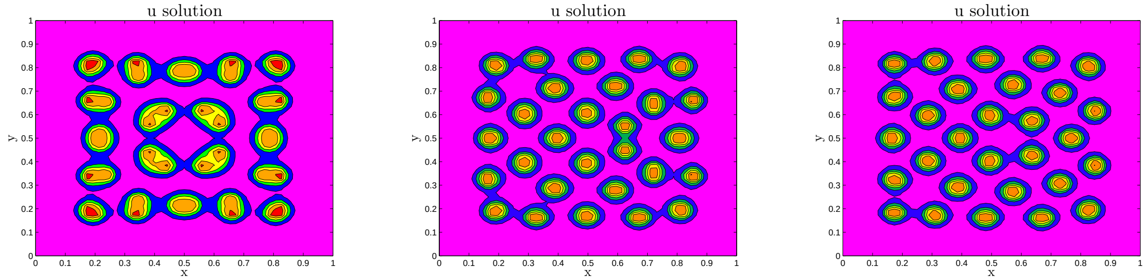
(a) $t = 1$ (b) $t = 10$ (c) $t = 100$

Figure 6.15: Dynamics of the solution of S-FSM (6.9)-(6.10) with $\gamma = 60$ and $\alpha = 2.0$.



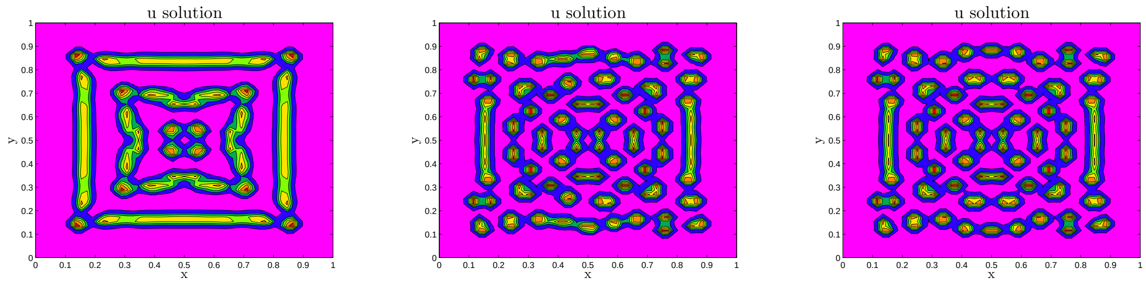
(a) $t = 1$ (b) $t = 10$ (c) $t = 100$

Figure 6.16: Dynamics of the solution of S-FSM (6.9)-(6.10) with $\gamma = 60$ and $\alpha = 1.8$.



(a) $t = 1$ (b) $t = 10$ (c) $t = 100$

Figure 6.17: Dynamics of the solution of S-FSM (6.9)-(6.10) with $\gamma = 60$ and $\alpha = 1.6$.



(a) $t = 1$ (b) $t = 10$ (c) $t = 100$

Figure 6.18: Dynamics of the solution of S-FSM (6.9)-(6.10) with $\gamma = 60$ and $\alpha = 1.5$.

Remark 6.3.3.

1. We observe from Figures 6.15-6.18, that the Turing pattern is exhibited for all different values of fractional order, α, over a period of time.

2. For the classical case $\alpha = 2.0$, an increase in the value of t has no effect on the pattern formation. However, as we decrease the value of α, the patterns are dynamic and the divisions are faster. Also, a smaller value of α gives aligned and completely different pattern. This is again a super-diffusion process, and so having fractional order in this model is imperative to see intrinsic properties of the model.

6.3.2 The Fractional Gray-Scott Model - Morphogenesis

We consider the nonlinear two-dimensional space-fractional Gray-Scott problem with homogeneous Dirichlet boundary conditions:

$$\frac{\partial u}{\partial t} = \lambda_1 \frac{\partial^\alpha u}{\partial |x|^\alpha} + \lambda_2 \frac{\partial^\alpha u}{\partial |y|^\alpha} - uv^2 + F(1-u), \quad (x,y) \in (0,1)\times(0,1), \quad t>0, \tag{6.11}$$
$$\frac{\partial v}{\partial t} = d_1 \frac{\partial^\alpha v}{\partial |x|^\alpha} + d_2 \frac{\partial^\alpha v}{\partial |y|^\alpha} + uv^2 - (F+\kappa)v, \quad (x,y) \in (0,1)\times(0,1), \quad t>0, \tag{6.12}$$

subject to initial conditions given as

$$u(x,y,0) = \begin{cases} 0.5 & 0.45 < x < 0.55,\ 0.45 < y < 0.55, \\ 1.0 & \text{otherwise,} \end{cases}$$

and

$$v(x,y,0) = \begin{cases} 0.25 & 0.45 < x < 0.55,\ 0.45 < y < 0.55 \\ 0.0 & \text{otherwise,} \end{cases}$$

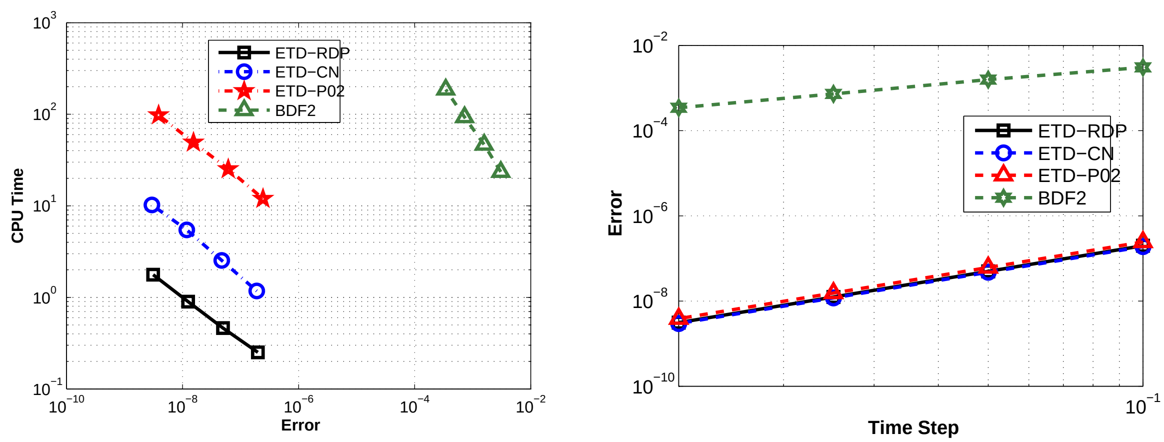
where F, κ, λ_1, λ_2, d_1 and d_2 are constants.

Comparison of RDP-FETD Scheme with other Second-order Schemes for S-FGSM

We choose $F = 0.03$, $\kappa = 0.055$, $\alpha = 1.6$, $\lambda_1 = \lambda_2 = 0.0002$, and $d_1 = d_2 = \frac{\lambda_1}{2}$ for our computation using the FETD-RDP scheme with the fractional centered difference method.

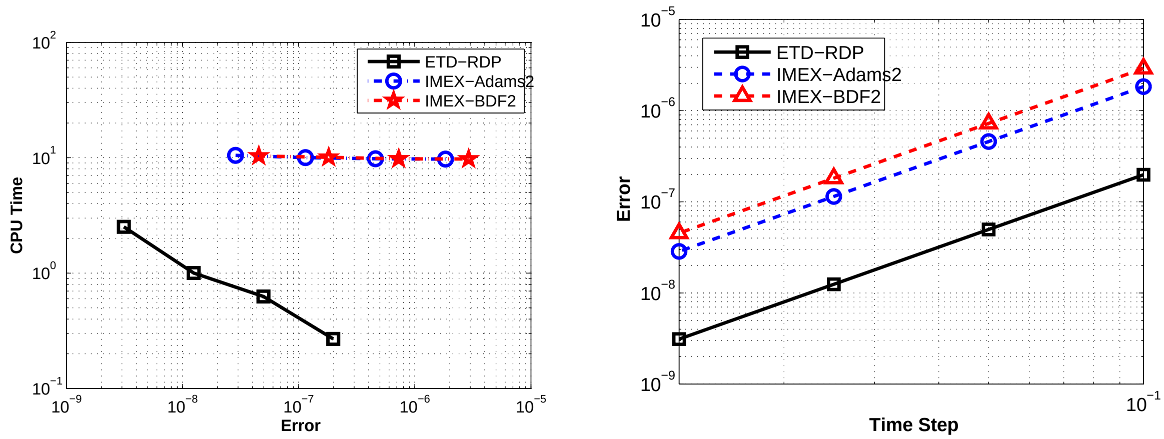
Table 6.5: Time rate of convergence of FETD-RDP for S-FGSM with $t = 2$

	k	h	L_∞ Error	Rate	Time (sec)
$\alpha = 1.3$	0.05000	0.05000	3.4387×10^{-9}	-	0.21520
	0.02500	0.05000	8.6129×10^{-10}	2.00	0.43001
	0.01250	0.05000	2.1559×10^{-10}	2.00	0.84732
	0.00625	0.05000	5.3749×10^{-11}	2.00	1.70784
$\alpha = 1.6$	0.1000	0.0250	1.9839×10^{-7}	-	0.25118
	0.0500	0.0250	4.9770×10^{-8}	1.99	0.46305
	0.0250	0.0250	1.2465×10^{-8}	2.00	0.89773
	0.0125	0.0250	3.1189×10^{-9}	2.00	1.77096
$\alpha = 1.8$	0.1000	0.0250	1.8462×10^{-6}	-	0.21732
	0.0500	0.0250	4.6382×10^{-7}	1.99	0.28265
	0.0250	0.0250	1.1626×10^{-7}	2.00	1.25619
	0.0125	0.0250	2.9105×10^{-8}	2.00	2.39355



(a) Efficiency (b) Convergence

Figure 6.19: Log-log plots showing convergence and efficiency of FETD-RDP with FETD-CN and FETD-P(0,2) for the S-FACE (6.11)-(6.12) with $\alpha = 1.6$ and $t = 2$



(a) Efficiency (b) Convergence

Figure 6.20: Log-log plots showing convergence and efficiency of FETD-RDP with IMEX-BDF2 and IMEX-Adams2 for the for S-FGSM (6.11)-(6.12) with $\alpha = 1.6$ and $t = 2$

Remark 6.3.4.

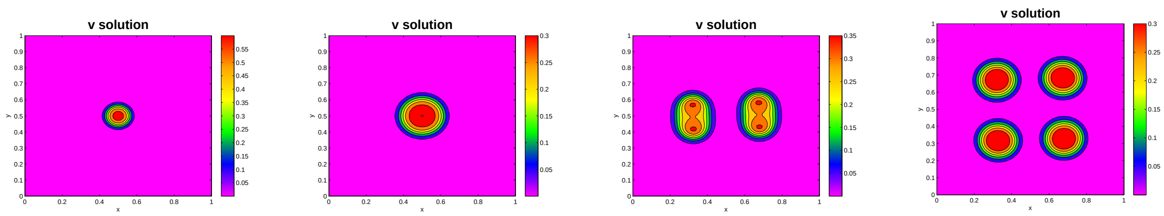
1. The second-order accuracy of FETD-RDP is again demonstrated in Table 6.5 for different values of α.

2. The FETD-RDP scheme applied to S-FGSM in Equations (6.11)-(6.12) is computationally more efficient than FETD-CN and FETD-P(0,2) as expected without compromising the accuracy see Figure 6.19. Furthermore, it is interesting to observe from Figure 6.19 that the FETD solutions of system of nonlinear space fractional Grey-Scott Model have comparable accuracy to BDF2 with much higher computational efficiency. This is due to the necessity of iterating at each step.

3. We also have a good comparison with the IMEX Schemes (IMEX-BDF2 and IMEX-Adams2) both in accuracy and computational efficiency see Figure 6.20.

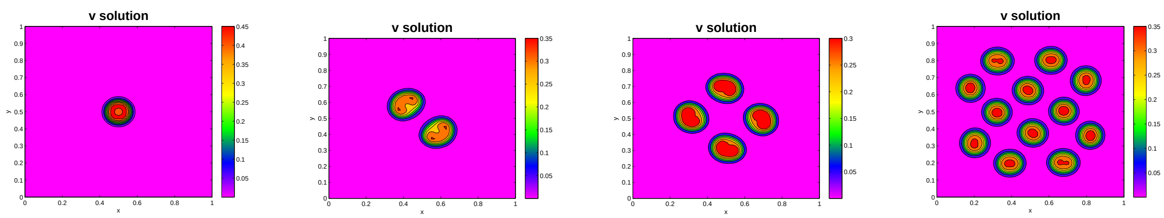
Effect of the fractional order, α, on the morphogenesis nature of the Gray-Scott model

We examine the effect of the fractional order, α, on the solution profile and how this affects the morphogenesis nature of the Gray-Scott model.



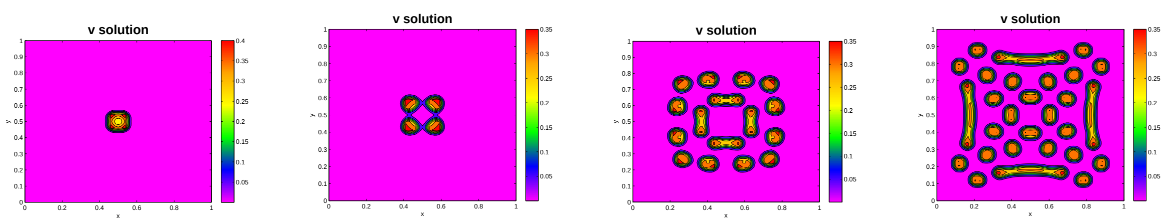
(a) $\alpha = 2.0$ and $t = 50$ (b) $\alpha = 2.0$ and $t = 4500$ (c) $\alpha = 2.0$ and $t = 6000$ (d) $\alpha = 2.0$ and $t = 6500$

Figure 6.21: V solution profiles for the S-FGSM with $\alpha = 1.6$.



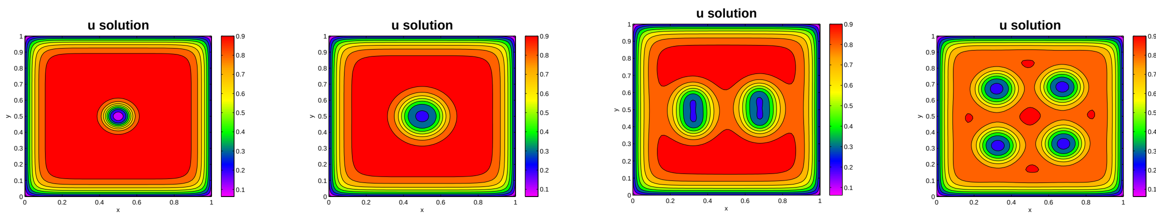
(a) $\alpha = 1.8$ and $t = 50$ (b) $\alpha = 1.8$ and $t = 3000$ (c) $\alpha = 1.8$ and $t = 3500$ (d) $\alpha = 1.8$ and $t = 6000$

Figure 6.22: V solution profiles for the S-FGSM with $\alpha = 1.8$.



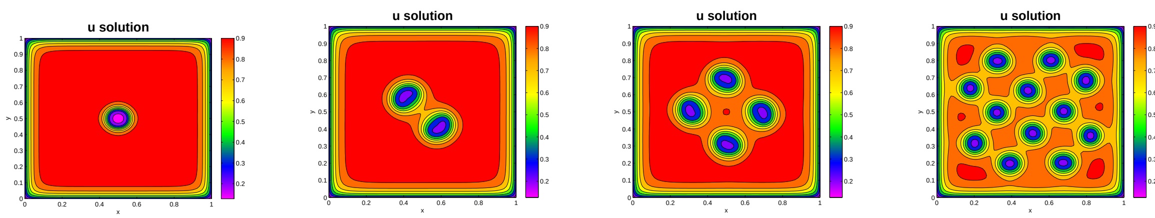
(a) $\alpha = 1.6$ and $t = 50$ (b) $\alpha = 1.6$ and $t = 500$ (c) $\alpha = 1.6$ and $t = 2500$ (d) $\alpha = 1.6$ and $t = 6000$

Figure 6.23: Morphogenesis nature of V solution profiles for the S-FGSM (6.11)-(6.12) over time.



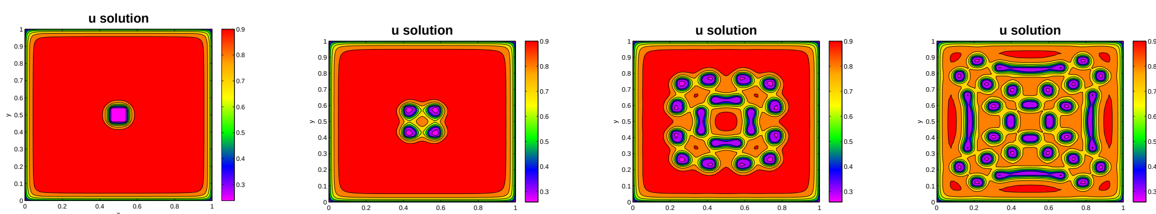
(a) $\alpha = 2.0$ and $t = 50$ (b) $\alpha = 2.0$ and $t = 4500$ (c) $\alpha = 2.0$ and $t = 6000$ (d) $\alpha = 2.0$ and $t = 6500$

Figure 6.24: V solution profiles for the S-FGSM with $\alpha = 1.6$.



(a) $\alpha = 1.8$ and $t = 50$ (b) $\alpha = 1.8$ and $t = 3000$ (c) $\alpha = 1.8$ and $t = 3500$ (d) $\alpha = 1.8$ and $t = 6000$

Figure 6.25: V solution profiles for the S-FGSM with $\alpha = 1.8$.



(a) $\alpha = 1.6$ and $t = 50$ (b) $\alpha = 1.6$ and $t = 500$ (c) $\alpha = 1.6$ and $t = 2500$ (d) $\alpha = 1.6$ and $t = 6000$

Figure 6.26: Morphogenesis nature of U solution profiles for the S-FGSM (6.11)-(6.12) over time.

Remark 6.3.5.

1. We observe from Figures 6.33-6.38, a morphogenesis pattern is exhibited for all different values of fractional order, α, over a period of time.

2. For the classical case $\alpha = 2.0$, an increase in the value of t has no effect on the morphogenesis pattern. However, as we decrease the value of α, the patterns are dynamic and the divisions are faster. Also, a smaller value of α gives an aligned and completely differ-

ent pattern. This is again a super-diffusion process and so having fractional order in this model is imperative to see intrinsic properties of the model.

6.3.3 The Fractional Brusselator Model - Turing Pattern

We consider the nonlinear two dimensional space fractional Brusselator (S-FBM) problem with homogeneous Dirichlet boundary conditions:

$$u_t = \zeta\left(\frac{\partial^\alpha u}{\partial|x|^\alpha} + \frac{\partial^\alpha u}{\partial|y|^\alpha}\right) + A + u^2 v - (B+1)u, \quad (x,y) \in (0,1)\times(0,1), \quad t>0, \tag{6.13}$$

$$v_t = \mathscr{K}\left(\frac{\partial^\alpha v}{\partial|x|^\alpha} + \frac{\partial^\alpha v}{\partial|y|^\alpha}\right) + Bu - u^2 v, \quad (x,y) \in (0,1)\times(0,1), \quad t>0, \tag{6.14}$$

subject to initial conditions given as

$$u(x,y,0) = 0.5 + y, \text{ and } v(x,y,0) = 1 + 5x, \; 0 \le x, y \le 1.$$

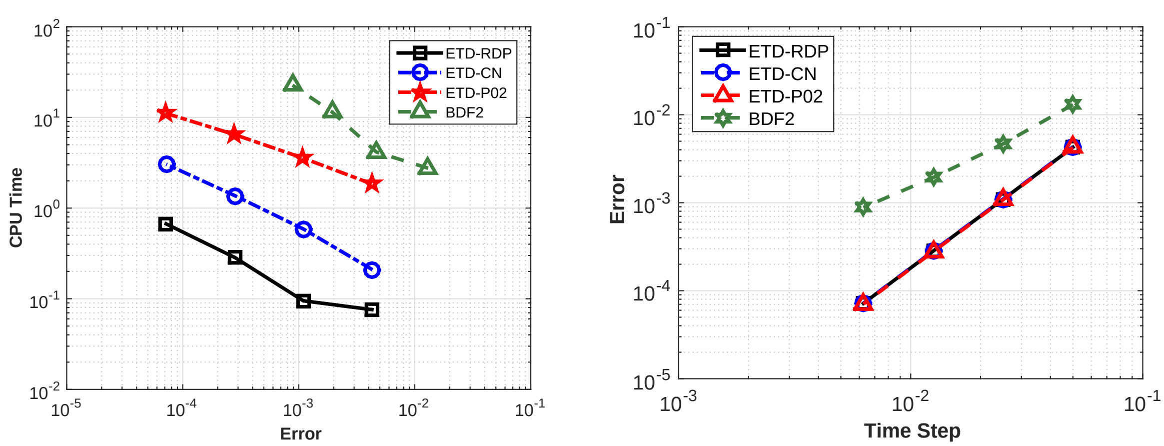
Here, u and v represent dimensionless concentrations of two chemical reactants, $\zeta, \mathscr{K}$ are the diffusion coefficients and A and B are constants concentrations of the two imput chemical reactants. Many physical problems are modeled using the Brusselator system such as the formation of ozone by atomic oxygen through a triple collision and enzymatic reactions, see [85]. This model is known to exhibit turing pattern, see [52, 86].

Comparison of RDP-FETD Scheme with other Second-order Schemes for S-FBM

We choose $A = 1$, $B = 3.4$, $\zeta = \mathscr{K} = 2 \times 10^{-3}$ for our computation using fractional centered difference method for the spatial discretization. The proposed FETD-RDP scheme is compared to some other second-order schemes for efficiency and accuracy.

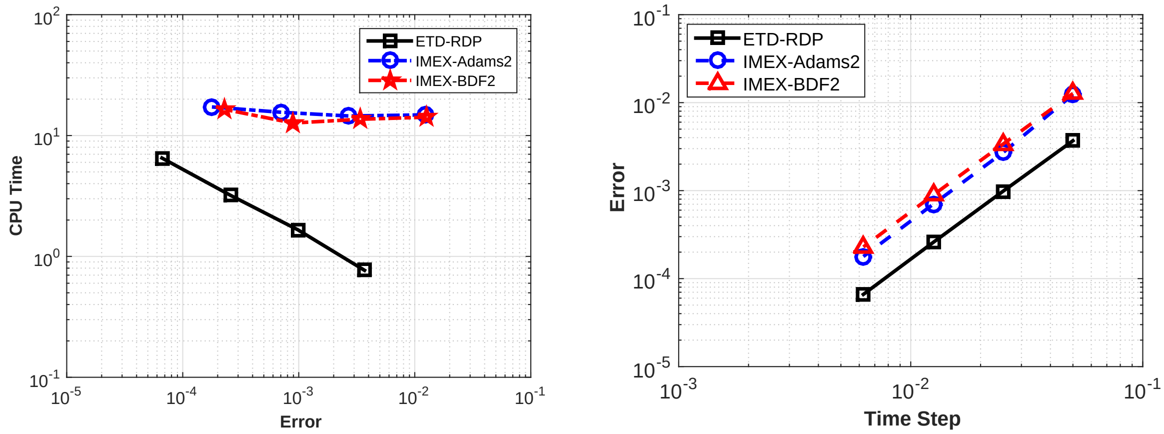
Table 6.6: Time rate of convergence of FETD-RDP for S-FBM with $t = 1$

	k	h	L_∞ Error	Rate	Time (sec)
$\alpha = 1.3$	0.05000	0.05000	4.8237×10^{-3}	-	0.03487
	0.02500	0.05000	1.1921×10^{-3}	2.02	0.06943
	0.01250	0.05000	3.0656×10^{-4}	1.96	0.13847
	0.00625	0.05000	7.8099×10^{-5}	1.97	0.27890
$\alpha = 1.5$	0.05000	0.05000	4.2697×10^{-3}	-	0.07582
	0.02500	0.05000	1.0944×10^{-3}	1.96	0.09496
	0.01250	0.05000	2.8215×10^{-4}	1.96	0.28431
	0.00625	0.05000	7.1846×10^{-5}	1.97	0.67017
$\alpha = 1.8$	0.05000	0.05000	3.4494×10^{-3}	-	0.04607
	0.02500	0.05000	9.1795×10^{-4}	1.91	0.13788
	0.01250	0.05000	2.4014×10^{-4}	1.93	0.19519
	0.00625	0.05000	6.1545×10^{-5}	1.96	0.45063



(a) Efficiency (b) Convergence

Figure 6.27: Log-log plots showing convergence and efficiency of FETD-RDP with FETD-CN and FETD-P(0,2) for the S-FBM (6.13)-(6.14)



(a) Efficiency (b) Convergence

Figure 6.28: Log-log plots showing convergence and efficiency of FETD-RDP with IMEX-BDF2 and IMEX-Adams2 for the for S-FBM (6.13)-(6.14)

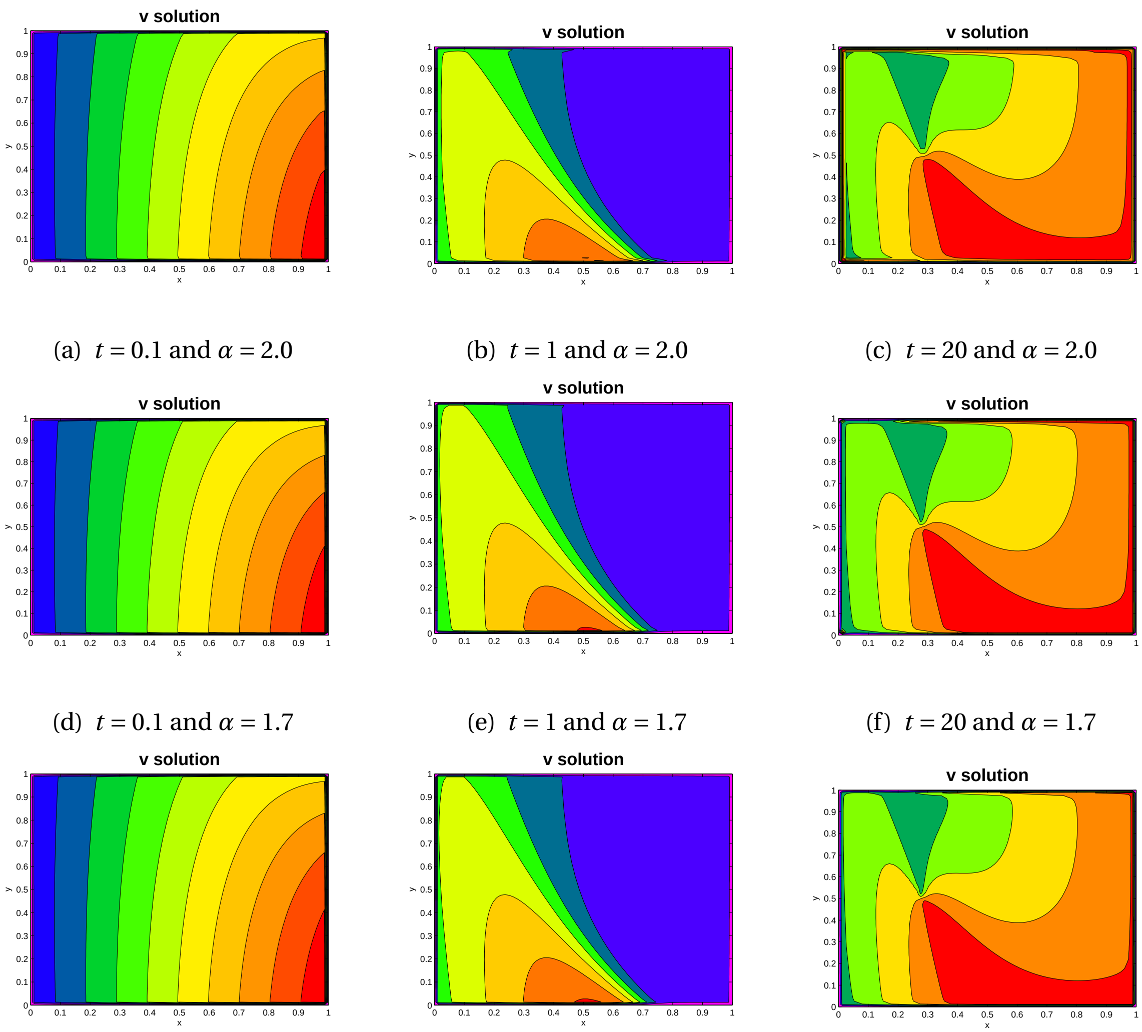
Remark 6.3.6.

1. Table 6.6 shows that the FETD-RDP scheme is second-order convergent by the grid refinement.

2. The FETD-RDP scheme is again computationally more efficient when compared with FETD-Pade(0,2), FETD-CN, BDF2, IMEX-BDF2 and IMEX-Adams second-order schemes, see Figures 6.27- 6.28.

The Turing Pattern Nature of Brusselator Model

As reported in the literature, see [52, 86], that the Brusselator system is used to model the Turing patterns, we exhibit this nature depending on the parameters chosen and the fractional order. For this purpose, we use the parameters $A = 1$, $B = 2.4$, $\zeta = \mathscr{K} = 10^{-5}$.

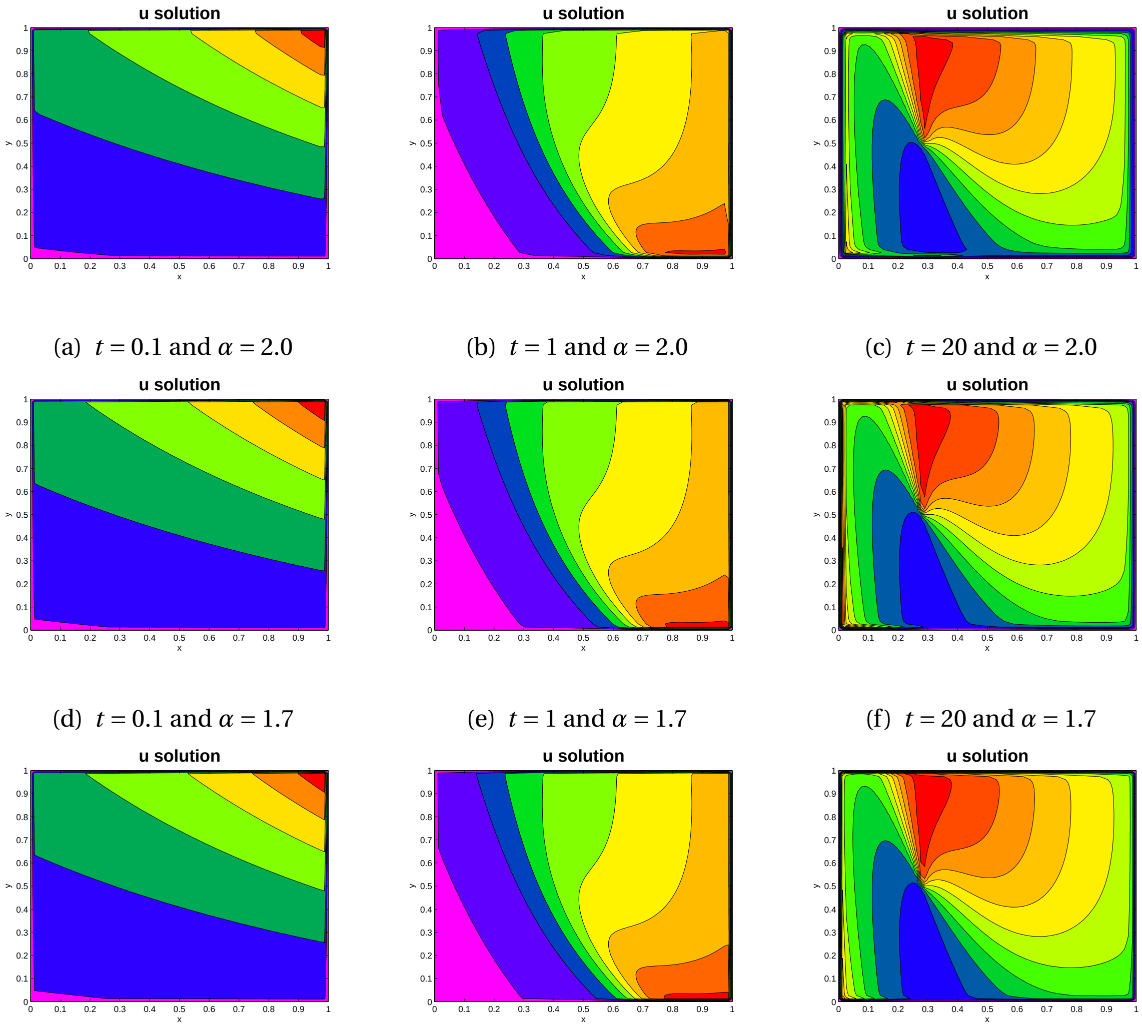


(a) $t = 0.1$ and $\alpha = 2.0$ (b) $t = 1$ and $\alpha = 2.0$ (c) $t = 20$ and $\alpha = 2.0$

(d) $t = 0.1$ and $\alpha = 1.7$ (e) $t = 1$ and $\alpha = 1.7$ (f) $t = 20$ and $\alpha = 1.7$

(g) $t = 0.1$ and $\alpha = 1.5$ (h) $t = 1$ and $\alpha = 1.5$ (i) $t = 20$ and $\alpha = 1.5$

Figure 6.29: V solutions profiles for the S-FBM (6.13)-(6.14) over a period of time for various values of α.



(a) $t = 0.1$ and $\alpha = 2.0$ (b) $t = 1$ and $\alpha = 2.0$ (c) $t = 20$ and $\alpha = 2.0$

(d) $t = 0.1$ and $\alpha = 1.7$ (e) $t = 1$ and $\alpha = 1.7$ (f) $t = 20$ and $\alpha = 1.7$

(g) $t = 0.1$ and $\alpha = 1.5$ (h) $t = 1$ and $\alpha = 1.5$ (i) $t = 20$ and $\alpha = 1.5$

Figure 6.30: U solutions profiles for the S-FBM (6.13)-(6.14) over a period of time for various values of α.

Remark 6.3.7.

We observe from Figure 6.29, that the Turing pattern is exhibited for all different values of α over a period of time.

6.3.4 The Fractional FitzHugh-Nagumo Model - Excitable Media

We consider the nonlinear two dimensional space fractional FitzHugh-Nagumo Model (S-FFNM) with homogeneous boundary conditions. The study of the excitable media is made possible using the FitzHugh Nagumo model see [35]. A cubic nonlinear reaction term is used to model the propagation of the transmembrane potential in the nerve axon. However, a single ordinary differential equation represents the recovery of the slow variable.

$$\frac{\partial u}{\partial t} = \lambda_1 \frac{\partial^\alpha u}{\partial |x|^\alpha} + \lambda_2 \frac{\partial^\alpha u}{\partial |y|^\alpha} + u(1-u)(u-a) - v,\ (x,y) \in (0,2.5)\times(0,2.5),\ t>0, \tag{6.15}$$

$$\frac{\partial v}{\partial t} = \varepsilon(\beta u - \gamma - \delta), \qquad (x,y) \in (0,2.5)\times(0,2.5),\ t>0, \tag{6.16}$$

subject to initial conditions given as

$$u(x,y,0) = \begin{cases} 1.0 & 0 < x \le 1.25,\ 0 < y < 1.25 \\ 0.0, & \text{otherwise} \end{cases}$$

and

$$v(x,y,0) = \begin{cases} 0.1 & 0 < x \le 2.5,\ 1.25 \le y < 2.5 \\ 0.0 & \text{otherwise,} \end{cases}$$

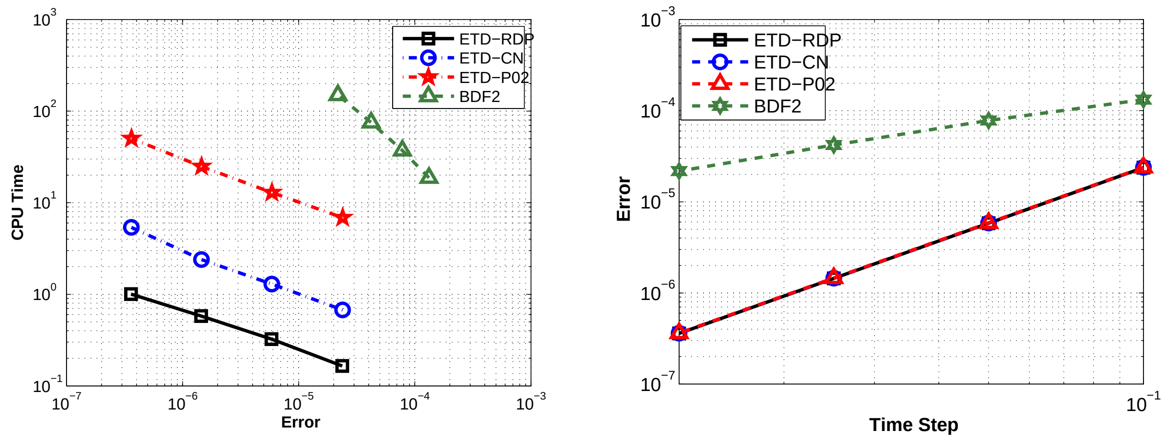
where the model parameters ε, β, γ, δ and a are constants and λ_1, λ_2 are the diffusion coefficients. This choice of initial conditions is such that the trivial state $(u,v) = (0,0)$ was perturbed by setting the lower-left quarter of the domain to $u = 1$ and the upper half part to $v = 0.1$. This allows the initial condition to curve and rotate clockwise generating the spiral pattern. This model has gained much popularity in terms of applications for many field of study. Such applications are in the study Ca^{+2} waves on Xenopus oocytes, the re-entry in heart tissue and Medaka eggs, see [20, 74, 83, 89, 99].

Comparison of RDP-FETD Scheme with other Second-order Schemes for S-FFNM

Here we choose $\varepsilon = 0.01$, $\beta = 0.5$, $\gamma = 1$, $\delta = 0$, $a = 0.1$, and $\lambda_1 = \lambda_2 = 10^{-4}$ for our computation using the FETD-RDP scheme with the fractional centered difference method.

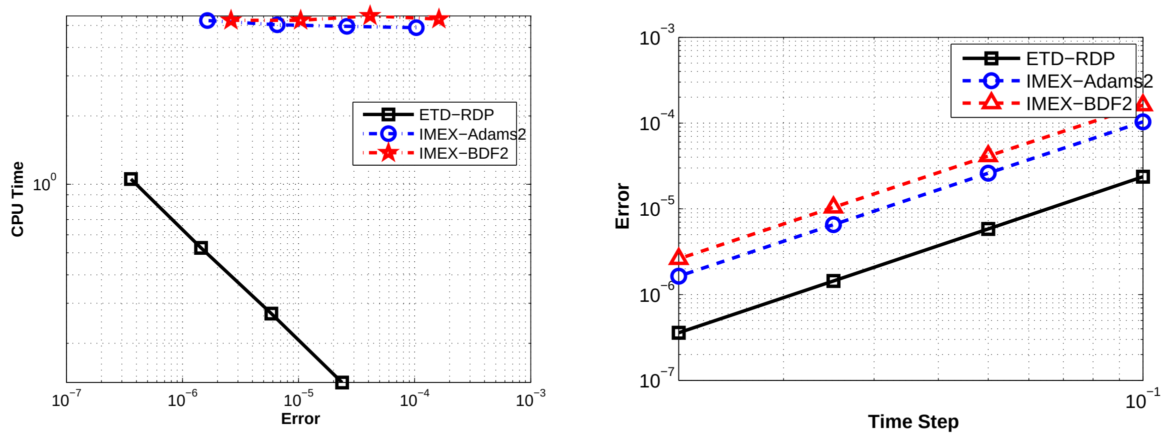
Table 6.7: Time rate of convergence of FETD-RDP for S-FFNM

	k	h	L_∞ Error	Rate	Time
$\alpha = 1.3$	0.1000	0.0250	2.3787×10^{-5}	-	0.13983
	0.0500	0.0250	5.8448×10^{-6}	2.02	0.34823
	0.0250	0.0250	1.4485×10^{-6}	2.01	0.69920
	0.0125	0.0250	3.6054×10^{-7}	2.01	1.34459
$\alpha = 1.5$	0.1000	0.0250	2.3704×10^{-5}	-	0.16468
	0.0500	0.0250	5.8246×10^{-6}	2.02	0.32439
	0.0250	0.0250	1.4435×10^{-6}	2.01	0.57872
	0.0125	0.0250	3.5930×10^{-7}	2.01	1.00632
$\alpha = 1.8$	0.1000	0.0250	2.3562×10^{-5}	-	0.14025
	0.0500	0.0250	5.7897×10^{-6}	2.02	0.26373
	0.0250	0.0250	1.4349×10^{-6}	2.01	0.56663
	0.0125	0.0250	3.5715×10^{-7}	2.01	1.08846



(a) Efficiency (b) Convergence

Figure 6.31: Log-log plots showing convergence and efficiency of FETD-RDP with FETD-CN, FETD-P(0,2) and BDF2 for the S-FFNM (6.15)-(6.16) with $\alpha = 1.5$



(a) Efficiency (b) Convergence

Figure 6.32: Log-log plots showing convergence and efficiency of FETD-RDP with IMEX-BDF2 and IMEX-Adams2 for the for S-FFNM (6.15)-(6.16) with $\alpha = 1.5$

Remark 6.3.8.

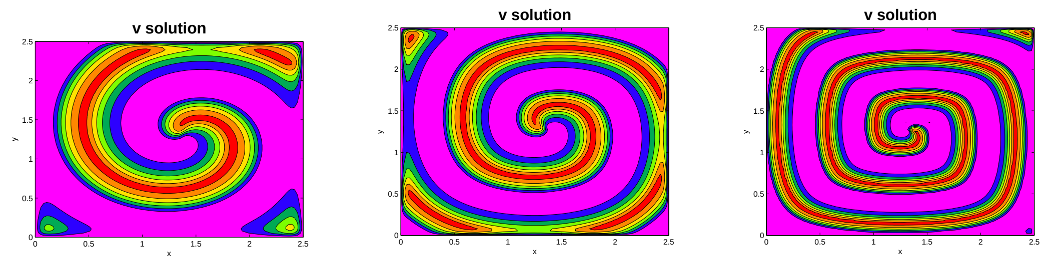
1. The second-order accuracy of the FETD-RDP is again demonstrated in Table 6.7.

2. The FETD-RDP scheme applied to S-FFNM, (6.15)-(6.16), is computationally more efficient compared to the FETD-CN, the FETD-P(0,2) without compromising accuracy.

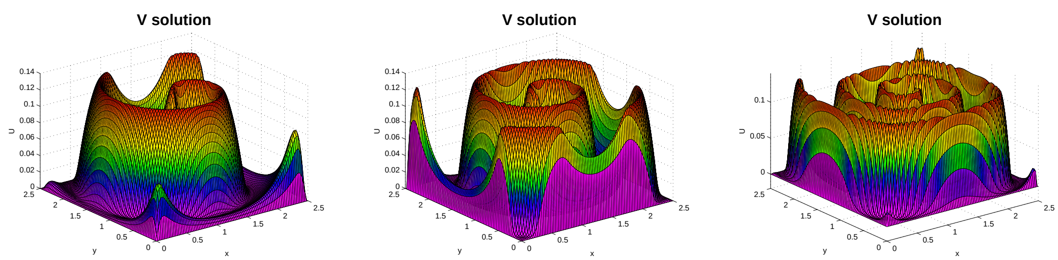
3. The same observation is seen when The FETD-RDP scheme is compared BDF2, IMEX-BDF2 and IMEX-Adams2 schemes both in accuracy and computational efficiency.

The Spiral Pattern Nature of The FitzHugh-Nagumo Model

FitzHugh-Nagumo Model has been observed to display spiral pattern for some choices of the parameter constants. Also, here we choose $\varepsilon = 0.01$, $\beta = 0.5$, $\gamma = 1$, $\delta = 0$, $a = 0.1$, and $\lambda_1 = \lambda_2 = 2 \times 10^{-4}$.

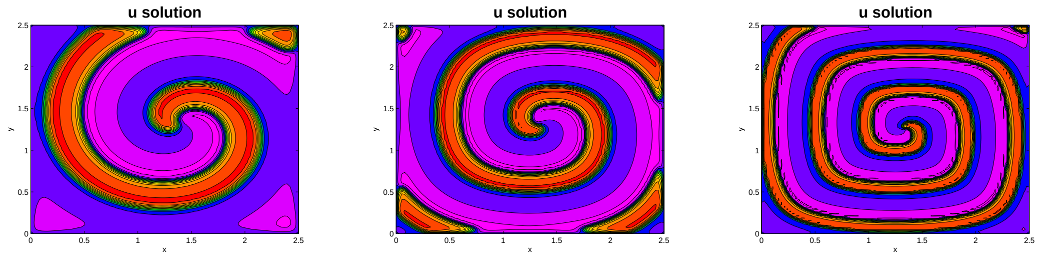


(a) $\alpha = 2.0$ (b) $\alpha = 1.8$ (c) $\alpha = 1.6$

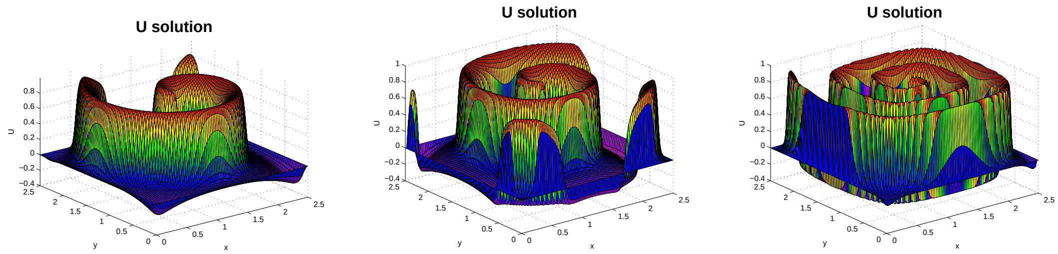


(d) $\alpha = 2.0$ (e) $\alpha = 1.8$ (f) $\alpha = 1.6$

Figure 6.33: Isotropic diffusion case: Spiral waves in V solutions profiles for the S-FFNM (6.15)-(6.16) with $t = 2500$.



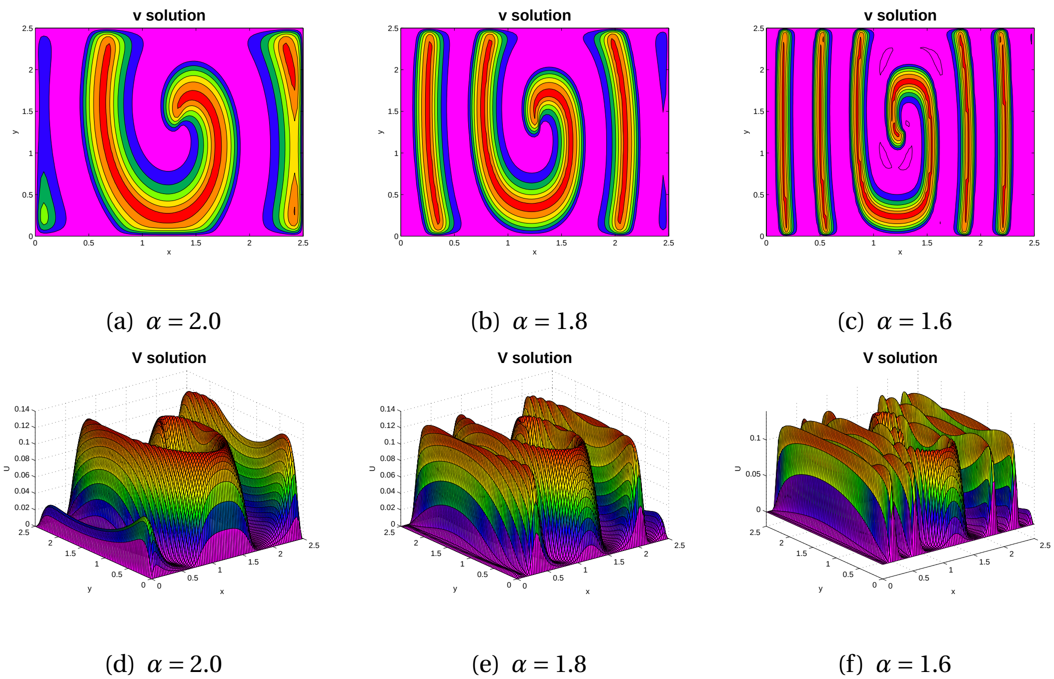
(a) $\alpha = 2.0$ (b) $\alpha = 1.8$ (c) $\alpha = 1.6$



(d) $\alpha = 2.0$ (e) $\alpha = 1.8$ (f) $\alpha = 1.6$

Figure 6.34: Isotropic diffusion case: Spiral waves in U solutions profiles for the S-FFNM (6.15)-(6.16) with $t = 2500$.

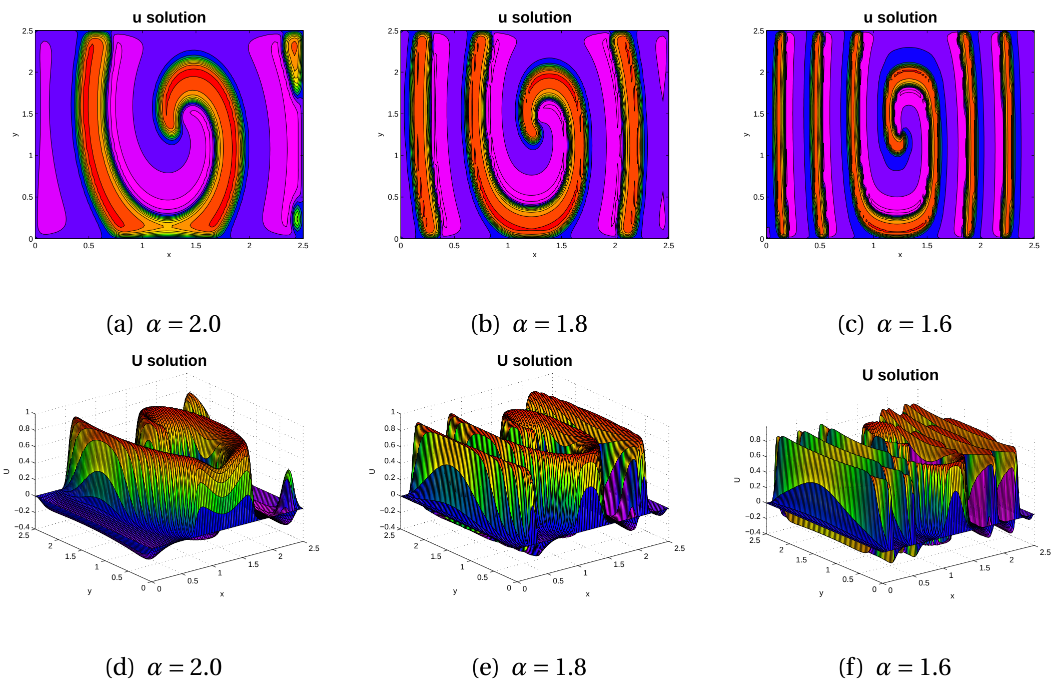
Considering different diffusion coefficients, we obtain different spiral pattern formations. This has been observed in []. We choose $\varepsilon = 0.01$, $\beta = 0.5$, $\gamma = 1$, $\delta = 0$, $a = 0.1$ using anisotropic diffusion ratios.



(a) $\alpha = 2.0$ (b) $\alpha = 1.8$ (c) $\alpha = 1.6$

(d) $\alpha = 2.0$ (e) $\alpha = 1.8$ (f) $\alpha = 1.6$

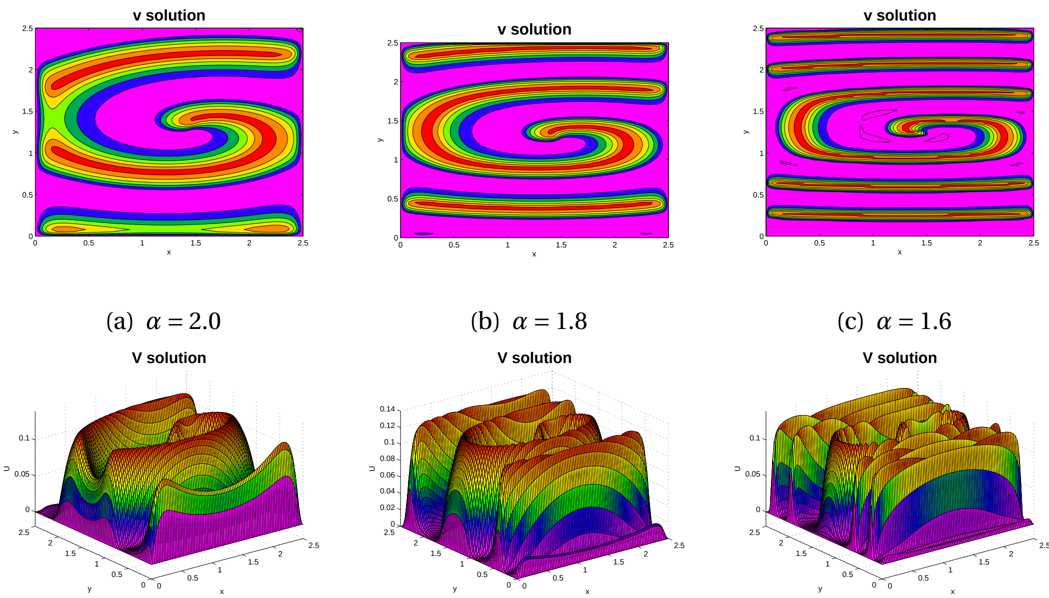
Figure 6.35: Anisotropic diffusion case: Spiral waves in V solutions profiles for the S-FFNM (6.15)-(6.16) with $t = 2500$, $\lambda_1 = 5 \times 10^{-5}$ and $\frac{\lambda_2}{\lambda_1} = 0.25 < 1$.



(a) $\alpha = 2.0$ (b) $\alpha = 1.8$ (c) $\alpha = 1.6$

(d) $\alpha = 2.0$ (e) $\alpha = 1.8$ (f) $\alpha = 1.6$

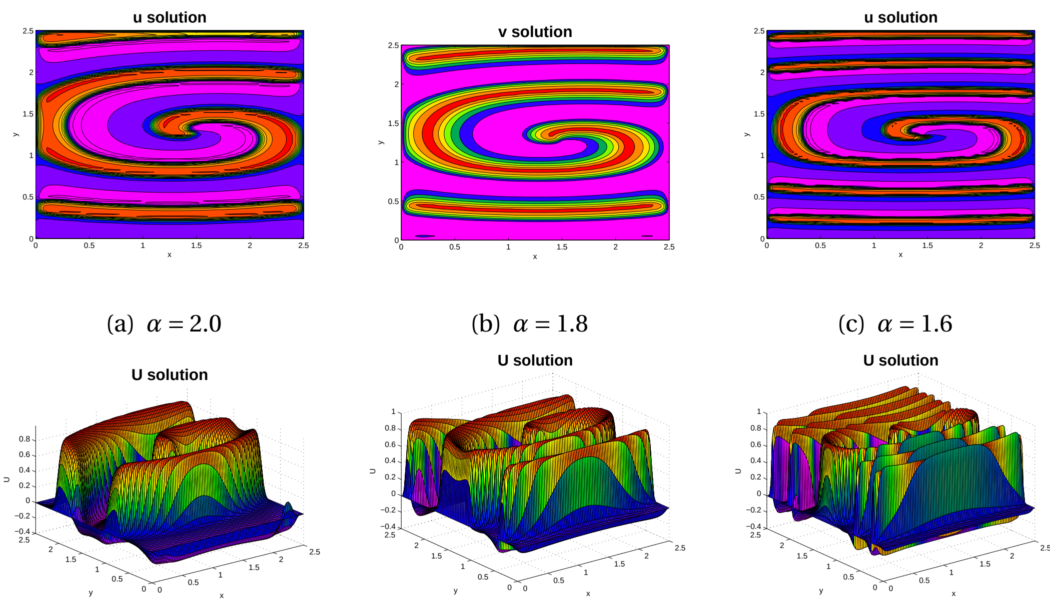
Figure 6.36: Anisotropic diffusion case: Spiral waves in U solutions profiles for the S-FFNM (6.15)-(6.16) with $t = 2500$, $\lambda_1 = 5 \times 10^{-5}$ and $\frac{\lambda_2}{\lambda_1} = 0.25 < 1$



(a) $\alpha = 2.0$ (b) $\alpha = 1.8$ (c) $\alpha = 1.6$

(d) $\alpha = 2.0$ (e) $\alpha = 1.8$ (f) $\alpha = 1.6$

Figure 6.37: Anisotropic diffusion case: Spiral waves in V solutions profiles for the S-FFNM (6.15)-(6.16) with $t = 2500$, $\lambda_2 = 5 \times 10^{-5}$ and $\frac{\lambda_1}{\lambda_2} = 0.25 < 1$.



(a) $\alpha = 2.0$ (b) $\alpha = 1.8$ (c) $\alpha = 1.6$

(d) $\alpha = 2.0$ (e) $\alpha = 1.8$ (f) $\alpha = 1.6$

Figure 6.38: Anisotropic diffusion case: Spiral waves in U solutions profiles for the S-FFNM (6.15)-(6.16) with $t = 2500$, $\lambda_2 = 5 \times 10^{-5}$ and $\frac{\lambda_1}{\lambda_2} = 0.25 < 1$

Remark 6.3.9.

1. Observe that in both the isotropic and anisotropic diffusion cases, the width of the excitation wavefront is reduced for decreasing fractional power α. The same for the wavelength of the system. This then allows the domain to accommodate a larger number of wavefronts for a smaller fractional power.

2. Also, when $\alpha = 2$, the spiral pattern is circular but the circular spiral pattern gradually becomes rectangular for reduced fractional order α.

3. When an anisotropic diffusion ratios $\frac{\lambda_2}{\lambda_1} = 0.25 < 1$ and $\frac{\lambda_1}{\lambda_2} = 0.25 < 1$ are considered, see Figures 6.35-6.38, the spiral wave follows an elliptical pattern. However, the have different orientations.

6.4 Centered Difference vs Matrix Transfer

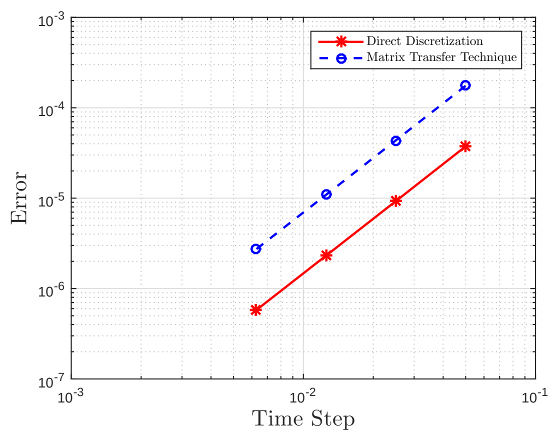
In this section, using the examples discussed above, we compare direct discretization of the Riesz space fractional derivative using fractional centered differencing with the matrix transfer technique discussed in the previous Chapter.

Centered Difference vs Matrix Transfer for the Enzyme Kinetic Model

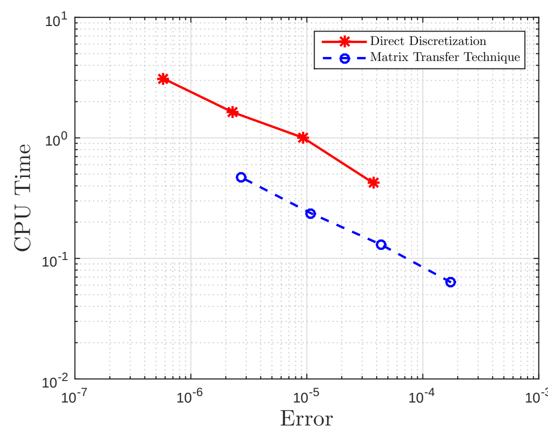
Through the fractional Enzyme kinetic Equation (S-FEK) above, we compare direct discretization of the Riesz space fractional derivative using fractional centered differencing with the matrix transfer technique discussed in section (2) with $\alpha = 1.6$, $\lambda = 0.001$.

		Centered Difference			Matrix Transfer Technique		
k	h	L_∞ Error	Rate	Time	L_∞ Error	Rate	Time
0.05000	0.0250	3.7408×10^{-5}	-	0.42248	1.7498×10^{-4}	-	0.06329
0.02500	0.0250	9.2612×10^{-6}	2.01	1.00467	4.3543×10^{-5}	2.01	0.13033
0.01250	0.0250	2.3041×10^{-6}	2.01	1.62988	1.0859×10^{-5}	2.00	0.23695
0.00625	0.0250	5.7462×10^{-7}	2.00	3.11806	2.7115×10^{-6}	2.00	0.47159

Table 6.8: Time rate of convergence of FETD-RDP for S-FEK with $\alpha = 1.6$, $\lambda = 0.001$



(a) Convergence



(b) Efficiency

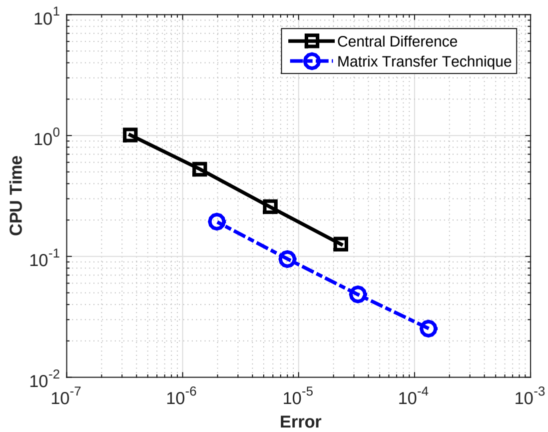
Figure 6.39: Log-log plots showing convergence and efficiency of FETD-RDP scheme comparing the fractional centered differencing and matrix transfer technique for S-FEK using $\alpha = 1.6$, $\lambda = 0.001$

Centered Difference vs Matrix Transfer for the FitzHugh-Nagumo Model

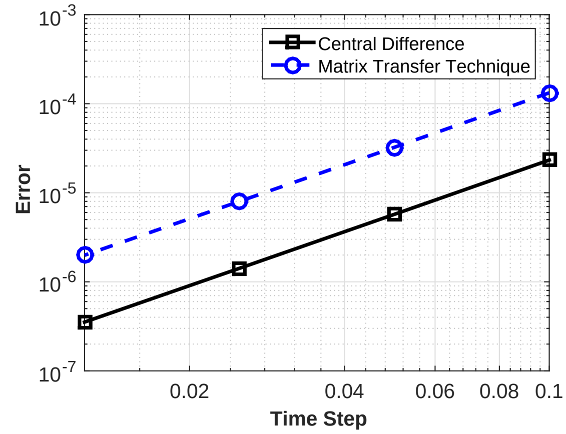
The merits of using a matrix transfer technique or a fractional centered differencing are examined for the system of space fractional FitzHugh-Nagumo model (S-FFNM) (6.15)-(6.16) with $\varepsilon = 0.01$, $a = 0.1$, $\beta = 0.5$, $\delta = 0$, $\gamma = 1$, and $\lambda_1 = \lambda_2 = 10^{-3}$.

Table 6.9: Time rate of convergence of FETD-RDP for S-FFNM with $t = 1$

	k	h	Centered Difference L_∞ Error	Rate	Time	Matrix Transfer Technique L_∞ Error	Rate	Time
$\alpha = 1.2$	0.1000	0.0250	2.3549×10^{-5}	-	0.12736	7.4332×10^{-5}	-	0.02513
	0.0500	0.0250	5.7872×10^{-6}	2.02	0.28040	1.7978×10^{-5}	2.05	0.04823
	0.0250	0.0250	1.4343×10^{-6}	2.01	0.61860	4.4214×10^{-6}	2.02	0.09588
	0.0125	0.0250	3.5702×10^{-7}	2.01	1.00418	1.0963×10^{-6}	2.01	0.18957
$\alpha = 1.4$	0.1000	0.0250	2.3295×10^{-5}	-	0.12579	1.3254×10^{-4}	-	0.02531
	0.0500	0.0250	5.7243×10^{-6}	2.02	0.25551	3.2378×10^{-5}	2.03	0.04842
	0.0250	0.0250	1.4187×10^{-6}	2.01	0.52547	8.0025×10^{-6}	2.02	0.09544
	0.0125	0.0250	3.5312×10^{-7}	2.01	1.01078	1.9893×10^{-6}	2.01	0.19255
$\alpha = 1.6$	0.1000	0.0250	2.3202×10^{-5}	-	0.12591	2.9512×10^{-4}	-	0.02504
	0.0500	0.0250	5.7002×10^{-6}	2.03	0.25399	7.3579×10^{-5}	2.00	0.04897
	0.0250	0.0250	1.4126×10^{-6}	2.01	0.49746	1.8375×10^{-5}	2.00	0.09428
	0.0125	0.0250	3.5159×10^{-7}	2.01	1.29404	4.5918×10^{-6}	2.00	0.18892
$\alpha = 1.8$	0.1000	0.0250	2.3660×10^{-5}	-	0.12604	6.0919×10^{-4}	-	0.02516
	0.0500	0.0250	5.8238×10^{-6}	2.02	0.25046	1.5542×10^{-4}	1.97	0.04879
	0.0250	0.0250	1.4447×10^{-6}	2.01	0.49733	3.9308×10^{-5}	1.98	0.09496
	0.0125	0.0250	3.5977×10^{-7}	2.01	0.99377	9.8878×10^{-6}	1.99	0.19052



(a) Efficiency



(b) Convergence

Figure 6.40: Log-log plots showing convergence and efficiency of FETD-RDP scheme comparing the centered differencing and matrix transfer technique for S-FFNM (6.15)-(6.16) with $\alpha = 1.6$

Centered Difference vs Matrix Transfer for the Schnakenberg Model

We examine the merits of using a matrix transfer technique or a fractional centered differencing for the system of space fractional Schnakenberg model (S-FSM) (6.9)-(6.10).

Table 6.10: Time rate of convergence of FETD-RDP for S-FSM (6.9)-(6.10) with $t = 1$ $a = 0.1305$, $b = 0.7695$, $\gamma = 1.5$, $\lambda_1 = \lambda_2 = 0.001$, and $d_1 = d_2 = 0.001$

			Centered Difference			Matrix Transfer Technique		
	k	h	L_∞ Error	Rate	Time	L_∞ Error	Rate	Time
$\alpha = 1.3$	0.1000	0.0250	5.3589×10^{-5}	-	0.24625	1.5989×10^{-3}	-	0.04052
	0.0500	0.0250	1.3293×10^{-5}	2.01	0.48398	4.0492×10^{-4}	1.98	0.08216
	0.0250	0.0250	3.3066×10^{-6}	2.01	0.98002	1.0163×10^{-4}	1.99	0.16416
	0.0125	0.0250	8.2431×10^{-7}	2.00	1.97822	2.5442×10^{-5}	2.00	0.32655
$\alpha = 1.5$	0.1000	0.0250	1.3059×10^{-4}	-	0.24426	2.3852×10^{-3}	-	0.04421
	0.0500	0.0250	3.3212×10^{-5}	1.98	0.49677	5.6399×10^{-4}	2.08	0.08108
	0.0250	0.0250	8.3703×10^{-6}	1.99	0.98015	1.3644×10^{-4}	2.05	0.16219
	0.0125	0.0250	2.1008×10^{-6}	1.99	1.96976	3.3505×10^{-5}	2.03	0.32798
$\alpha = 1.7$	0.1000	0.0250	1.7465×10^{-4}	-	0.44168	9.5076×10^{-3}	-	0.04223
	0.0500	0.0250	4.5045×10^{-5}	1.95	0.50186	2.3822×10^{-3}	2.00	0.08150
	0.0250	0.0250	1.1450×10^{-5}	1.98	0.98137	5.9731×10^{-4}	2.00	0.16338
	0.0125	0.0250	2.8872×10^{-6}	1.99	2.22876	1.4960×10^{-4}	2.00	0.32769

Centered Difference vs Matrix Transfer for the Grey-Scott Model

We examine the merits of using a matrix transfer technique or a fractional centered differencing for the system of space fractional Grey-Scott model (S-FGSM) (6.11)-(6.12).

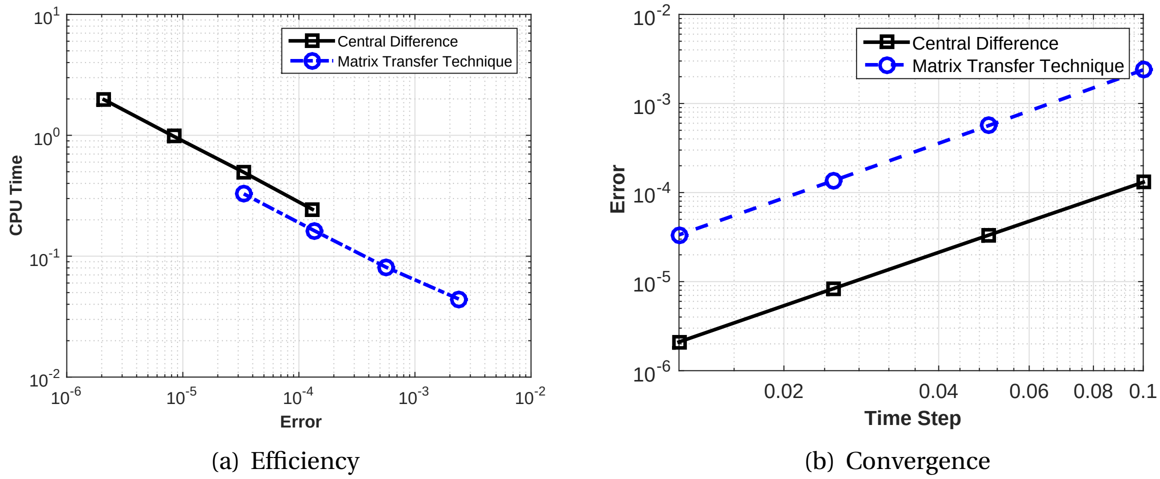
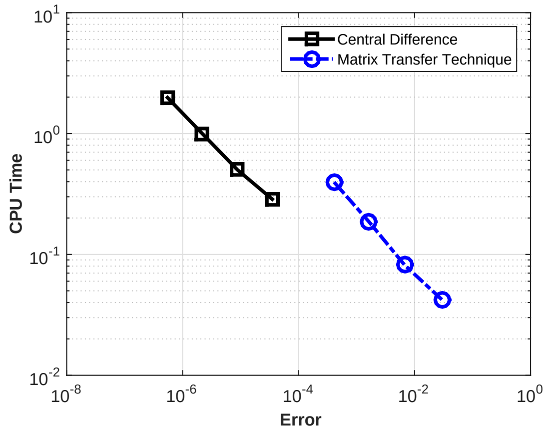


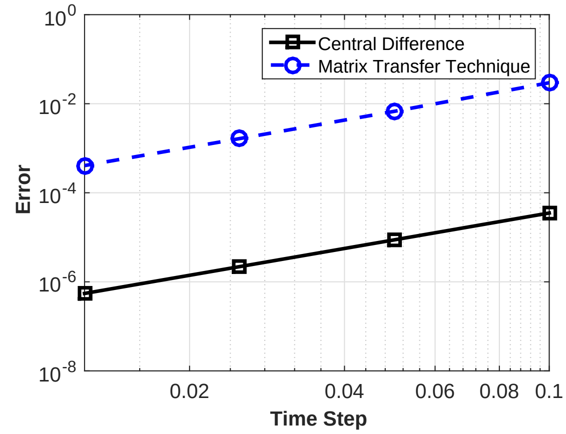
Figure 6.41: Log-log plots showing convergence and efficiency of FETD-RDP scheme comparing the fractional centered differencing and matrix transfer technique for S-FSM (6.9)-(6.10) with $t = 1$, $\alpha = 1.5$, $a = 0.1305$, $b = 0.7695$, $\gamma = 1.5$, $\lambda_1 = \lambda_2 = 0.001$, and $d_1 = d_2 = 0.001$

Table 6.11: Time rate of convergence of FETD-RDP for S-FGSM with $t = 1$, $\alpha = 1.5$, $F = 0.03$, $\kappa = 0.063$, and $\lambda_1 = \lambda_2 = d_1 = d_2 = 0.005$

			Centered Difference			Matrix Transfer Technique		
	k	h	L_∞ Error	Rate	Time	L_∞ Error	Rate	Time
$\alpha = 1.3$	0.1000	0.0250	3.3403×10^{-6}	-	0.24548	1.2382×10^{-2}	-	0.05082
	0.0500	0.0250	8.3802×10^{-7}	1.99	0.49113	3.0994×10^{-3}	2.00	0.08273
	0.0250	0.0250	2.0991×10^{-7}	2.00	0.98821	7.7586×10^{-4}	2.00	0.16217
	0.0125	0.0250	5.2532×10^{-8}	2.00	2.45318	1.9412×10^{-4}	2.00	0.33851
$\alpha = 1.5$	0.1000	0.0250	3.5112×10^{-5}	-	0.28624	2.9574×10^{-2}	-	0.04227
	0.0500	0.0250	8.7653×10^{-6}	2.00	0.50196	6.7515×10^{-3}	2.09	0.08159
	0.0250	0.0250	2.1913×10^{-6}	2.00	0.99604	1.6452×10^{-3}	2.03	0.18555
	0.0125	0.0250	5.4793×10^{-7}	2.00	1.98206	4.0805×10^{-4}	2.01	0.39644
$\alpha = 1.7$	0.1000	0.0250	8.5340×10^{-6}	-	0.24607	1.4084×10^{-4}	-	0.04329
	0.0500	0.0250	2.1215×10^{-6}	2.01	0.49175	3.5382×10^{-5}	1.97	0.08233
	0.0250	0.0250	5.2933×10^{-7}	2.00	0.97554	8.9432×10^{-5}	1.98	0.16487
	0.0125	0.0250	1.3224×10^{-7}	2.00	1.95107	2.2604×10^{-6}	1.98	0.32747



(a) Efficiency



(b) Convergence

Figure 6.42: Log-log plots showing convergence and efficiency of FETD-RDP scheme comparing the fractional centered differencing and matrix transfer technique for S-FGSM (6.11)-(6.12) with $t = 1$, $\alpha = 1.3$, $F = 0.03$, $\kappa = 0.063$, and $\lambda_1 = \lambda_2 = d_1 = d_2 = 0.005$

Remark 6.4.1.

1. The two methods (centered difference and matrix transfer technique) gave second-order convergence and are found to be effective in handling nonlinear space fractional reaction-diffusion with mismatched data for different values of α, see Tables 6.8-6.11.

2. The matrix transfer technique compares favourably over the centered difference approach in CPU time, see Tables 6.8-6.11. However, the centered difference approach compares favourably over the matrix transfer technique in terms of error produced, see Tables 6.8-6.11 and Figures 6.39-6.42.

3. It is therefore important to understand the trade-off in using any of these methods and based on the interest of the researcher.

Summary

The scheme proposed in this Chapter is shown to be second-order of convergence when applied to system of two-dimensional space-fractional reaction-diffusion models. The scheme is especially robust for problems with non-smooth/mismatched initial and boundary conditions. In terms of efficiency, the cpu time for our scheme compares favourably with second-order schemes such as FETD-CN, FETD-Padé(0,2), the BDF2, IMEX-BDF2 and IMEX-Adams2 schemes. The wider region of stability of our scheme allows for large time steps without losing stability of the solution. The algorithm could be easily implemented in parallel to take advantage of multiple processors for increased computational efficiency. Empirically, super-diffusion processes are displayed by investigating the effect of the fractional power of the underlying Laplacian operator on the pattern formation found in these models. Furthermore, we have discussed the trade-off between using fractional centered difference and matrix transfer technique in spatial discretization of Riesz fractional derivatives for different values of α.

Chapter 7

Rational Approximation of the Mittag-Leffler (M-L) Function and Its Inverse

7.1 Introduction

There have been many attempts to solve equations involving fractional derivatives both analytically and numerically. These include using the Laplace transform, Fourier transform and inverse Fourier transform, variational iteration method, homotopy analysis method, Adomian decomposition method, finite difference, finite element or finite volume discretisation of the fractional operator combined with a semi-implicit Euler formulation for the time evolution of the solution, exponential time differencing schemes and many others see [11, 33, 66, 67, 143–145, 147, 153]. Almost all these methods yield equations involving the (generalized) Mittag-Leffler functions. The role of the fundamental solution operator exponential function in the solution of integer-order differential equations is similar to the role of the generalized Mittag-Leffler functions in the solutions of fractional-order differential equations. In fact, the exponential function is a special case of the Mittag-Leffler type for a particular choice of the parameters. This has made Mittag-Leffler functions and their generalizations very important special functions and has drawn the attention of many researchers hoping to find efficient ways to numerically compute solutions. Recall from the earlier Section that the generalized Mittag-Leffler function (also called two-parameter Mittag-Leffler function) is defined as:

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k+\beta)}, \quad \beta, z \in \mathbb{C}, \quad \mathrm{Re}(\alpha) > 0. \tag{7.1}$$

A special case of this function, called a one-parameter Mittag-Leffler function, is given as:

$$E_{\alpha}(z) = E_{\alpha,1}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k+1)}, \quad z \in \mathbb{C}, \quad \mathrm{Re}(\alpha) > 0. \tag{7.2}$$

Straightforwardly, we see that this function represents many important special cases, such as:

$$\begin{aligned} E_{1,1}(z) &= e^z, & E_{1,2}(z) &= \frac{e^z-1}{z}, \\ E_{2,1}(z) &= \cosh(\sqrt{z}), & E_{2,2}(z) &= \frac{\sinh(\sqrt{z})}{\sqrt{z}}, \\ E_{2,1}(-z^2) &= \cos(z), & E_{0,1}(z) &= \frac{1}{1-z}, \quad |z|<1. \end{aligned}$$

We also recall that the generalized Mittag-Leffler function is an entire function [112], so bounded in any finite interval.

Lemma 7.1.1. *Let* $\beta, x \in \mathbb{R}$ *with* $0 < \beta \le 1$. *Then*

$$\frac{\Gamma(x)}{\Gamma(x+\beta)} \ge \frac{1}{x^\beta}. \tag{7.3}$$

Proof. Recall from the definition of the Gamma function that

$$\Gamma(x+\beta) = \int_0^\infty y^{x+\beta-1} e^{-y} dy,$$

and the Gamma identity holds:

$$\Gamma(x+1) = x\Gamma(x).$$

Let $0 < \beta < 1$. Define the following functions

$$f(y) := y^{\beta x} e^{-\beta y} \qquad \text{and} \qquad g(y) := y^{(1-\beta)x+\beta-1} e^{-(1-\beta)y}.$$

Let $p = \frac{1}{\beta}$ and $q = \frac{1}{1-\beta}$. Then we have

$$\frac{1}{p} + \frac{1}{q} = 1.$$

Hence, Hölder's inequality gives

$$\begin{aligned}
\Gamma(x+\beta) &= \int_0^\infty y^{x+\beta-1} e^{-y} dy \\
&= \int_0^\infty \left(y^{\beta x} e^{-\beta y}\right)\left(y^{(1-\beta)x+\beta-1} e^{-(1-\beta)y}\right) dy \\
&\le \left(\int_0^\infty f(y)^p\right)^{\frac{1}{p}} \left(\int_0^\infty g(y)^q\right)^{\frac{1}{q}} dy \\
&= \left(\int_0^\infty y^{\beta} e^{-y}\right)^{\beta} \left(\int_0^\infty y^{x-1} e^{-y}\right)^{1-\beta} dy \\
&= [\Gamma(x+1)]^{\beta} [\Gamma(x)]^{1-\beta} \\
&= [x\Gamma(x)]^{\beta} [\Gamma(x)]^{1-\beta} \\
&= x^{\beta}\Gamma(x).
\end{aligned}$$

That is

$$\frac{\Gamma(x)}{\Gamma(x+\beta)} \ge \frac{1}{x^{\beta}}, \qquad x \in \mathbb{R}, \quad 0 < \beta \le 1.$$

□

In [53], the computation of the generalized Mittag-Leffler function and its derivative are studied with $\alpha > 0$, $\beta \in \mathbb{R}$ and $z \in \mathbb{C}$. Later, an alternative seemingly simpler algorithm for computing the generalized Mittag-Leffler function was proposed in [63, 123]. This is based on mixed techniques such as asymptotic series, Taylor series, and integral representations. Subroutines for evaluating the generalized Mittag-Leffler function with any desired accuracy were provided in [46, 47, 110]. Numerical inversion of the Laplace transform of this function is instrumental in the development of these scripts.

A naive approach to evaluating the generalized Mittag-Leffler is by truncating the series representation of this function. Unfortunately, the convergence of the series can be very slow for arguments having moderate or large modulus, giving a huge amount of computation. Numerical cancellation could result, as well. One way out could be to use variable precision arithmetic [46]. Thus, a rational function approach such as a Padé approximation could be desirable and expected to be robust as far as accuracy and computationally efficient. The Padé approximations of the Mittag-Leffler function have been recently introduced in [126] on the compact set $\{|z| \leq 1\}$. In [91], upper and lower bounds for the Mittag-Leffler function with $t > 0$ are given using the Padé approximation. More works are done on this in [33] and a table of coefficients of the rational approximants to the M-L function for $0 < \alpha < 1$ is provided. On $[0.1, 15]$, these coefficients are calculated numerically to approximate the M-L function.

Furthermore, a global Padé approximation was previously proposed was used in [12] to construct a uniform rational approximation of the M-L function with $z > 0$ and $0 < \alpha < 1$ see also [4]. It is worth noting that most of these rational (Padé) approximations involve complex roots, which further slow down the computation. When solving multidimensional problems, it would be beneficial to utilize parallel techniques to speed up evolution. A good separation between the poles of the rational approximation is required, and most of the Padé approximations lack such property. It is therefore imperative to develop a real distinct pole rational approximation of M-L function to facilitate easy parallelization while ensuring computational accuracy and a relatively small error constant. This is the focus of the next section.

7.2 A Real Distinct Poles Rational Approximation of the Generalized Mittag-Leffler Functions

In this section, we develop a real distinct poles rational approximation (RDP) of the generalized Mittag-Leffler functions and prove some of the useful properties of this approximation which are applicable in solving fractional differential equations.

7.2.1 A Real Distinct Pole Rational Function

We seek to construct a rational function of the form [8, 9, 133]:

$$\mathscr{R}^*(z) = \frac{1+a_1 z}{(1-a_2 z)(1-a_3 z)}, \tag{7.4}$$

with $a_1, a_2, a_3 \in \mathbb{R}$, $a_2 \neq a_3$. This is not of Padé type.

Theorem 7.2.1. *Assume $a_1, a_2, a_3 \in \mathbb{R}$, $a_2 \neq a_3$ such that*

$$a_1 + a_2 + a_3 = \frac{\Gamma(\beta)}{\Gamma(\alpha+\beta)}, \quad a_3 - a_2 a_3 = \frac{\Gamma(\beta)}{\Gamma(2\alpha+\beta)} - \frac{\Gamma(\beta)}{\Gamma(\alpha+\beta)} a_2,$$

and $\mathscr{E}_{\alpha,\beta}(z) = \Gamma(\beta) E_{\alpha,\beta}(z)$. Then, $\mathscr{R}^*(z)$ is a second order approximation to $E_{\alpha,\beta}(z)$ i.e

$$\mathscr{R}^*(z) - \mathscr{E}_{\alpha,\beta}(z) = C z^3 + O\left(z^{p+2}\right), \quad as\ z \to 0,$$

with error constant

$$C = \left(\frac{\Gamma(\beta)}{\Gamma(\alpha+\beta)} - 1\right) a_3^2 + \left(\frac{\Gamma(\beta)}{\Gamma(2\alpha+\beta)} - 1\right) a_3 + \left(\frac{\Gamma(\beta)}{\Gamma(2\alpha+\beta)} - \frac{\Gamma(\beta)}{\Gamma(\alpha+\beta)}\right) a_2 + \frac{\Gamma(\beta)}{\Gamma(2\alpha+\beta)} - \frac{\Gamma(\beta)}{\Gamma(3\alpha+\beta)}.$$

Proof. We have from (7.1) that

$$\mathscr{E}_{\alpha,\beta}(z) = 1 + \frac{\Gamma(\beta)}{\Gamma(\alpha+\beta)} z + \frac{\Gamma(\beta)}{\Gamma(2\alpha+\beta)} z^2 + \frac{\Gamma(\beta)}{\Gamma(3\alpha+\beta)} z^3 + o(z^4). \tag{7.5}$$

Also, expanding the rational function, $\mathscr{R}^*(z)$, we obtain

$$\mathscr{R}^*(z) = 1 + (a_1 + a_2 + a_3)z + (a_3 + a_2(a_1 + a_2 + a_3) - a_2 a_3)z^2 + o(z^3). \tag{7.6}$$

Using the assumptions, the coefficients of z and z^2 clearly agree. In the expansion of $R(z)$ the coefficient of z^3 is calculated to be

$$\frac{\mathscr{R}^{*(3)}(0)}{3!} = a_1 a_2 a_3 + (a_2^2 + a_3^2)(a_1 + a_2 + a_3).$$

Hence, substituting the order equations and simplifying, the error constant is

$$\begin{aligned} C &= a_1 a_2 a_3 + (a_2^2 + a_3^2)(a_1 + a_2 + a_3) - \frac{\Gamma(\beta)}{\Gamma(3\alpha+\beta)} \\ &= a_1 \left(a_3 - \frac{\Gamma(\beta)}{\Gamma(2\alpha+\beta)} + \frac{\Gamma(\beta)}{\Gamma(\alpha+\beta)} a_2 \right) + \frac{\Gamma(\beta)}{\Gamma(\alpha+\beta)} (a_2^2 + a_3^2) - \frac{\Gamma(\beta)}{\Gamma(3\alpha+\beta)} \\ &= \left(\frac{\Gamma(\beta)}{\Gamma(\alpha+\beta)} - 1 \right) a_3^2 + \left(\frac{\Gamma(\beta)}{\Gamma(2\alpha+\beta)} - 1 \right) a_3 + \left(\frac{\Gamma(\beta)}{\Gamma(2\alpha+\beta)} - \frac{\Gamma(\beta)}{\Gamma(\alpha+\beta)} \right) a_2 \\ &\quad + \frac{\Gamma(\beta)}{\Gamma(2\alpha+\beta)} - \frac{\Gamma(\beta)}{\Gamma(3\alpha+\beta)}. \end{aligned}$$

□

Definition 7.2.2 (L-Acceptable)**.** A rational approximation $\mathscr{R}(z)$ of $\mathscr{E}_{\alpha,\beta}(z)$ is said to be A-acceptable, if $|\mathscr{R}(z)| < 1$ whenever $Re(z)$ is negative and L-acceptable if, in addition $|\mathscr{R}(z)| \to 0$ as $Re(z) \to -\infty$.

Lemma 7.2.3. *The rational approximation* (7.4) *is L-acceptable if* $a_2 > 0$ *and* $a_3 > 0$.

Proof. This follows from Maximum-Modulus principle. □

It is known that the smallest error constant, C, in Theorem (7.2.1) occurs when $a_2 = a_3$, [8, 9, 133], which is the case of repeated poles. Our aim is the construction of L-acceptable rational approximation to $E_{\alpha,\beta}(z)$, as oscillations are frequent in the methods arising from the A-acceptable diagonal Padé approximations. When such rational repeated pole approximations are used for the Mittag-Leffler function, $E_{\alpha,\beta}(z)$, it results in inherently serial algorithms. Alternatively, we construct the L-acceptable rational approximation:

$$\mathscr{R}(z) = \frac{1 + a_1 z}{\Gamma(\beta)(1 - a_2 z)(1 - a_3 z)}, \tag{7.7}$$

where

$$\begin{aligned} a_1 &= \frac{\Gamma(\beta)}{\Gamma(\alpha+\beta)} - a_2 - a_3, & (7.8)\\ a_2 &= \frac{\Gamma(\alpha+\beta)}{\Gamma(2\alpha+\beta)} - \frac{1}{4}, & (7.9)\\ a_3 &= \frac{\Gamma(\beta)\Gamma(2\alpha+\beta)}{\Gamma(\alpha+\beta)\left(5\Gamma(2\alpha+\beta) - 4\Gamma(\alpha+\beta)\right)}. & (7.10) \end{aligned}$$

Due to the fact that $\mathscr{R}(z)$ given above possesses real distinct poles, it admits a partial fraction expansion

$$\mathscr{R}(z) = \frac{a_1 + a_2}{\Gamma(\beta)(a_2 - a_3)(1 - a_2 z)} - \frac{a_1 + a_3}{\Gamma(\beta)(a_2 - a_3)(1 - a_3 z)}, \tag{7.11}$$

which permits the resulting algorithm to be implemented in a multiprocessor environment. We call this rational function the Real Distinct Poles (RDP) rational approximation of the Mittag-Leffler function, $E_{\alpha,\beta}(z)$.

Theorem 7.2.4. *Let* $0 < \alpha \le 1$, $\beta > 0$ *such that* $(\alpha+\beta)^\alpha < 4$, $\alpha + \beta \ge \frac{3}{2}$ *and* $\Gamma(\beta) \ge 1$. *Then the rational approximation* $\mathscr{R}(z)$ *given in* (7.7) *is L-acceptable.*

Proof. By Lemma (7.1.1) and $(\alpha+\beta)^\alpha < 4$, we have

$$a_2 = \frac{\Gamma(\alpha+\beta)}{\Gamma(2\alpha+\beta)} - \frac{1}{4} \quad \ge \quad \frac{1}{(\alpha+\beta)^\alpha} - \frac{1}{4} = \frac{4 - (\alpha+\beta)^\alpha}{4(\alpha+\beta)^\alpha} > 0.$$

Using the fact that Gamma function, Γ, is monotone increasing on $[1.5, +\infty)$ and that $\alpha + \beta \geq \frac{3}{2}$, we have that

$$\frac{\Gamma(\alpha+\beta)}{\Gamma(2\alpha+\beta)} < 1.$$

Hence, we obtain

$$\frac{5}{4} - \frac{\Gamma(\alpha+\beta)}{\Gamma(2\alpha+\beta)} > 0 \Longrightarrow 5\Gamma(2\alpha+\beta) - 4\Gamma(\alpha+\beta) > 0.$$

Therefore, $a_2 > 0$ and $a_3 > 0$. By Lemma (7.2.3) and the condition $\Gamma(\beta) \geq 1$, the proof is complete.

$\square$

We therefore obtain a real distinct pole rational approximation of the generalized Mittag-Leffler function

$$E_{\alpha,\beta}(-z) \approx \frac{1 - a_1 z}{\Gamma(\beta)(1 + a_2 z)(1 + a_3 z)}, \tag{7.12}$$

where a_1, a_2 and a_3 are given in (7.8), (7.9) and (7.10) respectively.

7.2.2 Special Cases

For a one parameter M-L function, which is usually encountered when solving a time fractional diffusion equation, our rational approximation reduces to:

$$E_{\alpha}(z) = E_{\alpha,1}(z) \approx \frac{1 + b_1 z}{(1 - b_2 z)(1 - b_3 z)}, \tag{7.13}$$

where

$$
\begin{aligned}
b_1 &= \frac{1}{\alpha\Gamma(\alpha)} - b_2 - b_3, && (7.14)\\
b_2 &= \frac{\Gamma(\alpha)}{2\Gamma(2\alpha)} - \frac{1}{4}, && (7.15)\\
b_3 &= \frac{\Gamma(2\alpha)}{\alpha\Gamma(\alpha)\,(5\Gamma(2\alpha) - 2\Gamma(\alpha))}. && (7.16)
\end{aligned}
$$

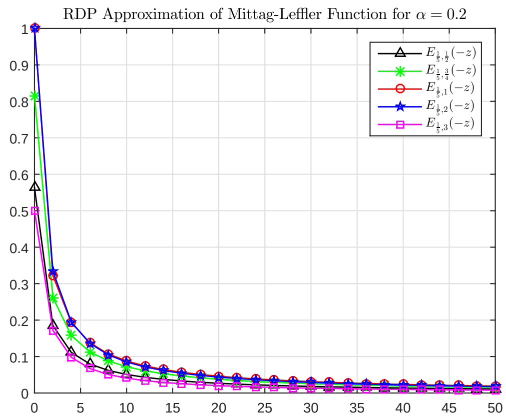
Also, we note that the M-L function considered here is a generalization of many important functions. For $\alpha = 1$,

$$a_2 = \frac{\Gamma(2)}{\Gamma(3)} - \frac{1}{4} = \frac{1}{4} \quad \text{and} \quad a_3 = \frac{\Gamma(3)}{\Gamma(2)(5\Gamma(3) - 4\Gamma(2))} = \frac{1}{3} \quad \text{and} \quad a_1 = \frac{1}{\Gamma(2)} - \frac{1}{3} - \frac{1}{4} = \frac{5}{12}.$$

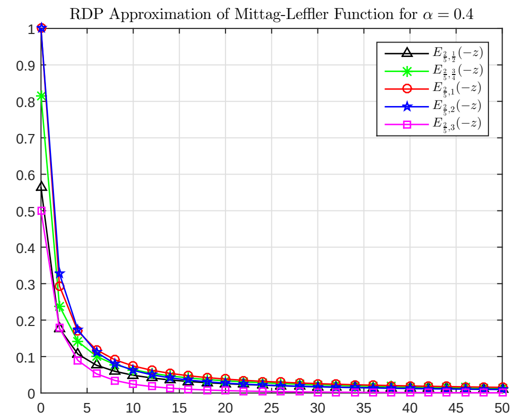
Thus we have as a special case,

$$e^z = E_{1,1}(z) \approx \frac{1 + \frac{5}{12}z}{(1 - \frac{1}{4}z)(1 - \frac{1}{3}z)}. \tag{7.17}$$

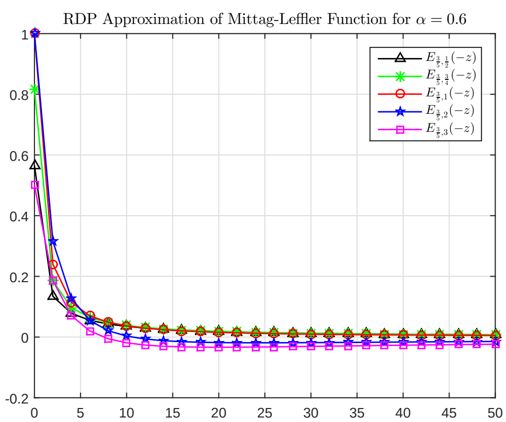
This corresponds to the rational approximation proposed in [8, 9] which has been very useful in developing an fractional exponential time differencing scheme for the solution of fractional reaction-diffusion equations. The FETD scheme developed using (7.17) in [9] was established to be stable, second order convergent and demonstrated to be robust for problems (integer-order) involving non-smooth initial and boundary conditions and steep solution gradients. These choices of coefficients are proven to give an error constant of $0.041\bar{6}$ which is near optimal in [8, 9, 133].



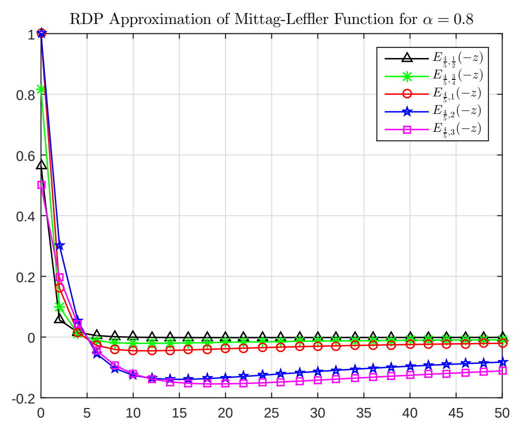
(a) $\alpha = 0.2$



(b) $\alpha = 0.4$



(c) $\alpha = 0.6$



(d) $\alpha = 0.8$

Figure 7.1: Empirical display of the L-acceptablity of RDP approximation of ML-fuction for different values of α and β.

7.3 Inverse Generalized Mittag-Leffler Function

In this section we introduce some notions useful to deal with the inverse generalized Mittag-Leffler function given in [63] and give the appropriate rational approximation on a suitable domain. The inverse Mittag-Leffler function $E^{-1}_{\alpha,\beta}(z)$ as the operator such that

$$E^{-1}_{\alpha,\beta}\left[E_{\alpha,\beta}(z)\right] = z. \tag{7.18}$$

In [63], the principal branch for the inverse M-L function in the complex plane is given satisfying the following conditions:

1. The function $E^{-1}_{\alpha,\beta}(z)$ is single valued and well defined on its principal branch.

2. Its principal branch reduces to the principal branch of the logarithm for $\alpha \longrightarrow 1$.

3. Its principal branch is a simply connected subset of the complex plane.

In order to be able to deal with the inverse Mittag-Leffler function, the following definition is essential.

Definition 7.3.1. A real function h defined on the interval I is completely monotone if it has derivatives of all orders on I and

$$(-1)^n h^{(n)}(t) \geq 0, \tag{7.19}$$

for all $t \in I$ and $n = 0, 1, 2, \cdots$.

In [111], it was shown that the Mittag-Leffler function $E_\alpha(-z)$ is completely monotone for all $z \geq 0$ if $0 \leq \alpha \leq 1$. Furthermore, in [121], using Hankel contour integration and corresponding probability measures, it was shown that the generalized Mittag-Leffler function $E_{\alpha,\beta}(-z)$ is completely monotone for all $z \geq 0$ if and only if $0 < \alpha \leq 1$ and $\beta \geq \alpha$. That is

$$(-1)^n \frac{d^n}{dz^n} E_{\alpha,\beta}(-z) \geq 0, \tag{7.20}$$

for all $z \in I$ and $n = 0, 1, 2, \cdots$ if and only if $0 < \alpha \leq 1$ and $\beta \geq \alpha$.

7.3.1 Rational Approximation of the Inverse Generalized M-L Function

Using the fact that the generalized Mittag- Leffler function $E_{\alpha,\beta}(-z)$ is completely monotone for all $z \in [0, \infty)$, we can conclude that it is a continuous and decreasing function on $[0, \infty)$. Hence, the corresponding inverse generalized Mittag-Leffler function $-E^{-1}_{\alpha,\beta}(z)$ is well defined on the interval $(0, \frac{1}{\Gamma(\beta)}]$ since we know by definition that $E_{\alpha,\beta}(0) = \frac{1}{\Gamma(\beta)}$. A global rational approximation of the inverse Mittag-Leffler function $-E_{\alpha}^{-1}(z)$ for all $z \in (0,1]$, $0 < \alpha < 1$ was given in [12]. Also, a global Padé approximation of the inverse generalized Mittag-Leffler function for some particular values of α and β appears in [148].

The simple nature of the proposed real distinct pole rational approximation of the generalized Mittag-Leffler function given in (7.7) makes it easy to derive its inverse. We rearrange (7.12) and solve the resulting quadratic equation to obtain a rational approximation of the inverse generalized Mittag-leffler function corresponding to $E_{\alpha,\beta}(-z)$ as:

$$-E_{\alpha,\beta}^{-1}(z) \approx \frac{\varepsilon_4}{z} + \varepsilon_3 - \sqrt{\frac{\varepsilon_1}{z} - \varepsilon_2 + \left(\varepsilon_3 + \frac{\varepsilon_4}{z}\right)^2}, \tag{7.21}$$

where

$$\varepsilon_1 = \frac{1}{a_2 a_3 \Gamma(\beta)}, \qquad \varepsilon_2 = \frac{1}{a_2 a_3}, \qquad \varepsilon_3 = \frac{a_2 + a_3}{2 a_2 a_3}, \qquad \varepsilon_4 = \frac{a_1}{a_2 a_3 \Gamma(\beta)},$$

and a_1, a_2, a_3 are given in (7.8), (7.9) and (7.10) respectively with $-E_{\alpha,\beta}^{-1}(z)|_{z\to 0^+} = +\infty$ and $-E_{\alpha,\beta}^{-1}(z)|_{z\to\frac{1}{\Gamma(\beta)}} = 0$.

7.4 Applications of the RDP Approximation of M-L Functions

We present some of the natural consequences of these approximations to the Mittag-Leffler function. In the cases where there are closed form solutions, we directly compare the RDP approximation. Otherwise, we make use of commonly used subroutines for evaluating the generalized Mittag-Leffler function with desired accuracy provided in [46, 47, 110] (*mlf*).

7.4.1 Application 1: The Complementary Error Function

For $\alpha = \frac{1}{2}$ and $\beta = 1$, we have a closed form representation as:

$$E_{\frac{1}{2},1}(-z) = \exp(z^2)erfc(z), \ z \geq 0, \tag{7.22}$$

where $erfc(z)$ is the complementary error function. Using RDP approximation for $E_{\frac{1}{2},1}(-z)$, we compare the result with the closed form (7.22) in Figure 7.2.

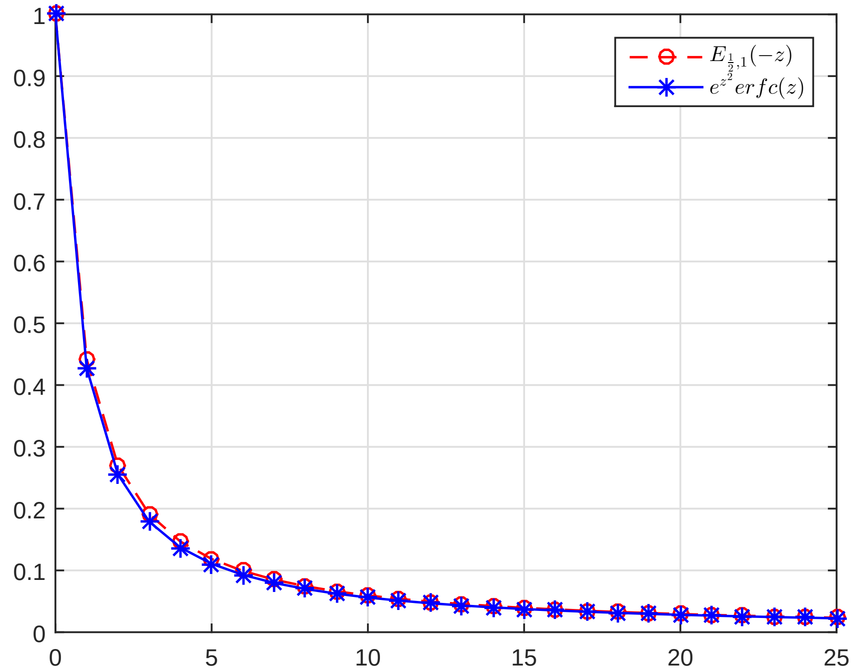


Figure 7.2: RDP Approximation of $e^{z^2}erfc(z)$ with $E_{\frac{1}{2},1}(-z)$ for $z \in [0, 25]$.

7.4.2 Application 2: Solution of Scalar Linear Fractional Differential Equations

We apply our proposed RDP approximation to the following scalar linear fractional differential equations:

1. Consider

$$ {}^{r}\mathscr{D}_t^{\alpha} u(t) + \sigma u(t) = 0, \quad t \geq 0, \tag{7.23} $$

with initial condition

$$ I^{\alpha} u(t)|_{t=0} = \kappa_1, $$

where $0 < \alpha \leq 1$, $\sigma > 0$, κ_1 is some constant, ${}^{r}\mathscr{D}_t^{\alpha}$ and I^{α} are, respectively, the Riemann-Liouville fractional derivative and integral of order α [78, 109]. Applying a Laplace transform to (7.23) and using the initial condition given, it is easy to obtain the analytical solution

$$ u(t) = \kappa_1 t^{-\alpha} E_{\alpha,\alpha}(-\sigma t^{\alpha}). \tag{7.24} $$

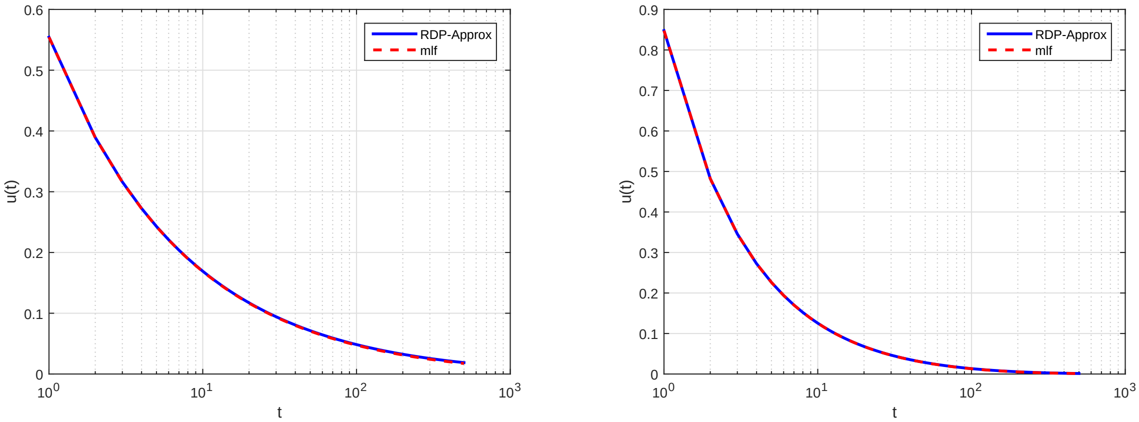
We can see that as simple as this equation seems to be, the solution is given in the form of the ML-function and computing it could be very involved when dealing with large arguments. The RDP rational approximation of the solution is given as:

$$ u(t) = \frac{\kappa_1 (1 - \lambda_1 \sigma t^{\alpha})}{\Gamma(\alpha) t^{\alpha} (1 + \lambda_2 \sigma t^{\alpha})(1 + \lambda_3 \sigma t^{\alpha})}, \tag{7.25} $$

where

$$ \lambda_1 = \frac{\Gamma(\alpha)}{\Gamma(2\alpha)} - \lambda_2 - \lambda_3, \; \lambda_2 = \frac{\Gamma(\alpha)}{\Gamma(3\alpha)} - \frac{1}{4}, \; \lambda_3 = \frac{\Gamma(\alpha)\Gamma(3\alpha)}{\Gamma(2\alpha)\,[5\Gamma(3\alpha) - 4\Gamma(2\alpha)]}. $$

The comparison between the RDP approximation (7.25) with the subroutine *mlf* is presented in Figure 7.3.



(a) $\alpha = 0.5$, $\sigma = 0.01$ and $\kappa = 1$.

(b) $\alpha = 0.8$, $\sigma = 0.01$ and $\kappa = 1$.

Figure 7.3: RDP approximation vs *mlf* of the solution (7.27).

2. Consider

$$ {}^{r}\mathscr{D}_t^{\alpha} u(t) + {}^{r}\mathscr{D}_t^{\beta} u(t) = \delta(t), \quad t \geq 0, \tag{7.26}$$

with initial condition

$$\left[I^{\alpha} u(t) + I^{\beta} u(t) \right] |_{t=0} = \kappa_2,$$

where $0 < \alpha < \beta \leq 1$, κ_2 is some constant. The analytical solution is given as, [148],

$$u(t) = (\kappa_2 + 1)\, t^{\beta-1} E_{\beta-\alpha,\beta}(-t^{\beta-\alpha}). \tag{7.27}$$

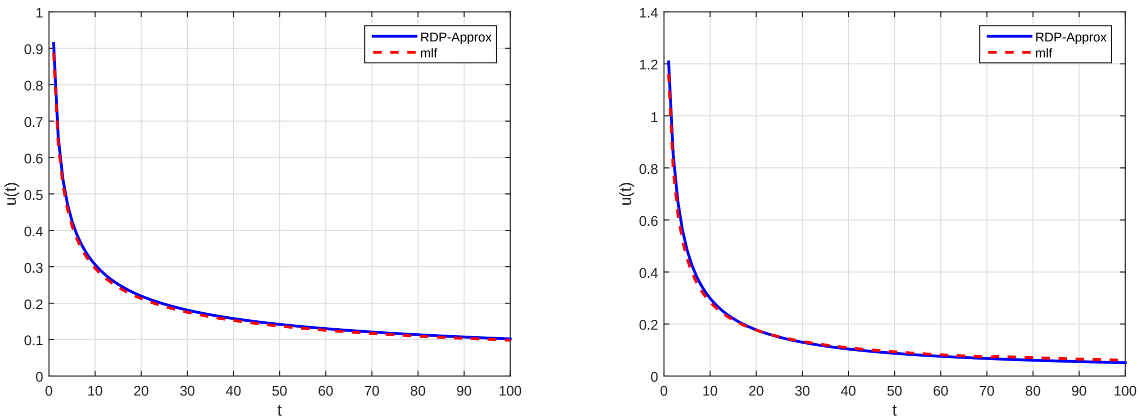
The RDP rational approximation of the solution is given as:

$$u(t) = \frac{\gamma\left(t^{\beta-1} - \zeta_1 t^{2\beta-\alpha}\right)}{(1+\zeta_2 t^{\beta-\alpha})(1+\zeta_3 t^{\beta-\alpha})}, \tag{7.28}$$

where $\gamma = \frac{\kappa_2+1}{\Gamma(\beta)}$ and

$$\zeta_1 = \frac{\Gamma(\beta)}{\Gamma(2\beta-\alpha)} - \zeta_2 - \zeta_3,\ \zeta_2 = \frac{\Gamma(2\beta-\alpha)}{\Gamma(3\beta-2\alpha)} - \frac{1}{4},\ \zeta_3 = \frac{\Gamma(\beta)\Gamma(3\beta-2\alpha)}{\Gamma(2\beta-\alpha)\left[5\Gamma(3\beta-2\alpha) - 4\Gamma(2\beta-\alpha)\right]}.$$

The comparison between the RDP approximation (7.28) with the subroutine *mlf* is presented in Figure 7.4.



(a) $\alpha = 0.5$, $\beta = 0.55$ and $\kappa = 2$.

(b) $\alpha = 0.35$, $\beta = 0.95$ and $\kappa = 2$.

Figure 7.4: RDP approximation vs *mlf* of the solution (7.27).

7.4.3 Application 3: Solution of the Space-Time Diffusion Equations

Consider the following space-time fractional diffusion problem, for which the analytical solution in the form of a Mittag-Leffler function is known.

$$\frac{\partial^{\alpha} u(x,t)}{\partial t^{\alpha}} = \frac{\partial^{\beta} u(x,t)}{\partial |x|^{\beta}}, \ 0 < x < \pi, \ 0 \leq t \leq 1, \tag{7.29}$$

with initial and boundary conditions

$$u(x,0) = x^4(\pi - x)^4, \ 0 \leq x \leq \pi,$$

$$u(0,t) = u(\pi,t) = 0, \ 0 \leq t \leq 1.$$

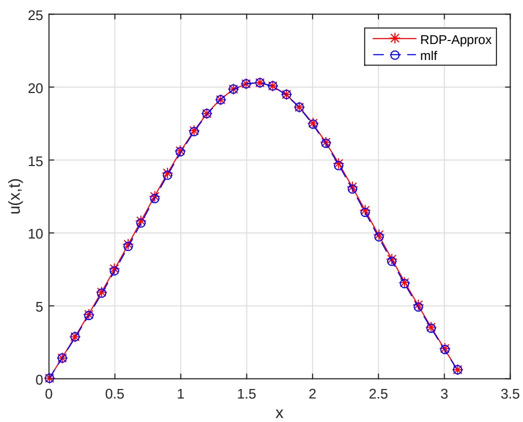
The analytical solution is given as, [34, 145],

$$u(x,t) = \sum_{k=1}^{\infty} \frac{48(1-(-1)^k)(\pi^4 k^4 - 180\pi^2 k^2 + 1680)}{\pi k^9} E_{\alpha,1}(-k^{\beta} t^{\alpha}) \sin(kx). \tag{7.30}$$

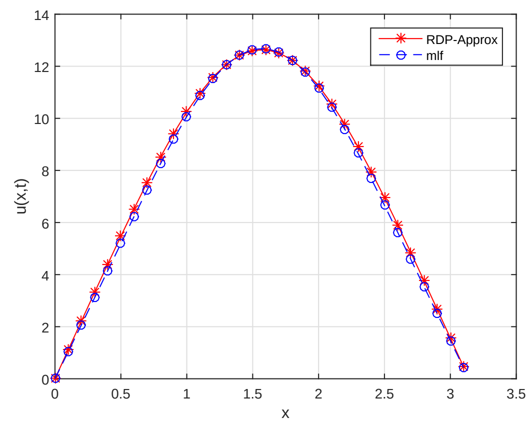
Observe that the solution involves a ML-function which is itself an infinite series, therefore giving a challenging computation. We apply the RDP rational function for the approximation of the ML-function and obtain:

$$u(x,t)=\sum_{k=1}^{\infty}\frac{48(1-(-1)^k)(\pi^4k^4-180\pi^2k^2+1680)(1-b_1k^{\beta}t^{\alpha})\sin(kx)}{\pi k^9(1+b_2k^{\beta}t^{\alpha})(1+b_3k^{\beta}t^{\alpha})}, \tag{7.31}$$

where b_1, b_2, b_3 are given in (7.14), (7.15) and (7.16) respectively. The approximation (7.31) is compared with *mlf*. Clearly from Figure 7.5-7.6, there is a good match.

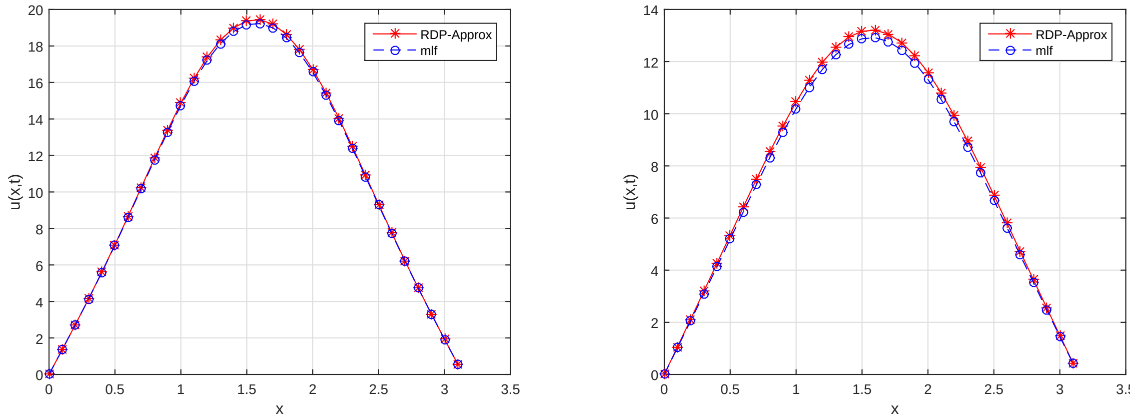


(a) $\alpha = 0.65$, $\beta = 1.9$ and $t = 0.2$.



(b) $\alpha = 0.65$, $\beta = 1.9$ and $t = 0.8$.

Figure 7.5: RDP approximation vs *mlf* of the solution (7.30) with $N = 20$, $\alpha = 0.65$, $\beta = 1.9$ for different values of t.



(a) $\alpha = 0.65$, $\beta = 1.9$ and $t = 0.2$.

(b) $\alpha = 0.65$, $\beta = 1.9$ and $t = 0.8$.

Figure 7.6: RDP approximation vs *mlf* of the solution (7.30) with $N = 20$, $\alpha = 0.55$, $\beta = 1.95$ for different values of t.

7.5 Applications of the RDP Approximation of The Inverse M-L Functions

In this section, we explore some applications of the inverses of generalized Mittag-Leffler functions and use the proposed rational approximation for its evaluation. It should be noted that as the Mittag-Leffler function is a generalization of the exponential function, so is the inverse Mittag-Leffler function is a generalization of the logarithm function for $\alpha = \beta = 1$.

7.5.1 Ultraslow Diffusion Model Using Structural Derivative Equations

It is well-known that some anomalous diffusion (sub-diffusion) models experience slow diffusion for which a fractional derivative in term of order $0 < \alpha < 1$ is used. Many laboratory experiments and observations have indicated ultraslow diffusion. This kind of diffusion is observed to behave completely differently from the standard anomalous diffusion. Researchers have ultilized in using the logarithmic diffusion model to describe the ultraslow diffusion but with very little outcome. Extensive work was done in [25], where the inverse Mittag-Leffler function was used as the structural function in modeling ultraslow diffusion of a random system of two interacting particles.

For a structural derivative modeling ultraslow diffusion, the probability of finding a diffusion particle at position x at time t is the solution to a diffusion equation

$$\frac{Sp(x,t)}{St} = D_\alpha \frac{\partial^2 p(x,t)}{\partial x^2}, \qquad x \in \mathbb{R}, \ \ t > 0, \tag{7.32}$$

where D_α is the generalized diffusion coefficient $(\frac{m^2}{s^\alpha})$. The corresponding structural derivative in time, using the inverse Mittag-Leffler function, is defined as:

$$\frac{Sp(x,t)}{St} = \lim_{t^* \to t} \frac{p(x,t^*) - p(x,t)}{E_{\alpha,1}^{-1}(t^*) - E_{\alpha,1}^{-1}(t)}. \tag{7.33}$$

Solving (7.33), using the kernel transform $\hat{t} = E_{\alpha,1}^{-1}(t)$, a Gaussian distribution is obtained as:

$$p(x,\hat{t}) = \frac{1}{\sqrt{4\pi D_\alpha \hat{t}}} e^{-\frac{x^2}{4D_\alpha \hat{t}}}. \tag{7.34}$$

The mean squared displacement of the ultraslow diffusion particle $x(t)$ and the characteristic function of $p(x,t)$ can be obtained from (7.34) respectively as

$$\langle x^2(t) \rangle = 2D_\alpha E_{\alpha,1}^{-1}(t), \tag{7.35}$$

$$p(x,q) = e^{-4D_\alpha q^2 E_{\alpha,1}^{-1}(t)}, \tag{7.36}$$

where q is the spatial frequency (wave number). In [25], a generalized mean squared displacement of the ultraslow diffusion particle $x(t)$ was proposed to contain classical Sinai anomalous diffusion law and its generalization (see [124, 125]) as:

$$\langle x^2(t) \rangle = 2D_\alpha \left[E_{\alpha,1}^{-1}(1+t) \right]^b, \qquad b > 0. \tag{7.37}$$

Note that this diffusion process describes a ballistic motion when $b > 4$, see [125].

When $\beta = 1$, we have the rational approximation of the inverse Mittag-Leffler function given as

$$E_\alpha^{-1}(z) \approx \omega_1 + \frac{\omega_2}{z} - \sqrt{\frac{\omega_3}{z} - \omega_3 + \left(\omega_1 + \frac{\omega_2}{z}\right)^2}, \tag{7.38}$$

where

$$\omega_1 = \frac{b_2 + b_3}{2b_2 b_3}, \qquad \omega_2 = \frac{b_1}{2b_2 b_3}, \qquad \omega_3 = \frac{1}{b_2 b_3},$$

and b_1, b_2, b_3 are given in (7.14), (7.15) and (7.16) respectively with $E_\alpha^{-1}(z)|_{z\to 0^+} = +\infty$ and $E_\alpha^{-1}(z)|_{z\to 1} = 0$. Using our proposed rational approximation to the inverse Mittag-Leffler function, $E_{\alpha,1}^{-1}(t)$ in (7.38), we obtain the generalized mean squared displacement of the ultraslow diffusion particle $x(t)$ and the characteristic function of $p(x,t)$ as

$$\begin{aligned} \langle x^2(t)\rangle &= 2D_\alpha\left(\omega_1 + \frac{\omega_2}{1+t} - \sqrt{\frac{\omega_3}{1+t} - \omega_3 + \left(\omega_1 + \frac{\omega_2}{1+t}\right)^2}\right)^b, & (7.39)\\ p(x,q) &= \exp\left\{-4D_\alpha q^2\left(\omega_1 + \frac{\omega_2}{t} - \sqrt{\frac{\omega_3}{t} - \omega_3 + \left(\omega_1 + \frac{\omega_2}{t}\right)^2}\right)\right\}, & (7.40)\end{aligned}$$

which is easily computed and does not involve truncation issues.

7.6 Generalized Exponential Time Discretization Scheme

In this section, we introduce the generalized exponential time discretization scheme (G-ETD), how clasical case is extended from integer order to non integer order and show how the proposed G-RDP for the M-L function is applicable. Consider a semilinear differential (reaction-diffusion) equation of time fractional order (FDEs) in the form:

$$\left\{\begin{aligned} \mathbb{D}_t^\alpha u + \mathscr{K}\Delta u &= f(u) \quad \text{in} \quad \Omega, \quad t \in (0,T), \\ u(0,\cdot) &= u_0, \end{aligned}\right. \tag{7.41}$$

where $\mathscr{K} > 0$, and $\mathbb{D}_t^\alpha$ denotes the Caputo derivative operator (with respect to t) of non-integer order $0 < \alpha \le 1$.

We state the following Lemmas which will be useful in the development of the scheme later.

Lemma 7.6.1. *[44] Let $a \le t$, $Re(\alpha) > 0$, and $\beta > 0$. Let $r \in \mathbb{R}$ such that $r > -1$. Then*

$$\int_a^t e_{\alpha,\beta}(t-\tau;\lambda)(\tau-a)^r d\tau = \Gamma(r+1)e_{\alpha,\beta+r+1}(t-a;\lambda), \tag{7.42}$$

where

$$e_{\alpha,\beta}(t;\lambda) = t^{\beta-1}E_{\alpha,\beta}(-t^\alpha\lambda).$$

Lemma 7.6.2. *[44] Let $a < b \le t$, $Re(\alpha) > 0$, and $\beta > 0$. Then*

$$\int_a^b e_{\alpha,\beta}(t-\tau;\lambda)d\tau = e_{\alpha,\beta+1}(t-a;\lambda) - e_{\alpha,\beta+1}(t-b;\lambda), \tag{7.43}$$

and

$$\int_a^b e_{\alpha,\beta}(t-\tau;\lambda)(\tau-a)d\tau = e_{\alpha,\beta+2}(t-a;\lambda) - (b-a)e_{\alpha,\beta+1}(t-b;\lambda) - e_{\alpha,\beta+2}(t-b;\lambda). \tag{7.44}$$

7.6.1 The Generalized ETD-RDP Scheme for Time Fractional Equations

In order to generalize the ETD methods to time fractional differential equations, we first discretize Equation (7.41) in the spatial direction using any finite difference approach to get:

$$\frac{d^\alpha}{dt^\alpha}U(t) + AU(t) = \mathscr{F}(U(t)). \tag{7.45}$$

Applying the Laplace transform, we obtain

$$s^\alpha\tilde{U}(s) - s^{\alpha-1}U_0 + A\tilde{U}(s) = \mathscr{F}(s) \Longleftrightarrow \tilde{U}(s) = \frac{s^{\alpha-1}}{(s^\alpha I + A)}U_0 + \frac{1}{(s^\alpha I + A)}\mathscr{F}(s).$$

Then applying the inverse Laplace transform, we get

$$U(t) = e_{\alpha,1}(t;A)U_0 + \int_0^t e_{\alpha,\alpha}(t-\tau;A)\mathscr{F}(U(\tau))d\tau, \tag{7.46}$$

where

$$e_{\alpha,\beta}(t;A) = \mathscr{L}^{-1}\left[\frac{s^{\alpha-\beta}}{(s^\alpha I + A)}\right] = t^{\beta-1}E_{\alpha,\beta}(-t^\alpha A).$$

Equation (7.46) represents a variation-of-constants formula for the fractional differential equation given in (7.41) which is the counterpart of Equation (5.4) for the fractional derivative case.

In the case of the exponential function, we have the semi-group property which is very helpful in developing the ETD scheme for integer order case. However, this property is not present in extension to the generalized Mittag-Leffler function, $e_{\alpha,\beta}(s+t;\lambda) \neq e_{\alpha,\beta}(s;\lambda)e_{\alpha,\beta}(t;\lambda)$ for $\alpha \neq 1$ and $\beta \neq 1$. Therefore, the variation-of constants formula given in (7.46) in a piecewise form:

$$U(t_n) = e_{\alpha,1}(t_n;A)U_0 + \sum_{j=0}^{n-1}\int_{t_j}^{t_{j+1}} e_{\alpha,\alpha}(t_n-\tau;A)\mathscr{F}(U(\tau))d\tau. \tag{7.47}$$

Following the same approach as in [45], we consider the piecewise first-order interpolating polynomials of the form:

$$P_{2,j}(s) = \mathscr{F}(U_j) + \frac{(s-t_j)}{h}(\mathscr{F}(U_{j+1} - \mathscr{F}(U_j)), \tag{7.48}$$

where

$$\mathscr{F}(U(s)) \approx \begin{cases} P_{2,j}(s) \text{ for } s \in [t_j, t_{j+1}],\ j = 0,1,2,\cdots,n-2 \\ P_{2,n-2}(s) \text{ for } s \in [t_{n-1}, t_n]. \end{cases} \tag{7.49}$$

Using Lemma (7.6.2), $\mathscr{B} = h^\alpha A$, and simplifying, the resulting semi-explicit scheme for $n \geq 2$ is given by

$$U_n = e_{\alpha,1}(n;\mathscr{B})U_0 + h^\alpha e^*_{\mathscr{B},n}\mathscr{F}(U_0) + h^\alpha\left[\sum_{j=1}^{n-1} e^{(2)}_{\mathscr{B},n-j}\mathscr{F}(U_j) - e^{(2)}_{\mathscr{B},0}\mathscr{F}(U_{n-2}) + 2e^{(2)}_{\mathscr{B},0}\mathscr{F}(U_{n-1})\right], \tag{7.50}$$

with

$$e^*_{\mathscr{B},n} = e_{\alpha,\alpha+2}(n-1;\mathscr{B}) + e_{\alpha,\alpha+1}(n;\mathscr{B}) - e_{\alpha,\alpha+2}(n;\mathscr{B}),$$

and

$$e^{(2)}_{\mathscr{B},n} = \begin{cases} e_{\alpha,\alpha+2}(1;\mathscr{B}), & n=0, \\ e_{\alpha,\alpha+2}(n-1;\mathscr{B}) - 2e_{\alpha,\alpha+2}(n;\mathscr{B}) + e_{\alpha,\alpha+2}(n+1;\mathscr{B}), & n \geq 1, \end{cases} \tag{7.51}$$

where

$$e_{\alpha,\beta}(t;\mathscr{B}) = h^{\beta-1}e_{\alpha,\beta}\left(\frac{t}{h}; h^\alpha\mathscr{B}\right), \quad h>0.$$

We call the scheme (7.54) semi-explicit since we have yet to approximate the matrix-argument ML-function involved. We have from the previous section, the partial fraction form of the rational approximation of the ML-function as:

$$\mathscr{R}(-z) = \frac{1}{\Gamma(\beta)}\left(\frac{a_1+a_2}{a_2-a_3}\right)(1+a_2z)^{-1} - \frac{1}{\Gamma(\beta)}\left(\frac{a_1+a_3}{a_2-a_3}\right)(1+a_3z)^{-1} \approx E_{\alpha,\beta}(-z), \tag{7.52}$$

and for the special case, we have

$$E_{\alpha,1}(-z) \approx \left(\frac{b_1+b_2}{b_2-b_3}\right)(1+b_2z)^{-1} - \left(\frac{b_1+b_3}{b_2-b_3}\right)(1+b_3z)^{-1}, \tag{7.53}$$

For convenience, denote

$$C_1 = \frac{1}{\Gamma(\alpha+1)}\left(\frac{a_1+a_2}{a_2-a_3}\right), \quad C_2 = \frac{1}{\Gamma(\alpha+1)}\left(\frac{a_1+a_3}{a_2-a_3}\right), \quad C_1^* = \left(\frac{b_1+b_2}{b_2-b_3}\right) \quad \text{and} \quad C_2^* = \left(\frac{b_1+b_3}{b_2-b_3}\right).$$

Using these approximations and simplifying, we have the following:

$$e_{\alpha,1}(t_n;\mathscr{B})U_0 \approx \left[C_1^*(I+b_2 t_n^\alpha \mathscr{B})^{-1} - C_2^*(I+b_3 t_n^\alpha \mathscr{B})^{-1}\right] U_0,$$

$$\begin{aligned} h^\alpha e^*_{\mathscr{B},n}\mathscr{F}(U_0) \quad &\approx \quad \frac{h^\alpha t_{n-1}^{\alpha+1}}{\alpha+1}\left[C_1(I+a_2 t_{n-1}^\alpha \mathscr{B})^{-1} - C_2(I+a_3 t_{n-1}^\alpha \mathscr{B})^{-1}\right]\mathscr{F}(U_0) \\ &\quad + h^\alpha t_n^\alpha \left(1-\frac{t_n}{\alpha+1}\right)\left[C_1(I+a_2 t_n^\alpha \mathscr{B})^{-1} - C_2(I+a_3 t_n^\alpha \mathscr{B})^{-1}\right]\mathscr{F}(U_0), \end{aligned}$$

$$h^\alpha\left[-e^{(2)}_{\mathscr{B},0}\mathscr{F}(U_{n-2}) + 2e^{(2)}_{\mathscr{B},0}\mathscr{F}(U_{n-1})\right] \approx \frac{h^\alpha}{(\alpha+1)}\left[C_1(I+a_2\mathscr{B})^{-1} - C_2(I+a_3\mathscr{B})^{-1}\right](2\mathscr{F}(U_{n-1}) - \mathscr{F}(U_{n-2})),$$

and

$$\begin{aligned} & h^\alpha e^{(2)}_{\mathscr{B},n-j}\mathscr{F}(U_j) \\ &\quad \approx \frac{C_1 h^\alpha}{\alpha+1}\left[t_{n-j-1}^{\alpha+1}(I+a_2 t_{n-j-1}^\alpha \mathscr{B})^{-1} - 2t_{n-j}^{\alpha+1}(I+a_2 t_{n-j}^\alpha \mathscr{B})^{-1} + t_{n-j+1}^{\alpha+1}(I+a_2 t_{n-j+1}^\alpha \mathscr{B})^{-1}\right]\mathscr{F}(U_j) \\ &\quad + \frac{C_2 h^\alpha}{\alpha+1}\left[t_{n-j-1}^{\alpha+1}(I+a_3 t_{n-j-1}^\alpha \mathscr{B})^{-1} - 2t_{n-j}^{\alpha+1}(I+a_3 t_{n-j}^\alpha \mathscr{B})^{-1} + t_{n-j+1}^{\alpha+1}(I+a_3 t_{n-j+1}^\alpha \mathscr{B})^{-1}\right]\mathscr{F}(U_j). \end{aligned}$$

Define the following as:

$$\begin{aligned} \mathscr{Q}(k_1;k_2;\mathscr{B}) &= C_1(I+k_1\mathscr{B})^{-1} - C_2(I+k_2\mathscr{B})^{-1}, \\ \mathscr{Q}(k_1;k_2;n;\mathscr{B}) &= C_1(I+k_1 t_n^\alpha \mathscr{B})^{-1} - C_2(I+k_2 t_n^\alpha \mathscr{B})^{-1}, \\ \mathscr{Q}^*(k_1;k_2;n;\mathscr{B}) &= C_1^*(I+k_1 t_n^\alpha \mathscr{B})^{-1} - C_2^*(I+k_2 t_n^\alpha \mathscr{B})^{-1}, \end{aligned}$$

$$\begin{aligned} & \mathscr{T}(k_1;k_2;k_3;k_4;n-j;\mathscr{B}) \\ &\quad = \frac{k_1 h^\alpha}{\alpha+1}\left[t_{n-j-1}^{\alpha+1}(I+k_3 t_{n-j-1}^\alpha \mathscr{B})^{-1} - 2t_{n-j}^{\alpha+1}(I+k_3 t_{n-j}^\alpha \mathscr{B})^{-1} + t_{n-j+1}^{\alpha+1}(I+k_3 t_{n-j+1}^\alpha \mathscr{B})^{-1}\right] \\ &\quad + \frac{k_2 h^\alpha}{\alpha+1}\left[t_{n-j-1}^{\alpha+1}(I+k_4 t_{n-j-1}^\alpha \mathscr{B})^{-1} - 2t_{n-j}^{\alpha+1}(I+k_4 t_{n-j}^\alpha \mathscr{B})^{-1} + t_{n-j+1}^{\alpha+1}(I+k_4 t_{n-j+1}^\alpha \mathscr{B})^{-1}\right]. \end{aligned}$$

$$\mathscr{T}(k_1;k_2;k_3;k_4;n-j;\mathscr{B})$$
$$= \frac{kh^\alpha}{\alpha+1}\left[t_{n-j-1}^{\alpha+1}(I+k_1 t_{n-j-1}^\alpha \mathscr{B})^{-1} - 2t_{n-j}^{\alpha+1}(I+k_1 t_{n-j}^\alpha \mathscr{B})^{-1} + t_{n-j+1}^{\alpha+1}(I+k_1 t_{n-j+1}^\alpha \mathscr{B})^{-1}\right].$$

Finally, the full explicit scheme for $n \geq 2$ is given by

$$\begin{aligned} U_n &= \mathscr{Q}^*(b_2;b_3;n;\mathscr{B})U_0 + \frac{h^\alpha t_{n-1}^{\alpha+1}}{\alpha+1}\mathscr{Q}(b_2;b_3;n-1;\mathscr{B})\mathscr{F}(U_0) + h^\alpha t_n^\alpha\left(1-\frac{t_n}{\alpha+1}\right)\mathscr{Q}(b_2;b_3;n;\mathscr{B})\mathscr{F}(U_0) \\ &\quad + \sum_{j=1}^{n-1}\mathscr{T}(C_1;C_2;a_2;a_3;n-j;\mathscr{B})\mathscr{F}(U_j) + \frac{h^\alpha}{(\alpha+1)}\mathscr{Q}(b_2;b_3;\mathscr{B})\left(2\mathscr{F}(U_{n-1})-\mathscr{F}(U_{n-2})\right). \end{aligned} \tag{7.54}$$

Summary

A real distinct pole rational approximation of the generalized Mittag-Leffler function is introduced. Under some mild conditions, this approximation is proven and empirically shown to be L-Acceptable. A complete monotonicity property of the Mittag-Leffler function enables us to derive a rational approximation for the inverse generalized Mittag-Leffler function by inversion. These approximations are especially useful in developing efficient and accurate numerical schemes partial differential equations of fractional order. Several applications are presented such as complementary error function, solution of fractional differential equations, and the ultraslow diffusion model using the structural derivative. Furthermore, we propose a generalized exponential integrator scheme for time-fractional nonlinear reaction-diffusion equation using the M-L RDP approximation.

Chapter 8

Conclusion and Recommendation

The scheme (FETD-RDP) proposed in this work is shown to be a second-order convergence when applied to systems of two-dimensional space-fractional reaction-diffusion models. The scheme is especially robust for problems with non-smooth/mismatched initial and boundary conditions. In terms of efficiency, the cpu time for our scheme compares favourably with second-order schemes such as FETD-CN, FETD-Padé(0,2), the BDF2, IMEX-BDF2 and IMEX-Adams2 schemes. The wider region of stability of our scheme allows for large time step without losing stability of the solution. One of the major benefits of the proposed scheme is that the algorithm could be easily implemented in parallel to take advantage of multiple processors for increased computational efficiency. Our approach is exhibited by solving many important nonlinear fractional reaction-diffusion models some of which exhibit pattern formations and have applications in cell-division. Empirically, super-diffusion processes are displayed by investigating the effect of the fractional power of the underlying Laplacian operator on the pattern formation found in these models. Furthermore, we have discussed the trade-off between using fractional centered differencing and matrix transfer technique in spatial discretization of Riesz fractional derivatives for different values of α.

Finally, a real distinct pole rational approximation of the generalized Mittag-Leffler function is introduced. Under some mild conditions, this approximation is proven and empirically shown to be L-Acceptable. A complete monotonicity property of the Mittag-Leffler function enables us to derive a rational approximation for the inverse generalized Mittag-Leffler function by inversion. These approximations are especially useful in developing efficient and accurate numerical schemes partial differential equations of fractional order. Several applications are presented such as complementary error function, solution of fractional differential equations, and the ultraslow diffusion model using the structural derivative. Furthermore, we propose a generalized exponential integrator scheme for time-fractional nonlinear reaction-diffusion equation using the M-L RDP approximation. However, the proposed scheme is still at the preliminary stage. Further work is required on the analysis of the efficiency and convergence results.

In the future, we recommend that efforts should be directed towards examining the performance of FETD-RDP scheme for problem with significant advection terms. The proposed real distinct pole rational approximation of the generalized Mittag-Leffler function has opened up a lot of work in this direction. Developing an efficient numerical scheme for nonlinear time-space fractional equations using the approximation should be a focus of future effort.

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Appendix

A: Some Commonly used Padé approximations

[k/j]	0	1	2
0	$\frac{1}{1}$	$\frac{1+z}{1}$	$\frac{1+z+\frac{z^2}{2!}}{1}$
1	$\frac{1}{1-z}$	$\frac{1+\frac{1}{2}z}{1-\frac{1}{2}z}$	$\frac{1+\frac{2}{3}z+\frac{1}{3}\frac{z^2}{2!}}{1-\frac{1}{3}z}$
2	$\frac{1}{1-z+\frac{z^2}{2!}}$	$\frac{1+\frac{1}{3}z}{1-\frac{2}{3}z+\frac{1}{3}\frac{z^2}{2!}}$	$\frac{1+\frac{1}{2}z+\frac{1}{6}\frac{z^2}{2!}}{1-\frac{1}{2}z+\frac{1}{6}\frac{z^2}{2!}}$
3	$\frac{1}{1-z+\frac{z^2}{2!}-\frac{z^3}{3!}}$	$\frac{1+\frac{1}{4}z}{1-\frac{3}{4}z+\frac{1}{2}\frac{z^2}{2!}-\frac{1}{4}\frac{z^3}{3!}}$	$\frac{1+\frac{2}{5}z+\frac{1}{10}\frac{z^2}{2!}}{1-\frac{3}{5}z+\frac{3}{10}\frac{z^2}{2!}-\frac{1}{10}\frac{z^3}{3!}}$

Table A1: Summary of some common Padé approximations

Curriculum Vitae

Olaniyi Samuel Iyiola

Education

August, 2017:

Ph.D., Applied and Computational Mathematics, (**CGPA: 3.969/4.00**)

University of Wisconsin-Milwaukee, Milwaukee, WI

Thesis Topic: *Exponential Integrator Method for Fractional Reaction-Diffusion Models*

Advisors: Bruce Wade, Ph.D

December, 2011:

M.S, Pure and Applied Mathematics, (**CGPA: 3.21/4.00**)

African University of Science and Technology, Abuja Nigeria

Thesis Topic: *Sobolev Spaces and Linear Elliptic Partial Differential Equations*

Advisors: Ngalla Djitte, Ph.D

August, 2008:

M.S, Mathematics, (**CGPA: 3.55/4.00**)

University of Nigeria, Nsukka Nigeria

Thesis Topic: *Iterative Approximation of Fixed Point of K-Strictly Pseudo-contractive Map in Hilbert Space*

Advisors: Micah O. Osilike, Ph.D & Felicia O. Isiogugu, Ph.D

Funded Research Projects Completed

2012–2014: Research Assistant

National Science, Technology and Innovation Plan (NSTIP)

King Abdulaziz City for Science and Tech., KACST - $459,379.54

Division of Mathematics & Statistics, King Fahd University of Petroleum & Minerals

Title: **Fluid transport through porous media with application to enhanced oil recovery**

Principal Investigator: Nadeem A. Malik, Ph.D

2013–2014: Research Assistant

Saudi Basic Chemical Industries (SABIC)

Saudi Basic Chemical Industries (SABIC) - $20,000

Division of Mathematics & Statistics, King Fahd University of Petroleum & Minerals

Title: **Inverse problems for fractional heat equation with Hilfer derivative**

Principal Investigator: Khaled M. Furati, Ph.D

2012–2013: Research Assistant

Saudi Basic Chemical Industries (SABIC)

Saudi Basic Chemical Industries (SABIC) - $20,000

Division of Mathematics & Statistics, King Fahd University of Petroleum & Minerals

Title: **A Study of Tumor Model with Treatment Profile**

Principal Investigator: F.D. Zaman, Ph.D

Refereed Journal Publications

1. K.M. Furati, **O.S Iyiola**, and K. Mustapha “An inverse source problem for a two-parameter anomalous diffusion with local time datum." *Computers and Mathematics with Applications*, 73(6), 1008-1015, (2017).

2. **O.S. Iyiola**, O. Tasbozan, A. Kurt, and Y. Cenesiz "On the analytical solutions of the system of conformable time-fractional Robertson equations with 1-D diffusion." *Chaos, Solitons and Fractals.* DOI: 10.1016/j.chaos.2016.11.003. (2017).

3. Y. Shehu, and **O.S. Iyiola** "Convergence Analysis for Proximal Split Feasibility Problem using Inertial Extrapolation Term Method" *Journal of Fixed Point Theory and Applications*, DOI: 10.1007/s11784-017-0435-z. (2017).

4. Y. Shehu, and **O.S. Iyiola** "Strong convergence result for monotone variational inequalities" *Numerical Algorithms.* DOI: 10.1007/s11075-016-0253-1 (2016).

5. **O.S. Iyiola**, and Y. Shehu "A cyclic iterative method for solving multiple sets split feasibility problems in Banach spaces." *Quaestiones Mathematicae*, 39(7):959–975, (2016).

6. **O.S. Iyiola**, and F.D. Zaman "A note on analytical solutions of nonlinear fractional 2D heat equation with non-local integral terms." *Pramana-Journal of Physics*, 87(4):51, DOI 10.1007/s12043-016-1239-1 (2016).

7. **O.S. Iyiola**, and E.R. Nwaeze "Some new results on the new conformable fractional calculus with application using D'Alambert approach." *Progress in fractional differentiation and applications*, 2(2):1–7, (2016).

8. Y. Shehu, F.U Ogbuisi, and **O.S. Iyiola** "Convergence Analysis of an iterative algorithm for fixed point problems and split feasibility problems in certain Banach spaces" *Optimization*, 65(2):299–323, (2016).

9. Y. Shehu, **O.S. Iyiola**, and C.D. Enyi "Iterative algorithm for split feasibility problems and fixed point problems in Banach spaces" *Numerical Algorithms*, 72(4):835–864, (2016).

10. **O.S. Iyiola** "Exact and Approximate Solutions of Fractional Diffusion Equations with Fractional Reaction Terms" *Progress in Fractional Differentiation and Applications*, 2(1):21–30, (2016).

11. G. Cai, Y. Shehu, and **O.S. Iyiola** "Iterative algorithms for solving variational inequalities and fixed point problems for asymptotically nonexpansive mappings in Banach spaces" *Numerical Algorithms* DOI: 10.1007/s11075-016-0121-z (2016).

12. Y. Shehu, G. Cai, and **O.S. Iyiola** "Iterative approximation of solutions for proximal split feasibility problems" *Fixed Point Theory and Applications* DOI: 10.1186/s13663-015-0375-5 (2015).

13. **O.S. Iyiola**, and G.O. Ojo "On the analytical solution of Fornberg-Whitham equation with the new fractional derivative." *Pramana-Journal of Physics*, 85(4):567–575, (2015).

14. **O.S. Iyiola**, and Y.U. Gaba "An Analytical Approach to Time-Fractional Harry Dym Equation." *Applied Mathematics and Information Sciences*, DOI: 10.18576/amis/10020 (2015).

15. K.M. Furati, **O.S. Iyiola**, and M. Kirane "An inverse problem for a generalized fractional diffusion." *Applied Mathematics and Computation*, 249:24–31, (2014).

16. **O.S. Iyiola**, and F.D. Zaman "A fractional diffusion equation model for cancer tumor." *American Institute of Physics Advances*, 4(10):107121, (2014).

17. Y. Shehu, **O.S. Iyiola**, and C.D. Enyi "On Proximal Split Feasibility Problems and Fixed Point Problem for Quasi-nonexpansive Multi-valued Mappings." *Advances in Nonlinear Variational Inequalities*, 17(2):71–87, (2014).

18. Y. Shehu, **O.S. Iyiola**, and C.D. Enyi "Iterative approximation of solutions for constrained convex minimization problem." *Arabian Journal of Mathematics*, 2(4):393–402, (2013).

Submitted Journal Publications

1. **O.S. Iyiola**, and B.A. Wade "Exponential Integrator Methods for System of Nonlinear Space-fractional Models with Super-diffusion Processes in Pattern Formation" 2017. Under review in *Computers & Mathematics with Applications*.

2. **O.S. Iyiola**, E.O. Asante-asamani, and B.A. Wade “A Real Distinct Poles Rational Approximation of Generalized Mittag-Leffler Functions and Thier Inverses: Applications to Fractional Calculus" 2017. Under review in *J. of Computational and Applied Mathematics.*

3. **O.S. Iyiola**, E.O. Asante-asamani, K.M. Furati, A.Q.M Khaliq and B.A. Wade “Efficient Time Discretization Scheme for Nonlinear Space Fractional Reaction-diffusion Equations" 2017. Under review in *Inter. J. of Computer Mathematics.*

4. G. Cai, A. Gibali, **O.S. Iyiola** and Y. Shehu “A New Double-Projection Method for Solving Variational Inequalities in Banach Space" 2017. Under review in *J. of Optimization Theory and Applications.*

5. Y. Shehu, and **O.S. Iyiola** “Another Strong Convergence Result for Proximal Split Feasibility Problem" 2016. Under review in *Optimization.*

Papers in Preparation

1. **O.S. Iyiola**, K.M. Furati, A.Q.M Khaliq and B.A. Wade “Solving System of Fractional Biological and Biochemical Models by the Means of Exponential Time Differencing.”

Book Chapters

1. **O.S. Iyiola** “Iterative Approximation of Fixed Points in Hilbert Space.” LAP LAMBERT Academic Publishing GmbH and Co. KG, (ISBN-9783844306095), (2012).

2. **O.S. Iyiola** “Sobolev Spaces and Linear Elliptic Partial Differential Equations." LAP LAMBERT Academic Publishing GmbH and Co. KG, (ISBN-978365914200), (2012).

Awards

Student Awards: University of Wisconsin-Milwaukee

1. Mark Lawrence Teply Award: Outstanding Research Potential — May 2017
2. Morris and Miriam Marden Award: High Quality Research Paper — May 2016
3. Chancellor's Award, University of Wisconsin-Milwaukee, WI — 2015/2016

Travel Awards:

1. SIAM student travel award for Conference on Computational Science and Engineering, Atlanta, GA, USA — Feb/Mar 2017
2. Conference on Current Developments in Mathematics, CDM, Harvard University, Cambridge, MA, USA — Nov 2016
3. QMath13: Mathematical Results in Quantum Physic, Mathematics Dept., Georgia Institute of Tech., Atlanta, GA, USA — Oct 2016
4. Industrial Math/Stat Modeling Workshop, **SAMSI**, North Carolina State University, NC, USA — Jul 2016
5. Workshop on Dynamics and Differential Equations **IMA**, University of Minnesota, MN, USA — Jun 2016
6. Workshop on Uncertainty, Sensitivity and Predictability in Ecology: Mathematical Challenges and Ecological Applications Mathematical Biosciences Institute, **MBI**, Ohio State Univ., OH, USA — Oct 2015
7. Conference on Waves, Spectral Theory and Applications Mathematics Department, Princeton University, Princeton, NJ, USA — Sept 2015
8. Winter Meeting Canada Mathematical Society, **CMS** Hamilton Ontario, Canada — Dec 2014

9. Summer School on Applied Analysis for Materials — Aug/Sept 2014
   Berlin Mathematical School **BMS**, Berlin, Germany

10. Summer School on Simulation, Optimization and Identification — Aug 2014
    in Solid Mechanics Gene Golub, **SIAM**, Linz, Austria

11. Short Course: Topics in Control Theory — May/Jun 2014
    IMA, University of Minnesota, MN, USA

12. Conference on Partial Differential Equations and Applications — May/Jun 2013
    SIAM APDE13 Orlando, FL, USA

Student Awards — African University of Science & Tech.

1. Best Project - World Bank Step-B Innovation Prize — Jan 2012

Conference/Colloquium Talks

1. “An Efficient Numerical Scheme for Space-Fractional Fitzhugh-Nagumo Model" SIAM Conference on Computational Science and Engineering, Atlanta, GA, USA — Feb/Mar 2017

2. “An overview on fractional calculus & fractional models" Graduate Student Colloquium, Math. Dept., UW-Milwaukee, WI, USA — Nov 2016

3. “Two-data points inverse source problem for a generalized time-fractional diffusion equation" Graduate Student Research Symposium, UW-Milwaukee, WI, USA — Oct 2016

4. “On the solution of fractional diffusion equation in the absence of source term" First AUS Regional Students' Conference on Mathematics (AUS-RSCM14), the American University of Sharjah, UAE — Mar 2014

5. “A Comparison Analysis of q-Homotopy Analysis Method q-HAM and Variational iterative method (VIM) to Fingero-Imbibition Phenomena in Double Phase Flow through Porous Media SIAM APDE13 Conference on Partial Differential Equations and Applications, FL, USA — Dec 2013

Conference Posters

1. “An Inverse Problem for a Fractional Diffusion Equation and the Associated Spectral Problems" Conference on Waves, Spectral Theory and Applications, Math. Dept, Princeton University, Princeton, NJ, USA — Sept 2015
2. “An Inverse Problem for a Fractional Diffusion" CMS Winter Meeting, Ontario, Canada — Dec 2014

Employment History

1. **Teaching Assistant:** — Jan 2015- Present
   University of Wisconsin-Milwaukee, WI
2. **Lecturer-B/Research Assistant:** — 2012- 2014
   King Fahd University of Petroleum and Minerals, Saudi Arabia
3. **Research Assistant/Teaching Assistant:** — Jan 2012- July 2012
   African University of Science and Technology, AUST, Nigeria
4. **Assistant Lecturer:** — Jan 2012- July 2012
   Nigeria Turkish Nile University, NTNU, Nigeria

5. **Mathematics Tutor** Jan 2009- July 2010

   Mainland Technical College, Nigeria

Certifications

1. Certificate in Responsible Conduct of Research, University of Wisconsin-Milwaukee, WI
2. Certificate in Business and Innovation, African University of Science and Technology
3. Certificate in Biological Sciences with Bio-energy and Agriculture track, African University of Science and Technology
4. Certificate in Energy and Environment, African University of Science and Technology

Professional Membership

1. Member of Canadian Mathematical Society, CMS, Canada 2014 – Present
2. Member of Society for Industrial and Applied Math, SIAM, USA 2013 – Present
3. Member of European Mathematical Society, EMS 2013 – Present
4. Member of American Mathematical Society, AMS, USA 2012 – Present

Referee Services

I review for the following journals:

1. Journal of Nonlinear Sciences and Applications 2017 – Present
2. American Institute of Physics, AIP Advances 2016 – Present
3. Algorithms 2016 – Present

4. Inverse Problems 2016 – Present
5. Applied Mathematics and Information Sciences 2016 – Present
6. SpringerPlus 2015 – Present
7. Kuwait Journal of Science 2014 – Present

Computer Skills

Basics: MS Word, MS Excel, Power-Point, Corel-Draw

Teaching Tools: MyMathLab, ALEKS, GATETWAY

Programming Language: Python, LaTex

Mathematical Software: MATLAB, Mathematica, Maple

Service and Activity

1. Member, Committee on Graduate Student Research Symposium, UW-Milwaukee, WI
2. Member, Panel of Judges: Badger State Science and Engineering Fair, Milwaukee, WI
3. Class Representative, Department of Mathematics, African University of Science and Technology, Nigeria for 2010-2011
4. Zonal Coordinator for Nigeria Christian Corpers' Fellowship (NCCF), Oron Zone, Akwa Ibom State Chapter, Nigeria
5. Class Representative, Department of Mathematics, University of Nigeria for 2004-2008
6. Publicity/Library Secretary for Anglican Students' Fellowship, University of Nigeria for 2005-2006

Languages

English

Interests

Table Tennis, Soccer