

TIME STEPPING SCHEMES WITH MATRIX
TRANSFORM TECHNIQUE FOR
SPACE-FRACTIONAL DIFFERENTIAL
EQUATIONS

BY

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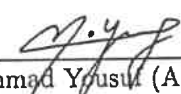
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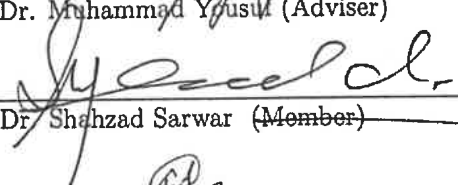
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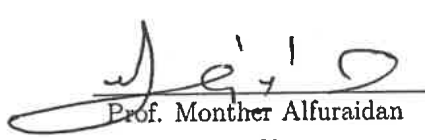
This thesis, written by **MUNIRAH MOHAMMED ALSHAYQI** under the direction of her thesis adviser and approved by her thesis committee, has been presented to and accepted by the Dean of Graduate Studies, in partial fulfillment of the requirements for the degree of **MASTER OF SCIENCE IN MATHEMATICS**.

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To my family, husband, and son.

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LIST OF ABBREVIATIONS

BCs	Boundary Conditions
CPU	Central Processing Unit
ETD	Exponential Time Differencing
ETDRK	Exponential Time Differencing Runge-Kutta
FDEs	Fractional Differential Equations
FPDEs	Fractional Partial Differential Equations
MTT	Matrix Transform Technique
ODEs	Ordinary Differential Equations

THESIS ABSTRACT

NAME: Munirah Mohammed Alshayqi

TITLE OF STUDY: Time Stepping Schemes with Matrix Transform Technique for Space-Fractional Differential Equations

MAJOR FIELD: Mathematics

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Non-linear time-dependent space-fractional differential equations are widely employed to simulate significant physical phenomena in diverse engineering and scientific fields. However, obtaining the exact solution for most of these systems is challenging because they are often represented in trigonometric series form. Therefore, the development of numerical solutions becomes crucial to addressing this complexity. Recently, there has been a growing interest in devising effective and reliable numerical approaches to solve these non-linear systems of fractional differential equations.

In this thesis, we have developed highly efficient high-order numerical schemes to solve space-fractional reaction-diffusion problems with homogeneous Neumann and Dirichlet boundary conditions. In the first part of the thesis, we developed numerical schemes that are based on the fourth-order Matrix Transform Technique (MTT) for spatial

discretization and third-order Exponential Time Differencing Runge-Kutta (ETDRK) type schemes. The ETDRK schemes are based on a single pole third order restricted Padé approximation and a third-order Padé (1,2) approximation. The partial fraction splitting approach is used to construct a computationally efficient version of the schemes. In the second part of the thesis, we have developed a robust framework for characterizing complex phenomena arising in space fractional reaction-diffusion systems. Highly efficient numerical schemes are developed by combining the power of the Fourier spectral approach in space and exponential time differencing schemes in time. The non-locality of the fractional operators results in full dense matrices. The advantage of the Fourier spectral approach is that a full diagonal representation of the fractional operator is obtained and we can extend the schemes to multi-dimensional problems with the same complexity as one-dimensional problems. Moreover, the proposed schemes exhibit stability, third-order convergence, and high efficiency due to their predictor-corrector nature. The efficiency of the schemes is further enhanced by applying powerful mathematical tools, namely, discrete sine and cosine transforms. Algorithms are developed to easily implement the methods on one and multidimensional systems with homogeneous Dirichlet as well as homogeneous Neumann boundary conditions. The computational efficiency, reliability and effectiveness of the presented methods are demonstrated through numerical experiments. Convergence results are computed to support the theoretical findings.

ملخص الرسالة

الاسم: منيرة محمد الشايعي

عنوان الدراسة: مخططات التدرج الزمني باستخدام تقنية تحويل المصفوفة للمعادلات التفاضلية الكسرية المكانية

التخصص: قسم الرياضيات

تاريخ الدرجة العلمية: مايو، 2024

تُستخدم المعادلات التفاضلية الكسرية المكانية غير الخطية المعتمدة على الزمن على نطاق واسع لمحاكاة الظواهر الفيزيائية المهمة في المجالات الهندسية والعلمية المتنوعة. ومع ذلك، فإن الحصول على الحلول الدقيقة لمعظم هذه الأنظمة يمثل تحديًا لأنها غالبًا ما يتم تمثيلها في شكل متسلسلة مثلثية. ولذلك، فإن تطوير الحلول العددية يصبح حاسماً لمعالجة هذا التعقيد. في الآونة الأخيرة، كان هناك اهتمام متزايد في ابتكار أساليب عددية فعالة وموثوقة لحل هذه الأنظمة غير الخطية من المعادلات التفاضلية الكسرية.

في هذه الأطروحة، قمنا بتطوير مخططات عددية عالية الكفاءة لحل مسائل تفاعل وانتشار التفاعل الكسري مع الشروط الحدودية المتجانسة لنيومان ودريشليت. في الجزء الأول من الأطروحة، قمنا بتطوير مخططات عددية تعتمد على تقنية تحويل المصفوفة من الدرجة الرابعة (MTT) للتمييز المكاني ومخططات من النوع الأسّي لاختلاف الوقت (Runge-Kutta) من الدرجة الثالثة. تعتمد مخططات ETDK على تقريب Padé المقيد من الدرجة الثالثة وتقريب (1,2) Padé من الدرجة الثالثة. يتم استخدام أسلوب تقسيم الكسور الجزئية لإنشاء نسخة فعالة من الناحية الحسابية للمخططات. في الجزء الثاني من الأطروحة، قمنا بتطوير إطار قوي لتوصيف الظواهر المعقدة التي تنشأ في أنظمة انتشار التفاعل الجزئي في المكان. تم تطوير مخططات عددية عالية الكفاءة من خلال الجمع بين قوة نهج فورييه الطيفي في المكان ومخططات التمييز الزمني الأسّي في الوقت. ينتج عن عدم محلية العوامل الكسرية مصفوفات كثيفة كاملة. تتمثل ميزة منهج فورييه الطيفي في الحصول على تمثيل قطري كامل للعامل الكسري ويمكننا توسيع المخططات لتشمل تمثيلات متعددة الأبعاد بنفس التعقيد مثل التمثيلات أحادية البعد. علاوة على ذلك، فإن المخططات المقترحة تظهر

الاستقرار والتقارب من الدرجة الثالثة والكفاءة العالية بسبب طبيعتها المتنبة والمصححة. يتم تعزيز كفاءة المخططات بشكل أكبر من خلال تطبيق أدوات رياضية قوية، وهي تحويلات الجيب وجيب التمام المنفصلة. تم تطوير الخوارزميات لتنفيذ الأساليب بسهولة على أنظمة أحادية ومتعددة الأبعاد مع شروط حدود ديريشليت المتجانسة وكذلك شروط حدود نيومان المتجانسة. يتم إثبات الكفاءة الحسابية والموثوقية والفعالية للطرق المقدمة من خلال التجارب العددية. يتم حساب نتائج التقارب لدعم النتائج النظرية.

CHAPTER 1

INTRODUCTION AND PRELIMINARIES RESULTS

Fractional calculus serves as an extension of conventional calculus, encompassing derivatives and integrals of non-integer orders. In 1695, Leibniz initiated discussions on the concept of fractional derivatives in correspondence with L'Hôpital, pondering the nature of the derivative when $n = \frac{1}{2}$ in the expression $\frac{d^n y}{dx^n}$ [1]. Subsequently, in a letter to J. Bernoulli, Leibniz further explored derivatives of arbitrary order, with additional insights contributed by Euler, Lagrange, and others. A formal definition for fractional derivatives was introduced by Laplace in 1812, that utilized the concept of integrals, while Lacroix proposed an alternative definition employing the gamma function, aligning with the Riemann-Liouville fractional derivative. Fourier contributed to the discourse in 1822 by introducing a definition of fractional derivatives based on the Fourier transform. Later, in 1930, Liouville extended the concept of fractional derivatives to arbitrary orders, For more information, see [2].

A class of differential equations with non-integer order derivatives are known as Fractional Differential Equations (FDEs). The significance of fractional calculus in various fields has drawn the attention of numerous scholars to this area of research. Many mathematical models have been modified using derivatives of fractional order instead of integer order, because the description of the hereditary and memory features of various substances is made possible by fractional-order derivatives and integrals [3]. The most frequent application of fractional integral and differential operators is in the study of viscoelasticity, where comprehensive surveys have been published [4]. Fractional derivatives have been effectively used to solve problems related to system biology [5], physics [6], [7], [8], chemistry and biochemistry, hydrology [9], [10], [11], and finance [12]. The exact solution to such a variety of problems is always a difficult challenge for researchers studying fractional differential equations. Finding numerical solution of such problems become more important when exact solution is not available. As a consequence, many researchers have tried various methods to discover the optimal solutions to several fractional order differential equations [13]. Numerous numerical techniques have been proposed to solve problems involving single term fractional operators. For further details about time and space fractional differential equations, see [14], [15], [16], [17] and [18], [19], [20] respectively. Fractional equations have many applications in engineering and science, including electrochemistry, diffusion-related diffusive transport, fluid flow, probability, electromagnetic theory, and many more. They are particularly useful in modeling mechanical systems, characterizing the rheological properties of rocks, and describing real materials electrical properties. In groundwater hydrology, for instance, we can demonstrate the mod-

ularity of tracer transfer via fluid flow by using the fractional advection-dispersion equation [11]. Nowadays, numerical solutions to fractional differential equations is an effective research area in finding optimal solutions for differential equations due to the lack of a definitive and effective methods to solve general fractional differential equations (FDEs) analytically. This deficiency motivates researchers to seek for new and effective numerical methods [13].

The fractional Laplacian is defined by describing it in multidimensional spaces [21], which presents a difficult non-local operator that necessitates complex analytical and computational methods

$$(-\Delta)^{\frac{\alpha}{2}}\Phi(y) = c_{\alpha,d}\text{P.V.} \int_{\mathbb{R}^d} \frac{\Phi(y) - \Phi(s)}{|y - s|^{\alpha+d}} ds \quad y \in \mathbb{R}^d.$$

In this expression, "P.V." denotes Cauchy principal value integration. Additionally, the normalization constant $c_{\alpha,d}$ is determined by

$$c_{\alpha,d} = \frac{2^\alpha \Gamma\left(\frac{d+\alpha}{2}\right)}{\pi^{d/2} \left|\Gamma\left(\frac{-\alpha}{2}\right)\right|}.$$

These formulations encapsulate the operational essence of the fractional Laplacian, highlighting its reliance on parameters α and d , as well as the integral representation involving Cauchy principal values.

In this framework, our primary focus lies in exploring the application of the fractional Laplacian within a bounded domain. We define the commonly used definitions of this non-local operator within such domains.

Integral Fractional Laplacian

The integral fractional Laplacian of $\Phi(y)$ for $y \in \Omega \subset \mathbb{R}^d$ is characterized by extending $\Phi(y)$ to a function in $\mathbb{R}^d$ as follows

$$\tilde{\Phi}(y) = \begin{cases} \Phi(y) & \text{if } y \in \Omega \\ 0 & \text{if } y \in \Omega^c \end{cases}$$

where Ω^c represents the complement of Ω .

Subsequently, the conventional definition of the fractional Laplacian is applied

$$-(-\Delta)^{\frac{\alpha}{2}}\Phi(y) := -(-\Delta)^{\frac{\alpha}{2}}\tilde{\Phi}(y).$$

An alternative definition is provided through the Fourier transform

$$-(-\Delta)^{\frac{\alpha}{2}}\Phi(y) := \mathcal{F}^{-1} \left(|\Phi|^\alpha \mathcal{F}\tilde{\Phi} \right)$$

Regional Fractional Laplacian

This definition is derived by confining the integration domain to Ω

$$-(-\Delta)^{\frac{\alpha}{2}}\Phi(y) := c_{\alpha,d} \int_{\Omega} \frac{\Phi(y) - \Phi(s)}{|y - s|^{\alpha+d}} ds$$

These distinct formulations offer diverse perspectives on the fractional Laplacian's behavior within bounded domains, shedding light on its various operational nuances.

Spectral Fractional Laplacian

The spectral fractional Laplacian is defined utilizing the spectral approach

$$-(-\Delta)^{\frac{\alpha}{2}}\Phi(y) := \sum_{k \in N} \Phi_k \lambda_k^{\frac{\alpha}{2}} \varphi_k(y)$$

In this case, the eigenfunctions and eigenvalues of the conventional Laplace operator within the domain Ω are represented by φ_k and λ_k . Δ , subject to homogeneous Dirichlet boundary conditions. Furthermore, Φ_k denotes the projection of Φ onto the direction e_k

$$\begin{cases} -\Delta \varphi_k = \lambda_k \varphi_k & \text{in } \Omega, \\ \varphi_k = 0 & \text{on } \partial\Omega. \end{cases}$$

1.1 Basic Definitions and Preliminaries Results

This section serves to introduce fundamental definitions and preliminary results essential for the understanding of the thesis.

Definition 1. [22] The Riesz fractional operator for α values between $n - 1$ and n on a bounded interval $a \leq y \leq b$ is expressed as

$$\frac{\partial^\alpha}{\partial |y|^\alpha} \Phi(y, t) = -\frac{1}{2 \cos(\frac{\pi\alpha}{2})} ({}_a D_y + {}_y D_b) \Phi(y, t), \quad \alpha \neq 1$$

where

$${}_a D_y \Phi(y, t) = \frac{1}{\Gamma(n - \alpha)} \frac{\partial^n}{\partial y^n} \int_a^y \frac{\Phi(s, t)}{(y - s)^{\alpha+1-n}} ds,$$

$${}_yD_b\Phi(y, t) = \frac{(-1)^n}{\Gamma(n - \alpha)} \frac{\partial^n}{\partial y^n} \int_y^b \frac{\Phi(s, t)}{(s - y)^{\alpha+1-n}} ds.$$

Definition 2. [23] Let the Laplacian $(-\Delta)$ has a complete set of orthonormal eigenfunctions ϕ_i associated with the eigenvalues λ_i within a bounded domain Ω under homogeneous boundary conditions, then

$$(-\Delta)^{\frac{\alpha}{2}}\Phi = \begin{cases} (-\Delta)^n\Phi & \text{if } \alpha = 2n, n \in \mathbb{N}_0 \\ (-\Delta)^{\frac{\alpha}{2}-n}(-\Delta)^n\Phi & \text{if } n-1 < \alpha \leq n, n \in \mathbb{N} \\ \sum_{i=1}^{\infty} \lambda_i^{\alpha} \langle \Phi, \phi_i \rangle \phi_i & \text{if } \alpha \leq 0 \end{cases}$$

Lemma 1. [24] For a function $\Phi(y)$ defined over the entire real line, $y \in (-\infty, \infty)$, we have

$$-(-\Delta)^{\frac{\alpha}{2}}\Phi(y) = -\frac{1}{2 \cos\left(\frac{\pi\alpha}{2}\right)} \left({}_{-\infty}D_y^{\alpha}\Phi(y) + {}_yD_{\infty}^{\alpha}\Phi(y) \right) = \frac{\partial^{\alpha}\Phi(y)}{\partial |y|^{\alpha}}.$$

This formulation showcases the application of the fractional Laplacian operator as a combination of the fractional derivatives of the left and right Riemann-Liouville. This encapsulates the operator's action on functions across unbounded domains.

The Tridiagonal Toeplitz Matrix

The symmetric tridiagonal Toeplitz matrix of size n is denoted by

$$M = \begin{pmatrix} r & q & & & \\ q & r & q & & \\ & \ddots & \ddots & \ddots & \\ & & q & r & q \\ & & & q & r \end{pmatrix} \quad (1.1)$$

Lemma 2. The tridiagonal Toeplitz matrix of the form (1.1) has the following eigenvalues and eigenvectors

$$\lambda_i = r + 2q \cos\left(\frac{i\pi}{n+1}\right), \quad i = 1, 2, \dots, n,$$

and

$$\mu_i = \begin{pmatrix} \sin\left(\frac{1i\pi}{n+1}\right) \\ \sin\left(\frac{2i\pi}{n+1}\right) \\ \sin\left(\frac{3i\pi}{n+1}\right) \\ \vdots \\ \sin\left(\frac{ni\pi}{n+1}\right) \end{pmatrix}, \quad i = 1, 2, \dots, n.$$

Proof. see [25].

Rational Approximations

Let $R_{a,b}(z)$ represent the (a, b) -Padé approximation, which denotes the $(a+b)^{\text{th}}$ order

Padé rational approximation of e^{-z} , defined as

$$R_{a,b}(z) = \frac{N_{a,b}(z)}{D_{a,b}(z)},$$

where

$$N_{a,b}(z) = \sum_{k=0}^a \frac{(b+a-k)!a!}{(a+b)!k!(a-k)!} (-z)^k,$$

$$D_{a,b}(z) = \sum_{k=0}^b \frac{(b+a-k)!b!}{(a+b)!k!(b-k)!} (z)^k.$$

Definition 3. A rational approximation $R_{a,b}(z)$ of e^z is said to be A -acceptable if $|R_{a,b}(z)| < 1$, whenever $\text{Re}(z) < 0$ and L -acceptable if it is A -acceptable and, additionally, $|R_{a,b}(z)| \rightarrow 0$ as $\text{Re}(z) \rightarrow -\infty$

- L -acceptable when $a = b - 2$ or $a = b - 1$.
- A -acceptable when $a = b$.

1.2 Problem Description

In this thesis, we consider the following space-fractional reaction-diffusion equation

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} = -\mathcal{K}(-\Delta)^{\frac{\alpha}{2}} u(\mathbf{x}, t) + f(u, t), \quad 1 < \alpha \leq 2, \quad (\mathbf{x}, t) \in \Omega \times (0, T], \quad (1.2)$$

$$u(\mathbf{x}, 0) = \Psi(\mathbf{x}) \quad \mathbf{x} \in \Omega \subset \mathbb{R}^m, \quad m = 1, 2, 3.$$

We consider the problems with homogeneous Neumann as well as homogeneous Dirichlet boundary conditions. Where $(-\Delta)^{\frac{\alpha}{2}}$ is the fractional Laplacian of order $1 < \alpha \leq 2$,

Ω is a bounded subset of $\mathbb{R}^m$, the constant $\mathcal{K}$ represents the diffusion coefficient and $f(u, t)$ represents the non-linear reaction term. Ensuring the existence of a unique solution of equation (1.2) under specified initial and boundary conditions requires certain assumptions. Specifically, the function f is assumed to be sufficiently smooth with respect to both u and t , and for constant $L > 0$ its partial derivative with respect to u must satisfies $f_u \geq -L$ [26].

In this thesis, we explore non-linear time-dependent Fractional Partial Differential Equations (FPDEs) systems, which are applied in diverse fields, including mathematical modeling of chemical, physical, biological phenomena. These equations typically include two important terms: the reaction term, which captures the interactions between different physical and biological species, and the diffusion term, which describes the random movement of each constituent[27]. Specifically, we delve into several reaction-diffusion models, including:

Fisher's Equation

Fisher's equation is a well-known reaction-diffusion model often discussed in the realm of non-linear time-dependent fractional partial differential equations. It serves as a classic representation of how populations spread spatially, incorporating a reaction term that reflects logistic growth [28]. The equation, commonly expressed as

$$\frac{\partial u}{\partial t} = -\mathcal{K}(-\Delta)^{\frac{\alpha}{2}}u + ru(1 - u),$$

where

- The population density at a given time t and position x is represented by $u(x, t)$.

- $\mathcal{K}$ represents the diffusion coefficient.
- r signifies the growth rate.
- The term $ru(1 - u)$ characterizes logistic growth or the reaction term.

Allen-Cahn Model

The Allen-Cahn model, established in 1958 by John E. Hilliard and John W. Cahn, describes the behavior of phase separation and interface movement at phase transitions [29].

$$\frac{\partial u}{\partial t} = -\mathcal{K}(-\Delta)^{\alpha/2}u + u - u^3.$$

It provides a mathematical framework for exploring phase separation and pattern formation across a range of physical and chemical systems. Widely applied in fields such as computational physics, materials science, solid-state physics, condensed matter physics, and the analysis of microstructure evolution.

FitzHugh-Nagumo model

The FitzHugh-Nagumo model, formulated by Richard FitzHugh and J. Nagumo in the 1960s, comprises fractional differential equations that describe dynamic processes in excitable cells [30], [31].

$$\begin{aligned}\frac{\partial u}{\partial t} &= -\mathcal{K}(\Delta)^{\frac{\alpha}{2}}u - v + u(1 - u)(u - a) \\ \frac{\partial v}{\partial t} &= \epsilon(\delta u - \beta v - \gamma).\end{aligned}$$

This system provides valuable insights into the generation and propagation of action potentials, the electrical signals crucial for neuron communication. Researchers em-

ploy this model to investigate phenomena such as excitability, oscillations, and wave propagation in neurons and other excitable cells. Excitable cells, a specialized cell type, possess the unique ability to produce and transmit electrical impulses, which are essential for transmitting signals within the nervous system and supporting various physiological functions.

1.3 Literature Review

Many numerical approaches for the fractional reaction-diffusion equations have been developed [32], [33], [34], [35]. By using the finite difference approach, Tadjeran and Meerschaert [36] were able to derive numerical solutions for the equation relating to fractional advection–dispersion flow in Caputo space. Shen et al. [37] and Liu and Shen [38] respectively, developed some numerical solutions for the fractional advection–dispersion equation in Riesz space and the space fractional diffusion equation.

In addition, for fractional derivatives in Riesz space, Yang et al. [24] derived numerical methods to solve fractional partial differential equations. Ding and Zhang in [39] developed numerical solutions for the advection–dispersion equation and fractional diffusion equation in Riesz space. Rahman et al. in [13] were able to find improved numerical solutions for the fractional advection–dispersion equation and fractional diffusion equation in Riesz space using Matrix Transform Technique (MTT) approach. Fourth order Runge-Kutta type L -stable and A -stable schemes were developed by Furati et al. in [40] for one dimensional and by Yousuf et al. in [41] for two di-

mensional problems. Fourth-order time stepping techniques with MTT approach for space-fractional reaction-diffusion equations were derived by Alzahrani et al. [42]. Recently, Yousuf and Sarwar [43] proposed a highly efficient numerical algorithm using Gaussian quadrature pole rational approximation for inhomogeneous space variable order fractional reaction-diffusion models.

1.4 Thesis Structure

In Chapter 2, we introduce highly efficient numerical schemes to solve space-fractional differential equations on finite domains. For spatial discretization, we utilize the fourth-order Matrix Transform Technique (MTT) to obtain the semi-discretized equation and use Exponential Time Differencing Runge-Kutta (ETDRK) type schemes to solve it in time. The ETDRK schemes are developed by using L -acceptable Padé (1,2) approximation and by using a single real pole rational approximation of the matrix exponential functions. Numerical experiments are explored to verify the convergence and stability. In Chapter 3, we extend our investigation by employing similar methodologies as in Chapter 2, but with a different approach for spatial discretization. Instead of utilizing the Matrix Transform Technique (MTT), we employ the Fourier spectral method to efficiently manage the numerical challenges posed by the non-local characteristics of the fractional Laplacian operator. We conduct numerical experiments to validate the convergence, stability, and effectiveness of the Fourier spectral approach in achieving accurate and reliable solutions. All the calculations are performed using an Intel iCore i7 Central Processing Unit (CPU) with 2.90GHz speed. In Chapter 4,

we present a comprehensive summary of the work conducted throughout the thesis.

CHAPTER 2

THIRD-ORDERED ETD

SCHEMES WITH

HOMOGENEOUS OR

NON-HOMOGENEOUS BCS

In this chapter, third-order numerical schemes were introduced for solving space-fractional reaction-diffusion equations, applicable to both non-homogeneous and homogeneous Boundary Conditions (BCs). We employ an enhanced version of the Matrix Transform Technique (MTT) tailored to accommodate non-homogeneous boundary conditions for the spatial discretization. For the temporal discretization, we combine the MTT approach with Exponential Time Differencing Runge-Kutta (ETDRK) method. Our ETDRK methods utilize a single pole third-order restricted Padé approximation and a third-order Padé (1,2) approximation for matrix exponential func-

tions. Because of the high-frequency components in the solution, we observe that the numerical A-stable scheme can lead to undesired oscillations. Interestingly, reducing the space-fractional derivative order helps mitigate these undesired oscillations. To address computational efficiency, we apply the partial fraction splitting approach, effectively reducing the computational demands of the schemes. Through numerical experimentation, we demonstrate the scheme's accuracy and reliability.

2.1 Matrix Transform Technique for Homogeneous BCs

Ilic et al[23] initially introduced the matrix transform method (MTT). They discretized the spatial derivative of the fractional Laplacian $(\Delta)^{\frac{\alpha}{2}}$ using a uniformly discretized mesh with step size h and a finite difference techniques. We consider the classical space diffusion equation

$$\begin{aligned}\frac{\partial u(x, t)}{\partial t} &= -\mathcal{K} \left[\frac{-\partial^2}{\partial x^2} u(x, t) \right], & x \in \Omega, \ t > 0, \\ u(x, 0) &= \Psi(x), & x \in \Omega \subset \mathbb{R}^m, m = 1, 2, 3.\end{aligned}$$

subject to the homogeneous Neumann or Dirichlet BCs. Let the discrete spatial step be denoted by h and $u_k(t) = u(x_k, t)$ for $k = 1, 2, \dots, M - 1$, where the constant M represents a positive integer. The spatial derivative is then approximated using the

following fourth-order approximation

$$\frac{du_k(t)}{dt} = -\mathcal{K} \left[-\frac{1}{h^2} \frac{\delta_x^2}{1 + \frac{1}{12}\delta_x^2} \right] u_k(t),$$

where $\delta_x^2 u_k(t) = u_{k-1}(t) - 2u_k(t) + u_{k+1}(t)$ represents the 2^{nd} order central difference operator.

Thus, a system of ODEs may be used to represent these finite difference approximation as follows

$$\frac{du_k(t)}{dt} = -\frac{\mathcal{K}}{h^2} \left[\frac{-u_{k-1}(t) + 2u_k(t) - u_{k+1}(t)}{\frac{1}{12}u_{k-1}(t) + \frac{5}{6}u_k(t) + \frac{1}{12}u_{k+1}(t)} \right]$$

which can be compactly expressed in form of matrices as

$$\begin{aligned} \frac{dU(t)}{dt} &= -\mathcal{K} \frac{A^{-1}B}{h^2} U(t), \\ U(0) &= U_0 \end{aligned} \tag{2.1}$$

where

$$U(t) = [u_1(t), u_2(t), \dots, u_{M-1}(t)]^T \text{ and } U_0 = U(0).$$

The following tridiagonal matrices A and B , each of size $M - 1 \times M - 1$, are both

diagonally dominant

$$A = \begin{pmatrix} \frac{5}{6} & \frac{1}{12} & 0 & \cdots & 0 & 0 \\ \frac{1}{12} & \frac{5}{6} & \frac{1}{12} & 0 & \cdots & 0 \\ 0 & \frac{1}{12} & \frac{5}{6} & \frac{1}{12} & 0 & \cdots \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & 0 & \frac{1}{12} & \frac{5}{6} & \frac{1}{12} & 0 \\ 0 & \cdots & 0 & \frac{1}{12} & \frac{5}{6} & \frac{1}{12} \\ 0 & 0 & \cdots & 0 & \frac{1}{12} & \frac{5}{6} \end{pmatrix}, \quad B = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & 0 & \cdots \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & 0 & -1 & 2 & -1 & 0 \\ 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & 0 & \cdots & 0 & -1 & 2 \end{pmatrix},$$

Based on Definition 2 in section (1.1), we can rewrite (1.2) as

$$\frac{\partial u(x, t)}{\partial t} = -\mathcal{K} \left(-\frac{\partial^2}{\partial x^2} \right)^{\frac{\alpha}{2}-1} \left(-\frac{\partial^2}{\partial x^2} \right) u(x, t) + f(u, t)$$

From equation (2.1), the above equation can be expressed as

$$\frac{dU(t)}{dt} = -\mathcal{K} \left(\frac{A^{-1}B}{h^2} \right)^{\frac{\alpha}{2}-1} \left(\frac{A^{-1}B}{h^2} \right) U(t)$$

Let $P = A^{-1}B$, where an invertible matrix E exists, allowing us to represent P as

$$P = E\Lambda E^{-1}$$

where the matrices representing the eigenvalues and eigenvectors of the matrix P are denoted by Λ and E , respectively. From lemma 2 in section (1.1), we can defined Λ

and E for homogeneous Dirichlet BCs as

$$\Lambda = \begin{pmatrix} \xi_1 & & & \\ & \xi_2 & & \\ & & \ddots & \\ & & & \xi_{M-1} \end{pmatrix}, \quad E = \begin{pmatrix} \vartheta_1 & \vartheta_2 & \cdots & \vartheta_{M-1} \end{pmatrix}$$

where for one-dimensional problems ξ_k and ϑ_k are calculated as

$$\xi_k = \frac{4 \sin^2 \left(\frac{k\pi}{2M} \right)}{1 - \frac{1}{3} \sin^2 \left(\frac{k\pi}{2M} \right)},$$

$$\vartheta_k = \begin{pmatrix} \sin \left(\frac{1k\pi}{M} \right) \\ \sin \left(\frac{2k\pi}{M} \right) \\ \vdots \\ \sin \left(\frac{(M-1)k\pi}{M} \right) \end{pmatrix},$$

for $k = 1, 2, \dots, M-1$, and for two-dimensional problems ξ_{kl} and ϑ_{kl} are calculated

as

$$\xi_{kl} = \frac{4 \sin^2 \left(\frac{k\pi}{2M} \right) + 4 \sin^2 \left(\frac{l\pi}{2M} \right)}{\left[1 - \frac{1}{3} \sin^2 \left(\frac{k\pi}{2M} \right) \right] + \left[1 - \frac{1}{3} \sin^2 \left(\frac{l\pi}{2M} \right) \right]},$$

$$\vartheta_{kl} = \begin{pmatrix} \sin \left(\frac{1k\pi}{M} \right) \sin \left(\frac{1l\pi}{M} \right) \\ \vdots \\ \sin \left(\frac{(M-1)k\pi}{M} \right) \sin \left(\frac{(M-1)l\pi}{M} \right) \end{pmatrix},$$

for $k, l = 1, 2, \dots, M-1$.

Whereas for homogeneous Neumann BCs, Λ and E are defined as

$$\Lambda = \begin{pmatrix} \xi_0 & & & \\ & \xi_1 & & \\ & & \ddots & \\ & & & \xi_M \end{pmatrix}, E = \begin{pmatrix} \vartheta_0 & \vartheta_1 & \cdots & \vartheta_M \end{pmatrix}$$

where for one-dimensional problems ξ_k and ϑ_k are calculated as

$$\xi_k = \frac{4 \cos^2 \left(\frac{k\pi}{2M} \right)}{1 - \frac{1}{3} \cos^2 \left(\frac{k\pi}{2M} \right)},$$

$$\vartheta_k = \begin{pmatrix} \sin \left(\frac{0k\pi}{M} \right) \\ \sin \left(\frac{1k\pi}{M} \right) \\ \vdots \\ \sin \left(\frac{(M)k\pi}{M} \right) \end{pmatrix},$$

for $k = 0, 1, \dots, M$, and for two-dimensional problems ξ_{kl} and ϑ_{kl} are calculated as

$$\xi_{kl} = \frac{4 \cos^2 \left(\frac{k\pi}{2M} \right) + 4 \cos^2 \left(\frac{l\pi}{2M} \right)}{\left[1 - \frac{1}{3} \cos^2 \left(\frac{k\pi}{2M} \right) \right] + \left[1 - \frac{1}{3} \cos^2 \left(\frac{l\pi}{2M} \right) \right]},$$

$$\vartheta_{kl} = \begin{pmatrix} \cos \left(\frac{0k\pi}{M} \right) \cos \left(\frac{0l\pi}{M} \right) \\ \vdots \\ \cos \left(\frac{(M)k\pi}{M} \right) \cos \left(\frac{(M)l\pi}{M} \right) \end{pmatrix},$$

for $k, l = 0, 1, 2, \dots, M$.

Therefore,

$$\frac{dU(t)}{dt} = -\frac{\mathcal{K}}{h^\alpha} P^{\alpha/2} U(t) = -\frac{\mathcal{K}}{h^\alpha} (E \Lambda^{\alpha/2} E^{-1}) U(t)$$

and the fractional Laplacian can be approximated as follows

$$(-\Delta)^{\frac{\alpha}{2}} u(x, t) \approx h^{-\alpha} P^{\frac{\alpha}{2}} u(t).$$

2.2 Matrix Transform Technique for Non-Homogeneous Dirichlet BCs

In this section, we consider the following one-dimensional non-homogeneous space-fractional reaction-diffusion problem

$$\begin{aligned} \frac{\partial u(x, t)}{\partial t} &= -\mathcal{K}(-\Delta)^{\frac{\alpha}{2}} u(x, t) + g(u, t), \quad 1 < \alpha \leq 2, \quad x \in (c, d), \quad t > 0, \\ u(x, 0) &= \psi(x), \quad c < x < d, \\ u(c, t) &= f(t) \text{ and } u(d, t) = h(t), \end{aligned} \tag{2.2}$$

where $(-\Delta)^{\frac{\alpha}{2}}$ represents the fractional Laplacian, which is established through the spectral decomposition methodology applied to the conventional Laplacian operator $(-\Delta)$. Ilic et al [23] initially introduced the matrix transform method (MTT) to approximate the fractional Laplacian using a uniformly discretized mesh with step size h for the homogeneous BCs. In this section, we extend this approach to handle non-homogeneous BCs. As we discussed in the previous Section (2.1) the fractional Laplacian operator with homogeneous boundary conditions can be discretized as follows

$$(-\Delta)^{\frac{\alpha}{2}} u(x, t) \approx h^{-\alpha} P^{\frac{\alpha}{2}} u(t)$$

The fractional Laplacian is represented in matrix form by using the eigenvectors and eigenvalues of the classical Laplace operator, as follows

$$P^{\frac{\alpha}{2}} = E\Lambda^{\frac{\alpha}{2}}E^{-1}.$$

where E represents the matrix of eigenvectors, while Λ represents the matrix of eigenvalues.

$$\Lambda = \text{diag}(\xi_1, \xi_2, \xi_3, \dots, \xi_{M-1}), \quad E = (\vartheta_1, \vartheta_2, \vartheta_3, \dots, \vartheta_{M-1}),$$

where $\xi_k = 4 \sin^2\left(\frac{k\pi}{2M}\right)$, and $\vartheta_k = \left(\sin\left(\frac{1k\pi}{M}\right), \sin\left(\frac{2k\pi}{M}\right), \sin\left(\frac{3k\pi}{M}\right), \dots, \sin\left(\frac{(M-1)k\pi}{M}\right)\right)^T$, $k = 1, 2, \dots, M-1$.

Using the finite difference approach, we obtain the matrix form of the classical Laplace operator, considering non-homogeneous BCs, as follows

$$(-\Delta)u \approx h^{-2}(Pu + \mathbf{v}_1 f(t) + \mathbf{v}_{m-1} h(t)).$$

In this context, $\mathbf{v}_i$ represents the $(i)^{\text{th}}$ standard basis vectors in $\mathbb{R}^{m-1}$. Using the definition in (1.1), we have

$$\begin{aligned} (-\Delta)^{\frac{\alpha}{2}}u &= (-\Delta)^{\frac{\alpha}{2}-1}(-\Delta)u \\ &\approx (h^{-2}P)^{\frac{\alpha}{2}-1} (h^{-2}(Pu + \mathbf{v}_1 f(t) + \mathbf{v}_{m-1} h(t))) \\ &= h^{-\alpha} P^{\frac{\alpha}{2}}u + h^{-\alpha} P^{\frac{\alpha}{2}-1} (\mathbf{v}_1 f(t) + \mathbf{v}_{m-1} h(t)) \end{aligned}$$

using the above MTT representation of the non-homogeneous boundary conditions, we can write (2.2) as

$$\frac{du}{dt} = -\frac{\mathcal{K}}{h^2}Pu + \frac{\mathcal{K}}{h^2}(\mathbf{v}_1 f(t) + \mathbf{v}_{m-1} h(t)) + g(u, t),$$

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

where Section (2.1) defines P .

2.3 Exponential Time Differencing

For the non-linear FPDEs, after discretizing the space-fractional derivative using an appropriate approximation methods, like finite element, spectral approach, finite difference, or another suitable approximation technique, we obtain a system of Ordinary Differential Equations (ODEs) with respect to time. The subsequent step involves solving these FPDEs by implementing an appropriate time-stepping method. Exponential Time Differencing (ETD) time-stepping schemes are renowned for their efficacy in time integration, offering compatibility with various spatial discretizations to achieve numerical solutions for semi-linear FPDEs. Exponential Time Differencing (ETD) schemes, initially introduced by Certaine [44] in the 1960s to solve partial differential equations, stand out for their precise handling of linear terms and the use of polynomial approximations for integral terms. This methodology significantly enhances computational efficiency by eliminating the requirement to solve non-linear systems at each time step. Further advancements were made by Cox and Mathews [45], who integrated these schemes with Runge-Kutta methods and polynomial expressions, thereby optimizing the approach for equations with integer-order derivatives and streamlining the solution process.

As mentioned in Section (2.1), the MTT approach can approximate the fractional Laplacian in form of matrix. This leads to the following system of ODEs

$$\begin{aligned}\frac{dU(t)}{dt} &= -\frac{\mathcal{K}}{h^\alpha} P^{\alpha/2} U(t) + F(U, t), \\ U(0) &= U_0\end{aligned}\tag{2.3}$$

where $U(t)$ and U_0 are defined as in (2.1), while $F(U, t)$ denotes the vector $[f(u_1(t), t), f(u_2(t), t), f(u_3(t), t), \dots, f(u_{M-1}(t), t)]^T$.

In case of the non-homogeneous BCs,

we consider $F(U, t) = \frac{\mathcal{K}}{h^2} (\mathbf{v}_1 f(t) + \mathbf{v}_{m-1} h(t)) + G(U, t)$, where $G(U, t)$ denotes the vector $[g(u_1(t), t), g(u_2(t), t), g(u_3(t), t), \dots, g(u_{M-1}(t), t)]^T$ and $\mathbf{v}_i$ represents the $(i)^{th}$ standard basis vectors in $\mathbb{R}^{m-1}$.

Let $B^{\frac{\alpha}{2}} = \frac{\mathcal{K}}{h^\alpha} P^{\alpha/2}$. by multiplying (2.3) by the integrating factor $e^{B^{\frac{\alpha}{2}} t}$ and integrate over t , we derive the following exact solution

$$U(t) = e^{-B^{\frac{\alpha}{2}} t} U_0 + \int_0^t e^{-(t-\tau)B^{\frac{\alpha}{2}}} F(U(\tau), \tau) d\tau\tag{2.4}$$

for the time discretization, let $t_n = nk$ where $n \in \mathbb{N}_0$ and k is the time step. By substituting t with $t+k$, and denoting $\tau - t$ as $k\mu$, we transform Equation (2.4) into the subsequent nonlinear Fredholm integral equation as

$$U(t+k) = e^{-kB^{\frac{\alpha}{2}}} U(t) + \int_0^1 k e^{-kB^{\frac{\alpha}{2}}(1-\mu)} F(u(t+\mu k), t+\mu k) d\mu,\tag{2.5}$$

we get the recurrence formula shown below

$$U(t_{n+1}) = e^{-kB^{\frac{\alpha}{2}}} U(t_n) + \int_0^1 k e^{-kB^{\frac{\alpha}{2}}(1-\mu)} F(u(t_n + \mu k), t_n + \mu k) d\mu. \quad (2.6)$$

2.3.1 The Third Order ETD Scheme

The integral in equation (2.6) involves the integral of the non-linear forcing term. Estimating the non-linear term $F(u(t_n + \mu k), t_n + \mu k)$ is the main purpose of the exponential time difference method. Cox and Mathews [45] introduced Runge-Kutta type time-stepping schemes for approximating the term $F(u(t_n + \mu k), t_n + \mu k)$. The first-order ETD scheme (ETD1) approximates $F(u(t_n + \mu k), t_n + \mu k)$ using a constant $\hat{F}_n$ over the interval $[t_n, t_{n+1}]$.

$$\begin{aligned} U_{n+1} &\approx e^{-\frac{k}{2}B^{\frac{\alpha}{2}}} U_n + \frac{k}{2} \int_0^1 e^{-\frac{k}{2}B^{\frac{\alpha}{2}}(1-\mu)} \hat{F}_n d\mu \\ &= e^{-\frac{k}{2}B^{\frac{\alpha}{2}}} U_n + (B^{\frac{\alpha}{2}})^{-1} \left(e^{-\frac{k}{2}B^{\frac{\alpha}{2}}} - I \right) \hat{F}_n \end{aligned}$$

Let

$$\alpha_n = \rho_0 \left(\frac{kB^{\frac{\alpha}{2}}}{2} \right) U_n + \frac{k}{2} \rho_1 \left(\frac{kB^{\frac{\alpha}{2}}}{2} \right) \hat{F}_n \quad (2.7)$$

where $\rho_0(kB^{\frac{\alpha}{2}}) = e^{-kB^{\frac{\alpha}{2}}}$ and $\rho_1(kB^{\frac{\alpha}{2}}) = (-kB^{\frac{\alpha}{2}})^{-1} (e^{-kB^{\frac{\alpha}{2}}} - I)$.

To obtain a higher-order approximation, we assume $F(u(t_n + \mu k), t_n + \mu k) \approx 2\hat{F}(\alpha_n, t_n + k/2) - \hat{F}_n$ for $t_n \leq t \leq t_{n+1}$. Thus, we obtain the second-order ETD

scheme (ETD2)

$$\begin{aligned} U_{n+1} &\approx e^{-\frac{k}{2}B^{\frac{\alpha}{2}}} U_n + \frac{k}{2} \int_0^1 e^{-\frac{k}{2}B^{\frac{\alpha}{2}}(1-\mu)} \left(2\hat{F}_n^\alpha - \hat{F}_n \right) d\mu \\ &= e^{-\frac{k}{2}B^{\frac{\alpha}{2}}} U_n + (B^{\frac{\alpha}{2}})^{-1} \left(e^{-\frac{k}{2}B^{\frac{\alpha}{2}}} - I \right) \left(2\hat{F}_n^\alpha - \hat{F}_n \right) \end{aligned}$$

where $\hat{F}(\alpha_n, t_n + k/2)$ denoted as $\hat{F}_n^\alpha$.

The ETD2 can be written as

$$\beta_n = \rho_0 \left(\frac{k}{2} B^{\frac{\alpha}{2}} \right) U_n + \frac{k}{2} \rho_1 \left(\frac{k}{2} B^{\frac{\alpha}{2}} \right) \left(2\hat{F}_n^\alpha - \hat{F}_n \right) \quad (2.8)$$

In addition, by using α_n and β_n defined in (2.7) and (2.8) to approximated the non-linear forcing term by a quadratic polynomial

$$F(u(t_n + \mu k), t_n + \mu k) \approx \hat{F}_n + (t - t_n) \left(4\hat{F}_n^\alpha - 3\hat{F}_n - \hat{F}_n^\beta \right) + \frac{(t - t_n)^2}{2} \left(\hat{F}_n - 2\hat{F}_n^\alpha + \hat{F}_n^\beta \right),$$

where $\hat{F}_n^\beta = \hat{F}(\beta_n, t_n + k)$. We arrived to the following third-order ETD scheme (ETD3)

$$\begin{aligned} U_{n+1} &= \rho_0(kB^{\frac{\alpha}{2}})U_n + k\rho_1(kB^{\frac{\alpha}{2}})\hat{F}_n + k\rho_2(kB^{\frac{\alpha}{2}}) \left(4\hat{F}_n^\alpha - 3\hat{F}_n - \hat{F}_n^\beta \right) \\ &\quad + 4k\rho_3(kB^{\frac{\alpha}{2}}) \left(\hat{F}_n - 2\hat{F}_n^\alpha + \hat{F}_n^\beta \right) \\ &= \rho_0(kB^{\frac{\alpha}{2}})U_n + \left(k\rho_1(kB^{\frac{\alpha}{2}}) - 3k\rho_2(kB^{\frac{\alpha}{2}}) + 4k\rho_3(kB^{\frac{\alpha}{2}}) \right) \hat{F}_n \\ &\quad + \left(4k\rho_2(kB^{\frac{\alpha}{2}}) - 8k\rho_3(kB^{\frac{\alpha}{2}}) \right) \hat{F}_n^\alpha + \left(4k\rho_3(kB^{\frac{\alpha}{2}}) - k\rho_2(kB^{\frac{\alpha}{2}}) \right) \hat{F}_n^\beta \end{aligned} \quad (2.9)$$

where

$$\begin{aligned}\rho_2(kB^{\frac{\alpha}{2}}) &= (-kB^{\frac{\alpha}{2}})^{-2} \left(e^{-kB^{\frac{\alpha}{2}}} + kB^{\frac{\alpha}{2}} - I \right), \\ \rho_3(kB^{\frac{\alpha}{2}}) &= (-kB^{\frac{\alpha}{2}})^{-3} \left(e^{-kB^{\frac{\alpha}{2}}} + kB^{\frac{\alpha}{2}} - \frac{(kB^{\frac{\alpha}{2}})^2}{2} - I \right).\end{aligned}$$

Computing matrix exponential is computationally intensive. Even for matrices with sparse representations, their exponentials may not retain the same sparsity. Particularly when dealing with a non-diagonal linear operator, direct implementation of this scheme may encounter numerical instability, especially if $B^{\frac{\alpha}{2}}$ possesses eigenvalues that approach zero. This challenge arises due to the requirement of computing, $e^{-kB^{\frac{\alpha}{2}}}$, $e^{-kB^{\frac{\alpha}{2}}/2}$, $(-B^{\frac{\alpha}{2}})^{-1}$, $(-B^{\frac{\alpha}{2}})^{-2}$, and $(-B^{\frac{\alpha}{2}})^{-3}$ are needed.

This chapter proposes a modification of equation (2.9) that utilizes third-order Padé(1,2) and single pole restricted Padé approximation for the matrix exponential function e^{-z} .

ETD-Padé(1,2) Scheme

Approximating a function by a rational function is called the Padé approximation. It frequently produces a better representation of the function than truncating its Taylor series. In this section, we use the Padé (1,2) approximation to approximate the matrix exponential functions $e^{-\frac{kB^{\frac{\alpha}{2}}}{2}}$ and $e^{-kB^{\frac{\alpha}{2}}}$. The Padé (1,2) approximation is of the third-order L-acceptable is defined by

$$R_{1,2}(z) = \frac{6 - 2z}{z^2 + 4z + 6} \quad (2.10)$$

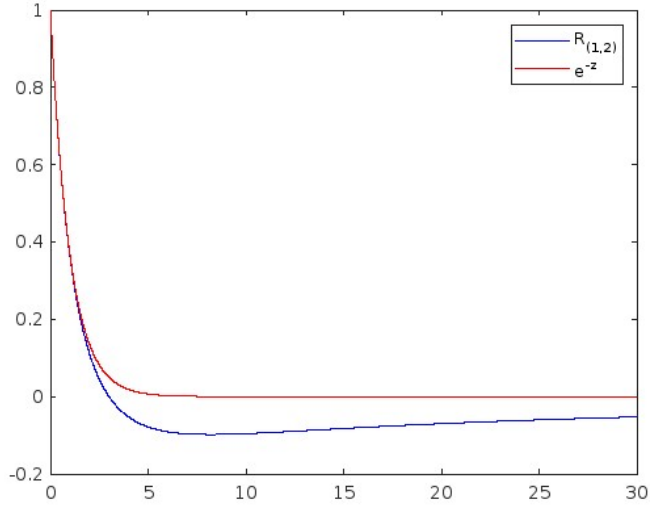


Figure 2.1: The behavior of $R_{1,2}(z)$ compared to e^{-z} over the interval $0 \leq z \leq 30$.

Based on definition 3 in Section (1.1), we can show that Padé (1,2) is L-acceptable by show the behavior of $R_{1,2}(z)$ and e^{-z} in figure (2.1) for $0 \leq z \leq 30$. The approximation provided in Equation (2.10) is verified to have third-order accuracy through the following demonstration

$$e^{-z} = 1 - z + \frac{1}{2}z^2 - \frac{1}{6}z^3 + \frac{1}{24}z^4 + \mathcal{O}(z^5),$$

$$R_{1,2}(z) = 1 - z + \frac{1}{2}z^2 - \frac{1}{6}z^3 + \frac{1}{36}z^4 + \mathcal{O}(z^5)$$

Then

$$\begin{aligned} \|e^{-z} - R_{1,2}(z)\| &= \left(\frac{1}{24} - \frac{1}{36}\right)z^4 + \mathcal{O}(z^5), \\ &= 0.013889z^4 + \mathcal{O}(z^5) \end{aligned}$$

as $z \rightarrow 0$ the approximation is of the third-order accuracy.

The modification of the third-order ETD scheme (ETD3) using Padé (1,2) approxi-

mation to approximate e^{-z} in (2.7)-(2.9) are obtained as

$$\begin{aligned}
\rho_0(kB^{\frac{\alpha}{2}}) &= R_{1,2}(kB^{\frac{\alpha}{2}}), \\
\rho_1(kB^{\frac{\alpha}{2}}) &= (-kB^{\frac{\alpha}{2}})^{-1} (R_{1,2}(kB^{\frac{\alpha}{2}}) - I) \\
&= \left(6I + 4kB^{\frac{\alpha}{2}} + kB^{\frac{\alpha}{2}2}\right)^{-1} (kB^{\frac{\alpha}{2}} + 6I), \\
\rho_2(kB^{\frac{\alpha}{2}}) &= (-kB^{\frac{\alpha}{2}})^{-2} (R_{1,2}(kB^{\frac{\alpha}{2}}) - I + kB^{\frac{\alpha}{2}}) \\
&= \left(6I + 4kB^{\frac{\alpha}{2}} + kB^{\frac{\alpha}{2}2}\right)^{-1} (kB^{\frac{\alpha}{2}} + 3I), \\
\rho_3(kB^{\frac{\alpha}{2}}) &= (-kB^{\frac{\alpha}{2}})^{-3} \left(R_{1,2}(kB^{\frac{\alpha}{2}}) - I + kB^{\frac{\alpha}{2}} - \frac{(kB^{\frac{\alpha}{2}})^2}{2}\right) \\
&= \left(12I + 8kB^{\frac{\alpha}{2}} + 2kB^{\frac{\alpha}{2}2}\right)^{-1} (kB^{\frac{\alpha}{2}} + 2I).
\end{aligned} \tag{2.11}$$

The advantages of using the rational approximation is not limited to approximate exponential functions, but also eliminating the inverse of the matrices $(-kB^{\frac{\alpha}{2}})^{-1}$, $(-kB^{\frac{\alpha}{2}})^{-1}$, and $(-kB^{\frac{\alpha}{2}})^{-3}$. Rearranging the terms using the approximation discussed above in (2.11) leads to the development of the new ETD-Padé(1,2) scheme

$$U_{n+1} = R_{1,2}(kB^{\frac{\alpha}{2}})U_n + \hat{\Phi}_1(kB^{\frac{\alpha}{2}})\hat{F}_n + \hat{\Phi}_2(kB^{\frac{\alpha}{2}})\hat{F}_n^\alpha + \hat{\Phi}_3(kB^{\frac{\alpha}{2}})\hat{F}_n^\beta, \tag{2.12}$$

where

$$\begin{aligned}\hat{\Phi}_1(z) &= \frac{k}{z^2 + 4z + 6}, \\ \hat{\Phi}_2(z) &= \frac{4k}{z^2 + 4z + 6}, \\ \hat{\Phi}_3(z) &= \frac{(z+1)k}{z^2 + 4z + 6}.\end{aligned}$$

and

$$\begin{aligned}\alpha_n &= \tilde{R}_{1,2}(kB^{\frac{\alpha}{2}})U_n + \tilde{\Psi}_1(kB^{\frac{\alpha}{2}})\hat{F}_n, \\ \beta_n &= R_{1,2}(kB^{\frac{\alpha}{2}})U_n + \tilde{\Psi}_2(kB^{\frac{\alpha}{2}})\left(2\hat{F}_n^\alpha - \hat{F}_n\right),\end{aligned}$$

where

$$\begin{aligned}\tilde{R}_{1,2}(z) &= \frac{24 - 4z}{z^2 + 8z + 24}, \\ \tilde{\Psi}_1(z) &= \frac{(z+12)k}{z^2 + 8z + 24}, \\ \tilde{\Psi}_2(z) &= \frac{(z+6)k}{z^2 + 4z + 6}.\end{aligned}$$

To enhance readability for readers, we replace $kB^{\frac{\alpha}{2}}$ by the variable z .

The scheme's partial fraction splitting approach

The scheme in (2.12) still require inverting quadratic matrix polynomials. The partial fraction splitting technique was employed to address this issue. The poles and weights below are determined using the partial fraction splitting approach and the MAPLESOFT program

$$R_{1,2}(\omega) = \frac{a_1}{(\omega + b_1)} + \frac{a_2}{(\omega + \bar{b}_1)},$$

$$\hat{\Phi}_1(\omega) = \frac{a_{11}}{(\omega + b_1)} + \frac{a_{12}}{(\omega + \bar{b}_1)},$$

$$\hat{\Phi}_2(\omega) = \frac{a_{21}}{(\omega + b_1)} + \frac{a_{22}}{(\omega + \bar{b}_1)},$$

$$\hat{\Phi}_3(\omega) = \frac{a_{31}}{(\omega + b_1)} + \frac{a_{32}}{(\omega + \bar{b}_1)},$$

where

$$a_1 = -1.0 + 3.53553390593273i, \quad a_2 = -1.0 + 3.53553390593273i = a_1,$$

$$a_{11} = -0.353553390593273i, \quad a_{12} = 0.353553390593273i,$$

$$a_{21} = -1.41421356237309i, \quad a_{22} = 1.41421356237309i,$$

$$a_{31} = 0.5 + 0.353553390593273i, \quad a_{32} = 0.5 - 0.353553390593273i,$$

$$b_1 = 2.0 - 1.41421356237310i, \quad \bar{b}_1 = 2.0 + 1.41421356237310i.$$

Also, the poles and weights of α_n and β_n are calculated as

$$\tilde{R}_{1,2}(\omega) = \frac{\tilde{a}_1}{(\omega + c_1)} + \frac{\tilde{a}_2}{(\omega + \bar{c}_1)},$$

$$\tilde{\Psi}_1(\omega) = \frac{\tilde{a}_{11}}{(\omega + c_1)} + \frac{\tilde{a}_{12}}{(\omega + \bar{c}_1)},$$

$$\tilde{\Psi}_2(\omega) = \frac{\tilde{a}_{21}}{(\omega + b_1)} + \frac{\tilde{a}_{22}}{(\omega + \bar{b}_1)},$$

where

$$\tilde{a}_1 = -2.000000000000001 + 7.07106781186548i,$$

$$\tilde{a}_2 = -1.999999999999999 + 7.07106781186548i,$$

$$\tilde{a}_{11} = 0.5 - 1.41421356237310i, \quad \tilde{a}_{12} = 0.5 + 1.41421356237310i,$$

$$\tilde{a}_{21} = 0.5 - 1.41421356237310i = \tilde{a}_{11}, \quad \tilde{a}_{22} = 0.5 + 1.41421356237310i = \tilde{a}_{12},$$

$$c_1 = 4.0 - 2.82842712474619i, \quad \bar{c}_1 = 4.0 + 2.82842712474619i.$$

The modified ETD-Padé(1,2) scheme for (2.12) becomes

$$\begin{aligned} U_{n+1} = & \left[\frac{a_1}{(\omega + b_1)} + \frac{a_2}{(\omega + \bar{b}_1)} \right] U_n + k \left[\frac{a_{11}}{(\omega + b_1)} + \frac{a_{12}}{(\omega + \bar{b}_1)} \right] \hat{F}_n \\ & + k \left[\frac{a_{21}}{(\omega + b_1)} + \frac{a_{22}}{(\omega + \bar{b}_1)} \right] \hat{F}_n^\alpha + k \left[\frac{a_{31}}{(\omega + b_1)} + \frac{a_{32}}{(\omega + \bar{b}_1)} \right] \hat{F}_n^\beta \end{aligned}$$

and

$$\begin{aligned} \alpha_n = & \left[\frac{\tilde{a}_1}{(\omega + c_1)} + \frac{\tilde{a}_2}{(\omega + \bar{c}_1)} \right] U_n + k \left[\frac{\tilde{a}_{11}}{(\omega + c_1)} + \frac{\tilde{a}_{12}}{(\omega + \bar{c}_1)} \right] \hat{F}_n, \\ \beta_n = & \left[\frac{a_1}{(\omega + b_1)} + \frac{a_2}{(\omega + \bar{b}_1)} \right] U_n + k \left[\frac{\tilde{a}_{21}}{(\omega + b_1)} + \frac{\tilde{a}_{22}}{(\omega + \bar{b}_1)} \right] \left(2\hat{F}_n^\alpha - \hat{F}_n \right). \end{aligned}$$

The ETD-Padé(1,2) Scheme Algorithm

Below is the algorithm for the ETD-Padé(1,2) scheme

Algorithm 1 The ETD-Padé(1,2) algorithm

```

1: for  $n = 1, 2, \dots, M = T/k$  do
2: Step I : Compute  $\alpha_n$ 
3:   Solve  $(kB^{\frac{\alpha}{2}} + c_1I)Y = (\tilde{a}_1U_n + k\tilde{a}_{11}\hat{F}_n)$  for  $Y$ .
4:   Compute  $\alpha_n = 2\operatorname{Re}(Y)$ .
5: Step II : Compute  $\beta_n$ 
6:   Solve  $(kB^{\frac{\alpha}{2}} + b_1I)X = (a_1U_n + k\tilde{a}_{21}(2\hat{F}_n^\alpha - \hat{F}_n))$  for  $X$ .
7:   Compute  $\beta_n = 2\operatorname{Re}(X)$ .
8: Step III : Compute  $U_{n+1}$ 
9:   Solve  $(kB^{\frac{\alpha}{2}} + b_1I)W = (a_1U_n + k(a_{11}\hat{F}_n + a_{21}\hat{F}_n^\alpha + a_{31}\hat{F}_n^\beta))$  for  $W$ 
10:  Compute  $U_{n+1} = 2\operatorname{Re}(W)$ .
11: end for

```

ETD-Restricted Padé Scheme

A single pole third order restricted Padé approximation is a technique employed to approximate exponential functions and make them more amenable to analysis. The restricted Padé approximation is defined as

$$\begin{aligned}
R_h(z) &= 1 - \frac{2z}{2 + (1 + \frac{\sqrt{3}}{3})z} - \frac{\sqrt{3}}{6} \left(\frac{2z}{2 + (1 + \frac{\sqrt{3}}{3})z} \right)^2 \\
&= \frac{6(6 + 2\sqrt{3}z - (1 + \sqrt{3})z^2)}{(6 + (3 + \sqrt{3})z)^2}
\end{aligned} \tag{2.13}$$

we note that $R_h(z)$ is a decreasing function over the interval $0 < z < \infty$. The approximation is intended to be stable throughout a wide range of z values. The stability is determined by examining the limit of $R_h(z)$ as z approaches infinity, guaranteeing that the scheme remains bounded and stable $R_h(\infty) = 1 - \sqrt{3} > -1$. Comparing the

restricted Padé approximation $R_h(z)$ to e^{-z} the exponential decay function to determine its accuracy. It is noticed that the difference between $R_h(z)$ and e^{-z} is of the order $O(z^4)$ as z approaches zero, which indicates that the scheme has a third-order accuracy [46].

$$\begin{aligned}
e^{-z} &= 1 - z + \frac{1}{2}z^2 - \frac{1}{6}z^3 + \frac{1}{24}z^4 + \mathcal{O}(z^5), \\
R_h(z) &= 1 - z + \frac{1}{2}z^2 - \frac{1}{6}z^3 - \frac{\sqrt{3}}{36}z^4 + \mathcal{O}(z^5), \\
||e^{-z} - R_h(z)|| &= \left(\frac{1}{24} - \frac{\sqrt{3}}{36}\right)z^4 + \mathcal{O}(z^5) \\
&= 0.0898z^4 + \mathcal{O}(z^5).
\end{aligned}$$

Figure (2.2) shows the behavior of $R_h(z)$ compared to e^{-z} for $0 \leq z \leq 30$, which demonstrate that the restricted Padé approximation is A-acceptable. Unlike other methods that may need complex arithmetic owing to complex conjugate roots in the denominator, the restricted Padé approximation is fully real arithmetic. This simplifies the implementation and lowers computational cost.

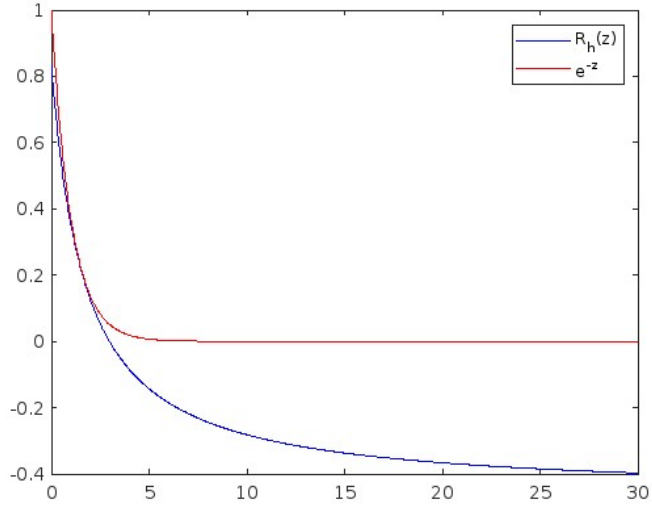


Figure 2.2: The behavior of $R_h(z)$ compared to e^{-z} over the interval $0 \leq z \leq 30$.

By replacing the exponential e^{-z} in (2.7)-(2.9) by $R_h(z)$, we have

$$\begin{aligned}
\rho_0(kB^{\frac{\alpha}{2}}) &= R_h(kB^{\frac{\alpha}{2}}), \\
\rho_1(kB^{\frac{\alpha}{2}}) &= (-kB^{\frac{\alpha}{2}})^{-1} (R_h(kB^{\frac{\alpha}{2}}) - I) \\
&= \left(6I + (3 + \sqrt{3})kB^{\frac{\alpha}{2}}\right)^{-2} \left((12\sqrt{3} + 18)kB^{\frac{\alpha}{2}} + 36I\right), \\
\rho_2(kB^{\frac{\alpha}{2}}) &= (-kB^{\frac{\alpha}{2}})^{-2} (R_h(kB^{\frac{\alpha}{2}}) - I + kB^{\frac{\alpha}{2}}) \\
&= \left(6I + (3 + \sqrt{3})kB^{\frac{\alpha}{2}}\right)^{-2} \left((6\sqrt{3} + 12)kB^{\frac{\alpha}{2}} + 18I\right), \\
\rho_3(kB^{\frac{\alpha}{2}}) &= (-kB^{\frac{\alpha}{2}})^{-3} \left(R_h(kB^{\frac{\alpha}{2}}) - I + kB^{\frac{\alpha}{2}} - \frac{(kB^{\frac{\alpha}{2}})^2}{2}\right) \\
&= \left(6I + (3 + \sqrt{3})kB^{\frac{\alpha}{2}}\right)^{-2} \left((3\sqrt{3} + 6)kB^{\frac{\alpha}{2}} + 6I\right).
\end{aligned} \tag{2.14}$$

By using the third-order restricted Padé A-stable approximation, we found that the

inverse of the matrices $(-kB^{\frac{\alpha}{2}})^{-1}$, $(-kB^{\frac{\alpha}{2}})^{-1}$, and $(-kB^{\frac{\alpha}{2}})^{-3}$ are cancelled. After rearranging the terms in (2.9) and using (2.14), we obtained the ETD- Restricted Padé scheme as follows

$$U_{n+1} = R_h(kB^{\frac{\alpha}{2}})U_n + \hat{\Phi}_1(kB^{\frac{\alpha}{2}})\hat{F}_n + \hat{\Phi}_2(kB^{\frac{\alpha}{2}})\hat{F}_n^\alpha + \hat{\Phi}_3(kB^{\frac{\alpha}{2}})\hat{F}_n^\beta, \quad (2.15)$$

where

$$\begin{aligned} \hat{\Phi}_1(z) &= \frac{6(1 + (\sqrt{3})z)k}{(6 + (3 + \sqrt{3})z)^2}, \\ \hat{\Phi}_2(z) &= \frac{24k}{(6 + (3 + \sqrt{3})z)^2}, \\ \hat{\Phi}_3(z) &= \frac{6(1 + (2 + \sqrt{3})z)k}{(6 + (3 + \sqrt{3})z)^2}, \end{aligned}$$

and

$$\begin{aligned} \alpha_n &= \tilde{R}_h(kB^{\frac{\alpha}{2}})U_n + \tilde{\Psi}_1(kB^{\frac{\alpha}{2}})\hat{F}_n, \\ \beta_n &= R_h(kB^{\frac{\alpha}{2}})U_n + \tilde{\Psi}_2(kB^{\frac{\alpha}{2}})\left(2\hat{F}_n^\alpha - \hat{F}_n\right), \end{aligned}$$

where

$$\begin{aligned} \tilde{R}_h(z) &= \frac{(144 + 24\sqrt{3}z - 6(1 + \sqrt{3})z^2)}{(12 + (3 + \sqrt{3})z)^2}, \\ \tilde{\Psi}_1(z) &= \frac{(72 + 6(3 + 2\sqrt{3})z)k}{(12 + (3 + \sqrt{3})z)^2}, \\ \tilde{\Psi}_2(z) &= \frac{(36 + 6(3 + 2\sqrt{3})z)k}{(6 + (3 + \sqrt{3})z)^2}. \end{aligned}$$

for simplicity, we write the previous expressions as functions of the variable z .

The scheme's partial fraction splitting approach

The inverses of higher-order matrix polynomials found in the considered ETD-Restricted Padé scheme (2.15) might lead to computational difficulties when calculating the power of these matrix polynomials, including roundoff errors and large condition numbers. As suggested by E. Gallopoulos and Y. Saad in [47] and Khaliq et al. in [48], the partial fraction decomposition approach was used to solve this issue. MATLAB is used to implement the partial fraction decomposition method to determine the following weights and poles

$$R_h(\omega) = a_0 + \frac{a_1}{(\omega + b_1)} + \frac{a_2}{(\omega + b_1)^2},$$

$$\hat{\Phi}_1(\omega) = \frac{a_{11}}{(\omega + b_1)} + \frac{a_{12}}{(\omega + b_1)^2},$$

$$\hat{\Phi}_2(\omega) = \frac{a_{22}}{(\omega + b_1)^2},$$

$$\hat{\Phi}_3(\omega) = \frac{a_{31}}{(\omega + b_1)} + \frac{a_{32}}{(\omega + b_1)^2},$$

where

$$a_0 = -0.7320508076, \quad a_1 = 2.784609691, \quad a_2 = -0.7461339179,$$

$$a_{11} = 0.7320508076, \quad a_{12} = -0.6602540378,$$

$$a_{21} = 0.0000000000, \quad a_{22} = 1.07179677,$$

$$a_{31} = 1.0000000000, \quad a_{32} = -1.0000000000,$$

$$b_1 = 1.267949192.$$

Also, the poles and weights of α_n and β_n are calculated

$$\begin{aligned}\tilde{R}_h(\omega) &= \tilde{a}_0 + \frac{\tilde{a}_1}{(\omega + \tilde{b}_1)} + \frac{\tilde{a}_2}{(\omega + \tilde{b}_1)^2}, \\ \tilde{\Psi}_1(\omega) &= \frac{\tilde{a}_{11}}{(\omega + \tilde{b}_1)} + \frac{\tilde{a}_{12}}{(\omega + \tilde{b}_1)^2}, \\ \tilde{\Psi}_2(\omega) &= \frac{\tilde{a}_{21}}{(\omega + \tilde{b}_2)} + \frac{\tilde{a}_{22}}{(\omega + \tilde{b}_2)^2}.\end{aligned}$$

where

$$\begin{aligned}\tilde{a}_0 &= -0.7320508076, \quad \tilde{a}_1 = 5.569219382, \quad \tilde{a}_2 = -2.984535672, \\ \tilde{a}_{11} &= 1.732050808, \quad \tilde{a}_{12} = -1.176914536, \\ \tilde{a}_{21} &= 1.732050808 = \tilde{a}_{11}, \quad \tilde{a}_{22} = -0.5884572681, \\ \tilde{b}_1 &= 2.535898385, \quad \tilde{b}_2 = 1.267949192 = b_1.\end{aligned}$$

The ETD-Restricted Padé scheme in (2.15) becomes

$$\begin{aligned}U_{n+1} &= \left[a_0 + \frac{a_1}{(\omega + b_1)} + \frac{a_2}{(\omega + b_1)^2} \right] U_n + k \left[\frac{a_{11}}{(\omega + b_1)} + \frac{a_{1,2}}{(\omega + b_1)^2} \right] \hat{F}_n \\ &\quad + k \left[\frac{a_{22}}{(\omega + b_1)^2} \right] \hat{F}_n^\alpha + k \left[\frac{a_{31}}{(\omega + b_1)} + \frac{a_{32}}{(\omega + b_1)^2} \right] \hat{F}_n^\beta,\end{aligned}$$

and

$$\alpha_n = \left[\tilde{a}_0 + \frac{\tilde{a}_1}{(\omega + \tilde{b}_1)} + \frac{\tilde{a}_2}{(\omega + \tilde{b}_1)^2} \right] U_n + k \left[\frac{\tilde{a}_{11}}{(\omega + \tilde{b}_1)} + \frac{\tilde{a}_{12}}{(\omega + \tilde{b}_1)^2} \right] \hat{F}_n,$$

$$\beta_n = \left[a_0 + \frac{a_1}{(\omega + b_1)} + \frac{a_2}{(\omega + b_1)^2} \right] U_n + k \left[\frac{\tilde{a}_{21}}{(\omega + b_1)} + \frac{\tilde{a}_{22}}{(\omega + b_1)^2} \right] (2\hat{F}_n^\alpha - \hat{F}_n).$$

The ETD-Restricted Padé Scheme Algorithm

Below is the algorithm for the ETD-Restricted Padé scheme

Algorithm 2 The ETD-Restricted Padé algorithm

```

for  $n = 1, 2, \dots, M = T/k$  do
2: Step I : Compute  $\alpha_n$ 
   Solve  $(kB^{\frac{\alpha}{2}} + \tilde{b}_1 I) Y = \tilde{a}_2 U_n + k\tilde{a}_{12} \hat{F}_n$  for  $Y$ .
4:   Solve  $(kB^{\frac{\alpha}{2}} + \tilde{b}_1 I) X = \tilde{a}_1 U_n + k\tilde{a}_{11} \hat{F}_n + Y$  for  $X$ .
   Compute  $\alpha_n = \tilde{a}_0 U_n + X$ .
6: Step II : Compute  $\beta_n$ 
   Solve  $(kB^{\frac{\alpha}{2}} + b_1 I) Y = a_2 U_n + k\tilde{a}_{22} (2\hat{F}_n^\alpha - \hat{F}_n)$  for  $Y$ .
8:   Solve  $(kB^{\frac{\alpha}{2}} + b_1 I) X = a_1 U_n + k\tilde{a}_{21} (2\hat{F}_n^\alpha - \hat{F}_n) + Y$  for  $X$ .
   Compute  $\beta_n = a_0 U_n + X$ .
10: Step III : Compute  $U_{n+1}$ 
   Solve  $(kB^{\frac{\alpha}{2}} + b_1 I) Y = a_2 U_n + ka_{12} \hat{F} + ka_{22} \hat{F}_n^\alpha + ka_{32} \hat{F}_n^\beta$  for  $Y$ .
12:   Solve  $(kB^{\frac{\alpha}{2}} + b_1 I) X = a_1 U_n + ka_{11} \hat{F} + ka_{31} \hat{F}^\beta + Y$  for  $X$ .
   Compute  $U_{n+1} = a_0 U_n + X$ .
14: end for

```

2.4 Stability Regions and Linear Error Analysis

In this section, we examine the linear stability of our proposed methods by showing the graphs of their regions of stability, following the approach outlined in [45]. Our focus is on the nonlinear ordinary differential equation (ODE)

$$u_t = -au + f(u).$$

with $f(u)$ represents a non-linear function operating on u the complex-valued function.

Let us consider the existence of a fixed point u_0 such that the equation $-au_0 + f(u_0) = 0$ holds. After linearizing around the fixed point u_0 , we derive the following

$$u_t = au + \mu u \tag{2.16}$$

where u represents the perturbation from u_0 , and $\mu = f'(u_0)$ is the derivative of f evaluated at u_0 . The fixed point u_0 is stable for all μ if the real component of $(\mu - a)$ is negative. Let $x = \mu k$ and $y = -ak$ are new variables that we declare and the time step is indicated by k . We define the amplification factor using the A -stable ETD-Restricted Padé and the L -stable ETD-Padé(1,2) schemes on Equation (2.16). For the ETD-Padé(1,2) scheme in (2.12)

$$R(x, y) = \frac{U_{n+1}}{U_n} = \frac{b_3 x^3 + b_2 x^2 + b_1 x + b_0}{den} \tag{2.17}$$

where

$$b_3 = y^3 + 38y^2 + 180y + 144$$

$$b_2 = -y^4 - 19y^3 - 30y^2 + 288y + 432$$

$$b_1 = -y^4 - 16y^3 + 84y^2 + 576y + 864$$

$$b_0 = -2y^5 - 18y^4 - 52y^3 + 84y^2 + 576y + 864$$

$$den = (z^2 + 4z + 6)^2 (z^2 + 8z + 24).$$

similarly, for the ETD-Restricted Padé scheme in (2.15)

$$R(x, y) = \frac{U_{n+1}}{U_n} = \frac{d_3x^3 + d_2x^2 + d_1x + d_0}{den}$$

where

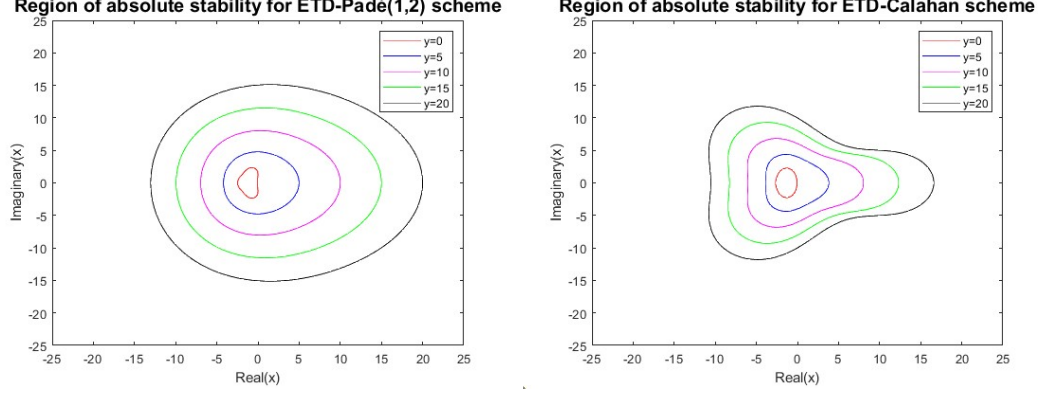
$$d_3 = (19440\sqrt{3} + 33696)y^3 + (59616\sqrt{3} + 102384)y^2 + (46656\sqrt{3} + 85536)y + 31104,$$

$$d_2 = (-4104\sqrt{3} - 7128)y^4 + (27432\sqrt{3} + 47952)y^3 + (125712\sqrt{3} + 439344)y^2 + 124416\sqrt{3}y + 124416,$$

$$d_1 = (-4104\sqrt{3} - 7128)y^5 + (5400\sqrt{3} + 9504)y^4 + (115344\sqrt{3} + 198288)y^3 + (290304\sqrt{3} + 479520)y^2 + (248832\sqrt{3} + 435456)y + 248832$$

$$d_0 = -(2376\sqrt{3} + 4104)y^6 - (15120\sqrt{3} + 25920)y^5 - (22032\sqrt{3} + 36288)y^4 + (44064\sqrt{3} + 77760)y^3 + (163296\sqrt{3} + 264384)y^2 + (155520\sqrt{3} + 279936)y + 186624,$$

$$den = (12 + (3 + \sqrt{3})y)^2 (6 + (3 + \sqrt{3})y)^4.$$



(a) Region of absolute stability of L -stable ETD-Padé(1,2) scheme (b) Region of absolute stability of A -stable ETD-Restricted Padé scheme.

Figure 2.3: The absolute stability regions for the L -stable ETD-Padé(1,2) and A -stable ETD-Restricted Padé schemes.

For different values of y , the stability region of the L -stable ETD-Padé(1,2) and A -stable ETD-Restricted Padé schemes is displayed in Figures (2.3). This demonstrates that as $y \rightarrow \infty$, the stability regions of the L -stable ETD-Padé(1,2) and A -stable ETD-Restricted Padé schemes expand, thereby confirming the schemes' stability.

2.4.1 Linear Error Analysis

In this section, we demonstrate the third-order rate of convergence of our proposed methods. We establish that the novel approaches achieve a local truncation error of third order in time, achieved through the linearization of $\mathbf{F}(\mathbf{u})$ with $(H\mathbf{u})$. This is illustrated by examining the linear semi-discretized model given as

$$\frac{d\mathbf{u}}{dt} = -B\mathbf{u} + H\mathbf{u} \quad (2.18)$$

where B and H represent matrices derived from the spatial discretization. Multiply equation (2.18) by the integrating factor e^{B-Ht} , we have the exact solution

$$\mathbf{u}(t_{n+1}) = e^{B-Hk} \mathbf{u}(t_n) \quad (2.19)$$

To demonstrate the third-order convergence for the ETD-Padé(1,2) scheme (2.12), we apply the scheme to the equation (2.18)

$$\begin{aligned} \mathbf{u}_{n+1} = & ((kB)^2 + 4kB + 6I)^{-2} \times [6I - 2kB + kH] u_n \\ & + ((kB)^2 + 4kB + 6I)^{-2} [4kH\alpha_n + (k^2BH + kH)\beta_n] \end{aligned}$$

where

$$\begin{aligned} \alpha_n = & ((kB)^2 + 8kB + 24I)^{-2} \times [24I - 4kB + k^2BH + 12kH] u_n, \\ \beta_n = & ((kB)^2 + 4kB + 6I)^{-2} \times [6I - 2kB] u_n \\ & + ((kB)^2 + 4kB + 6I)^{-2} \times [k^2BH + 6kH] (2\alpha_n - u_n) \end{aligned}$$

Employing the Taylor series expansion technique for

$$\begin{aligned} \frac{1}{z^2 + 8z + 24} &= \frac{1}{24} - \frac{1}{72}z + \frac{5}{1728}z^2 - \frac{1}{2592}z^3 \\ &\quad + \frac{1}{124416}z^4 + \mathcal{O}(z^5), \\ \frac{1}{z^2 + 4z + 6} &= \frac{1}{6} - \frac{1}{9}z + \frac{5}{108}z^2 - \frac{1}{81}z^3 \\ &\quad + \frac{1}{1944}z^4 + \mathcal{O}(z^5) \end{aligned} \quad (2.20)$$

using the obtained Taylor expansions (2.20), we have

$$\begin{aligned} \mathbf{u}_{n+1} = & \left[I + (H - B)k + k^2 \left(\frac{1}{2}B^2 - BH + \frac{1}{2}H^2 \right) + k^3 \left(\frac{1}{6}H^3 - \frac{1}{6}B^3 + \frac{1}{2}B^2H - \frac{1}{2}BH^2 \right) \right. \\ & \left. + k^4 \left(\frac{1}{36}B^4 - \frac{1}{8}B^3H + \frac{1}{6}B^2H^2 - \frac{5}{72}BH^3 \right) + \mathcal{O}(k^5) \right] \mathbf{u}_n \end{aligned} \quad (2.21)$$

The exact solution in equation (2.19) is reformulated using the Taylor series expansion of $e^{(H-B)k}$

$$\begin{aligned} \mathbf{u}_{n+1} = & \left[I + k(H - B) + k^2 \left(\frac{H^2}{2} - HB + \frac{B^2}{2} \right) + k^3 \left(\frac{H^3}{6} - \frac{H^2B}{2} + \frac{HB^2}{2} - \frac{B^3}{6} \right) \right. \\ & \left. + k^4 \left(\frac{H^4}{24} - \frac{H^3B}{6} + \frac{H^2B^2}{4} - \frac{HB^3}{6} + \frac{B^4}{24} \right) + \mathcal{O}(k^5) \right] \mathbf{u}_n \end{aligned} \quad (2.22)$$

Based on the derivations from equations (2.21) and (2.22), we derive the local truncation error

$$e_{n+1} = \|\mathbf{u}_{n+1} - e^{(H-B)k}\mathbf{u}_n\| = \mathcal{O}(k^4)$$

similarly, for the ETD-Restricted Padé Scheme, we apply (2.15) to (2.19)

$$\begin{aligned} \mathbf{u}_{n+1} = & (6I + (3 + \sqrt{3})kB)^{-2} \times \\ & \left[6 \left(6I + 2\sqrt{3}kB - (1 + \sqrt{3})k^2B^2 \right) + 6 \left(kH + (1 + \sqrt{3})k^2HB \right) \right] u_n \quad (2.23) \\ & + (6I + (3 + \sqrt{3})kB)^{-2} \left[24kH\alpha_n + 6kH \left(1 + (2 + \sqrt{3})kB \right) \beta_n \right] \end{aligned}$$

where

$$\begin{aligned}
\alpha_n &= (12I + (3 + \sqrt{3})kB)^{-2} \times \\
&\quad \left[6 \left(24I + 4\sqrt{3}kB - (1 + \sqrt{3})k^2B^2 \right) + 6 \left(12kH + (3 + 2\sqrt{3})kHB \right) \right] u_n, \\
\beta_n &= (6I + (3 + \sqrt{3})kB)^{-2} \times \left(36I + 12\sqrt{3}kB - 6(1 + \sqrt{3})k^2B^2 \right) u_n \\
&\quad + (6I + (3 + \sqrt{3})kB)^{-2} \times \left[\left(36kH + 6(3 + 2\sqrt{3})k^2HB \right) \right] (2\alpha_n - u_n),
\end{aligned}$$

Employing the Taylor series expansion technique for

$$\begin{aligned}
\frac{1}{(12 + (3 + \sqrt{3})z)^2} &= \frac{1}{144} - \left(\frac{1}{288} \frac{\sqrt{3}}{864} \right) z + \left(\frac{1}{576} + \frac{\sqrt{3}}{1152} \right) z^2 \\
&\quad - \left(\frac{1}{1152} + \frac{5\sqrt{3}}{10368} \right) z^3 + \left(\frac{35}{82944} + \frac{5\sqrt{3}}{20736} \right) z^4 + \mathcal{O}(z^5), \\
\frac{1}{(6 + (3 + \sqrt{3})z)^2} &= \frac{1}{36} - \left(\frac{1}{36} \frac{\sqrt{3}}{108} \right) z + \left(\frac{1}{36} + \frac{\sqrt{3}}{72} \right) z^2 \\
&\quad - \left(\frac{1}{36} + \frac{5\sqrt{3}}{324} \right) z^3 + \left(\frac{35}{1296} + \frac{5\sqrt{3}}{324} \right) z^4 + \mathcal{O}(z^5)
\end{aligned}$$

we can write (2.23) as

$$\begin{aligned}
\mathbf{u}_{n+1} &= \left[I + (H - B)k + k^2 \left(\frac{1}{2}B^2 - BH + \frac{1}{2}H^2 \right) + k^3 \left(\frac{1}{6}H^3 - \frac{1}{6}B^3 + \frac{1}{2}B^2H - \frac{1}{2}BH^2 \right) \right. \\
&\quad \left. + k^4 \left(-\frac{H^4}{24} + \left(\frac{1}{24} + \frac{\sqrt{3}}{9} \right) H^3B - \left(\frac{1}{24} - \frac{\sqrt{3}}{12} \right) HB^3 - \frac{\sqrt{3}}{6} H^2B^2 - \frac{\sqrt{3}}{36} B^4 \right) \right. \\
&\quad \left. + \mathcal{O}(k^5) \right] \mathbf{u}_n
\end{aligned} \tag{2.24}$$

from (2.24) and (2.22), we derive the third order convergence of the scheme

$$e_{n+1} = \left\| \mathbf{u}_{n+1} - e^{(H-B)k} \mathbf{u}_n \right\| = \mathcal{O}(k^4)$$

2.5 Numerical Experiments

The numerical test problems presented in this section encompass both initial conditions with irregular features and those characterized by smoothness. We solve a one-dimensional test problem with smooth initial data, for which an exact solution is available, to confirm the third-order accuracy of our time-stepping methods. In order to verify our third-order accuracy, we also address several problems involving non-smooth data. The L_2 or L_∞ norms are indicated in the following by $||\cdot||$. The L_2 norm of a vector is determined by taking the square root of the sum of the squares of its components. In contrast, the L_∞ norm of a vector is calculated by identifying the maximum absolute value among its components.

The following formula determines the convergence order in both space and time, where the spatial step size is h and the temporal step size is k .

$$\mathcal{R} = \log_2 (E(h, k))$$

where

$$E(h, k) = \frac{\|(u_{exact} - u_{h,k})\|}{\|(u_{exact} - u_{h/2,k/2})\|}$$

where the numerical solution is denoted as $u_{h,k}$ and the exact solution is denoted as u_{exact} . If the exact solution is unknown, we fix h and determine the order of convergence in time as follows

$$\mathcal{R} = \log_2 (E)$$

where

$$E = \frac{\|(u_{h,k} - u_{h,2k})\|}{\|(u_{h,k/2} - u_{h,k})\|}$$

2.5.1 A test problem with exact solution

In order to verify the third-order accuracy of our modified ETD schemes, we examine the following artificially constructed space-fractional reaction-diffusion Benchmark equation [49]

$$\begin{aligned} \frac{\partial u}{\partial t} &= -\mathcal{K}(-\Delta)^{\frac{\alpha}{2}}u + g(u, x, t), \quad 1 < \alpha \leq 2, \quad 0 < x < 1, \\ u(x, 0) &= 0, \quad 0 < x < 1, \\ u(0, t) &= u(1, t) = 0, \quad t > 0, \end{aligned} \tag{2.25}$$

where

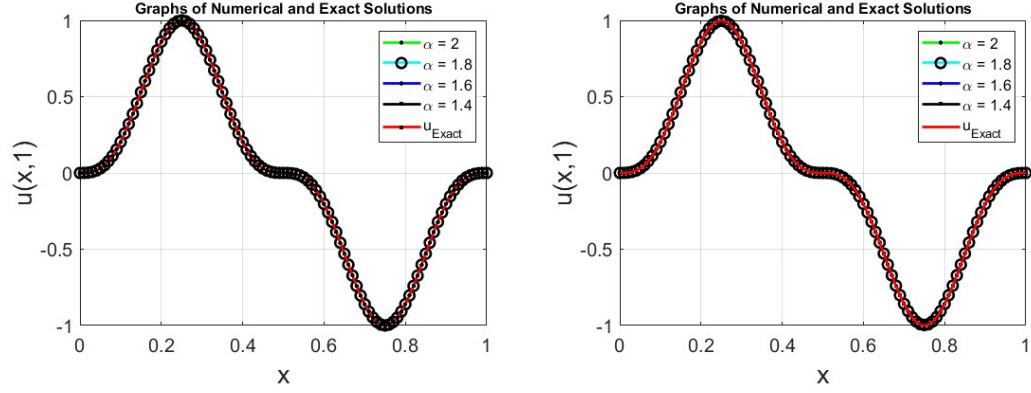
$$g(u, x, t) = \alpha t^{\alpha-1} \sin^3(2\pi x) + \frac{\mathcal{K}}{4} t^\alpha \{3[(2\pi)^\alpha + 1] \sin(2\pi x) - [(6\pi)^\alpha + 6] \sin(6\pi x)\} - \mathcal{K}u,$$

and $\mathcal{K} > 0$.

For problem (2.5.1), The exact solution is

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

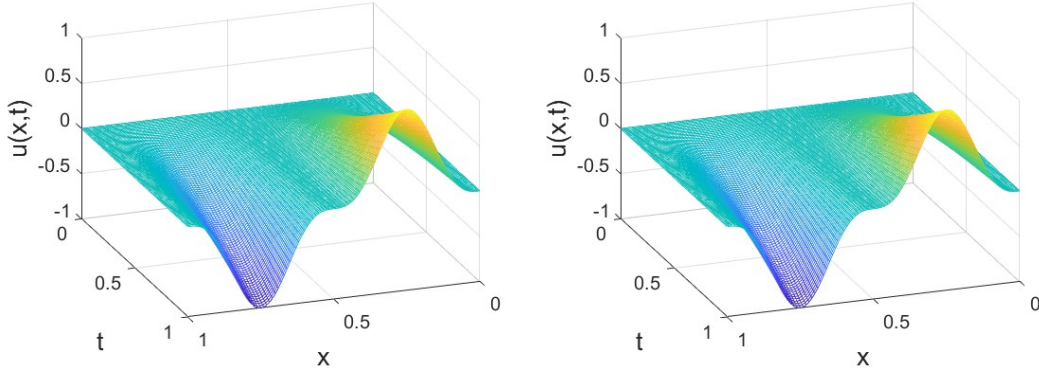
The Benchmark problem has been selected to verify that our modified methods demonstrate third-order temporal accuracy and fourth-order spatial accuracy. Figure (2.4) illustrates the solutions obtained up to $T = 1$ for $\mathcal{K} = 1$, $k = h = 0.01$, and various



(a) The exact solution vs. ETD-Padé(1,2) scheme. (b) The exact solution vs. ETD-Restricted Padé scheme.

Figure 2.4: Problem 2.5.1: The L -stable and A -stable schemes compared to the exact solution.

α values, using the L -stable ETD-Padé(1,2) and A -stable ETD-Restricted Padé numerical schemes compared to the exact solution. Figure (2.5) show the time evolution solutions obtained for $\mathcal{K} = 1$, $h = k = 0.01$, and $\alpha = 1.4$, using the A -stable ETD-Restricted Padé and L -stable ETD-Padé(1,2) schemes. Table (2.1) shows The L_2 errors, convergence orders in space for the Padé (1,2) scheme. The convergence orders for L_2 and L_∞ errors for a series of temporal steps for ETD-Restricted Padé scheme, beginning with $k = 0.025$, with each subsequently halved are represented in table (2.2) and table (2.3) with CPU time. In the same manners, the convergence orders for L_2 and L_∞ errors for ETD-Padé(1,2) scheme are represented in table (2.4) and table (2.5) with CPU time. From the tables, the ETD-Restricted Padé scheme required less CPU time compared to the ETD-Padé(1,2) scheme. whereas the ETD-Padé(1,2) scheme converge to the third- order accuracy faster than the ETD-Restricted Padé scheme.



(a) Time evolution solution using ETD-Padé(1,2) scheme. (b) Time evolution solution using ETD-Restricted Padé scheme.

Figure 2.5: Problem 2.5.1: The time evolution solution using both of the L -stable and A -stable schemes.

Table 2.1: Problem 2.5.1: L_2 Convergence results in space for the L -stable scheme.

α	h	k	error	order- L_2	CPU Time
1.4	0.10000	0.0010	9.5003e-03	—	0.0577
	0.05000	0.0010	5.9109e-04	4.0065	0.0839
	0.02500	0.0010	3.6008e-05	4.0370	0.1568
	0.01250	0.0010	2.2348e-06	4.0101	0.4102
	0.00625	0.0010	1.3812e-07	4.0161	1.4686
1.6	0.10000	0.0010	1.1060e-02	—	0.0577
	0.05000	0.0010	6.8672e-04	4.0095	0.0838
	0.02500	0.0010	4.1826e-05	4.0370	0.1571
	0.01250	0.0010	2.5949e-06	4.0106	0.4192
	0.00625	0.0010	1.5950e-07	4.0241	1.4811

Table 2.2: Problem 2.5.1: L_2 Convergence results in time and for the A -stable scheme.

α	h	k	error	order- L_2	CPU Time
1.4	0.01250	0.02500	1.5031e-04	-	0.0290
	0.00625	0.01250	3.2057e-05	2.2292	0.0235
	0.00313	0.00625	5.5964e-06	2.5181	0.0599
	0.00156	0.00313	8.5137e-07	2.7166	0.3998
1.6	0.01250	0.02500	1.9279e-04	-	0.0278
	0.00625	0.01250	4.7699e-05	2.0150	0.0204
	0.00313	0.00625	9.4872e-06	2.3299	0.0440
	0.00156	0.00313	1.5936e-06	2.5737	0.2963

Table 2.3: Problem 2.5.1: L_∞ Convergence results in time for the A -stable scheme.

α	h	k	error	order- L_∞	CPU Time
1.4	0.01250	0.02500	1.5031e-04	-	0.0261
	0.00625	0.01250	3.2057e-05	2.2292	0.0170
	0.00313	0.00625	5.5964e-06	2.5181	0.0432
	0.00156	0.00313	8.5137e-07	2.7166	0.1943
1.6	0.01250	0.02500	1.9279e-04	-	0.0262
	0.00625	0.01250	4.7699e-05	2.0150	0.0156
	0.00313	0.00625	9.4872e-06	2.3299	0.0398
	0.00156	0.00313	1.5936e-06	2.5737	0.1911

Table 2.4: Problem 2.5.1: L_2 Convergence results in time for L -stable scheme.

α	h	k	error	order- L_2	CPU Time
1.4	0.01000	0.10000	1.5278e-03	-	0.0315
	0.01000	0.05000	3.1273e-04	2.2885	0.0221
	0.01000	0.02500	5.3277e-05	2.5533	0.0307
	0.01000	0.01250	6.7471e-06	2.9812	0.0584
1.6	0.01000	0.10000	1.6249e-03	-	0.0308
	0.01000	0.05000	3.9027e-04	2.0578	0.0210
	0.01000	0.02500	7.2507e-05	2.4283	0.0311
	0.01000	0.01250	1.0459e-05	2.7933	0.0616

2.5.2 A Biochemistry Problem

We consider the following one-dimensional space fractional Enzyme Kinetics problem

$$\frac{\partial u}{\partial t} = -\mathcal{K}(-\Delta)^{\frac{\alpha}{2}}u - \frac{u}{1+u}, \quad 0 < x < 1, \quad 1 < \alpha \leq 2,$$

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

$$u(0, t) = u(1, t) = 0, \quad t > 0,$$

Table 2.5: Problem 2.5.1: L_∞ Convergence results in time for the L -stable scheme.

α	h	k	error	order- L_∞	CPU Time
1.4	0.01000	0.10000	2.4268e-04	-	0.0317
	0.01000	0.05000	5.4707e-05	2.1493	0.0211
	0.01000	0.02500	9.9975e-06	2.4521	0.0315
	0.01000	0.01250	9.5897e-07	3.3820	0.0597
1.6	0.01000	0.10000	2.4263e-04	-	0.0322
	0.01000	0.05000	6.2520e-05	1.9564	0.0217
	0.01000	0.02500	1.2673e-05	2.3026	0.0303
	0.01000	0.01250	1.5840e-06	3.0001	0.0600

The above problem exhibits a discontinuity between its boundary and initial conditions. Figures (2.6) and (2.7) show the time evolution solutions using both of the A -stable ETD-Restricted Padé and L -stable ETD-Padé(1,2) methods for $\mathcal{K} = 1, k = h = 0.01$ and different α values over the interval $t \in [0, 1]$. The convergence orders for L_2 and L_∞ errors for ETD-Restricted Padé scheme are represented in table (2.6) and table (2.7) with CPU time. In the same manners, The convergence orders for L_2 and L_∞ errors for ETD-Padé(1,2) scheme are represented in table (2.8) and table (2.9) with CPU time. When employing the A -stable scheme, undesired oscillations become apparent near the boundaries at α values of 2, 1.8, and 1.6. As the fractional order diminishes to $\alpha = 1.4$, the undesired oscillations decrease. Conversely, solutions obtained through the L -stable numerical scheme show no oscillations and consistently maintains the expected third-order temporal accuracy, irrespective of the α value.

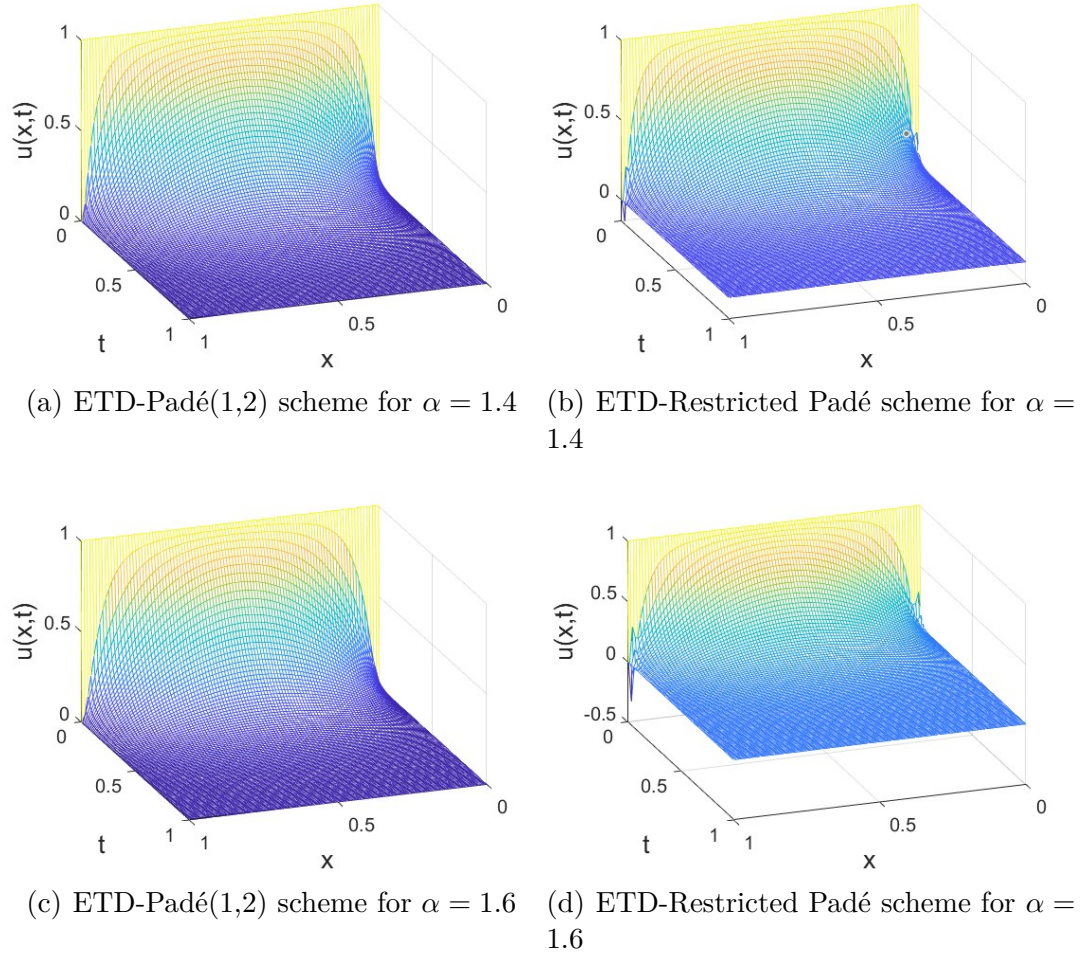
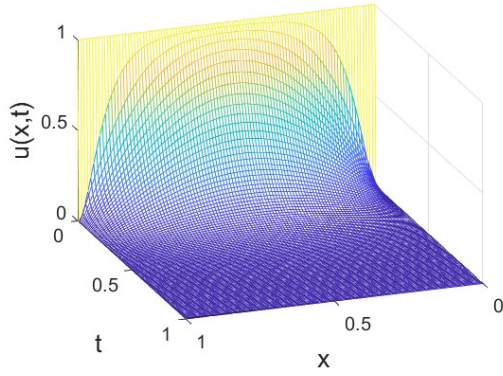


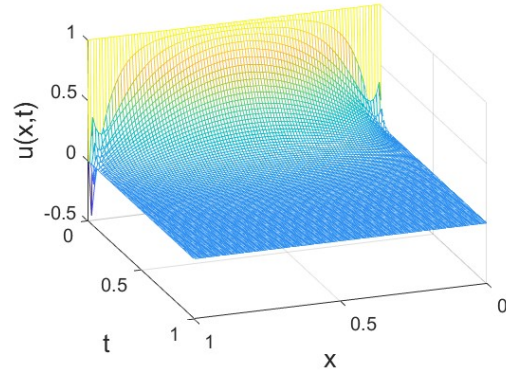
Figure 2.6: Problem 2.5.2: The numerical schemes solutions for $\alpha = 1.4, 1.6$.

Table 2.6: Problem 2.5.2: L_2 Convergence results in time for the A -stable scheme.

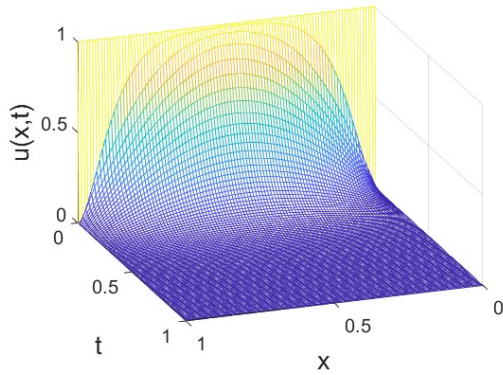
α	h	k	error	order- L_2	CPU Time
1.4	0.01250	0.02500	2.1710e-04	-	0.0060
	0.01250	0.01250	2.7450e-05	2.9835	0.0040
	0.01250	0.00625	3.4581e-06	2.9887	0.0050
	0.01250	0.00313	4.6054e-07	2.9086	0.0120
1.6	0.01250	0.02500	4.0043e-04	-	0.0074
	0.01250	0.01250	3.3028e-05	3.5998	0.0038
	0.01250	0.00625	4.1231e-06	3.0019	0.0051
	0.01250	0.00313	5.1488e-07	3.0014	0.0117



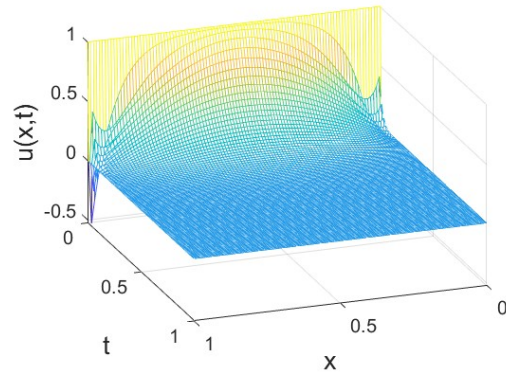
(a) ETD-Padé(1,2) scheme for $\alpha = 1.8$



(b) ETD-Restricted Padé scheme for $\alpha = 1.8$



(c) ETD-Padé(1,2) scheme for $\alpha = 2$



(d) ETD-Restricted Padé scheme for $\alpha = 2$

Figure 2.7: Problem 2.5.2: The numerical schemes solutions for $\alpha = 1.8, 2$.

Table 2.7: Problem 2.5.2: L_∞ Convergence results in time for the A -stable scheme.

α	h	k	error	order- L_∞	CPU Time
1.4	0.01250	0.02500	3.3121e-05	-	0.0058
	0.01250	0.01250	4.2957e-06	2.9468	0.0034
	0.01250	0.00625	5.4025e-07	2.9912	0.0047
	0.01250	0.00313	7.1936e-08	2.9088	0.0110
1.6	0.01250	0.02500	2.0428e-04	-	0.0064
	0.01250	0.01250	5.2251e-06	5.2889	0.0036
	0.01250	0.00625	6.5227e-07	3.0019	0.0045
	0.01250	0.00313	8.1453e-08	3.0014	0.0109

Table 2.8: Problem 2.5.2: L_2 Convergence results in time for the L -stable scheme.

α	h	k	error	order- L_2	CPU Time
1.4	0.01250	0.02500	4.3276e-06	-	0.0392
	0.01250	0.01250	5.3844e-07	3.0067	0.0693
	0.01250	0.00625	6.6232e-08	3.0232	0.1393
	0.01250	0.00313	8.1164e-09	3.0286	0.2883
1.6	0.01250	0.02500	2.6681e-06	-	0.0396
	0.01250	0.01250	3.3285e-07	3.0029	0.0713
	0.01250	0.00625	4.0649e-08	3.0336	0.1376
	0.01250	0.00313	4.8570e-09	3.0651	0.2812

Table 2.9: Problem 2.5.2: L_∞ Convergence results in time for the L -stable scheme.

α	h	k	error	order- L_∞	CPU Time
1.4	0.01250	0.02500	6.8436e-07	-	0.0392
	0.01250	0.01250	8.5146e-08	3.0067	0.0692
	0.01250	0.00625	1.0474e-08	3.0232	0.1377
	0.01250	0.00313	1.2835e-09	3.0286	0.2783
1.6	0.01250	0.02500	4.2188e-07	-	0.0395
	0.01250	0.01250	5.2629e-08	3.0029	0.0730
	0.01250	0.00625	6.4273e-09	3.0336	0.1422
	0.01250	0.00313	7.6797e-10	3.0651	0.2854

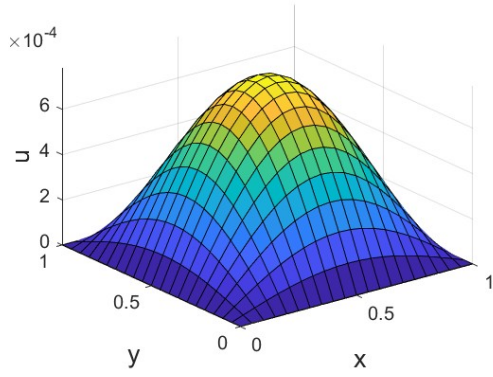
2.5.3 Fisher's equation

Consider the two-dimensional space-fractional Fisher's problem

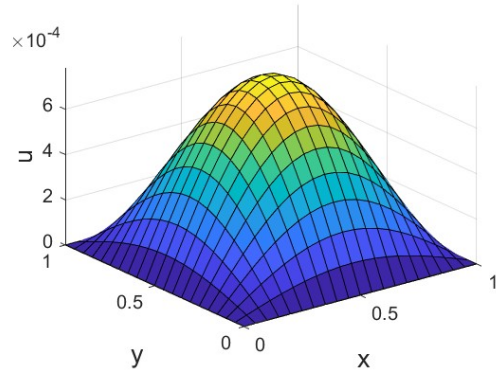
$$\frac{\partial u}{\partial t} = -\mathcal{K}(-\Delta)^{\frac{\alpha}{2}}u + u - u^2, \quad (x, y) \in (0, 1) \times (0, 1)$$

$$u(x, y, 0) = \sin\left(\frac{\pi y}{2}\right)$$

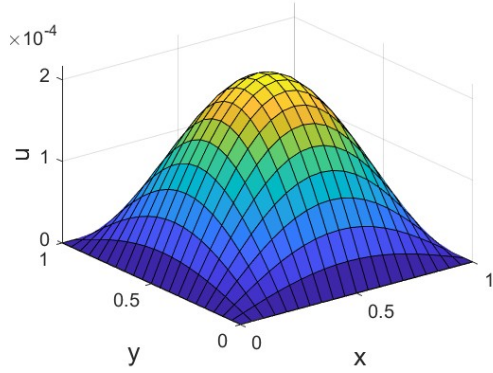
with homogeneous Dirichlet boundary condition and $\mathcal{K} = 1$. The issue of mismatched boundary and initial conditions arises in this problem. The solution profiles in figure (2.8) computed with $h = 0.5, k = 0.0125$ at $T = 1$ for $\alpha = 1.4, 1.8$. The convergence orders for L_2 and L_∞ errors for ETD-Restricted Padé scheme are represented in table



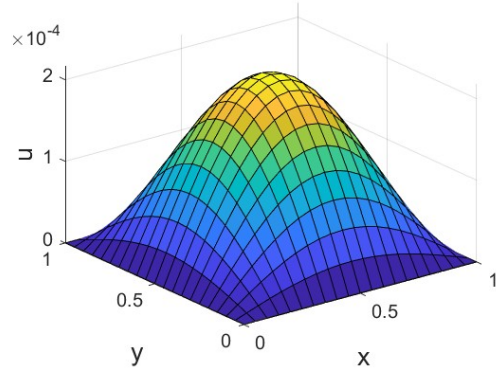
(a) ETD-Padé(1,2) scheme for $\alpha = 1.4$



(b) ETD-Restricted Padé scheme for $\alpha = 1.4$



(c) ETD-Padé(1,2) scheme for $\alpha = 1.8$



(d) ETD-Restricted Padé scheme for $\alpha = 1.8$

Figure 2.8: Problem 2.5.3: The L -stable and A -stable schemes solutions for $\alpha = 1.4, 1.8$.

(2.10) and table (2.11) with CPU time. The convergence orders for L_2 and L_∞ errors for ETD-Padé(1,2) scheme are represented in table (2.12) and table (2.13) with CPU time. As we observed in the first numerical experiment the A -stable scheme demonstrated lower CPU time requirements compared to the L -stable scheme.

Table 2.10: Problem 2.5.3: L_2 Convergence results in time for the A -stable scheme.

α	h	k	error	order- L_2	CPU Time
1.4	0.1000	0.05000	4.5758e-03	-	0.0145
	0.1000	0.02500	6.7392e-04	2.7634	0.0110
	0.1000	0.01250	9.2840e-05	2.8598	0.0131
	0.1000	0.00625	1.2296e-05	2.9166	0.0205
1.8	0.1000	0.05000	4.4843e-03	-	0.0144
	0.1000	0.02500	6.7401e-04	2.7340	0.0118
	0.1000	0.01250	9.7620e-05	2.7875	0.0160
	0.1000	0.00625	1.3707e-05	2.8322	0.0257

Table 2.11: Problem 2.5.3: L_∞ Convergence results in time for the A -stable scheme.

α	h	k	error	order- L_∞	CPU Time
1.4	0.10000	0.05000	5.2391e-03	-	0.0177
	0.10000	0.02500	7.5852e-04	2.7881	0.0134
	0.10000	0.01250	1.0331e-04	2.8762	0.0157
	0.10000	0.00625	1.3597e-05	2.9256	0.0248
1.8	0.10000	0.05000	5.5303e-03	-	0.0138
	0.10000	0.02500	8.3450e-04	2.7284	0.0115
	0.10000	0.01250	1.2055e-04	2.7912	0.0144
	0.10000	0.00625	1.6917e-05	2.8332	0.0251

Table 2.12: Problem 2.5.3: L_2 Convergence results in time for the L -stable scheme.

α	h	k	error	order- L_2	CPU Time
1.4	0.10000	0.05000	2.4662e-04	-	0.0129
	0.10000	0.02500	3.3802e-05	2.8671	0.0154
	0.10000	0.01250	4.4503e-06	2.9251	0.0298
	0.10000	0.00625	5.7199e-07	2.9598	0.0615
1.8	0.10000	0.05000	9.0929e-05	-	0.0128
	0.10000	0.02500	1.2834e-05	2.8247	0.0156
	0.10000	0.01250	1.7224e-06	2.8975	0.0297
	0.10000	0.00625	2.2401e-07	2.9428	0.0607

Table 2.13: Problem 2.5.3: L_∞ Convergence results in time for the L -stable scheme.

α	h	k	error	order- L_∞	CPU Time
1.4	0.10000	0.05000	3.1070e-04	-	0.0161
	0.10000	0.02500	4.2570e-05	2.8676	0.0197
	0.10000	0.01250	5.6039e-06	2.9253	0.0376
	0.10000	0.00625	7.2022e-07	2.9599	0.0720
1.8	0.10000	0.05000	1.1482e-04	-	0.0132
	0.10000	0.02500	1.6206e-05	2.8247	0.0163
	0.10000	0.01250	2.1749e-06	2.8975	0.0299
	0.10000	0.00625	2.8286e-07	2.9428	0.0618

2.5.4 Allen-Cahn Problem

We experiment the Allen-Cahn problem with non-homogeneous BCs by converting the problem into homogeneous BCs and solve the problem using the proposed numerical L -stable ETD-Padé(1,2) and A -stable ETD-Restricted Padé schemes. We examine the one-dimensional non-homogeneous space-fractional Allen-Cahn problem

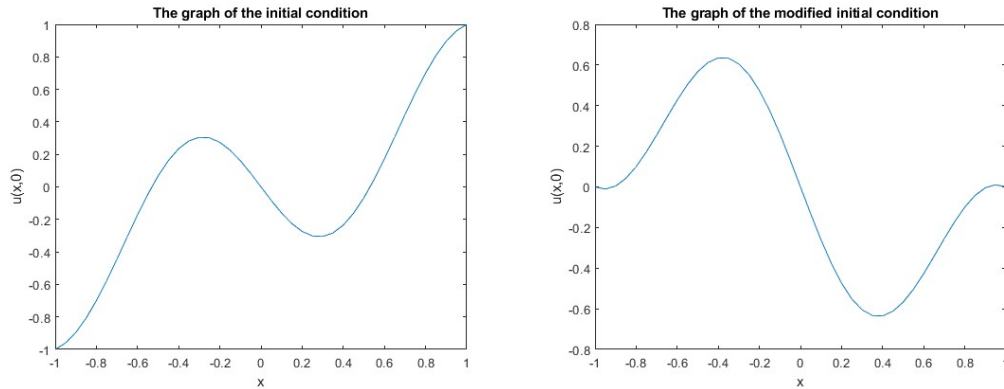
$$\frac{\partial u}{\partial t} = -\mathcal{K}(-\Delta)^{\alpha/2}u + u(1 - u^2), \quad (x, t) \in [-1, 1] \times [0, 100], \quad 1 < \alpha \leq 2$$

$$u(x, 0) = 0.47 \sin(-1.5\pi x) + 0.53x$$

$$u(-1, t) = -1,$$

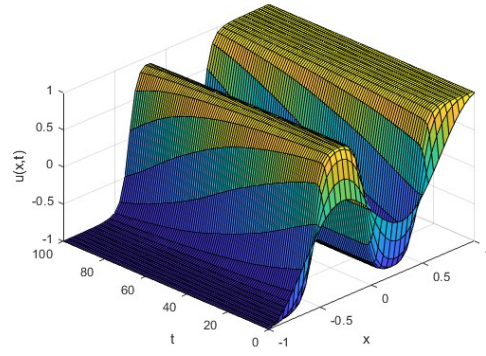
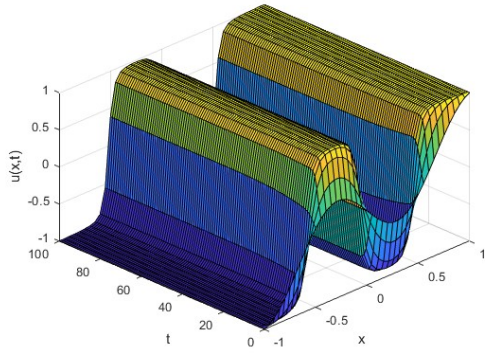
$$u(1, t) = 1$$

The graph of the initial condition represented in figure (2.9(a)). By applying the linear transformation technique, we obtained a homogeneous BCs as in figure (2.9(b)). Figures (2.10) and (2.11) illustrate the behavior of the numerical solutions using L -stable and A -stable schemes for various values of α and $k = 1, h = 0.05$ respectively.

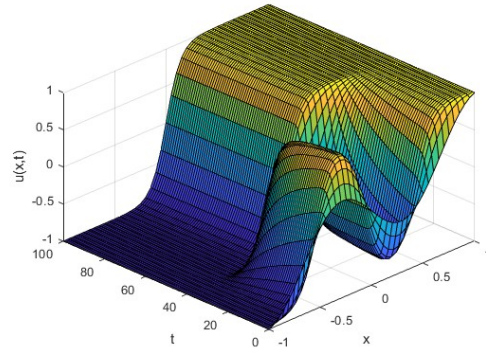
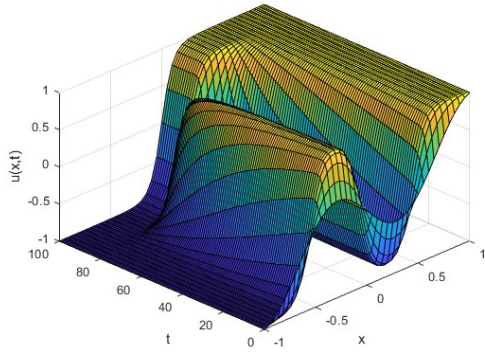


(a) The graph of the initial condition (b) The graph of the modified initial condition

Figure 2.9: Problem 2.5.4: The graph of the IC and modified IC.

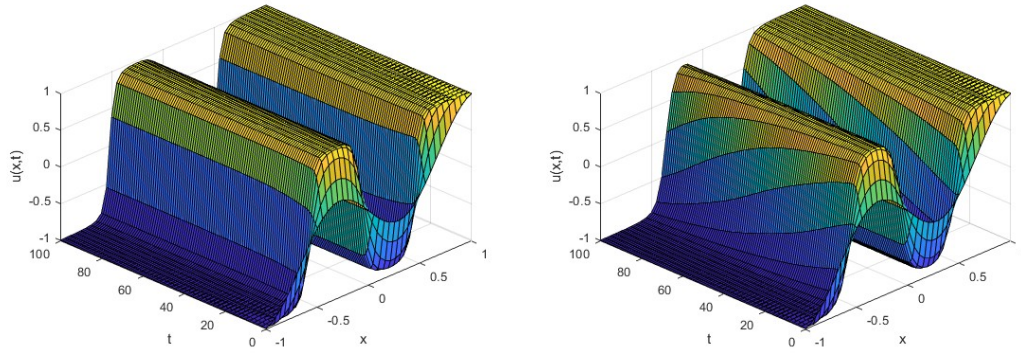


(a) ETD-Padé(1,2) Scheme when $\alpha = 1.4$ (b) ETD-Padé(1,2) Scheme when $\alpha = 1.6$

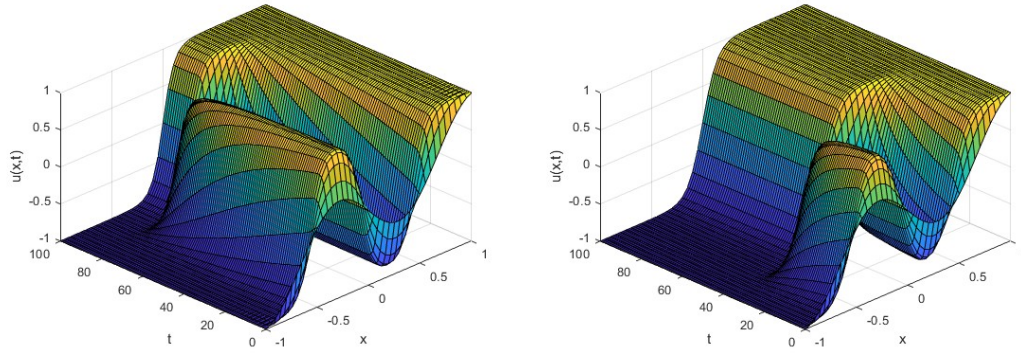


(c) ETD-Padé(1,2) Scheme when $\alpha = 1.8$ (d) ETD-Padé(1,2) Scheme when $\alpha = 2$

Figure 2.10: Problem 2.5.4: The solution using ETD-Padé(1,2) Scheme.



(a) ETD-Restricted Padé scheme when $\alpha = 1.4$ (b) ETD-Restricted Padé scheme when $\alpha = 1.6$



(c) ETD-Restricted Padé scheme when $\alpha = 1.8$ (d) ETD-Restricted Padé scheme when $\alpha = 2$

Figure 2.11: Problem 2.5.4: The solution using ETD-Restricted Padé scheme.

2.6 Conclusion

The difficulties presented by space-fractional reaction-diffusion equations have spurred the development of two novel third-order numerical schemes. The proposed numerical L -stable ETD-Padé(1,2) and A -stable ETD-Restricted Padé schemes are obtained by employing the forth-order MTT approach for space discretization and ETD for temporal discretization. It was found that the A -stable approach might exhibit unwanted spurious oscillations, especially when dealing with non-smooth initial data. The L -stable approach, on the other hand reliably preserves its expected third-order

accuracy across all value of α . Furthermore, through numerical experimentation, it has been observed that the ETD-Padé(1,2) scheme requires more computational time compared to the ETD-Restricted Padé schemes.

CHAPTER 3

FOURIER SPECTRAL THIRD-ORDER ETD SCHEMES

In this chapter, the main goal is to combine the power of Fourier spectral methods with the advantages of the restricted Padé rational approximations to develop a robust framework for characterizing complex phenomenon arising in space fractional reaction-diffusion systems. The fractional Laplacian operator has a diagonal representation when Fourier spectral approach is applied. This approach can easily be extended to address multi-dimensional problems in the same way that it can solve one-dimensional problems and make it possible to achieve spectral convergence for multidimensional cases. Highly efficient time stepping schemes are developed using third order single pole Restricted Padé and padé (1,2) rational approximations to the exponential matrix functions. Efficiency of the proposed schemes is further en-

hanced by applying powerful mathematical tools, namely discrete sine and cosine transforms. Algorithms are developed to easily implement the methods on one and multidimensional systems with homogeneous Dirichlet as well as homogeneous Neumann boundary conditions. Computational efficiency, reliability and effectiveness of the proposed methods is demonstrated through numerical experiments. Convergence results are computed to support the theoretical findings.

3.1 Space Discretisation

To formulate a spatial fractional reaction-diffusion equation, we can substitute the standard Laplace operator with its fractional counterpart. Consider the following problem

$$\frac{\partial v(\mathbf{x}, t)}{\partial t} = -\mathcal{K}(-\Delta)^{\alpha/2}v(\mathbf{x}, t) + F(v, t), \quad t \in [0, T], \quad 1 < \alpha \leq 2 \quad (3.1)$$

$$v(\mathbf{x}, 0) = \phi(\mathbf{x}), \quad \mathbf{x} \in \Omega$$

with homogeneous Dirichlet as well as homogeneous Neumann boundary conditions. where Ω is contained within the d -dimensional real space and $d = 1, 2, 3$. In order to understand the fractional Laplacian, spectral decomposition is essential tool, see [24] and [50]. The fractional Laplacian $(-\Delta)^{\alpha/2}$ has the same spectral decomposition as the classical Laplace operator $(-\Delta)$, which is the eigenvalues of $(-\Delta)$ raised to the power of $(\alpha/2)$ [51]. Based on definition 2 in Section (1.1) for the spectral decomposition, we can extend it to 3-dimensional space. Given a bounded region $\Omega \subset \mathbb{R}^d$, Let the

Laplacian $(-\Delta)$ possess a complete set of orthonormal eigenfunctions, denoted as $\psi_k, \psi_{k,l}$, or $\psi_{k,l,n}$, in accordance with standard boundary conditions. Correspondingly, it is associated with eigenvalues $\mu_k, \mu_{k,l}$, or $\mu_{k,l,n}$.

$$\begin{aligned} (-\Delta)\psi_k &= \mu_k\psi_k, & \text{if } d = 1, \\ (-\Delta)\psi_{k,l} &= \mu_{k,l}\psi_{k,l}, & \text{if } d = 2, \\ (-\Delta)\psi_{k,l,n} &= \mu_{k,l,n}\psi_{k,l,n}, & \text{if } d = 3, \end{aligned}$$

for $k, l, n = 0, 1, 2, \dots$, on Ω . Let

$$\begin{aligned} v_1 &= \sum_{k=0}^{\infty} \hat{v}_k \psi_k, & \hat{v}_k &= \langle v_1, \psi_k \rangle, & \sum_{k=0}^{\infty} |\hat{v}_k|^2 |\mu_k|^\alpha &< \infty, \\ v_2 &= \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \hat{v}_{k,l} \psi_{k,l}, & \hat{v}_{n,m} &= \langle v_2, \psi_{k,l} \rangle, & \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} |\hat{v}_{k,l}|^2 |\mu_{k,l}|^\alpha &< \infty, \\ v_3 &= \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \sum_{n=0}^{\infty} \hat{v}_{k,l,n} \psi_{k,l,n}, & \hat{v}_{k,l,n} &= \langle v_3, \psi_{k,l,n} \rangle, & \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \sum_{n=0}^{\infty} |\hat{v}_{k,l,n}|^2 |\mu_{k,l,n}|^\alpha &< \infty. \end{aligned}$$

Then,

$$\begin{aligned} (-\Delta)^{\frac{\alpha}{2}} v_1 &= \sum_{k=0}^{\infty} \hat{v}_k \mu_k^{\frac{\alpha}{2}} \psi_k, \\ (-\Delta)^{\frac{\alpha}{2}} v_2 &= \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \hat{v}_{k,l} \mu_{k,l}^{\frac{\alpha}{2}} \psi_{k,l}, \\ (-\Delta)^{\frac{\alpha}{2}} v_3 &= \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \sum_{n=0}^{\infty} \hat{v}_{k,l,n} \mu_{k,l,n}^{\frac{\alpha}{2}} \psi_{k,l,n}. \end{aligned}$$

The specified boundary conditions determine the eigenvalues and eigenvectors of the classical Laplace operator. For the dimension $d = 1, 2, 3$ and $\mathbf{x} \in \Omega = (a, b)^d$, we have the eigenvalues and eigenvectors under the homogeneous Dirichlet BCs are given by

$$\mu_{k_1, \dots, k_d} = \sum_{m=k_1}^{k_d} \left(\frac{(m+1)\pi}{b-a} \right)^2,$$

$$\psi_{k_1, \dots, k_d} = \left(\sqrt{\frac{2}{b-a}} \right)^d \prod_{m=k_1}^{k_d} \sin \left(\frac{(m+1)\pi (x_m - a)}{b-a} \right), k_i = 0, 1, 2, \dots,$$

and the eigenvalues and eigenvectors under the homogeneous Neumann BCs are given by

$$\mu_{k_1, \dots, k_d} = \sum_{m=k_1}^{k_d} \left(\frac{m\pi}{b-a} \right)^2$$

$$\psi_{k_1, \dots, k_d} = \left(\sqrt{\frac{2}{b-a}} \right)^d \prod_{m=k_1}^{k_d} \cos \left(\frac{m\pi (x_m - a)}{b-a} \right), k_i = 0, 1, 2, \dots$$

If we restrict our analysis to a finite number of orthonormal trigonometric eigenfunctions ψ_k , the fractional Laplacian can be estimated using a truncated series

$$(-\Delta)^{\frac{\alpha}{2}} v \approx \sum_{m=0}^{N_x-1} \hat{v}_m \mu_m^{\frac{\alpha}{2}} \psi_m \quad (3.2)$$

To outline the foundational basis of the technique, let's focus on considering the one-dimensional space problem of (3.1) in Fourier space for some $x \in [a, b]$. Using the Fourier transform and the definition of the fractional Laplacian in Section (1.1), we obtain

$$\frac{d}{dt} \mathcal{F}[v(x, t)] = -\mathcal{K} M \mathcal{F}[v(x, t)] + \mathcal{F}[F(v, t)]$$

where $M = \mathcal{K}(\mu^2)^{\alpha/2}$.

For the homogeneous Dirichlet BCs, the eigenvalues are computed as

$$\mu_i = \frac{(i)\pi}{L}$$

$$\text{for } x_i = a + ih, \quad h = \frac{L}{(N_x + 1)}$$

and for the homogeneous Neumann BCs, the eigenvalues are computed as

$$\mu_i = \frac{(i-1)\pi}{L}$$

$$\text{for } x_i = a + (i-1)h + \frac{h}{2}, \quad h = \frac{L}{N_x}$$

Where $L = b - a$ and $i = 1, 2, \dots, N_x$, where the spatial step size is represented by h , and the number of spatial mesh points is indicated by N_x . Discrete Cosine or Sine transforms and their inverses are efficient methods we employ to compute the coefficients $\hat{v}_n$ and carry out the inverse reconstruction of v in physical space. These techniques depend on the given homogeneous BCs [52], [53].

3.2 Time Discretisation

Using the aforementioned Fourier spectral method, the following ordinary differential equations system (ODEs) is established, considering homogeneous boundary conditions

$$\frac{d}{dt}\mathcal{F}[v(x, t)] = -M\mathcal{F}[v(x, t)] + \mathcal{F}[F(v, t)]$$

let $\hat{v} = \mathcal{F}[v(x, t)]$ and $\hat{F}(\hat{v}, t) = \mathcal{F}[F(v, t)]$, then the ODEs system can be expressed as

$$\frac{d\hat{v}}{dt} = -M\hat{v} + \hat{F}(\hat{v}, t) \quad (3.3)$$

By multiplying Equation (3.3) by the integrating factor e^{Mt} and integrating over t , we derive the following exact solution

$$\hat{v}(t) = e^{-Mt}\hat{v}_0 + \int_0^t e^{-M(t-\tau)}\hat{F}(\hat{v}(\tau), \tau) d\tau \quad (3.4)$$

Therefore, the solution satisfied the recurrence formula

$$\hat{v}(t_{n+1}) = e^{-kM}\hat{v}(t_n) + \int_0^1 k e^{-kM(1-\mu)}\hat{F}(\hat{v}(t_n + \mu k), t_n + \mu k) d\mu \quad (3.5)$$

Cox and Mathews formulated time-stepping schemes that offer higher-order approximations schemes of Runge-Kutta type [45]. Let $\hat{v}(t_n) = \hat{v}_n$ and $\hat{F}(\hat{v}(t_n), t_n) = \hat{F}_n$.

Within this framework, our attention is directed towards the ETDRK3 scheme

$$\begin{aligned} \hat{v}_{n+1} &= e^{-kM}\hat{v}_n + k(-kM)^{-1} (e^{-kM} - I) \hat{F}_n \\ &+ k(-kM)^{-2} (e^{-kM} - I + kM) \left(-3\hat{F}_n + 4\hat{F}_n^\alpha - \hat{F}_n^\beta \right) \\ &+ 4k(-kM)^{-3} \left(e^{-kM} - I + kM - \frac{(kM)^2}{2} \right) \left(\hat{F}_n - 2\hat{F}_n^\alpha + \hat{F}_n^\beta \right), \end{aligned} \quad (3.6)$$

where

$$\begin{aligned}\alpha_n &= e^{\frac{kM}{2}} \hat{v}_n + \frac{k}{2} \left(-\frac{kM}{2}\right)^{-1} \left(e^{-\frac{kM}{2}} - I\right) \hat{F}_n, \\ \beta_n &= e^{-kM} \hat{v}_n + k(-kM)^{-1} (e^{-kM} - I) \left(2\hat{F}_n^\alpha - \hat{F}_n\right),\end{aligned}$$

and

$$\begin{aligned}\hat{F}_n &= F(\hat{v}_n, t_n), \\ \hat{F}_n^\alpha &= F(\alpha_n, t_n + k/2), \\ \hat{F}_n^\beta &= \hat{F}(\beta_n, t_n + k).\end{aligned}$$

For further details on the scheme's derivation, see to section (2.3.1).

Computing the matrix exponential of sparse matrix representations don't necessarily result in a sparse form. This chapter suggests modifying equation (3.6) for the matrix exponential function e^{-z} by using the third-order Restricted Padé and Padé(1,2) approximations.

3.2.1 ETD-Padé(1,2) Scheme

The Padé (1,2) approximation (2.10) is of the third-order L-acceptable approximation. The exponential matrix functions $e^{-\frac{kM}{2}}$ and e^{-kM} are approximated using the Padé (1,2) approximation. Approximating e^{-kM} is given by

$$R_{1,2}(kM) = (k^2M^2 + 4kM + 6I)^{-1}(6I - 2kM) \quad (3.7)$$

Therefor, the ETD scheme in (3.6) becomes

$$\hat{v}_{n+1} = R_{1,2}(kM)\hat{v}_n + \hat{\Phi}_1(kM)\hat{F}_n + \hat{\Phi}_2(kM)\hat{F}_n^\alpha + \hat{\Phi}_3(kM)\hat{F}_n^\beta, \quad (3.8)$$

where

$$\hat{\Phi}_1(kM) = k(k^2M^2 + 4kM + 6I)^{-1}$$

$$\hat{\Phi}_2(kM) = 4k(k^2M^2 + 4kM + 6I)^{-1}$$

$$\hat{\Phi}_3(kM) = k(k^2M^2 + 4kM + 6I)^{-1} (kM + I)$$

and

$$\alpha_n = \tilde{R}_{1,2}(kM)\hat{v}_n + \tilde{\Psi}_1(kM)\hat{F}_n,$$

$$\beta_n = R_{1,2}(kM)\hat{v}_n + \tilde{\Psi}_2(kM) \left(2\hat{F}_n^\alpha - \hat{F}_n \right),$$

where

$$\tilde{R}_{1,2}(kM) = (k^2M^2 + 8kM + 24I)^{-1}(24I - 4kM)$$

$$\tilde{\Psi}_1(kM) = k(k^2M^2 + 8kM + 24I)^{-1} (kM + 12I)$$

$$\tilde{\Psi}_2(kM) = k(k^2M^2 + 4kM + 6I)^{-1} \cdot (kM + 6I)$$

3.2.2 ETD-Restricted Padé Scheme

The Restricted Padé approximation is of the third-order A-acceptable approximation.

The approximation of e^{-kM} using-Restricted Padé approximation is defined as

$$R_h(kM) = 6 \left(6 + \left(3 + \sqrt{3} \right) kM \right)^{-2} \left(6I + 2\sqrt{3}kM - \left(1 + \sqrt{3} \right) k^2M^2 \right) \quad (3.9)$$

Approximating the exponential matrix functions $\exp(-\frac{kM}{2})$ and e^{-kM} in (3.6) and rearranging terms, we obtain the following third-order ETD-Restricted Padé Scheme

$$\hat{v}_{n+1} = R_h(kM^{\frac{\alpha}{2}})\hat{v}_n + \hat{\Phi}_1(kM)\hat{F}_n + \hat{\Phi}_2(kM)\hat{F}_n^\alpha + \hat{\Phi}_3(kM)\hat{F}_n^\beta, \quad (3.10)$$

where

$$\hat{\Phi}_1(kM) = 6k(6I + (3 + \sqrt{3})kM)^{-2}(I + (1 + \sqrt{3})kM)$$

$$\hat{\Phi}_2(kM) = 24k(6I + (3 + \sqrt{3})kM)^{-2}$$

$$\hat{\Phi}_3(kM) = 6k(6I + (3 + \sqrt{3})kM)^{-2}(I + (2 + \sqrt{3})kM)$$

and

$$\alpha_n = \tilde{R}_h(kM)\hat{v}_n + \tilde{\Psi}_1(kM)\hat{F}_n,$$

$$\beta_n = R_h(kM)\hat{v}_n + \tilde{\Psi}_2(kM)\left(2\hat{F}_n^\alpha - \hat{F}_n\right),$$

where

$$\tilde{R}_h(kM) = 6(12I + (3 + \sqrt{3})kM)^{-2}\left(24I + 4\sqrt{3}kM - (1 + \sqrt{3})k^2M^2\right),$$

$$\tilde{\Psi}_1(kM) = 6k(12I + (3 + \sqrt{3})kM)^{-2}(12I + (3 + 2\sqrt{3})kM),$$

$$\tilde{\Psi}_2(kM) = 6k(6I + (3 + \sqrt{3})kM)^{-2}(6I + (3 + 2\sqrt{3})kM).$$

3.3 The Third-Order ETD Algorithms

The algorithms for the modified numerical schemes, the L -stable ETD-Padé(1,2) and

A -stable ETD-Restricted Padé schemes is presented below

Algorithm 3 Three-Dimensional ETD-Padé(1,2) Algorithm for Neumann BCs

```

Initialize: grid points  $Nx = Ny = Nz$ ,  $h = \frac{b-a}{N_x}$ , time step  $k$ ,  $T, \mathcal{K}$ ,  $\alpha$ , initial
condition  $v$ .
for  $i = 1, 2, \dots, N_x$  do
3:   Calculate  $\mu_i = \left( \left( \frac{(i-1)\pi}{b-a} \right)^2 + \left( \frac{(i-1)\pi}{b-a} \right)^2 + \left( \frac{(i-1)\pi}{b-a} \right)^2 \right)^{\alpha/2}$ ,
      Calculate  $x_i, y_i, z_i$  as  $a + (i-1)h + \frac{h}{2}$ .
end for
6: Calculate  $A_1 = ((k\mathcal{K}\mu)^2 + 4k\mathcal{K}\mu + 6)$  and  $A_2 = ((k\mathcal{K}\mu)^2 + 8k\mathcal{K}\mu + 24)$ .
for  $n = 1$  to  $\text{round}(T/k)$  do
  Transform  $v$  to discrete cosine space:  $vdct = \text{dctn}(v)$ .
9:   Update time:  $t = nk$ .
      Calculate  $\alpha_n = \text{idctn}[(24 - 4k\mathcal{K}\mu) \cdot vdct + k(k\mathcal{K}\mu + 12) \cdot \text{dctn}(F_n)/A_2]$ .
      Calculate  $\beta_n = \text{idctn}[(6 - 2k\mathcal{K}\mu) \cdot vdct + k(k\mathcal{K}\mu + 6) \cdot \text{dctn}(2F_n^\alpha - F_n)/A_1]$ .
  Update  $v$  using discrete cosine transforms:
12:   $v = \text{idctn}((\text{dctn}((6 - 2k\mathcal{K}\mu) \cdot vdct) + k \cdot \text{dctn}(F_n) \cdot + 4k \cdot \text{dctn}(F_n^\alpha)
      + (k\mathcal{K}\mu + 1) \cdot \text{dctn}(F_n^\beta))/A_1)$ .
end for

```

For problems with homogeneous Dirichlet BCs, the computation of μ becomes

$$\mu = \left(\left(\frac{(1 : Nx)\pi}{b-a} \right)^2 + \left(\frac{(1 : Ny)\pi}{b-a} \right)^2 + \left(\frac{(1 : Nz)\pi}{b-a} \right)^2 \right)^{\frac{\alpha}{2}}.$$

Furthermore, the grid spacing h is changed to $\frac{b-a}{N_x+1}$. Instead of **idctn** and **dctn**,

the functions **idstn1** and **dstn** are used, respectively. These are the Discrete Co-

sine/Sine Transforms for one- and two-dimensional situations. Moreover, the notations

dctn/dstn indicate the Discrete Cosine/Sine Transforms for arbitrary n dimensions,

whereas **idctn/idstn** denote their inverse.

Algorithm 4 Three-Dimensional ETD-Restricted Padé Algorithm for Neumann BCs

Initialize: grid points $Nx = Ny = Nz$, $h = \frac{b-a}{N_x}$, time step k , $T, \mathcal{K}$, α , initial condition v .

for $i = 1, 2, \dots, N_x$ **do**

Calculate $\mu_i = \left(\left(\frac{(i-1)\pi}{b-a} \right)^2 + \left(\frac{(i-1)\pi}{b-a} \right)^2 + \left(\frac{(i-1)\pi}{b-a} \right)^2 \right)^{\alpha/2}$,

4: Calculate x_i, y_i, z_i as $a + (i-1)h + \frac{h}{2}$.

end for

Calculate $A_1 = (6 + (3 + \sqrt{3})k\mathcal{K}\mu)^2$ and $A_2 = (12 + (3 + \sqrt{3})k\mathcal{K}\mu)^2$.

for $n = 1$ to $\text{round}(T/k)$ **do**

8: Transform v to discrete cosine space: $vdct = \text{dctn}(v)$.
Update time: $t = nk$.
Calculate $\alpha_n = \text{idctn} [(24 + 4k\sqrt{3}\mathcal{K}\mu - (1 + \sqrt{3})(k\mathcal{K}\mu)^2) \cdot vdct + 6k(12 + (3 + 2\sqrt{3})k\mathcal{K}\mu) \cdot \text{dctn}(F_n)/A_2]$.

12: Calculate $\beta_n = \text{idctn} [6(6 + 2k\sqrt{3}\mathcal{K}\mu - (1 + \sqrt{3})(k\mathcal{K}\mu)^2) \cdot vdct + 6k(6 + (3 + 2\sqrt{3})k\mathcal{K}\mu) \cdot \text{dctn}(2F_n^\alpha - F_n)/A_1]$.

Update v using discrete cosine transforms:
 $v = \text{idctn} ((\text{dctn}(6(6 + 2k\sqrt{3}\mathcal{K}\mu - (1 + \sqrt{3})(k\mathcal{K}\mu)^2) \cdot vdct + (1 + (1 + \sqrt{3})k\mathcal{K}\mu) \cdot \text{dctn}(F_n) + 4k \cdot \text{dctn}(F_n^\alpha) + 6k(1 + (2 + \sqrt{3})k\mathcal{K}\mu) \cdot \text{dctn}(F_n^\beta))/A_1)$.

16: $+4k \cdot \text{dctn}(F_n^\alpha) + 6k(1 + (2 + \sqrt{3})k\mathcal{K}\mu) \cdot \text{dctn}(F_n^\beta))/A_1$.

end for

3.4 The Stability Regions and Linear Error Analysis

To investigate the linear stability of the suggested approaches, detailed in section (2.4). We begin with the fundamental non-linear ordinary differential equation

$$u_t = -au + f(u)$$

with $f(u)$ represents a non-linear function operating on u the complex-valued function.

After establishing a fixed point u_0 such that $-au_0 + f(u_0) = 0$, we proceed to linearize around u_0 , obtaining $u_t = au + \lambda u$, with $\lambda = f'(u_0)$ which indicates the derivative of f evaluated at u_0 . For the stability analysis, we introduce new variables $y = -ak$

and $x = \lambda k$, for time step k , facilitating the expression of the amplification factor through the Exponential Time Differencing (ETD) techniques, namely the L -stable ETD-Padé(1,2) and A -stable ETD-Restricted Padé schemes. The amplification factor for each method is delineated as follows

- **The L -stable ETD-Padé(1,2) scheme:**

The amplification factor is defined as

$$R(x, y) = \frac{b_3x^3 + b_2x^2 + b_1x + b_0}{\text{den}}$$

where the coefficients b_3, b_2, b_1 , and b_0 are defined by the scheme's parameters and den signifies the denominator, as in section (2.4).

- **The A -stable ETD-Restricted Padé scheme:**

Similarly, the amplification factor is

$$R(x, y) = \frac{d_3x^3 + d_2x^2 + d_1x + d_0}{\text{den}}$$

with d_3, d_2, d_1 , and d_0 representing coefficients unique to the Restricted Padé method and den the corresponding denominator, see section (2.4).

The depiction of stability regions in figure (2.3) for both the L -stable ETD-Padé(1,2) and A -stable ETD-Restricted Padé methods reveals that as $y \rightarrow \infty$, their stability regions broaden, affirming the robustness of these approaches.

In demonstrating the third-order convergence rate of our novel methods, we first

established the local truncation error as third-order in time by linearizing $\mathbf{F}(\mathbf{u})$ with $(H\mathbf{u})$.

$$\frac{d\mathbf{u}}{dt} = -M\mathbf{u} + H\mathbf{u} \quad (3.11)$$

The numerical solution, represented by Equation (2.21) and (2.23) for both of the L -stable ETD-Padé(1,2) and A -stable ETD-Restricted Padé methods and the exact solution, given by Equation (2.19). As in section (2.4), the local truncation error was computed to be

$$\|\mathbf{u}_{n+1} - e^{(H-M)k}\mathbf{u}_n\| = \mathcal{O}(k^4)$$

We conclude that, both schemes are of the third-order convergence.

3.5 Numerical Experiments

In this section, we apply our new methods to some well-known test problems to discuss and compute the numerical solutions. First, we solve a one dimensional test problem whose exact solution is available. The second problem we considered is a two-dimensional Allen-Cahn problem with an initial condition that is not smooth. Using absolute errors between the successive iterations, the order of convergence is calculated as

$$\mathcal{R} = \log_2 \frac{E(2k)}{E(k)},$$

where the error $E(k)$ is computed as the difference between the solutions at time steps $2k$ and k , represented as $|u(2k) - u(k)|$. This method calculates the order of convergence in cases where analytical solutions are not available, as discussed in [41], [54].

Convergence errors are determined using both the L_2 and L_∞ norms. The convergence tables provide information on the new method's computational efficiency, which is demonstrated by keeping track of CPU time during each iteration. As observed, the CPU time remains small even with a high number of time steps.

3.5.1 A test problem with exact solution

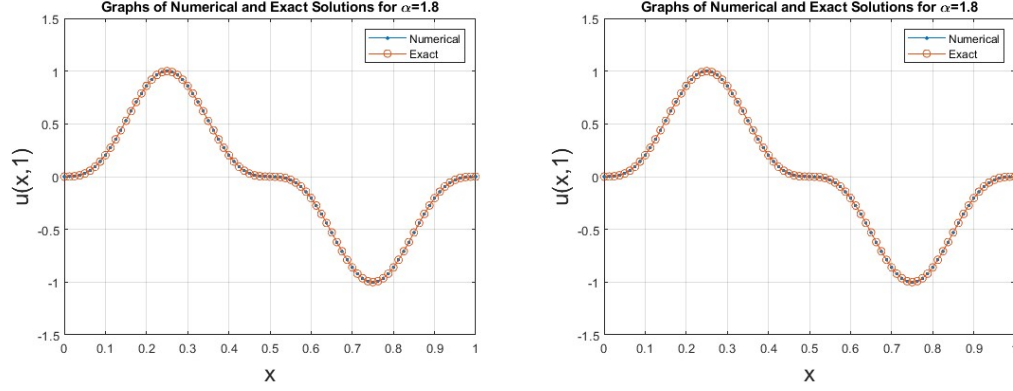
The exact solution of the following reaction-diffusion problem from Zhai et al. [49] is available. This test problem is being used to show the convergence order of the new modified methods.

$$\begin{aligned}\frac{\partial u}{\partial t} &= -\mathcal{K}(\Delta)^{\frac{\alpha}{2}} + f(u, x, t), & (x, t) \in (0, 1) \times (0, \infty), \quad 1 < \alpha \leq 2, \\ u(x, 0) &= 1, & 0 < x < 1, \\ u(0, t) &= 0, \quad u(1, t) = 0, & t > 0, \\ f(u, x, t) &= \alpha t^{\alpha-1} \sin^3(3\pi x) + \frac{\mathcal{K}}{4} t^\alpha (3[1 + (2\pi)^\alpha] \sin(2\pi x) - [1 + (6\pi)^\alpha] \sin(6\pi x)) - \mathcal{K}u\end{aligned}$$

For problem (3.5.1), The exact solution is

$$u(x, t) = t^\alpha \sin^3(2\pi x). \quad (3.12)$$

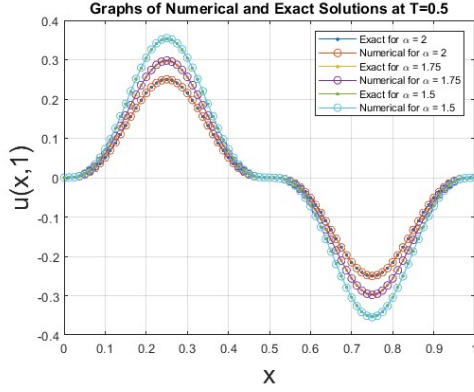
Problem (3.5.1) has been solved for various values of α . Graph of the numerical and exact solutions are shown in the figure (3.1) for both the L -stable ETD-Padé(1,2) and A -stable ETD-Restricted Padé methods. Since exact solution contains t^α , therefore graphs of the exact solution will vary depending on the value of α for $T \neq 1$. For $T = 0.5$, we have calculated numerical solutions for several values of α to demonstrate



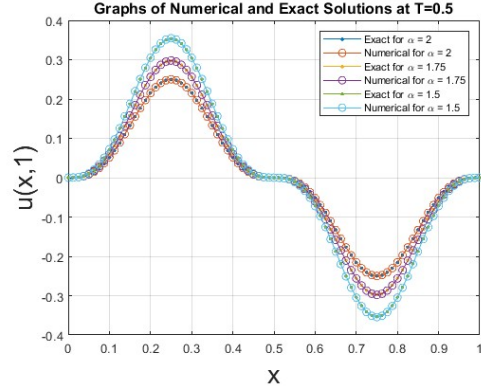
(a) Problem 3.5.1: Graph of numerical and exact solutions at $T = 1$ for ETD-Padé(1,2) scheme. (b) Problem 3.5.1: Graph of numerical and exact solutions at $T = 1$ for ETD-Restricted Padé scheme.

Figure 3.1: Problem 3.5.1: The L -stable and A -stable schemes compared to the exact solution.

the accuracy of our numerical approach. The figure (3.2) displays the graphs of both the numerical and exact solutions. Reliability of the numerical scheme for $0 \leq t \leq 1$ is shown by plotting the time evolution graph in figure (3.3). The convergence orders for L_∞ errors for different temporal steps are represented in table (3.1) with CPU time. The A -stable time stepping method is observed to require less computational time than the L -stable method.

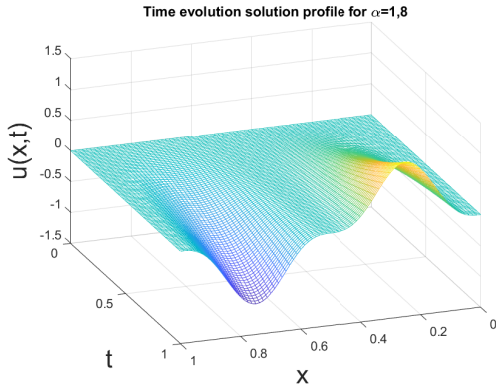


(a) Problem 3.5.1: Graphs of numerical and exact solutions at $T = 0.5$ for ETD-Padé(1,2) scheme.

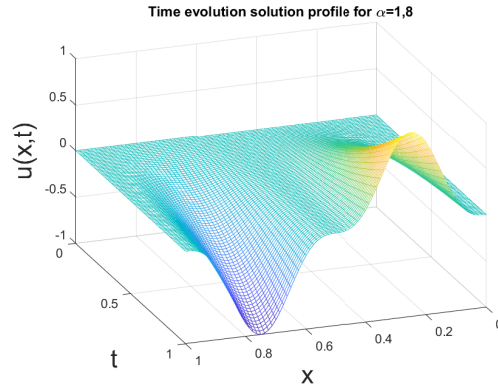


(b) Problem 3.5.1: Graphs of exact and numerical solution at $T = 0.5$ for ETD-Restricted Padé scheme.

Figure 3.2: Problem 3.5.1: Graphs of the exact solution and L -stable and A -stable numerical schemes at $T = 0.5$ for various values of α .



(a) Problem 3.5.1: Time evolution graph for L -stable ETD-Padé(1,2) scheme.



(b) Problem 3.5.1: Time evolution graph for A -stable ETD-Restricted Padé scheme.

Figure 3.3: Problem 3.5.1: Time evolution solution of the L -stable and A -stable schemes.

Table 3.1: Problem 3.5.1: L_∞ Convergence results for the L -stable and A -stable numerical schemes for $\alpha = 1.5$.

Method	h	k	error	order- L_∞	CPU Time
ETD-Padé(1,2)	0.01000	0.01000	2.4756e-04	-	0.0102
	0.00500	0.00500	3.0991e-05	2.9979	0.0003
	0.00250	0.00250	3.8753e-06	2.9995	0.0003
	0.00125	0.00125	4.8446e-07	2.9999	0.0006
	0.00063	0.00063	6.0559e-08	3.0000	0.0051
ETD-Restricted Padé	0.01000	0.01000	2.4756e-04	-	0.0163
	0.00500	0.00500	3.0991e-05	2.9979	0.0004
	0.00250	0.00250	3.8753e-06	2.9995	0.0003
	0.00125	0.00125	4.8446e-07	2.9999	0.0003
	0.00063	0.00063	6.0559e-08	3.0000	0.0032

3.5.2 Allen Cahn Equation with Nonsmooth Data

The Allen-Cahn equation (3.13) serves as a reaction-diffusion model for capturing the phase segregation dynamics within multi-component alloy systems. This includes detailing the movements of boundaries between phases and the formation of microstructural patterns.

$$\begin{aligned}
\frac{\partial u}{\partial t} &= -\mathcal{K}(\Delta)^{\frac{\alpha}{2}} - u(u^2 - 1), \quad (x, y) \in [0, 1] \times [0, 1], \quad t \in [0, T], \quad (3.13) \\
u(x, y, 0) &= \begin{cases} x^2 y(1 - x^3)(1 - y), & 0 < x < 0.5, \quad 0 < y < 1 \\ \frac{7}{16} xy(1 - x)(1 - y), & 0.5 \leq x < 1, \quad 0 < y < 1 \end{cases} \\
u(., t) &= 0, \quad (x, y) \in [0, 1] \times [0, 1], \quad t > 0,
\end{aligned}$$

Handling nonsmooth initial data within the Allen-Cahn equation framework poses numerous computational difficulties. This type of data may obstruct the achievement of numerical stability and accuracy, especially in regions near interfaces where there are abrupt changes in the solution's gradient. In the context of the Allen-Cahn equation

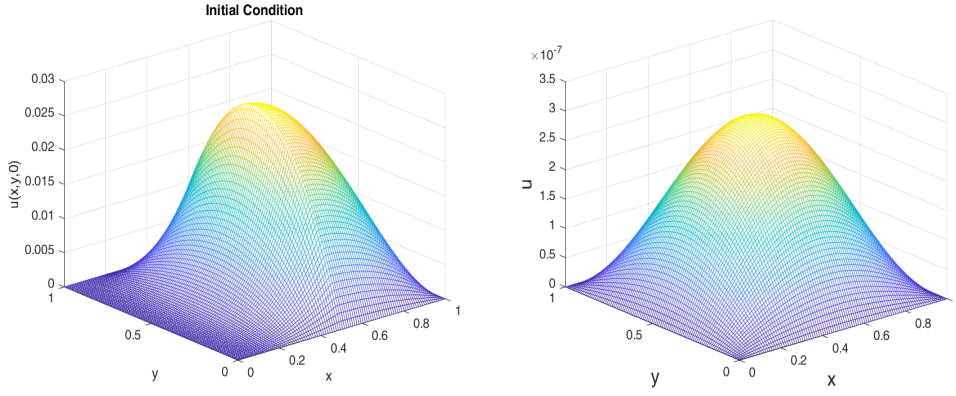


Figure 3.4: Problem 3.5.2: The Initial condition (left) and solution using L -stable scheme with 10 time steps only (right).

with nonsmooth initial conditions, it is noteworthy that L-stable schemes often provide solutions more expeditiously compared to A-stable schemes , see figures (3.4) and (3.5). This efficiency is attributed to the inherent attributes of L-stable methods, which prioritize stability while ensuring relatively swift convergence, particularly in scenarios involving nonsmooth data.

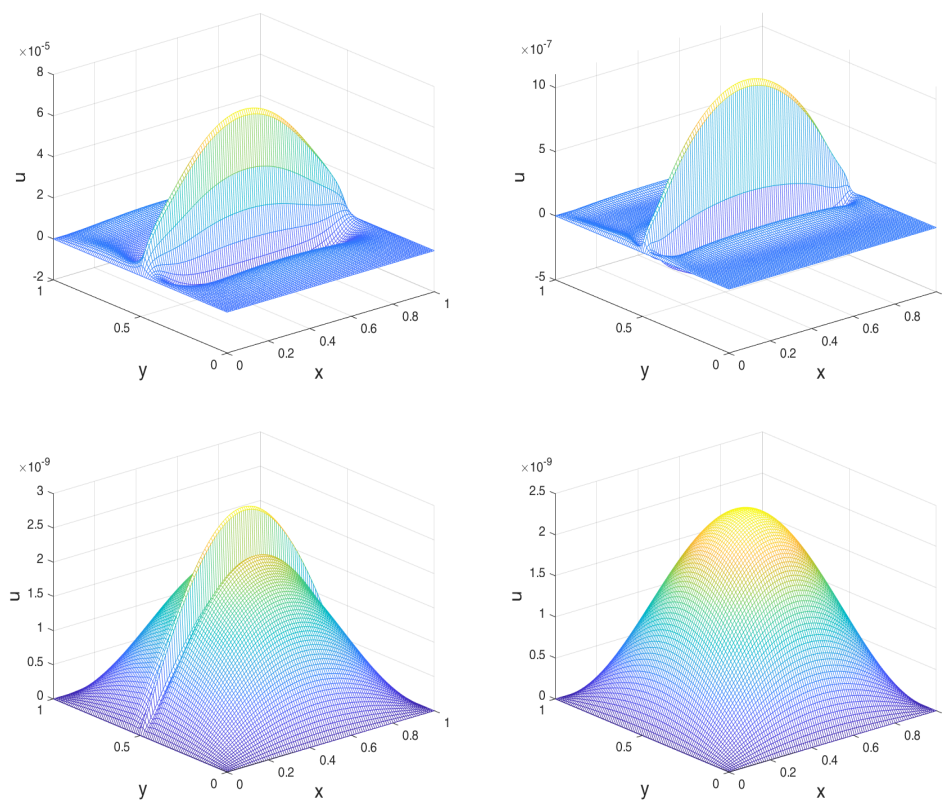


Figure 3.5: Problem 3.5.2: Numerical solution using A -stable method with 10, 20, 40, and 80 time steps.

3.5.3 3D Fisher's Equation

Consider the three-dimensional space-fractional Fisher's problem

$$\frac{\partial u}{\partial t} = -\mathcal{K}(-\Delta)^{\frac{\alpha}{2}}u + u - u^2, \quad (x, y, z) \in \Omega, \quad 1 < \alpha \leq 2$$

with the initial condition

$$u(x, y, z, 0) = \sin(\pi y) \sin(\pi z)$$

with homogeneous Dirichlet boundary condition.

Where $\Omega = (0, 1) \times (0, 1) \times (0, 1)$ and $\mathcal{K} = 1/5$. The issue of mismatched boundary and initial conditions arises in this problem. The numerical solutions obtained by the L-stable scheme computed with $k = 0.1, h = 0.0125$ at $T = 1$ for $\alpha = 1.4, 1.8$ are shown in figures (3.6) and (3.7), respectively. In the same manners, the numerical solutions obtained by the A-stable scheme for $\alpha = 1.4, 1.8$ are shown in figures (3.8) and (3.9), respectively. When employing the A-stable scheme, undesired oscillations for appears $\alpha = 1.8$,. As the fractional order diminishes to $\alpha = 1.4$, the undesired oscillations decrease. Additionally, in Figure (3.10), it can be observed that reducing the time step to $k = 0.05$ for $\alpha = 1.8$ further decreases the undesired oscillations. However, this reduction in time step results in an increase in CPU time to 12.832983 seconds, compared to 6.515076 seconds for $k = 0.1$.

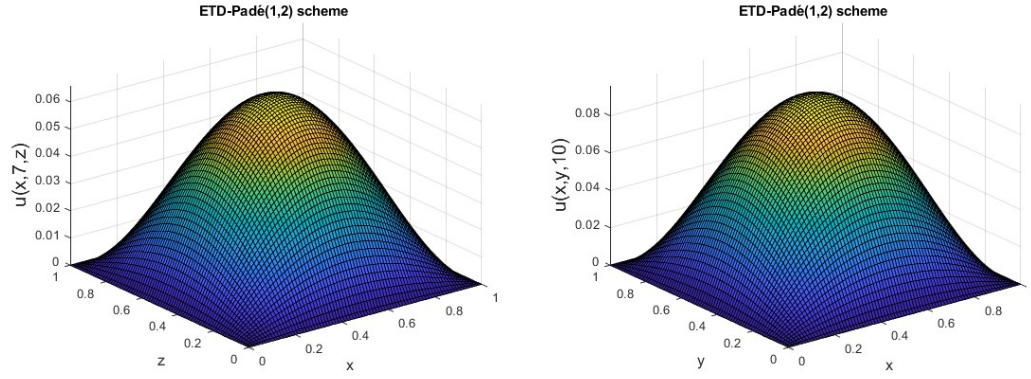


Figure 3.6: Problem 3.5.3: The L -stable scheme solutions for $\alpha = 1.4$.

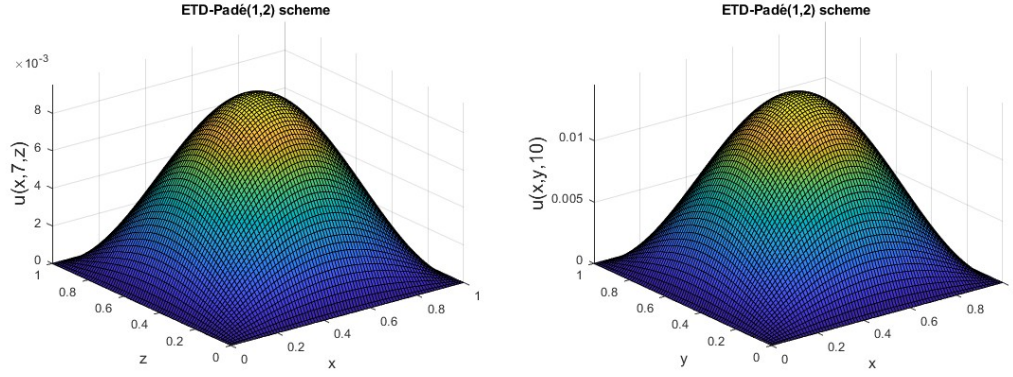


Figure 3.7: Problem 3.5.3: The L -stable scheme solutions for $\alpha = 1.8$.

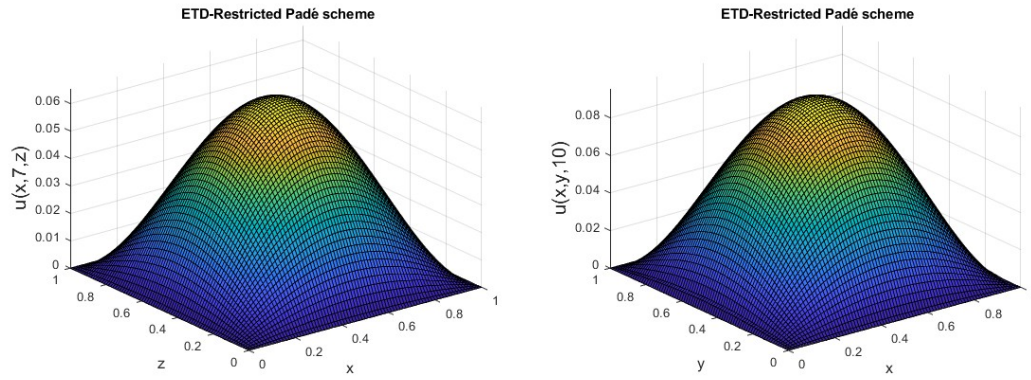


Figure 3.8: Problem 3.5.3: The A -stable scheme solutions for $\alpha = 1.4$.

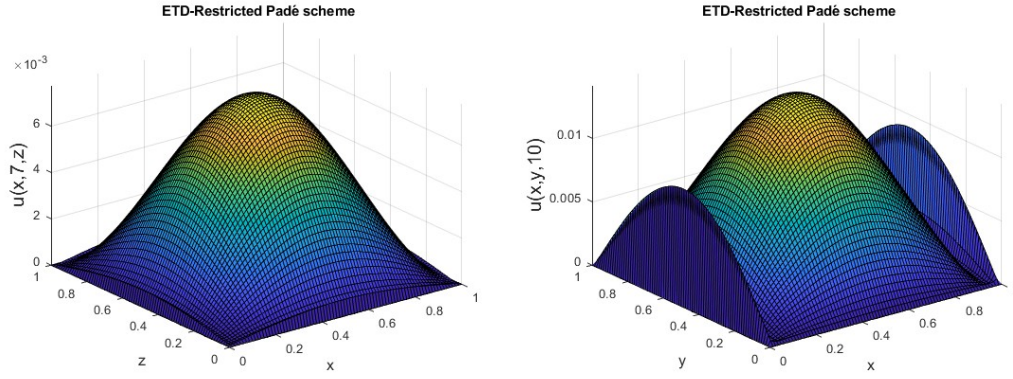


Figure 3.9: Problem 3.5.3: The A -stable scheme solutions for $\alpha = 1.8$.

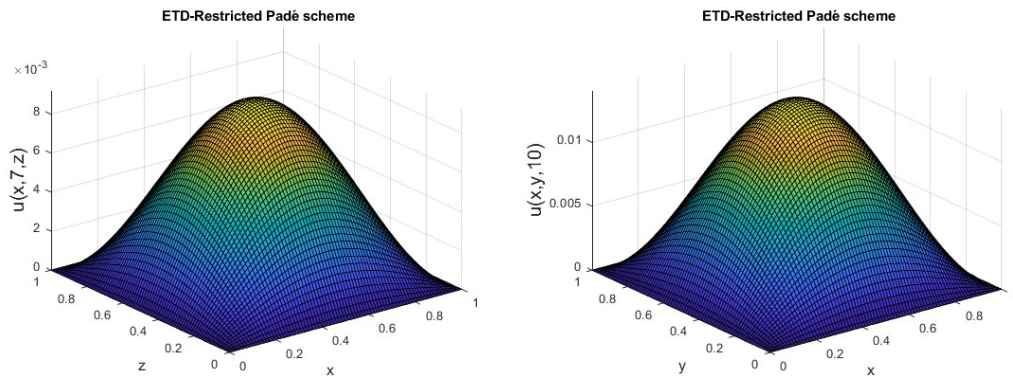


Figure 3.10: Problem 3.5.3: The A -stable scheme solutions for $k = 0.05$ and $\alpha = 1.8$.

3.5.4 Fitzhugh–Nagumo model

The FitzHugh–Nagumo reaction-diffusion model is an extension of the basic FitzHugh–Nagumo model. This model is used to account for the spatial dynamics, particularly diffusion, in addition to temporal dynamics. The behavior of excitable media such as chemical reactions or the propagation of action potentials in excitable tissues like neurons are described by this model [30], [31].

$$\begin{aligned}\frac{\partial u}{\partial t} &= -\mathcal{K}_\alpha(\Delta)^{\frac{\alpha}{2}}u - v + u(u - a)(1 - u), \\ \frac{\partial v}{\partial t} &= \epsilon(\beta u - \gamma v - \delta),\end{aligned}$$

where the parameters values taken are: $\mathcal{K} = 10^{-4}$, $a = 0.1$, $\epsilon = 0.01$, $\gamma = 1$, $\beta = 0.5$ and $\delta = 0$. The problem (3.5.4) is solved on the spatial domain $[0, 2.5] \times [0, 2.5]$ with homogeneous Neumann boundary conditions. We perturb the initial state $(u, v) = (0, 0)$ by assigning $u = 1$ to the lower-left quarter of the spatial domain and $v = 0.1$ to the upper half part. This perturbation will cause the initial condition to curve and rotate clockwise and generate the spiral waves. Figure (3.11) and (3.12) show the graphs of the numerical solutions of both v and u computed for various values of α .

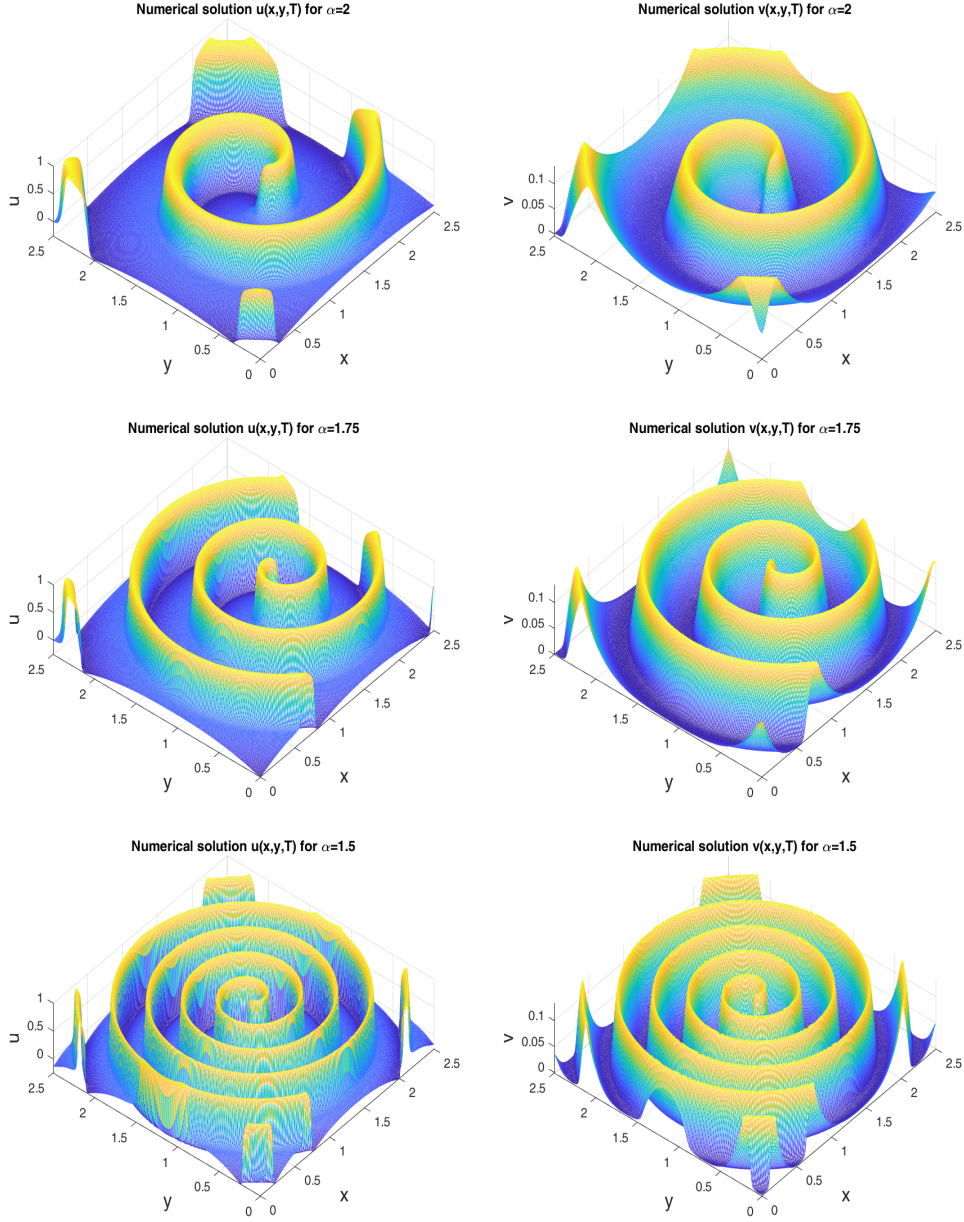


Figure 3.11: Problem 3.5.4: Numerical solutions of Fitzhugh–Nagumo model using ETD-Restricted Padé scheme for various values of α

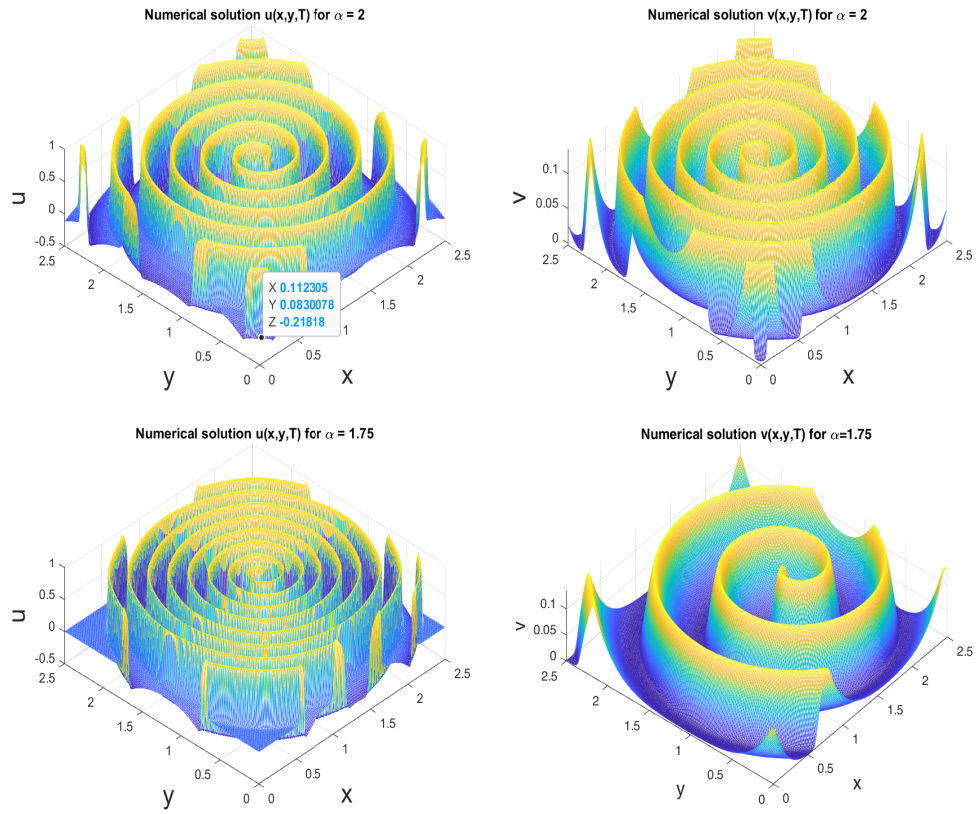


Figure 3.12: Problem 3.5.4: Numerical solutions of Fitzhugh–Nagumo model using ETD- $\text{Padé}(1,2)$ scheme for various values of α

3.5.5 Allen Cahn Equation for Phase Separation Phenomena

In this problem, we consider the two-dimensional Allen-Chan equation starting from a random initial configuration. Phase separation can occur, for instance, between domains with different magnetizations in a ferromagnet, or in mixtures of ice and water, [55]. It also occurs in mixtures of two substances with different properties, such as metals in certain alloys, water and oil, or oil and vinegar in mayonnaise missing egg yolk. However, the Allen-Cahn equation does not conserve the total amount of each phase, which is why other equations, such as the Cahn-Hilliard equation are used. Figure (3.13) shows the contour plot and 3-dimensional plot of the random initial condition. The patterned dynamics of Allen-Cahn model for different values of α using ETD-Restricted Padé scheme shown in the figure (3.14) are computed at $T = 20$. Phase change phenomena is further explored and shown in the figures (3.15).

$$\begin{aligned}\frac{\partial u}{\partial t} &= -\mathcal{K}_\alpha(\Delta)^{\frac{\alpha}{2}} - u(u^2 - 1), \quad (x, y) \in \Omega, \quad 0 < t \leq T, \quad (3.14) \\ u(x, y, 0) &= [-0.1\text{Random}(N) + 0.1\text{Random}(N)]/2 \\ u(., t) &= 0, \quad (x, y) \in \Omega, \quad t > 0,\end{aligned}$$

where $\Omega = [-1, 1] \times [-1, 1]$

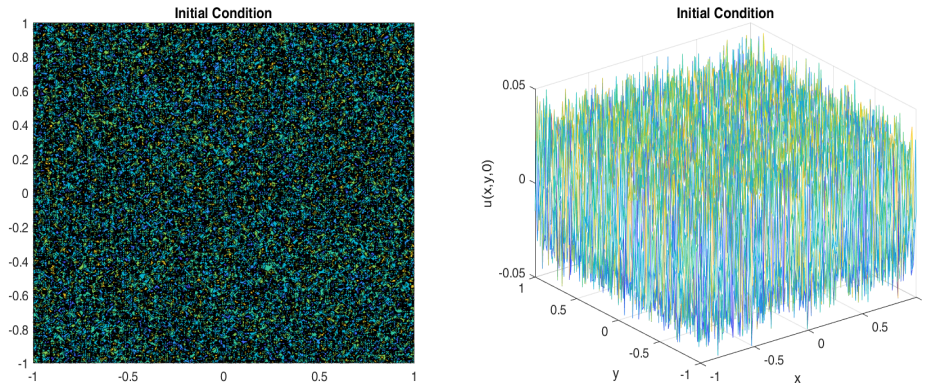


Figure 3.13: Problem 3.5.5: Initial condition contour plot (left) and 3-Dimensional plot (right) with random noise.

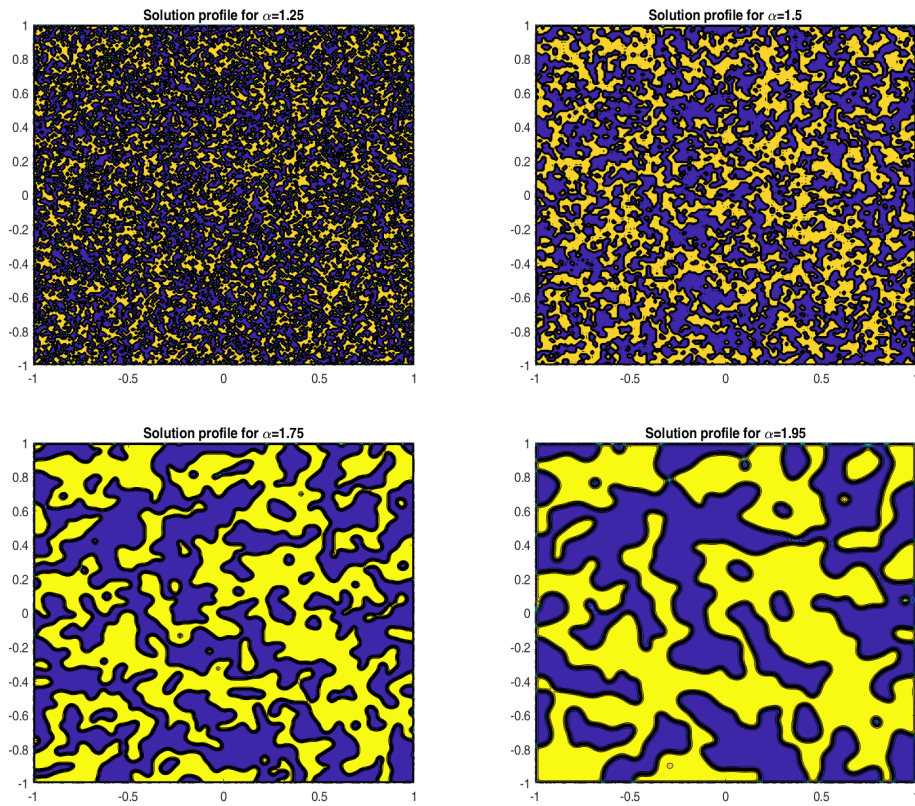


Figure 3.14: Problem 3.5.5: Solution profiles at $t = 20$ for various values of α

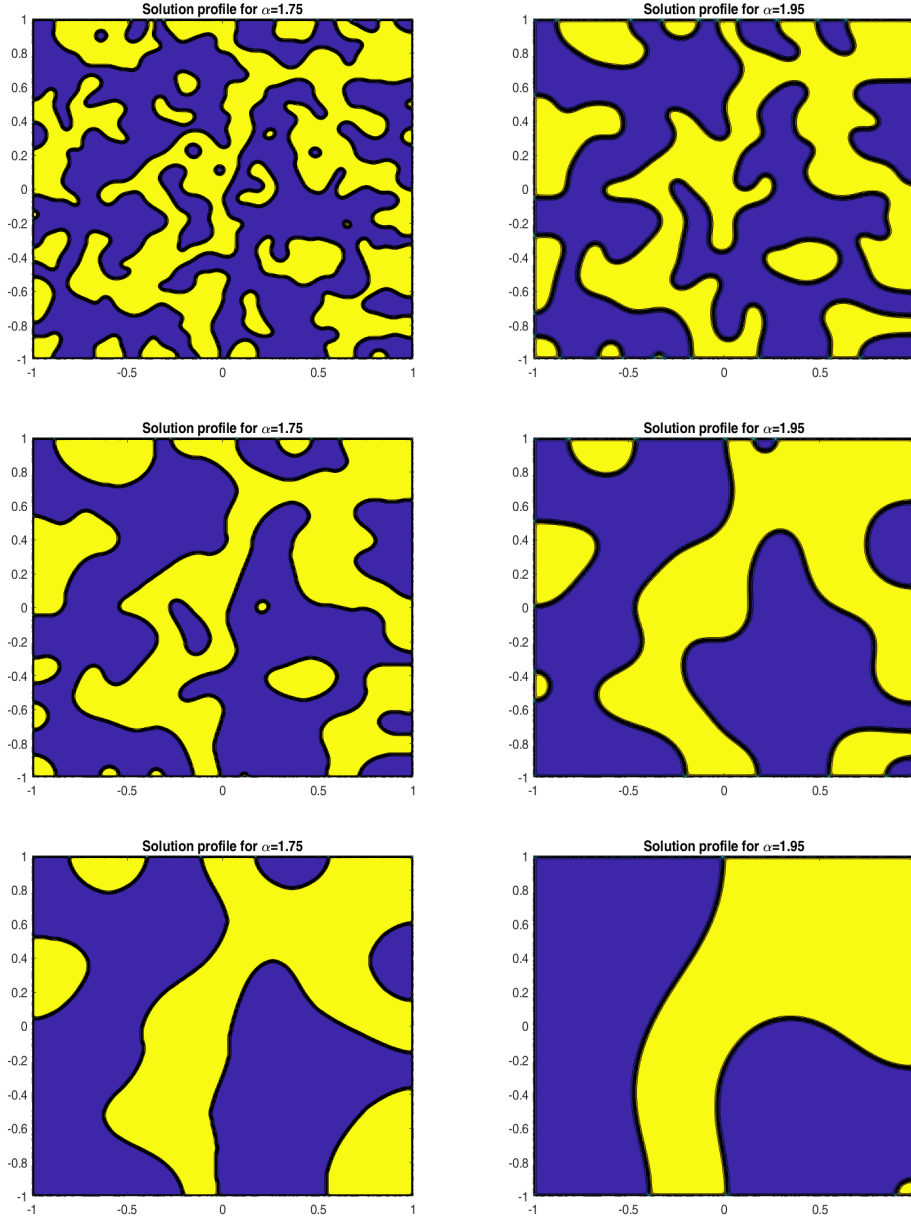


Figure 3.15: Problem 3.5.5: Solution profiles at $t = 50$, $t = 200$, and $t = 1000$ for various values of α

3.6 Conclusion

Two highly efficient methods, characterized as A-stable and L-stable, have been developed to solve nonlinear fractional reaction-diffusion systems. These schemes utilize the Fourier spectral approach for spatial discretization and the Exponential Time Differencing (ETD) approach for temporal discretization. Additionally, a novel approach utilizing a single Gaussian quadrature pole rational approximation of the matrix exponential function has been introduced. Through analytical proof and numerical verification, the third-order convergence of these methods has been established. Furthermore, solution profiles have been plotted to illustrate the impact of order of diffusion in some two-dimensional problems.

CHAPTER 4

CONCLUSION AND FUTURE WORK

In our study, we introduced two highly efficient numerical schemes designed for solving nonlinear fractional reaction-diffusion problems on finite domains with either homogeneous Neumann or homogeneous Dirichlet boundary conditions. These schemes combine the Matrix Transform Technique (MTT) for spatial discretization with Exponential Time Differencing Runge-Kutta (ETDRK) approach to solve the semi-discretized equations. Furthermore, we extended our study to include the solution of problems involving non-homogeneous Dirichlet boundary conditions. Additionally, we developed a new time-stepping numerical scheme based on real poles rational approximation of matrix exponential functions, comparing it with the Padé (1,2) approximation method which involves complex arithmetic poles. To enhance computational efficiency, we employed the partial fraction splitting approach. Moreover, we utilized the Fourier Spectral approach for space discretization, which can be extended to solve

multi-dimensional problems in the same manner as it solves one-dimensional problems, thereby enabling spectral convergence for multidimensional cases. We thoroughly discussed the convergence and stability of the schemes and conducted numerical experiments to illustrate their accuracy, reliability, and efficiency. Our study underscores the significance of selecting appropriate numerical schemes, as the A-stable approach may exhibit unwanted spurious oscillations, especially with non-smooth initial data, while the L-stable approach consistently maintains its expected third-order accuracy. As future work, it would be beneficial to explore the impact of different boundary conditions on the performance and accuracy of the numerical schemes. This investigation could involve analyzing how variations in boundary conditions, such as mixed or time-dependent boundary conditions, influence the stability and convergence properties of the schemes. By conducting such an analysis, valuable insights can be gained into optimizing the schemes for a broader range of practical applications and boundary conditions.

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