Numerical treatment of certain fractional and non-fractional differential equations

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Numerical Treatment of Certain Fractional and Non-fractional Differential Equations

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School of Electrical & Electronic Engineering

A thesis submitted to the Nanyang Technological University
in partial fulfillment of the requirements for the degree of
Doctor of Philosophy

2020

Statement of Originality

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Patricia Wg

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Prof Wong Jia Yiing, Patricia

Authorship Attribution Statement

This thesis contains material from 4 papers published in the following peer-reviewed journal / from papers accepted at conferences in which I am listed as an author.

Chapter 3 is published as Q. Ding and P. J. Y. Wong, “Mid-knot cubic non-polynomial spline for a system of second-order boundary value problems,” *Boundary Value Problems*, 2018, Paper No. 156, 16 pp.

The contributions of the co-authors are as follows:

- Prof Wong provided the initial project direction and edited the manuscript drafts.
- I prepared the manuscript drafts.
- I derived the numerical algorithm and analyzed the theoretical results with the help of Prof Wong.
- I co-designed the numerical simulation with Prof Wong and analyzed the data.

Chapter 4 is published as Q. Ding and P. J. Y. Wong, “Numerical method for fractional Bagley-Torvik equation,” *Proceedings of the International Conference on Numerical Analysis and Applied Mathematics 2018 (ICNAAM-2018), AIP Conference Proceedings 2116, 240007 (2019)*.

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- I co-designed the numerical simulation with Prof Wong and analyzed the data.

Chapter 5 is published as Q. Ding and P. J. Y. Wong, “An efficient numerical approach for a new generalized fractional diffusion equation,” *Proceedings of the International Conference on Numerical Analysis and Applied Mathematics 2018 (ICNAAM-2018)*, AIP Conference Proceedings 2116, 240009 (2019).

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- Prof Wong provided the initial project direction and edited the manuscript drafts.
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- I derived the numerical algorithm and analyzed the theoretical results with the help of Prof Wong.
- I co-designed the numerical simulation with Prof Wong and analyzed the data.

Chapter 7 is published as Q. Ding and P. J. Y. Wong, “Non-polynomial spline method for time-fractional nonlinear Schrödinger equation,” *Proceedings of the 15th International Conference on Control, Automation, Robotics and Vision, Singapore (2018)*.

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14 April 2020

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Ding Qinxu

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Qinxu Ding

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“Life is like a sea, only the strong will of people, to reach the other shore.”

—Karl Marx

To my dear family

Abstract

Differential equations with integer order or fractional order derivatives have attracted much attention for a long time, as they are very useful in modelling phenomena that arise from various fields such as physics, chemistry, biology, mechanics, finance and engineering. Indeed, the ‘memory’ property of fractional derivatives enhances the accuracy of the models. However, it is a fact that finding analytical solutions of differential equations, fractional or non-fractional, is nearly impossible in many instances. The development of efficient numerical schemes for such equations is therefore very important, and this will be the focus of our work in this thesis.

In this thesis, we shall investigate the numerical treatment of differential equations in two categories: (i) ordinary differential equations; (ii) partial differential equations. In the first category, we consider two problems – a second-order boundary value problem with discontinuous second order derivative at some breakup points; and a fractional Bagley-Torvik equation. For both problems, we propose new numerical methods that give more accurate solutions than other methods in the literature. In fact, the numerical scheme for the second-order boundary value problem is based on cubic non-polynomial spline deployed over the mid-knots of a uniform mesh, while discrete cubic spline and weighted shifted Grünwald-Letnikov difference operator are used to solve the fractional Bagley-Torvik equation. We also present theoretical proofs of the stability and convergence of the numerical schemes, and confirm the theoretical results by numerical experiments.

In the second category of partial differential equations, we consider a fractional nonlinear Schrödinger equation and a *generalized* fractional diffusion equation. For the fractional nonlinear Schrödinger equation, our proposed method, which employs quintic non-polynomial spline, improves the spatial convergence achieved so far in the literature. As for the *generalized* fractional diffusion equation, here the fractional derivative is ‘generalized’ in the sense that it features a scale function and a weight function, which can scale up/down the time domain or assign different

weights at different time points. With specific scale functions and weight functions, the generalized fractional derivative reduces to well known fractional derivatives in the literature. The approximation of the generalized fractional derivative as well as the numerical treatment of generalized fractional problems have been scarcely researched in the literature. In this thesis, we shall derive higher order approximations for the generalized fractional derivative and then apply them in the numerical schemes proposed for a generalized fractional diffusion problem. In all the problems that we considered above, both theoretical analysis and numerical simulation are presented to support and illustrate the efficiency of our methods.

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Notations

P	uniform mesh of $[a, b]$ in (2.1)
P'	mesh of $[0, T]$ in (2.18)
P''	uniform mesh of $[\mathcal{Z}(0), \mathcal{Z}(T)]$ in (5.12)
h	grid step size in x dimension
τ	grid step size in t dimension
$D_t^k(\frac{\partial^k}{\partial t^k})$	k -th derivative with respect to t
$D_x^m(\frac{\partial^m}{\partial x^m})$	m -th derivative with respect to x
u_{xx}	second order derivative of u with respect to variable x
$u_{zzz}(u_{zzzz})$	third order (fourth order) derivative of u with respect to variable z

$\mathcal{R}$	set of real numbers
$\mathcal{R}^+$	set of positive real numbers
$\mathcal{N}$	set of positive integer numbers
$\lceil \gamma \rceil$	the smallest integer larger than γ
$y^{(k)}(\cdot)$	k -th derivative of $y(\cdot)$
$\mathcal{C}^k(\cdot)$	$\{y(\cdot) \mid y^{(k)}(\cdot) \text{ is continuous, } 0 \leq i \leq k\}$
$\mathcal{C}^{m,k}(\cdot)$	$\{y(\cdot) \mid D_x^i D_t^j y \text{ is continuous, } 0 \leq i \leq m, 0 \leq j \leq k\}$
$L^1(\mathcal{R})$	$\{y(t) \mid \int_{-\infty}^{\infty} y(s) ds < +\infty\}$
$\tilde{y}(\varpi)$	Fourier transform of $y(t)$
$\mathcal{C}^{\gamma+m}(\mathcal{R})$	$\{y(t) \mid \int_{-\infty}^{\infty} (1 + \varpi ^{\gamma+m}) \tilde{y}(\varpi) d\varpi < \infty\}$
$\mathcal{U}_P$	$\{u \mid u = (u_0, u_1, \dots, u_M) \text{ and } u_0 = u_M = 0\}$
δ_x^i	x dimension difference notations (5.4)

$(\cdot, \cdot)_1$	semi inner product in (5.5)
$(\cdot, \cdot)$	inner product in (5.5)
$ \cdot _1$	semi norm in (5.6)
$\ \cdot\ $	$L2$ norm in (5.6)
$\ \cdot\ _\infty$	maximum norm in (5.6)
$E_{av}(h, N)$	average norm error at $t = t_N$ with step sizes h, τ (5.74)
$E_\infty(h, N)$	maximum norm error at $t = t_N$ with step sizes h, τ (5.74)
$E_2(h, \tau)$	maximum $L2$ norm error with step sizes h, τ (7.64)
$E_\infty(h, \tau)$	maximum modulus error with step sizes h, τ (7.65)
$E_\infty^{Re}(h, \tau)$	maximum real part absolute error with step sizes h, τ (7.66)
$E_\infty^{Im}(h, \tau)$	maximum imaginary part absolute error with step sizes h, τ (7.66)
S_{av}	spatial convergence order in average norm (5.75)
T_{av}	temporal convergence order in average norm (5.75)
S_∞	spatial convergence order in maximum norm
T_∞	temporal convergence order in maximum norm
S_2	spatial convergence order in $L2$ norm (7.67)
T_2	temporal convergence order in $L2$ norm (7.68)

Chapter 1

Introduction

1.1 Background

There is a long history in the development of differential equations, which first came into existence from 1671 during the invention of calculus by Newton and Leibniz. Differential equations include ordinary differential equations and partial differential equations. An ordinary differential equation is an equation containing an unknown function of one real or complex variable, while a partial differential equation contains more than one independent variable. Since derivatives and differential equations are very powerful in describing how changes take place, they are widely used to model the phenomena in various fields, such as physics, biology, finance, engineering and so on.

In the past few decades, fractional differential equations have increasingly been employed to propose more accurate models for different systems of science [38, 70, 103, 104, 111]. Due to the nonlocal property of fractional derivative, those systems which require ‘memory’ property can be described more accurately. Actually, fractional derivative has its roots in 1695, from the letter between de l’Hospital and Leibniz. It is just an operator which generalizes the ordinary derivative, and it will reduce to the ordinary derivative when the order is an integer. Until now, there are many different ways to define a fractional derivative, such as Grünwald-Letnikov derivative [104], Riemann-Liouville fractional derivative [104], Caputo fractional derivative [38, 104], Katugampola derivative [63], local fractional operator [135, 147], Risez fractional derivative [137] and tempered fractional derivative [112]. However, the

most famous among them are Riemann-Liouville fractional derivative and Caputo fractional derivative, which are widely used by researchers. Recently, to unify the various type of fractional derivatives, Agrawal [4] has proposed a new generalized fractional derivative, which includes a scale function $\mathcal{Z}(t)$ and a weight function $\mathcal{W}(t)$. By choosing specific scale and weight functions, the generalized fractional derivative will reduce to known fractional derivative in the literature. Besides the purpose of unification, the scale and weight functions have practical applications, such as stretch or contract the time domain with scale function and weigh an event differently at different time points with weight function.

Although fractional and non-fractional differential equations are both powerful to model the phenomena and systems, it is difficult to obtain the analytical solutions for most of them. Under this situation, developing efficient and stable numerical schemes becomes necessary. Actually, the development of numerical treatment for differential equations is a classical problem in mathematics. In 1768, Leonhard Euler was the first to publish his famous method, the Euler method. Till now, there are many well known methods to solve the differential equations such as multistep methods, Runge-Kutta method, finite difference method, spline method, finite element method, collocation method and so on. In particular, discrete spline was first introduced by Mangasarian and Schumaker [88] in 1971. Subsequently, Lyche [86, 87] developed the theory of discrete spline. Chen and Wong [27–31] further developed the discrete spline and applied it to various problems. On the other hand, non-polynomial spline methods have also attracted attentions. A survey of this method was presented by Khan et al. [66]. Actually, we shall focus on using discrete and non-polynomial spline methods to approximate the integer (second) order derivatives in the problems.

In this thesis, we aim to propose efficient and highly accurate numerical methods to solve various differential equations. We shall also present rigorous stability and convergence analysis for our numerical schemes and provide numerical experiments to verify the theoretical results.

1.2 Major Contribution

The objective of this thesis is to develop efficient and accurate numerical schemes for fractional and non-fractional differential equations in the following two parts:

- (a) two classes of ordinary differential equations;
- (b) two classes of partial differential equations.

The first problem of part (a) is a system of second-order boundary value problems. This type of system arises in the study of obstacle, unilateral, moving and free boundary value problems [16, 33, 34, 71, 110]. To avoid the points of discontinuity of the second order derivative, we apply a mid-knot cubic non-polynomial spline to obtain the numerical solution. We prove that our scheme is stable and second order convergent by matrix analysis method. From the numerical experiments, our method performs better than literature works. The second problem of part (a) is the fractional Bagley-Torvik equation, which is first discussed by Bagley and Torvik [14, 15] who have used fractional derivatives to put forward some viscoelastic models. We derive a fourth order weighted shifted Grünwald-Letnikov difference operator to approximate the Riemann-Liouville fractional derivative and extend it to the Caputo fractional derivative. Together with a discrete cubic spline method, we derive a numerical scheme to solve the fractional Bagley-Torvik equation. Using the matrix analysis method, we claim our method is fourth order convergent, which achieves the best result to date.

The first problem of part (b) is a generalized fractional diffusion equation that has also been considered in [133]. The generalized fractional derivative includes a scale function and a weight function that can be changed and hence generate many types of fractional derivatives. However, there are limited approximation methods proposed for this kind of generalized fractional derivative. Till now, the best result is $(2-\gamma)$ th order, where γ is the fractional order. Therefore, we derive a third order approximation for it based on the generalized weighted shifted Grünwald-Letnikov difference operator. Together with central finite difference method, we derive a numerical scheme to solve the generalized fractional diffusion equation. We seriously demonstrate the stability and convergence of our scheme by energy method. Later on, we further derive a fourth order approximation for the generalized fractional

derivative. To achieve high accuracy in both time and space, we combine a compact finite difference scheme to solve the generalized fractional diffusion equation this time. From the theoretical result, the convergence orders of time and space are both four.

The second problem of part (b) is a time-fractional nonlinear Schrödinger equation, which is used to describe fractional quantum mechanical behavior. It is derived by replacing the first order time derivative by the Caputo fractional derivative. We apply quintic non-polynomial spline to approximate the second order derivative in it. The previous best result is a fourth order convergence in space, and we improve it to sixth order. The theoretical analysis is completed by Fourier method.

1.3 Outline of the Thesis

The main contributions of the thesis are presented in Chapters 3-7. The relationships among these chapters can be summarized in two aspects. The first aspect is about the types of differential equations considered in the chapters. We consider more and more complicated differential equations as we progress in the thesis, from integer order ordinary differential equation (Chapter 3) to fractional order ordinary differential equation on real space domain (Chapter 4), to generalized fractional order partial differential equation on real space domain (Chapters 5-6), to fractional order partial differential equation on complex space domain (Chapter 7). The second aspect is about the types of approximation methods used in these chapters. To approximate the second order derivative, we employ spline methods in three chapters, namely the mid-knot cubic non-polynomial spline (Chapter 3), discrete cubic spline (Chapter 4) and quintic non-polynomial spline (Chapter 7); and we use finite difference methods in two chapters, namely the central finite difference (Chapter 5) and compact finite difference (Chapter 6). To approximate the fractional derivative, we employ the well known L1 discretization (Chapter 7) and develop the weighted shifted Grunwald-Letnikov (WSGD) methods in three chapters, namely 4-WSGD (Chapter 4), third order generalized WSGD (Chapter 5) and fourth order generalized WSGD (Chapter 6).

The thesis is organized as follows.

In Chapter 2, we will introduce discrete spline, non-polynomial spline, basic fractional calculus and review related work in the literature.

In Chapter 3, a *mid-knot cubic non-polynomial spline* is applied to obtain the numerical solution of a system of second-order boundary value problems. The numerical method is proved to be uniquely solvable and is of second-order accuracy. We further include three examples to illustrate the accuracy of our method and to compare with other methods in the literature.

In Chapter 4, we develop a higher order numerical method for the fractional Bagley-Torvik equation. The main tools used include a *new* fourth order approximation for the fractional derivative based on the weighted shifted Grünwald-Letnikov difference operator and a discrete cubic spline approach. We show that the theoretical convergence order *improves* those of previous work. Four examples are further presented to illustrate the efficiency of our method and to compare with other methods in the literature.

In Chapter 5, we develop a higher order approximation for the *generalized* fractional derivative that includes a scale function $\mathcal{Z}(t)$ and a weight function $\mathcal{W}(t)$. This is then used to solve a generalized fractional diffusion problem numerically. The stability and convergence analysis of the numerical scheme are conducted by the energy method. It is proven that the temporal convergence order is 3 and the spatial convergence order is 2. Finally, we provide three examples to confirm the theoretical results.

In Chapter 6, we derive a fourth order approximation for the *generalized* fractional derivative that is characterized by a scale function $\mathcal{Z}(t)$ and a weight function $\mathcal{W}(t)$. Combining the new approximation with compact finite difference method, we develop a numerical scheme for a generalized fractional diffusion problem. The stability and convergence of the numerical scheme are proved by the energy method, and it is shown that the temporal and spatial convergence orders are both 4. Several numerical experiments are provided to illustrate the efficiency of our scheme.

In Chapter 7, we shall solve a time-fractional nonlinear Schrödinger equation by using the quintic non-polynomial spline and the $L1$ formula. The unconditional stability, unique solvability and convergence of our numerical scheme are proved by Fourier method. It is shown that our method is sixth order accurate in the spatial dimension and $(2 - \gamma)$ th order accurate in the temporal dimension, where γ

is the fractional order. The efficiency of the proposed numerical scheme is further illustrated by numerical experiments, meanwhile the simulation results indicate better performance over previous work in the literature.

Finally, Chapter 8 summarizes our work and provides some future work.

Chapter 2

Literature Review

In this chapter, we begin with the introduction of discrete spine and non-polynomial spline. We shall focus on the spline relations for the approximation of second order derivative, which are used in Chapters 3, 4 and 7. We also give a review about other existing methods for the approximation of second order derivative. Next, we shall introduce basic definitions of fractional integrals and derivatives. We also give a review about the approximation methods for the Riemann-Liouville and Caputo fractional derivatives. In the last, we give some physical meanings about the equations we consider in Chapter 3-7.

2.1 Approximation of the Second Order Derivative

In this section, we shall introduce some basic concepts of discrete and non-polynomial spline methods. We also derive the spline relations which are useful to approximate the second order derivative. After that, we would list other existing methods used to solve problems involving second order derivative. We consider $x \in [a, b]$ of a given function $y(x)$ without loss of generality and assume that the function $y(x)$ is sufficiently smooth. First, we will give the following mesh which will be used throughout this section. Let

$$P : a = x_0 < x_1 < \cdots < x_M = b \tag{2.1}$$

be a uniform mesh of $[a, b]$ with $x_m - x_{m-1} = h$, $1 \leq m \leq M$, and the step size $h = \frac{b-a}{M}$.

2.1.1 Discrete Spline Method

The discrete spline has been carefully discussed in [27–31, 86–88]. In this section, we shall only focus on introducing discrete cubic spline to approximate the second order derivative.

Let $h_c \in (0, h]$ be a given constant. The *central difference operator* $D_{h_c}^{\{k\}}$, $k = 0, 1, 2$ applying to a function $y(x)$ gives

$$D_{h_c}^{\{0\}} y(x) = y(x), \quad D_{h_c}^{\{1\}} y(x) = \frac{1}{2h_c} [y(x + h_c) - y(x - h_c)],$$

$$D_{h_c}^{\{2\}} y(x) = \frac{1}{h_c^2} [y(x + h_c) - 2y(x) + y(x - h_c)].$$

Lyche [87] has introduced the *basic polynomials* $x^{\{j\}}$, $j = 0, 1, 2, 3$ as

$$x^{\{j\}} = x^j, \quad j = 0, 1, 2, \quad x^{\{3\}} = x(x^2 - h_c^2).$$

Clearly, we have $D_{h_c}^{\{1\}} x^{\{j\}} = jx^{\{j-1\}}$, $j = 0, 1, 2, 3$.

Right now, we give the definition of discrete cubic spline.

Definition 2.1. [28] Let $S(x, h, h_c)$ be a piecewise continuous function defined over $[a, b]$ (with mesh P) and $S_m(x)$ be its restriction in $[x_{m-1}, x_m]$, $1 \leq m \leq M$ passing through the points (x_{m-1}, S_{m-1}) and (x_m, S_m) . We say $S(x, h, h_c)$ is a *discrete cubic spline* if $S_m(x)$, $1 \leq m \leq M$ is a polynomial of degree 3 or less and

$$(S_{m+1} - S_m)(x_m + jh_c) = 0, \quad j = -1, 0, 1, \quad 1 \leq m \leq M - 1$$

or equivalently

$$D_{h_c}^{\{j\}} S_m(x_m) = D_{h_c}^{\{j\}} S_{m+1}(x_m), \quad j = 0, 1, 2, \quad 1 \leq m \leq M - 1.$$

Note that [87] has the same definition for discrete spline.

First, we shall obtain an explicit expression of $S_m(x)$ for $x \in [x_{m-1}, x_m]$, $1 \leq m \leq M$. Denote $D_{h_c}^{\{2\}} S_m(x_m) = W_m$. Since $D_{h_c}^{\{2\}} S_m(x)$ is piecewise linear, we have for $x \in [x_{m-1}, x_m]$, $1 \leq m \leq M$,

$$D_{h_c}^{\{2\}} S_m(x) = \frac{x_m - x}{h} W_{m-1} + \frac{x - x_{m-1}}{h} W_m,$$

which leads to

$$S_m(x) = \frac{(x_m - x)^{\{3\}}}{6h} W_{m-1} + \frac{(x - x_{m-1})^{\{3\}}}{6h} W_m + \frac{x_m - x}{h} C_{1,m} + \frac{x - x_{m-1}}{h} C_{2,m}, \quad (2.2)$$

where $C_{1,m}$ and $C_{2,m}$ are constants that can be determined using the interpolation conditions $S_m(x_{m-1}) = S_{m-1}$ and $S_m(x_m) = S_m$. It is found that

$$C_{1,m} = S_{m-1} - \frac{h^2 - h_c^2}{6} W_{m-1}, \quad C_{2,m} = S_m - \frac{h^2 - h_c^2}{6} W_m.$$

Next, upon substituting $C_{1,m}$ and $C_{2,m}$ into (2.2) and then taking central difference, we get

$$\begin{aligned} D_{h_c}^{\{1\}} S_m(x) = & \frac{-(x_m - x)^{\{2\}}}{2h} W_{m-1} + \frac{(x - x_{m-1})^{\{2\}}}{2h} W_m + \frac{S_m - S_{m-1}}{h} \\ & - \frac{h^2 - h_c^2}{6h} (W_{m-1} - W_m). \end{aligned} \quad (2.3)$$

Using the continuity condition $D_{h_c}^{\{1\}} S_m(x_m) = D_{h_c}^{\{1\}} S_{m+1}(x_m)$, from (2.3) we obtain the ‘spline relation’

$$S_{m-1} - 2S_m + S_{m+1} = \alpha W_{m-1} + \beta W_m + \alpha W_{m+1}, \quad 1 \leq m \leq M-1, \quad (2.4)$$

where

$$\alpha = \frac{h^2 - h_c^2}{6}, \quad \beta = \frac{2h^2 + h_c^2}{3}. \quad (2.5)$$

Remark 2.1. The spline relation (2.4) is used to approximate the second order derivative [28, 143]. For a specified $h_c = \frac{1}{\sqrt{2}}h$, this relation gives fourth order accuracy. For $h_c \neq \frac{1}{\sqrt{2}}h$, the relation gives second order accuracy.

2.1.2 Non-polynomial Spline Methods

The non-polynomial spline methods have been discussed in a very good survey paper [66]. In this section, we shall introduce cubic and quintic non-polynomial spline methods.

First, we shall introduce the cubic non-polynomial spline. Consider the uniform mesh P .

Definition 2.2. For a given mesh P , we say $\bar{S}(x)$ is the *cubic non-polynomial spline with parameter ξ (> 0)* if $\bar{S}(x) \in C^{(2)}[a, b]$, $\bar{S}(x)$ has the form $\text{span}\{1, x, \sin \xi x, \cos \xi x\}$, and its restriction $\bar{S}_m(x)$ on $[x_{m-1}, x_m]$, $1 \leq m \leq M$ satisfies

$$\begin{cases} \bar{S}_m(x_{m-1}) = \bar{S}_{m-1}, & \bar{S}_m(x_m) = \bar{S}_m, \\ \bar{S}_m''(x_{m-1}) = \bar{W}_{m-1}, & \bar{S}_m''(x_m) = \bar{W}_m. \end{cases} \quad (2.6)$$

From the above definition, for $x \in [x_{m-1}, x_m]$, $1 \leq m \leq M$, we can express $\bar{S}_m(x)$ as

$$\bar{S}_m(x) = \bar{C}_{1,m} \sin \xi(x - x_{m-1}) + \bar{C}_{2,m} \cos \xi(x - x_{m-1}) + \bar{C}_{3,m}(x - x_{m-1}) + \bar{C}_{4,m}. \quad (2.7)$$

Using (2.6), a direct computation gives

$$\begin{aligned} \bar{S}_m(x) = & \frac{-\bar{W}_m + \bar{W}_{m-1} \cos \xi h}{\xi^2 \sin \xi h} \sin \xi(x - x_{m-1}) - \frac{\bar{W}_{m-1}}{\xi^2} \cos \xi(x - x_{m-1}) \\ & + \left(\frac{\bar{S}_m - \bar{S}_{m-1}}{h} + \frac{\bar{W}_m - \bar{W}_{m-1}}{\xi^2 h} \right) (x - x_{m-1}) + \bar{S}_{m-1} + \frac{\bar{W}_{m-1}}{\xi^2}. \end{aligned} \quad (2.8)$$

Then, using the continuity of the first derivative of the spline, namely, $\bar{S}_m'(x_m) = \bar{S}_{m+1}'(x_m)$, $1 \leq m \leq M - 1$, we obtain from (2.8)

$$\bar{S}_{m-1} - 2\bar{S}_m + \bar{S}_{m+1} = h^2 (\bar{\alpha} \bar{W}_{m-1} + 2\bar{\beta} \bar{W}_m + \bar{\alpha} \bar{W}_{m+1}), \quad 1 \leq m \leq M - 1, \quad (2.9)$$

where

$$\bar{\alpha} = \frac{1}{\xi h \sin \xi h} - \frac{1}{\xi^2 h^2}, \quad \bar{\beta} = \frac{1}{\xi^2 h^2} - \frac{\cos \xi h}{\xi h \sin \xi h}. \quad (2.10)$$

Remark 2.2. The spline relation (2.9) is used to approximate the second order derivative [44, 65, 66, 76, 116]. For $\bar{\alpha} = \frac{1}{12}h^2$, the spline relation gives fourth order accuracy. For other choice of $\bar{\alpha}$, it gives second order accuracy.

Right now, we shall introduce the quintic non-polynomial spline method.

Definition 2.3. For a given mesh P , we say $\hat{S}(x)$ is the quintic non-polynomial spline with parameter $\xi(> 0)$ if $\hat{S}(x) \in C^{(4)}[a, b]$, $\hat{S}(x)$ has the form span $\{1, x, x^2, x^3, \sin \xi x, \cos \xi x\}$ and its restriction $\hat{S}_m(x)$ on $[x_{m-1}, x_m]$, $1 \leq m \leq M$ satisfies

$$\begin{cases} \hat{S}_m(x_{m-1}) = \hat{S}_{m-1}, & \hat{S}_m(x_m) = \hat{S}_m, \\ \hat{S}_m^{(2)}(x_{m-1}) = \hat{W}_{m-1}, & \hat{S}_m^{(2)}(x_m) = \hat{W}_m, \\ \hat{S}_m^{(4)}(x_{m-1}) = \hat{F}_{m-1}, & \hat{S}_m^{(4)}(x_m) = \hat{F}_m. \end{cases} \quad (2.11)$$

From the above definition, for each segment $[x_{m-1}, x_m]$, $1 \leq m \leq M$, the quintic non-polynomial spline $\hat{S}_m(x)$ is defined by

$$\begin{aligned} \hat{S}_m(x) = & \hat{C}_{1,m} + \hat{C}_{2,m}(x - x_{m-1}) + \hat{C}_{3,m}(x - x_{m-1})^2 + \hat{C}_{4,m}(x - x_{m-1})^3 \\ & + \hat{C}_{5,m} \sin \xi(x - x_{m-1}) + \hat{C}_{6,m} \cos \xi(x - x_{m-1}). \end{aligned} \quad (2.12)$$

Using (2.11), a direct computation gives

$$\begin{aligned} \hat{C}_{1,m} &= \hat{S}_{m-1} - \frac{\hat{F}_{m-1}}{\xi^4}, \\ \hat{C}_{2,m} &= \frac{\hat{S}_m - \hat{S}_{m-1}}{h} + \frac{\hat{F}_{m-1} - \hat{F}_m}{\xi^4 h} - \frac{h}{6}(2\hat{W}_{m-1} + \hat{W}_m) - \frac{h}{6\xi^2}(2\hat{F}_{m-1} + \hat{F}_m), \\ \hat{C}_{3,m} &= \frac{1}{2} \left(\hat{W}_{m-1} + \frac{\hat{F}_{m-1}}{\xi^2} \right), \\ \hat{C}_{4,m} &= \frac{\hat{W}_m - \hat{W}_{m-1}}{6h} + \frac{\hat{F}_m - \hat{F}_{m-1}}{6\xi^2 h}, \\ \hat{C}_{5,m} &= \frac{\hat{F}_m - \hat{F}_{m-1} \cos \xi h}{\xi^4 \sin \xi h}, \\ \hat{C}_{6,m} &= \frac{\hat{F}_{m-1}}{\xi^4}, \end{aligned} \quad (2.13)$$

where $m = 0, 1, 2, \dots, M-1$.

Using the continuity of the first and third derivatives of the spline at $x = x_m$, that is $\hat{S}_m^{(1)}(x_m) = \hat{S}_{m+1}^{(1)}(x_m)$ and $\hat{S}_m^{(3)}(x_m) = \hat{S}_{m+1}^{(3)}(x_m)$, we obtain the following relations

$$\begin{aligned} (a) \hat{W}_{m-1} + 4\hat{W}_m + \hat{W}_{m+1} &= \frac{6}{h^2} \left(\hat{S}_{m-1} - 2\hat{S}_m + \hat{S}_{m+1} \right) \\ &\quad - 6h^2 \left(\alpha_1 \hat{F}_{m-1} + 2\beta_1 \hat{F}_m + \alpha_1 \hat{F}_{m+1} \right), \quad (2.14) \\ (b) \hat{W}_{m-1} - 2\hat{W}_m + \hat{W}_{m+1} &= h^2 \left(\hat{\alpha} \hat{F}_{m-1} + 2\hat{\beta} \hat{F}_m + \hat{\alpha} \hat{F}_{m+1} \right), \end{aligned}$$

where

$$\begin{aligned} \hat{\alpha} &= \frac{1}{\xi^2 h^2} \left(\frac{\xi h}{\sin \xi h} - 1 \right), \quad \hat{\beta} = \frac{1}{\xi^2 h^2} \left(1 - \frac{\xi h \cos \xi h}{\sin \xi h} \right), \\ \alpha_1 &= \frac{1}{6\xi^2 h^2} + \frac{1}{\xi^4 h^4} - \frac{1}{\xi^3 h^3 \sin \xi h}, \quad \beta_1 = \frac{1}{3\xi^2 h^2} - 1 + \frac{\cos \xi h}{\xi^3 h^3 \sin \xi h}. \end{aligned} \quad (2.15)$$

Applying (2.14)(a) and (2.14)(b), we can easily get

$$\begin{aligned} &\frac{1}{h^2} \left[\hat{\alpha} \hat{S}_{m+2} + 2(\hat{\beta} - \hat{\alpha}) \hat{S}_{m+1} + 2(\hat{\alpha} - 2\hat{\beta}) \hat{S}_m + 2(\hat{\beta} - \hat{\alpha}) \hat{S}_{m-1} + \hat{\alpha} \hat{S}_{m-2} \right] \\ &= p \hat{W}_{m+2} + q \hat{W}_{m+1} + s \hat{W}_m + q \hat{W}_{m-1} + p \hat{W}_{m-2}, \quad 2 \leq m \leq M-2, \end{aligned} \quad (2.16)$$

where

$$p = \alpha_1 + \frac{\hat{\alpha}}{6}, \quad q = 2 \left[\frac{2\hat{\alpha} + \hat{\beta}}{6} - (\alpha_1 - \beta_1) \right], \quad s = 2 \left[\frac{\hat{\alpha} + 4\hat{\beta}}{6} + (\alpha_1 - 2\beta_1) \right]. \quad (2.17)$$

Remark 2.3. The spline relation (2.16) is used to approximate the second order derivative [79, 82, 83]. Noted that the consistency relation for (2.14)(b) will lead to $2(\hat{\alpha} + \hat{\beta}) = 1$.

2.1.3 Other Methods

To approximate the second order derivative, there are also some other methods besides discrete spline and non-polynomial spline methods. For non-fractional differential equations, there are finite difference [8], compact finite difference [102], polynomial spline [5–7, 9, 13], B-spline [99], decomposition [96] and iteration method [100]. For fractional differential equations, there are finite difference [24, 32, 122, 133, 134, 138, 139], compact finite difference [25, 35, 36, 49, 57], polynomial spline [56, 141, 142], B-spline [45], collocation [17, 18], discontinuous Galerkin [62, 80], iteration [91], differential transform [11], decomposition [108] and homotopy perturbation method [151].

2.2 Fractional Calculus

In this section, we shall first introduce some essential concepts of fractional integrals and derivatives. After that, we shall introduce some approximation methods for Riemann-Liouville fractional derivative and Caputo fractional derivative. In this thesis, we mainly focus on the approximations of time-fractional derivatives. Therefore, we consider $t \in [0, T]$ for a given function $y(t)$ without loss of generality. Let

$$P' : 0 = t_0 < t_1 < \cdots < t_N = T \quad (2.18)$$

be a uniform mesh of $[0, T]$ with $t_n - t_{n-1} = \tau$, $1 \leq n \leq N$, and the step size $\tau = \frac{T}{N}$.

2.2.1 Fractional Integrals and Derivatives

First, we shall introduce the concepts of fractional integrals including definitions of Riemann-Liouville fractional integral and a new generalized fractional integral.

Definition 2.4. [38, 103, 104] Let $\gamma \in \mathcal{R}^+ \setminus \mathcal{N}$. The Riemann-Liouville fractional integral of $y(t)$ is defined by

$${}^{RL}_0 I_t^\gamma y(t) = \frac{1}{\Gamma(\gamma)} \int_0^t (t-s)^{\gamma-1} y(s) ds. \quad (2.19)$$

Actually, the above definition coincides with the classical definition of a n -fold integral with $n \in \mathcal{N}$. Besides the above classical Riemann-Liouville fractional integral, Agrawal [4] proposed a new generalized fractional integral with a weight function $\mathcal{W}(t)$ and a scale function $\mathcal{Z}(t)$. Here, we give the following definition.

Definition 2.5. [4] Let $\gamma \in \mathcal{R}^+ \setminus \mathcal{N}$. The *generalized Riemann-Liouville fractional integral* of $y(t)$ with scale function $\mathcal{Z}(t)$ and weight function $\mathcal{W}(t)$ is defined by

$${}^{RL}_0 I_{t;[\mathcal{Z},\mathcal{W}]}^\gamma y(t) = \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(\gamma)} \int_0^t [\mathcal{Z}(t) - \mathcal{Z}(s)]^{\gamma-1} \mathcal{W}(s) \mathcal{Z}'(s) y(s) ds. \quad (2.20)$$

Remark 2.4. It is obvious that (2.20) reduces to the classical fractional integral (2.19) when $\mathcal{Z}(t) = t$, $\mathcal{W}(t) \equiv 1$.

Next, we shall introduce the fractional derivatives considered in this thesis including Riemann-Liouville fractional derivative, Caputo fractional derivative and a new generalized fractional derivative.

Definition 2.6. [38, 103, 104] Let $\gamma \in \mathcal{R}^+ \setminus \mathcal{N}$ and $k = \lceil \gamma \rceil$. The γ -th order Riemann-Liouville fractional derivative of $y(t)$ is given by

$${}^{RL}_0 D_t^\gamma y(t) = D_t^k ({}^{RL}_0 I_t^{k-\gamma} y(t)) = \frac{1}{\Gamma(k-\gamma)} \frac{d^k}{dt^k} \int_0^t (t-s)^{k-\gamma-1} y(s) ds. \quad (2.21)$$

Definition 2.7. [38, 103, 104] Let $\gamma \in \mathcal{R}^+ \setminus \mathcal{N}$ and $k = \lceil \gamma \rceil$. The γ -th order Caputo fractional derivative of $y(t)$ is given by

$${}_0^C D_t^\gamma y(t) = {}^{RL}_0 I_t^{k-\gamma} (D_t^k y(t)) = \frac{1}{\Gamma(k-\gamma)} \int_0^t (t-s)^{k-\gamma-1} y^{(k)}(s) ds. \quad (2.22)$$

Lemma 2.1. [38] Let $\gamma \in \mathcal{R}^+ \setminus \mathcal{N}$ and $k = \lceil \gamma \rceil$. We have

$${}_0^C D_t^\gamma y(t) = {}^{RL}_0 D_t^\gamma y(t) - \sum_{j=1}^{k-1} \frac{y^{(j)}(0)}{\Gamma(j-\gamma+1)} t^{j-\gamma}. \quad (2.23)$$

Remark 2.5. From Lemma 2.1, it is obvious that ${}_0^C D_t^\gamma y(t) = {}^{RL}_0 D_t^\gamma y(t)$ if and only if $y^{(j)}(0) = 0$, $0 \leq j \leq k-1$.

Finally, we shall introduce two new generalized fractional derivatives in [4]. For simplicity, we shall first introduce a notation as

$$D_{[\mathcal{Z}, \mathcal{W}]}^k y(t) = [\mathcal{W}(t)]^{-1} \left[\left(\frac{1}{\mathcal{Z}'(t)} D_t \right)^k (\mathcal{W}(t)y(t)) \right] (t), \quad (2.24)$$

where $\mathcal{Z}(t)$ is the scale function and $\mathcal{W}(t)$ is the weight function.

Now, we can give the definitions of the new generalized Riemann-Liouville and new generalized Caputo fractional derivatives.

Definition 2.8. Let $\gamma \in \mathcal{R}^+ \setminus \mathcal{N}$ and $k = \lceil \gamma \rceil$. The γ -th order generalized Riemann-Liouville fractional derivative of $y(t)$ is given by

$${}^{RL}_0 D_{t;[\mathcal{Z}, \mathcal{W}]}^\gamma y(t) = D_{[\mathcal{Z}, \mathcal{W}]}^k ({}^{RL}_0 I_{t;[\mathcal{Z}, \mathcal{W}]}^{k-\gamma} y(t)). \quad (2.25)$$

Definition 2.9. Let $\gamma \in \mathcal{R}^+ \setminus \mathcal{N}$ and $k = \lceil \gamma \rceil$. The γ -th order generalized Caputo fractional derivative of $y(t)$ is given by

$${}_0^C D_{t;[\mathcal{Z}, \mathcal{W}]}^\gamma y(t) = {}^{RL}_0 I_{t;[\mathcal{Z}, \mathcal{W}]}^{k-\gamma} (D_{[\mathcal{Z}, \mathcal{W}]}^k y(t)). \quad (2.26)$$

2.2.2 Approximation of Fractional Derivatives

In this section, we shall discuss the approximation methods for fractional derivatives. We focus on the approximation when the fractional order $\gamma \in (0, 1)$ and $\gamma \in (1, 2)$. These will be used in the later chapters of this thesis. Actually, there are many methods for approximating the fractional derivatives in the literature. For fractional order $\gamma \in (0, 1)$, there are $L1$ discretization [49, 56, 79, 97, 123], $L1 - 2$ method [50], $L1 - 3$ method [19], $L1 - r$ method ($r \geq 4$) [75], $L2 - 1_\sigma$ method [10], Grünwald-Letnikov method [125, 139], WSGD method [57, 125], fractional Crank-Nicolson method [61] and convolution quadrature [60]. For $\gamma \in (1, 2)$, there are $L1$ discretization [123], Grünwald-Letnikov method [89], WSGD method [55, 125], forward finite difference [136] and fractional trapezoid [144]. We just introduce $L1$ discretization and WSGD method in this section, as we shall apply them in the numerical schemes of later chapters. Readers can refer to the above references for other methods.

First, we shall present the $L1$ discretization. To our best knowledge, Sun and Wu [123] first proposed $L1$ discretization to solve a fractional diffusion-wave system. In that system, the order of Caputo fractional derivative is $\gamma \in (1, 2)$. Therefore, they used an indirect method to complete the approximation. Later on, they applied it on fractional sub-diffusion equations [49] where $\gamma \in (0, 1)$. Now, we only give the definition and accuracy of this method for $\gamma \in (0, 1)$, which will be used in Chapter 7.

Lemma 2.2. [49, 123] *Let $y(t) \in \mathcal{C}^2[0, t_n]$. The $L1$ discretization approximation of the Caputo fractional derivative is given by*

$${}_0^C D_t^\gamma y(t_n) = \mu \sum_{j=0}^{n-1} R_{n,j}^\gamma (y_{j+1} - y_j) + O(\tau^{2-\gamma}), \quad (2.27)$$

where $0 < \gamma < 1$, $\mu = \frac{1}{\Gamma(2-\gamma)\tau^\gamma}$ and $R_{n,j}^\gamma = (n-j)^{1-\gamma} - (n-j-1)^{1-\gamma}$, $0 \leq j \leq n-1$.

Next, we shall introduce the WSGD method [55, 57, 125]. Actually, the WSGD method is normally used to approximate the Riemann-Liouville fractional derivative. Suppose that $y(t)$ is a properly defined function over $\mathcal{R}$. We begin with the shifted Grünwald-Letnikov difference operator in [89, 125], defined by

$$J_{\tau,l}^\gamma y(t) = \frac{1}{\tau^\gamma} \sum_{n=0}^{\infty} g_n^\gamma y(x - (n-l)\tau), \quad (2.28)$$

where l is an integer, τ is the step size and $g_n^\gamma = (-1)^n \binom{\gamma}{n}$ is the Grünwald-Letnikov weight, which can be computed iteratively by

$$g_0^\gamma = 1, \quad g_n^\gamma = \left(1 - \frac{\gamma+1}{n}\right) g_{n-1}^\gamma, \quad n \geq 1. \quad (2.29)$$

Now, we shall introduce 2-WSGD and 3-WSGD approximations for the Riemann Liouville fractional derivative.

Lemma 2.3. [125] *Let $y(t) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+2}(\mathcal{R})$. For any given $t \in \mathcal{R}$, it holds that*

$${}_{-\infty}^{RL} D_t^\gamma y(t) = \frac{\gamma - 2\bar{l}}{2(l - \bar{l})} J_{\tau,l}^\gamma y(t) + \frac{2l - \gamma}{2(l - \bar{l})} J_{\tau,\bar{l}}^\gamma y(t) + O(\tau^2), \quad (2.30)$$

where $l, \bar{l}$ are integers and τ is the step size.

Remark 2.6. The 2-WSGD approximation is derived in [125]. It is then applied to solve a fractional diffusion equation. Normally, one takes $(l, \bar{l}) = (0, -1)$ or $(-1, 0)$ to obtain an implicit scheme.

Lemma 2.4. [57, 125] Let $y(t) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+3}(\mathcal{R})$. For any given $t \in \mathcal{R}$, it holds that

$${}_{-\infty}^RL_t^\gamma y(t) = \mathfrak{S}_1 J_{\tau,l}^\gamma y(t) + \mathfrak{S}_2 J_{\tau,\hat{l}}^\gamma y(t) + \mathfrak{S}_3 J_{\tau,\bar{l}}^\gamma y(t) + O(\tau^3), \quad (2.31)$$

where $l, \bar{l}, \hat{l}$ are integers, τ is the step size and

$$\begin{aligned} \mathfrak{S}_1 &= \frac{12\bar{l}\hat{l} - (6\bar{l} + 6\hat{l} + 1)\gamma + 3\gamma^2}{12(\bar{l}\hat{l} - \bar{l}\bar{l} - \hat{l}\hat{l} + \bar{l}^2)}, \quad \mathfrak{S}_2 = \frac{12\bar{l}\hat{l} - (6l + 6\hat{l} + 1)\gamma + 3\gamma^2}{12(\hat{l}\bar{l} - \bar{l}\bar{l} - \hat{l}\hat{l} + \bar{l}^2)} \\ \mathfrak{S}_3 &= \frac{12\bar{l}\bar{l} - (6l + 6\bar{l} + 1)\gamma + 3\gamma^2}{12(\bar{l}\bar{l} - \hat{l}\bar{l} - \bar{l}\hat{l} + \bar{l}^2)}. \end{aligned} \quad (2.32)$$

Remark 2.7. The 3-WSGD approximation is derived in [125]. Later on, [57] extended it to approximate the Caputo fractional derivative and applied it to solve a fractional diffusion equation with $(l, \bar{l}, \hat{l}) = (0, -1, -2)$.

2.3 Physical Meanings of Equations

In this section, we shall introduce the physical meanings of the equations we consider in Chapters 3-7. We also describe the derivations of these equations from real physical problems. We just summarize the idea and important steps of these derivations here. Readers can refer to the cited references for more details.

2.3.1 A System of Second Order Boundary Value Problems

In this section, we shall introduce a system of second order boundary value problems, which arises in the study of obstacle, unilateral, moving and free boundary value problems [16, 33, 34, 71, 110]. For example, the obstacle problem is to find the equilibrium position of an elastic material whose boundary is held fixed, and which is constrained to lie above a given obstacle. It is deeply related to the study of minimal surfaces and the capacity of a set in potential theory as well. Here, we just consider one dimension situation. The equilibrium configuration of an elastic

string pulled at the ends and lying over an obstacle. As stated in [71], the elastic string should satisfy the following conditions at equilibrium

$$\begin{aligned}
-u''(x) &\geq f(x), & \text{on } \bar{\Omega} = [0, \pi], \\
u(x) &\geq \psi(x), & \text{on } \bar{\Omega} = [0, \pi], \\
[u''(x) - f(x)][u(x) - \psi(x)] &= 0, & \text{on } \bar{\Omega} = [0, \pi], \\
u(0) &= u(\pi) = 0,
\end{aligned} \tag{2.33}$$

where $u(x)$ is the vertical position of the string, $f(x)$ is a given force on the string and $\psi(x)$ is the elastic obstacle function.

Noor and Khalifa [99] first discussed it using the variational inequality approach and showed that the problem (2.33) is equivalent to the variational inequality problem (also see [16, 33, 71, 101])

$$\bar{\rho}(u, v - u) \geq \langle f, v - u \rangle, \quad \text{for all } u \in C, \tag{2.34}$$

where $\bar{\rho}(\cdot, \cdot)$ is a coercive continuous bilinear form and C is the closed convex set given by $C = \{v \in H_0^1(\bar{\Omega}) \mid v \geq \psi \text{ on } \bar{\Omega}\}$ and $H_0^1(\bar{\Omega})$ is a Sobolev space.

Following the idea and technique of Lewy and Stampacchia [73], the variational inequality (2.34) can be written as

$$\begin{aligned}
u'' - [\bar{\mu}(u - \psi)](u - \psi) &= f, \quad 0 < x < \pi, \\
u(0) &= u(\pi) = 0,
\end{aligned} \tag{2.35}$$

where $\bar{\mu}(t)$, known as the penalty function, is the discontinuous function defined by

$$\bar{\mu}(t) = \begin{cases} 1, & t \geq 0, \\ 0, & t < 0, \end{cases} \tag{2.36}$$

and ψ is the given obstacle function defined by

$$\psi(x) = \begin{cases} -1, & 0 \leq x \leq \frac{\pi}{4}, \\ 1, & \frac{\pi}{4} \leq x \leq \frac{3\pi}{4}, \\ -1, & \frac{3\pi}{4} \leq x \leq \pi. \end{cases} \quad (2.37)$$

From equations (2.35)–(2.37), one obtains the following system of second-order boundary value problems

$$u'' = \begin{cases} f, & 0 \leq x \leq \frac{\pi}{4} \text{ and } \frac{3\pi}{4} \leq x \leq \pi, \\ u + f - 1, & \frac{\pi}{4} \leq x \leq \frac{3\pi}{4}, \end{cases} \quad (2.38)$$

$$u(0) = u(\pi) = 0$$

with continuity conditions of u and u' at $\frac{\pi}{4}$ and $\frac{3\pi}{4}$.

2.3.2 Fractional Bagley-Torvik Equation

In this section, we introduce the fractional Bagley-Torvik equation. The equation is first discussed by Bagley and Torvik to describe the motion of viscoelastically damped structures and the motion of fluids [14, 15, 126].

They consider a rigid plate of mass m immersed in a Newtonian fluid of infinite extent and connected by a massless spring of stiffness K to a fixed point. They assume that the small motions of the spring do not disturb the fluid, and that the area of the plate A is sufficiently large. They first show that the resulting shear stress $\sigma(x, t)$ at any point in the fluid can be expressed directly in terms of a fractional order time derivative of the fluid velocity profile as the following equation

$$\sigma(x, t) = \sqrt{\mu\rho} {}^C D_t^{\frac{1}{2}} v(x, t), \quad (2.39)$$

where ρ is the fluid density, μ is the viscosity, and v is the profile of the transverse fluid velocity.

Summing forces on the plate, they find the differential equation describing the

displacement, $u(t)$, of the plate to be

$$mu''(t) = F_x = -Ku(t) - 2A\sigma(0, t). \quad (2.40)$$

Substituting the stress from equation (2.39), and using $v(0, t) = u'(t)$, we can obtain the fractional Bagley-Torvik equation

$$mu''(t) + 2A\sqrt{\mu\rho} {}^C D_t^{\frac{3}{2}} u(t) + Ku(t) = 0. \quad (2.41)$$

2.3.3 New Generalized Fractional Diffusion Equation

In this section, we shall introduce a *generalized* fractional diffusion equation of order γ , where $0 < \gamma < 1$. Such an equation describes the physical phenomenon of a *slow diffusion* process [3, 92], noting that ordinary diffusion occurs when $\gamma = 1$. In a slow diffusion process, the mean square displacement of particles from the original starting site is nonlinear in time and follows a generalized Fick's second law. In fact, the asymptotic behavior of the mean square displacement is such that (assume that $\mathcal{Z}(t) \rightarrow \infty$ as $t \rightarrow \infty$)

$$\langle x(\mathcal{Z}(t)) \rangle \sim \mathcal{Z}(t)^\gamma, \quad t \rightarrow \infty,$$

where γ ($0 < \gamma < 1$) is the anomalous diffusion exponent. Let $\tilde{V}(x, \mathcal{Z}(t))$ be the density function of diffusing material at location x and time $\mathcal{Z}(t)$ that describes this diffusion motion. Following the derivation in [146], we have

$${}_0^C D_z^\gamma \tilde{V}(x, \mathcal{Z}(t)) = \frac{\partial^2 \tilde{V}(x, \mathcal{Z}(t))}{\partial x^2}, \quad t > 0, \quad (2.42)$$

where ${}_0^C D_z^\gamma \tilde{V}(x, \mathcal{Z}(t))$ is the classical Caputo fractional derivative defined by

$${}_0^C D_z^\gamma \tilde{V}(x, \mathcal{Z}(t)) = \frac{1}{\Gamma(1-\gamma)} \int_0^{\mathcal{Z}(t)} \frac{1}{(\mathcal{Z}(t) - \tilde{z})^\gamma} \frac{\partial \tilde{V}(x, \tilde{z})}{\partial \tilde{z}} d\tilde{z}.$$

Let $\tilde{z} = \mathcal{Z}(s)$ and $V(x, t) = \tilde{V}(x, \mathcal{Z}(t))$. It is easy to check that

$${}_0^C D_z^\gamma \tilde{V}(x, \mathcal{Z}(t)) = {}_0^C D_{t;[\mathcal{Z}(t), 1]}^\gamma V(x, t)$$

(refer to (2.26) for the definition of ${}_0^C D_{t;[\mathcal{Z}(t),1]}^\gamma V(x,t)$). Hence, (2.42) gives rise to a *generalized* fractional diffusion equation

$${}_0^C D_{t;[\mathcal{Z}(t),1]}^\gamma V(x,t) = \frac{\partial^2 V(x,t)}{\partial x^2}, \quad t > 0. \quad (2.43)$$

2.3.4 Fractional Nonlinear Schrödinger Equation

In this section, we shall introduce the time-fractional nonlinear Schrödinger equation of order γ , where $0 < \gamma < 1$. Such an equation describes fractional quantum mechanical behavior, which describes the evolution of the position-space wave function of a particle [98]. The derivation of standard form of the Schrödinger equation in one space and one time dimension is given in [52],

$$i\hbar \frac{\partial u(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 u(x,t)}{\partial x^2} + F(x,t)u(x,t), \quad (2.44)$$

where i is the imaginary unit, $\hbar$ is the Planck constant, $u(x,t)$ is the state vector of the quantum system, m is the particle's mass and $F(x,t)$ is the potential. This can be expressed in Planck units as follows

$$iT_p \frac{\partial u(x,t)}{\partial t} = -\frac{L_p^2 M_p}{2m} \frac{\partial^2 u(x,t)}{\partial x^2} + \frac{F(x,t)}{E_p} u(x,t), \quad (2.45)$$

where T_p , L_p , M_p and E_p are Planck time, length, mass and energy.

When the time derivative is fractionalized by Caputo fractional derivative, we obtain the time fractional nonlinear Schrödinger equation,

$$i(T_p)^\gamma {}_0^C D_t^\gamma u(x,t) = -\frac{L_p^2 M_p}{2m} \frac{\partial^2 u(x,t)}{\partial x^2} + \frac{F(x,t)}{E_p} u(x,t). \quad (2.46)$$

Part I

Ordinary Differential Equation

Chapter 3

A System of Second Order Boundary Value Problems

In this chapter, we consider a system of second-order boundary value problems of the type

$$u''(x) = \begin{cases} f(x), & a \leq x \leq \bar{a}, \\ \bar{g}(x)u(x) + f(x) + r, & \bar{a} \leq x \leq \bar{b}, \\ f(x), & \bar{b} \leq x \leq b, \end{cases} \quad (3.1)$$

$$u(a) = \hat{a}, \quad u(b) = \hat{b}$$

with continuity conditions of u and u' at $\bar{a}$ and $\bar{b}$. Here, f and $\bar{g}$ are continuous functions on $[a, b]$ and $[\bar{a}, \bar{b}]$ respectively, r , $\hat{a}$ and $\hat{b}$ are real finite constants. This type of systems arise in the study of obstacle, unilateral, moving and free boundary value problems [16, 33, 34, 71, 110]. For instance, in modelling an elastic string lying over an elastic obstacle, it has been first shown in [99] that a variational inequality can be transformed to equation (3.1) by using the penalty function technique of Lewy and Stampacchia [73].

There are substantial interests on the numerical treatment of the problem (3.1). Noor and Khalifa [99] have used a collocation method with cubic B-splines as basis functions to solve (3.1), while the well known Numerov method and finite difference schemes based on the central difference have been employed in [102]. Thereafter,

Al-Said et al. [9] show that cubic spline method gives numerical solutions that are more accurate than that computed by quintic spline and finite difference techniques. The numerical results of [9, 99, 102] indicate *first-order* accuracy for these methods. In [8], a two-stage method is developed where a finite difference scheme is first employed to obtain the numerical solutions at mid-knots of a uniform mesh, then a second-order interpolation is used to obtain the numerical solutions at the knots. This method is of *second-order* accuracy. Other proven *second-order* accurate methods include polynomial spline methods that employ quadratic spline [5], cubic spline [6, 7] and quintic spline [13]. The numerical solutions are obtained at mid-knots of a uniform mesh in [5–7], while numerical solutions are obtained at the knots in [13]. These polynomial spline methods use ‘continuous’ spline, and derivatives of the spline are involved in the spline relations. On the other hand, *discrete spline* uses differences instead of derivatives in the spline relations. In [29], Chen and Wong have developed a *deficient discrete cubic spline* method for (3.1). It is proved that the accuracy of the method is two, and the numerical experiments demonstrate better accuracy over polynomial spline methods.

Besides continuous polynomial splines, non-polynomial splines have also been applied to solve (3.1). *Non-polynomial spline*, also known as parametric spline [66], depends on a parameter $\xi > 0$, and reduces to the ordinary cubic or quintic spline when $\xi \rightarrow 0$. Due to the parameter ξ , the numerical solutions obtained by non-polynomial splines in the literature are observed to be more accurate than that computed by polynomial splines. In fact, a cubic non-polynomial spline method has been proposed by Khan and Aziz [65] and subsequently by Siraj-ul-Islam and Tirmizi [116] to solve (3.1) at the knots of a uniform mesh. The method is shown to be of order two, and numerical results indicate better accuracy over polynomial spline methods. Higher degree non-polynomial splines have also been used in higher order boundary value problems, for example quartic non-polynomial spline for third-order boundary value problem [115, 118], quintic non-polynomial spline for fourth-order boundary value problem [67] and sextic non-polynomial spline for fifth-order boundary value problem [68]. Out of all these work, only [118] gives the numerical solutions of the third-order boundary value problem at mid-knots of a uniform mesh while the rest obtains the numerical solutions at the knots. The methods mentioned so far yield discrete numerical schemes. There are also iterative methods such as Adomian decomposition method [96] and variational iteration method [100]. Both of these methods do not require discretization.

Motivated by the above work especially those involving the use of non-polynomial splines, in this chapter we shall develop a *cubic non-polynomial spline* scheme at *mid-knots* of a uniform mesh for the problem (3.1).

This chapter is organized as follows. We develop the numerical scheme based on mid-knot cubic non-polynomial spline in Section 3.1. Then the stability and convergence of the proposed scheme are proposed in Section 3.2. In Section 3.3, experiments are presented to illustrate the numerical efficiency and the better performance over other methods. Finally, a brief conclusion is given in Section 3.4.

3.1 Numerical Scheme

Consider the mesh P in (2.1). Without loss of generality, let

$$\bar{a} = \frac{3a+b}{4} = x_{M/4} \quad \text{and} \quad \bar{b} = \frac{a+3b}{4} = x_{3M/4},$$

and we require the positive integer M (≥ 12) to be divisible by 4. Thus, the points $\bar{a}$ and $\bar{b}$ are in mesh P .

Define the *mid-knots* of the mesh P as

$$x_{m-1/2} = a + \left(m - \frac{1}{2}\right)h, \quad 1 \leq m \leq M. \quad (3.2)$$

Note that the breakup points $\bar{a}$ and $\bar{b}$ are *not* any of the mid-knots defined above, in fact $\bar{a} \in [x_{M/4-1/2}, x_{M/4+1/2}]$ and $\bar{b} \in [x_{3M/4-1/2}, x_{3M/4+1/2}]$.

In the following, we define the cubic non-polynomial spline in terms of *mid-knots* of the mesh P . Note that Chapter 2 gives a similar definition in terms of the *knots* of P .

Definition 3.1. For a given mesh P , we say $\bar{S}(x)$ is the *cubic non-polynomial spline* with parameter ξ (> 0) if $\bar{S}(x) \in C^{(2)}[a, b]$, $\bar{S}(x)$ has the form $\text{span}\{1, x, \sin \xi x, \cos \xi x\}$, and its restriction $\bar{S}_m(x)$ on $[x_{m-1/2}, x_{m+1/2}]$, $1 \leq m \leq M-1$ satisfies

$$\begin{cases} \bar{S}_m(x_{m-1/2}) = \bar{S}_{m-1/2}, & \bar{S}_m(x_{m+1/2}) = \bar{S}_{m+1/2}, \\ \bar{S}_m''(x_{m-1/2}) = \bar{W}_{m-1/2}, & \bar{S}_m''(x_{m+1/2}) = \bar{W}_{m+1/2}. \end{cases} \quad (3.3)$$

Then, using the similar technique of Definition 2.2, we obtain the following spline relation for $2 \leq m \leq M-1$,

$$\bar{S}_{m-3/2} - 2\bar{S}_{m-1/2} + \bar{S}_{m+1/2} = h^2 (\bar{\alpha}\bar{W}_{m-3/2} + 2\bar{\beta}\bar{W}_{m-1/2} + \bar{\alpha}\bar{W}_{m+1/2}), \quad (3.4)$$

where $\bar{\alpha}$ and $\bar{\beta}$ are defined in (2.10).

Remark 3.1. When $\xi \rightarrow 0$, we have $(\bar{\alpha}, \bar{\beta}) \rightarrow (\frac{1}{6}, \frac{1}{3})$ and the cubic non-polynomial spline relation (3.4) reduces to the well known cubic spline relation. Further, for the consistency of relation (3.4), we have $2\bar{\alpha} + 2\bar{\beta} = 1$ [66].

We shall approximate a solution $u(x)$ of (3.1) by the non-polynomial spline $\bar{S}_m(x)$ over the subinterval $[x_{m-1/2}, x_{m+1/2}]$, $1 \leq m \leq M-1$. Hence, it follows from (3.4) that

$$u_{m-3/2} - 2u_{m-1/2} + u_{m+1/2} = h^2 (\bar{\alpha}u''_{m-3/2} + 2\bar{\beta}u''_{m-1/2} + \bar{\alpha}u''_{m+1/2}) + T_m, \quad (3.5)$$

where $2 \leq m \leq M-1$ and T_m is the truncation error. By Taylor expansion, the truncation error is found to be

$$\begin{aligned} T_m = & h^2(1 - 2\bar{\alpha} - 2\bar{\beta})u''_{m-1/2} + h^4 \left(\frac{1}{12} - \bar{\alpha} \right) u^{(4)}_{m-1/2} + h^6 \left(\frac{1}{360} - \frac{\bar{\alpha}}{12} \right) u^{(6)}_{m-1/2} \\ & + O(h^7), \quad 2 \leq m \leq M-1. \end{aligned} \quad (3.6)$$

Remark 3.2. Due to the consistency relation $2\bar{\alpha} + 2\bar{\beta} = 1$, (3.6) immediately gives $T_m = O(h^4)$, $2 \leq m \leq M-1$. If, in addition, $\bar{\alpha} = \frac{1}{12}$ (which implies $\bar{\beta} = \frac{5}{12}$), then (3.6) yields $T_m = O(h^6)$, $2 \leq m \leq M-1$.

Next, since we approximate a solution $u(x)$ of (3.1) by the non-polynomial spline $\bar{S}(x)$, it is natural to set the second derivative of the spline as

$$\bar{W}_{m-1/2} = \begin{cases} f_{m-1/2}, & 1 \leq m \leq \frac{M}{4}, \\ \bar{g}_{m-1/2}\bar{S}_{m-1/2} + f_{m-1/2} + r, & \frac{M}{4} + 1 \leq m \leq \frac{3M}{4}, \\ f_{m-1/2}, & \frac{3M}{4} + 1 \leq m \leq M. \end{cases} \quad (3.7)$$

Note that in (3.7), by considering the second derivative at mid-knots, we *avoid* the breakup points $\bar{a}$ and $\bar{b}$ at which u'' is discontinuous.

Substituting (3.7) into (3.4) yields the following equations:

- for $2 \leq m \leq \frac{M}{4} - 1$,

$$\bar{S}_{m-3/2} - 2\bar{S}_{m-1/2} + \bar{S}_{m+1/2} = h^2 (\bar{\alpha}f_{m-3/2} + 2\bar{\beta}f_{m-1/2} + \bar{\alpha}f_{m+1/2}); \quad (3.8)$$

- for $m = \frac{M}{4}$,

$$\begin{aligned} & \bar{S}_{M/4-3/2} - 2\bar{S}_{M/4-1/2} + (1 - \bar{\alpha}h^2\bar{g}_{M/4+1/2})\bar{S}_{M/4+1/2} \\ &= h^2 [\bar{\alpha}f_{M/4-3/2} + 2\bar{\beta}f_{M/4-1/2} + \bar{\alpha}(f_{M/4+1/2} + r)]; \end{aligned} \quad (3.9)$$

- for $m = \frac{M}{4} + 1$,

$$\begin{aligned} & \bar{S}_{M/4-1/2} + (-2 - 2\bar{\beta}h^2\bar{g}_{M/4+1/2})\bar{S}_{M/4+1/2} + (1 - \bar{\alpha}h^2\bar{g}_{M/4+3/2})\bar{S}_{M/4+3/2} \\ &= h^2 [\bar{\alpha}f_{M/4-1/2} + 2\bar{\beta}(f_{M/4+1/2} + r) + \bar{\alpha}(f_{M/4+3/2} + r)]; \end{aligned} \quad (3.10)$$

- for $\frac{M}{4} + 2 \leq m \leq \frac{3M}{4} - 1$,

$$\begin{aligned} & (1 - \bar{\alpha}h^2\bar{g}_{m-3/2})\bar{S}_{m-3/2} + (-2 - 2\bar{\beta}h^2\bar{g}_{m-1/2})\bar{S}_{m-1/2} \\ &+ (1 - \bar{\alpha}h^2\bar{g}_{m+1/2})\bar{S}_{m+1/2} \\ &= h^2 [\bar{\alpha}(f_{m-3/2} + r) + 2\bar{\beta}(f_{m-1/2} + r) + \bar{\alpha}(f_{m+1/2} + r)]; \end{aligned} \quad (3.11)$$

- for $m = \frac{3M}{4}$,

$$\begin{aligned} & (1 - \bar{\alpha}h^2\bar{g}_{3M/4-3/2})\bar{S}_{3M/4-3/2} + (-2 - 2\bar{\beta}h^2\bar{g}_{3M/4-1/2})\bar{S}_{3M/4-1/2} + \bar{S}_{3M/4+1/2} \\ &= h^2 [\bar{\alpha}(f_{3M/4-3/2} + r) + 2\bar{\beta}(f_{3M/4-1/2} + r) + \bar{\alpha}f_{3M/4+1/2}]; \end{aligned} \quad (3.12)$$

- for $m = \frac{3M}{4} + 1$,

$$\begin{aligned} & (1 - \bar{\alpha}h^2\bar{g}_{3M/4-1/2})\bar{S}_{3M/4-1/2} - 2\bar{S}_{3M/4+1/2} + \bar{S}_{3M/4+3/2} \\ & = h^2 [\bar{\alpha} (f_{3M/4-1/2} + r) + 2\bar{\beta}f_{3M/4+1/2} + \bar{\alpha}f_{3M/4+3/2}] ; \end{aligned} \quad (3.13)$$

- for $\frac{3M}{4} + 2 \leq m \leq M - 1$,

$$\bar{S}_{m-3/2} - 2\bar{S}_{m-1/2} + \bar{S}_{m+1/2} = h^2 (\bar{\alpha}f_{m-3/2} + 2\bar{\beta}f_{m-1/2} + \bar{\alpha}f_{m+1/2}). \quad (3.14)$$

To set up a system of M equations for the unknown $\bar{S}_{m-1/2}$, $1 \leq m \leq M$, we need two more equations besides (3.8)–(3.14). Using the method of undetermined coefficients, we obtain the following two equations which have truncation errors of $O(h^6)$:

$$\left\{ \begin{aligned} 2\bar{S}_0 - 3\bar{S}_{1/2} + \bar{S}_{3/2} &= h^2 \left(-\frac{1}{120}\bar{W}_0 + \frac{5}{8}\bar{W}_{1/2} + \frac{7}{48}\bar{W}_{3/2} - \frac{1}{80}\bar{W}_{5/2} \right), \\ 2\bar{S}_M - 3\bar{S}_{M-1/2} + \bar{S}_{M-3/2} &= h^2 \left(-\frac{1}{120}\bar{W}_M + \frac{5}{8}\bar{W}_{M-1/2} + \frac{7}{48}\bar{W}_{M-3/2} \right. \\ &\quad \left. - \frac{1}{80}\bar{W}_{M-5/2} \right). \end{aligned} \right. \quad (3.15)$$

Since $M \geq 12$, from (3.7) we have $\bar{W}_{m-1/2} = f_{m-1/2}$ for $m = 1, 2, 3, M-2, M-1, M$. Hence, the above two equations become

$$\left\{ \begin{aligned} 2\bar{S}_0 - 3\bar{S}_{1/2} + \bar{S}_{3/2} &= h^2 \left(-\frac{1}{120}f_0 + \frac{5}{8}f_{1/2} + \frac{7}{48}f_{3/2} - \frac{1}{80}f_{5/2} \right), \\ 2\bar{S}_M - 3\bar{S}_{M-1/2} + \bar{S}_{M-3/2} &= h^2 \left(-\frac{1}{120}f_M + \frac{5}{8}f_{M-1/2} + \frac{7}{48}f_{M-3/2} \right. \\ &\quad \left. - \frac{1}{80}f_{M-5/2} \right). \end{aligned} \right. \quad (3.16)$$

We have now derived the *mid-knot cubic non-polynomial spline scheme* which comprises the equations (3.8)–(3.14) and (3.16) with $2\bar{\alpha} + 2\bar{\beta} = 1$. The solvability of the system and the convergence analysis will be tackled in the next section.

3.2 Solvability and Convergence

In this section, we shall establish the unique solvability of the mid-knot cubic non-polynomial spline scheme (3.8)–(3.14) and (3.16) and also conduct a convergence analysis. To begin, we define the norms of a column vector $T = [T_m]$ and a matrix $A = [a_{mj}]$ as follows:

$$\|T\|_\infty = \max_m |T_m| \quad \text{and} \quad \|A\|_\infty = \max_m \sum_j |a_{mj}|.$$

Let $e_{m-1/2} = u_{m-\frac{1}{2}} - \bar{S}_{m-\frac{1}{2}}$, $1 \leq m \leq M$ be the errors. Let $U = [u_{m-1/2}]$, $\bar{S} = [\bar{S}_{m-1/2}]$, $\tilde{F} = [\tilde{F}_m]$, $T = [T_m]$ and $E = [e_{m-1/2}]$ be M -dimensional column vectors. The system (3.8)–(3.14) and (3.16) can be written as

$$A\bar{S} = \tilde{F}, \quad (3.17)$$

where

$$A = A_0 + h^2 Q \bar{G}. \quad (3.18)$$

Here, A_0 , Q and $\bar{G}$ are $M \times M$ matrices given by

$$A_0 = \begin{pmatrix} 3 & -1 & & & \\ -1 & 2 & -1 & & \\ & & \ddots & & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 3 \end{pmatrix}, \quad (3.19)$$

$$Q = \begin{pmatrix} \frac{5}{8} & \frac{7}{48} & -\frac{1}{80} & & \\ \bar{\alpha} & 2\bar{\beta} & \bar{\alpha} & & \\ & & \ddots & & \\ & & & \bar{\alpha} & 2\bar{\beta} & \bar{\alpha} \\ & & & -\frac{1}{80} & \frac{7}{48} & \frac{5}{8} \end{pmatrix} \quad (3.20)$$

and $\bar{G} = \text{diag}[v_{m-1/2}]$ where

$$v_{m-1/2} = \begin{cases} 0, & 1 \leq m \leq \frac{M}{4}, \\ \bar{g}_{m-1/2}, & \frac{M}{4} + 1 \leq m \leq \frac{3M}{4}, \\ 0, & \frac{3M}{4} + 1 \leq m \leq M. \end{cases} \quad (3.21)$$

Further, $\tilde{F} = [\tilde{F}_m]$, $1 \leq m \leq M$ is given by:

- for $m = 1$,

$$\tilde{F}_m = 2\hat{a} - h^2 \left(-1/120 f_{m-1} + 5/8 f_{m-1/2} + 7/48 f_{m+1/2} - 1/80 f_{m+3/2} \right); \quad (3.22)$$

- for $2 \leq m \leq \frac{M}{4} - 1$ and $\frac{3M}{4} + 2 \leq m \leq M - 1$,

$$\tilde{F}_m = -h^2 \left(\bar{\alpha} f_{m-3/2} + 2\bar{\beta} f_{m-1/2} + \bar{\alpha} f_{m+1/2} \right); \quad (3.23)$$

- for $m = \frac{M}{4}$ and $m = \frac{3M}{4}$,

$$\tilde{F}_m = -h^2 \left(\bar{\alpha} f_{m-3/2} + 2\bar{\beta} f_{m-1/2} + \bar{\alpha} f_{m+1/2} + \bar{\alpha} r \right); \quad (3.24)$$

- for $m = \frac{M}{4} + 1$ and $m = \frac{3M}{4} + 1$,

$$\tilde{F}_m = -h^2 \left[\bar{\alpha} f_{m-3/2} + 2\bar{\beta} f_{m-1/2} + \bar{\alpha} f_{m+1/2} + (\bar{\alpha} + 2\bar{\beta}) r \right]; \quad (3.25)$$

- for $\frac{M}{4} + 2 \leq m \leq \frac{3M}{4} - 1$,

$$\tilde{F}_m = -h^2 \left[\bar{\alpha} f_{m-3/2} + 2\bar{\beta} f_{m-1/2} + \bar{\alpha} f_{m+1/2} + (2\bar{\alpha} + 2\bar{\beta}) r \right]; \quad (3.26)$$

- for $m = M - 1$,

$$\tilde{F}_m = 2\hat{b} - h^2 \left(-1/120 f_m + 5/8 f_{m-1/2} + 7/48 f_{m-3/2} - 1/80 f_{m-5/2} \right). \quad (3.27)$$

It follows from (3.17) that

$$AU = \tilde{F} + T, \quad (3.28)$$

where

$$T = AE. \quad (3.29)$$

Remark 3.3. Noting Remark 3.2, we see that for $2 \leq m \leq M - 1$,

$$T_m = \begin{cases} O(h^4), & \text{if } 2\bar{\alpha} + 2\bar{\beta} = 1, \\ O(h^6), & \text{if } \bar{\alpha} = \frac{1}{12}, \bar{\beta} = \frac{5}{12}. \end{cases}$$

Coupling with the fact that the truncation error in another two equations (3.16) is $O(h^6)$, we get

$$\|T\|_\infty = \begin{cases} O(h^4), & \text{if } 2\bar{\alpha} + 2\bar{\beta} = 1, \\ O(h^6), & \text{if } \bar{\alpha} = \frac{1}{12}, \bar{\beta} = \frac{5}{12}. \end{cases} \quad (3.30)$$

Lemma 3.1. [127] *The matrix A_0 is nonsingular and*

$$\|A_0^{-1}\|_\infty \leq \frac{M^2 + 1}{8} = \frac{(b - a)^2 + h^2}{8h^2}. \quad (3.31)$$

Lemma 3.2. [48] *Let D be a square matrix such that $\|D\|_\infty < 1$. Then, $(I + D)$ is nonsingular and*

$$\|(I + D)^{-1}\|_\infty \leq \frac{1}{1 - \|D\|_\infty}. \quad (3.32)$$

We are now ready to establish the unique solvability and the convergence of the mid-knot cubic non-polynomial spline scheme in the following theorem.

Theorem 3.1. *Suppose*

$$K = \frac{1}{8} [(b - a)^2 + h^2] \hat{g} < 1, \quad (3.33)$$

where $\hat{g} = \max_{x \in [\bar{a}, \bar{b}]} |\bar{g}(x)|$. Then, the system (3.17) has a unique solution and

$$\|E\|_\infty = O(h^2). \quad (3.34)$$

Proof. Suppose (3.17) has a unique solution, then it can be written as

$$\bar{S} = A^{-1}\tilde{F} = (A_0 + h^2 Q \bar{G})^{-1} \tilde{F} = [A_0(I + A_0^{-1} h^2 Q \bar{G})]^{-1} \tilde{F} = (I + A_0^{-1} h^2 Q \bar{G})^{-1} A_0^{-1} \tilde{F}. \quad (3.35)$$

By Lemma 3.1, the inverse A_0^{-1} exists, hence for the existence of the unique solution S it remains to show that $(I + A_0^{-1}h^2Q\overline{G})$ is nonsingular.

From the definitions of matrices Q and $\overline{G}$, it is clear that

$$\|Q\|_\infty = 1, \quad \|\overline{G}\|_\infty = \max_{\frac{M}{4}+1 \leq m \leq \frac{3M}{4}} \left| \overline{g}_{m-\frac{1}{2}} \right| \leq \hat{g}. \quad (3.36)$$

Using (3.31) and (3.36), we find

$$\|A_0^{-1}h^2Q\overline{G}\|_\infty \leq h^2\|A_0^{-1}\|_\infty \cdot \|Q\|_\infty \cdot \|\overline{G}\|_\infty \leq \frac{1}{8} [(b-a)^2 + h^2] \hat{g} = K. \quad (3.37)$$

Since $K < 1$, it follows immediately from Lemma 3.2 that $(I + A_0^{-1}h^2Q\overline{G})$ is nonsingular. It is hence proven that (3.17) has a unique solution given by (3.35).

Next, we consider the error E , which from (3.29) can be written as

$$E = A^{-1}T = (I + A_0^{-1}h^2Q\overline{G})^{-1}A_0^{-1}T.$$

From (3.30), we note that $\|T\|_\infty = O(h^4)$ in the general case, i.e., $2\overline{\alpha} + 2\overline{\beta} = 1$. Together with Lemma 3.2, (3.37) and (3.31), it follows that

$$\begin{aligned} \|E\|_\infty &\leq \|(I + A_0^{-1}h^2Q\overline{G})^{-1}\|_\infty \cdot \|A_0^{-1}\|_\infty \cdot \|T\|_\infty \\ &\leq \frac{\|A_0^{-1}\|_\infty \cdot \|T\|_\infty}{1 - \|A_0^{-1}h^2Q\overline{G}\|_\infty} \\ &\leq \frac{(b-a)^2 + h^2}{8h^2(1-K)} O(h^4) \\ &= \frac{K}{\hat{g}(1-K)} O(h^2) \\ &= O(h^2). \end{aligned}$$

This shows that (3.17) is a second-order convergence method. If we choose parameter $\overline{\alpha} = 1/12$, $\overline{\beta} = 5/12$, this shows that (3.17) is a fourth-order convergence method from (3.30). However, the solution exists continuously only up to the second derivative as referred in [13]. Therefore the method is only second-order accurate over the whole interval, which results in a second-order convergence from numerical solution. Actually, a similar conclusion can be observed in [8, 9, 29] ■

Remark 3.4. Besides equation (3.15) and (3.16), we have obtained two following equations by coefficient undetermined method, which can be verified as $O(h^4)$ truncation error from Taylor expansion.

$$\begin{cases} 2\bar{S}_0 - 3\bar{S}_{1/2} + \bar{S}_{3/2} = h^2 \left(-\frac{1}{4}\bar{W}_0 + \bar{W}_{1/2} \right), \\ 2\bar{S}_M - 3\bar{S}_{M-1/2} + \bar{S}_{M-3/2} = h^2 \left(-\frac{1}{4}\bar{W}_M + \bar{W}_{M-1/2} \right). \end{cases} \quad (3.38)$$

Also for $M \geq 12$, from (3.7) we have $\bar{W}_{m-1/2} = f_{m-1/2}$ for $m = 1, 2, 3, M-2, M-1, M$. Hence, the above two equations become

$$\begin{cases} 2\bar{S}_0 - 3\bar{S}_{1/2} + \bar{S}_{3/2} = h^2 \left(-\frac{1}{4}f_0 + f_{1/2} \right), \\ 2\bar{S}_M - 3\bar{S}_{M-1/2} + \bar{S}_{M-3/2} = h^2 \left(-\frac{1}{4}f_M + f_{M-1/2} \right). \end{cases} \quad (3.39)$$

We have used (3.8)–(3.14) and (3.39) to get a second order scheme for parameter $2\bar{\alpha} + 2\bar{\beta} = 1$ excepts $\bar{\alpha} = 1/12, \bar{\beta} = 5/12$. The numerical error would be bigger than numerical scheme (3.8)–(3.14) and (3.16) as observed in numerical simulation, although it is also second-order accurate.

3.3 Experiment

To illustrate the application of the mid-knot cubic non-polynomial spline scheme (3.8)–(3.14) and (3.16), we consider the following second-order boundary value problems

$$u'' = \begin{cases} f, & 0 \leq x \leq \frac{\pi}{4} \text{ and } \frac{3\pi}{4} \leq x \leq \pi, \\ u + f - 1, & \frac{\pi}{4} \leq x \leq \frac{3\pi}{4}, \end{cases} \quad (3.40)$$

$$u(0) = u(\pi) = 0$$

with continuity conditions of u and u' at $\frac{\pi}{4}$ and $\frac{3\pi}{4}$.

In Example 3.1, we shall consider a well known special case of the system (3.40) when $f = 0$. This special case is first discussed in [99] and subsequently considered in almost every paper on system of second-order boundary value problems.

Example 3.1. [99] *We consider the system (3.40) when $f = 0$, i.e.,*

$$u'' = \begin{cases} 0, & 0 \leq x \leq \frac{\pi}{4} \text{ and } \frac{3\pi}{4} \leq x \leq \pi, \\ u - 1, & \frac{\pi}{4} \leq x \leq \frac{3\pi}{4}, \end{cases} \quad (3.41)$$

$$u(0) = u(\pi) = 0.$$

The analytical solution of (3.41) is given by

$$u(x) = \begin{cases} \frac{4}{\gamma_1}x, & 0 \leq x \leq \frac{\pi}{4}, \\ 1 - \frac{4}{\gamma_2} \cosh\left(\frac{\pi}{2} - x\right), & \frac{\pi}{4} \leq x \leq \frac{3\pi}{4}, \\ \frac{4}{\gamma_1}(\pi - x), & \frac{3\pi}{4} \leq x \leq \pi, \end{cases} \quad (3.42)$$

where $\gamma_1 = \pi + 4 \coth \frac{\pi}{4}$ and $\gamma_2 = \pi \sinh \frac{\pi}{4} + 4 \cosh \frac{\pi}{4}$.

In Table 3.1, we present the maximum absolute errors $\|E\|_\infty = \max_{1 \leq m \leq M} |e_{m-1/2}|$ obtained from our mid-knot cubic non-polynomial spline scheme for various values of $\bar{\alpha}$ and $\bar{\beta}$, and also the maximum absolute errors obtained from other methods. A brief description of the methods listed in Table 3.1 is given below:

- (a) The mid-knot cubic non-polynomial spline scheme is (3.8)–(3.15) developed in this chapter. This is shown to be a second-order method.
- (b) In [65, 116], parametric cubic spline has been used to obtain numerical solutions of (3.1) at the knots x_m . The value of the second derivative at the breakup point $\bar{a}$ is taken to be the mean of $u''(\bar{a}-)$ and $u''(\bar{a}+)$, likewise at the breakup point $\bar{b}$. This method is of second order.
- (c) In [29], a deficient discrete cubic spline method based on central difference has been developed. This method is shown to be a second-order method.

- (d) In [5–7], quadratic and cubic spline methods have been developed at mid-knots to avoid the breakup points $\bar{a}$ and $\bar{b}$, these methods are of second order.
- (e) In [8], a second-order modified Numerov method is proposed. First, a finite difference scheme is developed to obtain approximate solutions at the mid-knots. Then, using a second-order interpolation, these approximations are used to compute the solutions at the knots x_m .
- (f) In [13], quintic spline is used to solve (3.1). Here, at the two points of discontinuity $\bar{a}$ and $\bar{b}$, the mean of the left- and right-hand limits of u'' has been used. The method developed is second-order accurate.
- (g) In [99], a collocation method is employed with cubic B-splines as basic functions. The method is of first order.
- (h) In [9], the authors have proposed first-order accurate methods based on the cubic spline and quintic spline methods.
- (i) In [102], the authors have employed the well known Numerov method as well as finite difference schemes based on the central difference. Both methods are shown to be first-order accurate.

From Table 3.1, the numerical results confirm that our method is of second order. Compared to the parametric cubic spline method [65, 116], our method gives the *smallest errors* for all cases of $(\bar{\alpha}, \bar{\beta})$. Furthermore, our method *outperforms* all other methods [5–9, 13, 29, 99, 102] in all cases.

To illustrate graphically, in Figures 3.1 and 3.2, we plot the exact solution, the numerical solution obtained from the mid-knot cubic non-polynomial spline method, and the associated absolute errors when $(\bar{\alpha}, \bar{\beta}, h) = (\frac{1}{12}, \frac{5}{12}, \frac{\pi}{80})$. It is observed from the figures that this method gives a good approximation to the exact solution.

Finally, to investigate the effect of $\bar{\alpha}$ on the maximum absolute error $\|E\|_\infty$, in Figure 3.3 we plot the maximum absolute errors for different values of $\bar{\alpha} \in (0, 0.5)$ (in steps of $\frac{1}{32}$) when $h = \frac{\pi}{80}$. It is observed that the minimum $\|E\|_\infty$ is achieved at about $\bar{\alpha} = \frac{1}{8}$.

In the next two examples, unlike Example 3.1, we consider the problem (3.1) with nonzero f .

TABLE 3.1: (Example 3.1) Maximum absolute errors

Methods	$h = \pi/20$	$h = \pi/40$	$h = \pi/80$
Mid-knot cubic non-polynomial spline $\bar{\alpha} = 1/8, \bar{\beta} = 3/8$	$2.40e-04$	$6.34e-05$	$1.63e-05$
Mid-knot cubic non-polynomial spline $\bar{\alpha} = 1/10, \bar{\beta} = 2/5$	$3.44e-04$	$9.11e-05$	$2.34e-05$
Mid-knot cubic non-polynomial spline $\bar{\alpha} = 1/12, \bar{\beta} = 5/12$	$4.14e-04$	$1.09e-04$	$2.81e-05$
Mid-knot cubic non-polynomial spline $\bar{\alpha} = 1/14, \bar{\beta} = 3/7$	$4.64e-04$	$1.23e-04$	$3.15e-05$
Mid-knot cubic non-polynomial spline $\bar{\alpha} = 1/16, \bar{\beta} = 7/16$	$5.01e-04$	$1.33e-04$	$3.40e-05$
Parametric cubic spline [65] $\bar{\alpha} = 1/8, \bar{\beta} = 3/8$	$8.62e-04$	$2.47e-04$	$6.57e-05$
Parametric cubic spline [65] $\bar{\alpha} = 1/10, \bar{\beta} = 2/5$	$7.74e-04$	$2.21e-04$	$5.89e-05$
Parametric cubic spline [65] $\bar{\alpha} = 1/12, \bar{\beta} = 5/12$	$7.16e-04$	$2.04e-04$	$5.43e-05$
Parametric cubic spline [65] $\bar{\alpha} = 1/14, \bar{\beta} = 3/7$	$6.74e-04$	$1.92e-04$	$5.11e-05$
Parametric cubic spline [65, 116] $\bar{\alpha} = 1/16, \bar{\beta} = 7/16$	$6.43e-04$	$1.83e-04$	$4.87e-05$
Deficient discrete cubic spline [29]	$1.19e-03$	$3.04e-04$	$7.68e-05$
Cubic spline [7]	$1.26e-03$	$3.29e-04$	$8.43e-05$
Modified Numerov method [8]	$1.65e-03$	$4.33e-04$	$1.11e-04$
Cubic spline [6]	$1.94e-03$	$4.99e-04$	$1.27e-04$
Quadratic spline [5]	$2.20e-03$	$5.87e-04$	$1.51e-04$
Quintic spline [13]	$2.57e-03$	$7.31e-04$	$1.94e-04$
Collocation-cubic B spline [99]	$1.40e-02$	$7.71e-03$	$4.04e-03$
Cubic spline [9]	$1.80e-02$	$9.13e-03$	$4.60e-03$
Quintic spline [9]	$1.82e-02$	$9.17e-03$	$4.61e-03$
Numerov [102]	$2.32e-02$	$1.21e-02$	$6.17e-03$
Finite difference scheme [102]	$2.50e-02$	$1.29e-02$	$6.58e-03$

FIGURE 3.1: (Example 3.1) Exact solution and numerical solution when $(\bar{\alpha}, \bar{\beta}, h) = (\frac{1}{12}, \frac{5}{12}, \frac{\pi}{80})$

FIGURE 3.2: (Example 3.1) Absolute error when $(\bar{\alpha}, \bar{\beta}, h) = (\frac{1}{12}, \frac{5}{12}, \frac{\pi}{80})$ FIGURE 3.3: (Example 3.1) Maximum absolute error for different $\bar{\alpha}$ when $h = \frac{\pi}{80}$

Example 3.2. We consider the boundary value problem

$$u'' = \begin{cases} 2, & 0 \leq x \leq \frac{\pi}{4}, \\ -u + \frac{\pi^2}{16} + \frac{7}{4}\pi + 1, & \frac{\pi}{4} \leq x \leq \frac{3\pi}{4}, \\ 2, & \frac{3\pi}{4} \leq x \leq \pi, \end{cases} \quad (3.43)$$

$$u(0) = 0, \quad u(\pi) = \frac{\pi^2}{2} + \frac{5\pi}{2} + 2.$$

TABLE 3.2: (Example 3.2) Maximum absolute errors and convergence orders

h	MCNS $\bar{\alpha} = 1/16$ $\bar{\beta} = 7/16$		MCNS $\bar{\alpha} = 1/14$ $\bar{\beta} = 3/7$		MCNS $\bar{\alpha} = 1/12$ $\bar{\beta} = 5/12$		MCNS $\bar{\alpha} = 1/10$ $\bar{\beta} = 2/5$		MCNS $\bar{\alpha} = 1/8$ $\bar{\beta} = 3/8$		DDCS	
	$\ E\ _\infty$	order	$\ E\ _\infty$	order	$\ E\ _\infty$	order	$\ E\ _\infty$	order	$\ E\ _\infty$	order	$\ E\ _\infty$	order
$\frac{\pi}{20}$	$7.10e-03$		$7.19e-03$		$7.30e-03$		$7.46e-03$		$8.43e-03$		$7.91e-02$	
$\frac{\pi}{40}$	$1.86e-03$	1.93	$1.88e-03$	1.94	$1.91e-03$	1.93	$1.96e-03$	1.93	$2.12e-03$	1.99	$1.98e-02$	2.00
$\frac{\pi}{80}$	$4.76e-04$	1.97	$4.82e-04$	1.96	$4.90e-04$	1.96	$5.02e-04$	1.97	$5.30e-04$	2.00	$4.93e-03$	2.01
$\frac{\pi}{160}$	$1.21e-04$	1.98	$1.22e-04$	1.98	$1.24e-04$	1.98	$1.27e-04$	1.98	$1.33e-04$	1.99	$1.23e-03$	2.00
$\frac{\pi}{320}$	$3.03e-05$	2.00	$3.07e-05$	1.99	$3.12e-05$	1.99	$3.19e-05$	1.99	$3.32e-05$	2.00	$3.07e-04$	2.00
h	PCS $\bar{\alpha} = 1/16$ $\bar{\beta} = 7/16$		PCS $\bar{\alpha} = 1/14$ $\bar{\beta} = 3/7$		PCS $\bar{\alpha} = 1/12$ $\bar{\beta} = 5/12$		PCS $\bar{\alpha} = 1/10$ $\bar{\beta} = 2/5$		PCS $\bar{\alpha} = 1/8$ $\bar{\beta} = 3/8$			
	$\ E\ _\infty$	order	$\ E\ _\infty$	order	$\ E\ _\infty$	order	$\ E\ _\infty$	order	$\ E\ _\infty$	order		
$\frac{\pi}{20}$	$1.32e-02$		$1.31e-02$		$1.30e-02$		$1.29e-02$		$1.36e-02$			
$\frac{\pi}{40}$	$3.69e-03$	1.84	$3.67e-03$	1.84	$3.64e-03$	1.84	$3.61e-03$	1.84	$3.55e-03$	1.94		
$\frac{\pi}{80}$	$9.71e-04$	1.93	$9.66e-04$	1.93	$9.59e-04$	1.92	$9.48e-04$	1.93	$9.33e-04$	1.93		
$\frac{\pi}{160}$	$2.49e-04$	1.96	$2.47e-04$	1.97	$2.46e-04$	1.96	$2.43e-04$	1.96	$2.39e-04$	1.96		
$\frac{\pi}{320}$	$6.30e-05$	1.98	$6.26e-05$	1.98	$6.21e-05$	1.99	$6.14e-05$	1.98	$6.04e-05$	1.98		

Here, $f(x) = 2$, $\bar{g}(x) = -1$ and $r = \frac{\pi^2}{16} + \frac{7}{4}\pi - 1$. The analytical solution of (3.43) is given by

$$u(x) = \begin{cases} x^2 + x, & 0 \leq x \leq \frac{\pi}{4}, \\ -\frac{\sqrt{2}\pi}{2} \sin x - \sqrt{2}(\pi + 1) \cos x + \frac{\pi^2}{16} + \frac{7\pi}{4} + 1, & \frac{\pi}{4} \leq x \leq \frac{3\pi}{4}, \\ x^2 + x - \frac{\pi^2}{2} + \frac{3\pi}{2} + 2, & \frac{3\pi}{4} \leq x \leq \pi. \end{cases} \quad (3.44)$$

In this example, we focus on comparing the three more accurate methods observed in Table 3.1, namely (i) mid-knot cubic non-polynomial spline (MCNS), (ii) parametric cubic spline (PCS) [65, 116], and (iii) deficient discrete cubic spline (DDCS) [29]. In Table 3.2, we present the maximum absolute errors and the convergence orders of these methods. It is clear that the mid-knot cubic non-polynomial spline scheme achieves the *smallest errors* in all the cases.

Next, the effect of $\bar{\alpha}$ on the maximum absolute error is illustrated in Figure 3.4, where we plot the maximum absolute errors for different values of $\bar{\alpha} \in (0, 0.5)$ (in steps of $\frac{1}{32}$) when $h = \frac{\pi}{80}$. We notice that the minimum $\|E\|_\infty$ is achieved at about $\bar{\alpha} = \frac{1}{16}$, which is different from Example 3.1.

FIGURE 3.4: (Example 3.2) Maximum absolute error for different $\bar{\alpha}$ when $h = \frac{\pi}{80}$

Example 3.3. We consider the the boundary value problem

$$u'' = \begin{cases} 2, & 0 \leq x \leq \frac{1}{4}, \\ u + \frac{3}{16}, & \frac{1}{4} \leq x \leq \frac{3}{4}, \\ 2, & \frac{3}{4} \leq x \leq 1, \end{cases} \quad (3.45)$$

$$u(0) = 1, \quad u(1) = \frac{15}{8}e^{\frac{1}{2}} - \frac{1}{8}.$$

In this example, $f(x) = 2$, $\bar{g}(x) = 1$ and $r = -\frac{29}{16}$. The analytical solution of (3.45) is given by

$$u(x) = \begin{cases} x^2 + x + 1, & 0 \leq x \leq \frac{1}{4}, \\ \frac{3}{2}e^{x-\frac{1}{4}} - \frac{3}{16}, & \frac{1}{4} \leq x \leq \frac{3}{4}, \\ x^2 + \left(\frac{3}{2}e^{\frac{1}{2}} - \frac{3}{2}\right)x + \frac{3}{8}e^{\frac{1}{2}} + \frac{3}{8}, & \frac{3}{4} \leq x \leq 1. \end{cases} \quad (3.46)$$

Once again we compare the three better methods arising from Table 3.1, namely (i) mid-knot cubic non-polynomial spline (MCNS), (ii) parametric cubic spline (PCS) [65, 116], and (iii) deficient discrete cubic spline (DDCS) [29]. In Table 3.3, we present the maximum absolute errors of these methods and it is clear that the mid-knot cubic non-polynomial spline scheme *outperforms* in all the cases.

TABLE 3.3: (Example 3.3) Maximum absolute errors and convergence orders

h	MCNS $\bar{\alpha} = 1/16$ $\bar{\beta} = 7/16$		MCNS $\bar{\alpha} = 1/14$ $\bar{\beta} = 3/7$		MCNS $\bar{\alpha} = 1/12$ $\bar{\beta} = 5/12$		MCNS $\bar{\alpha} = 1/10$ $\bar{\beta} = 2/5$		MCNS $\bar{\alpha} = 1/8$ $\bar{\beta} = 3/8$		DDCS	
	$\ E\ _\infty$	order	$\ E\ _\infty$	order	$\ E\ _\infty$	order	$\ E\ _\infty$	order	$\ E\ _\infty$	order	$\ E\ _\infty$	order
$\frac{1}{20}$	$5.68e-05$		$5.68e-05$		$5.67e-05$		$5.67e-05$		$5.66e-05$		$2.60e-04$	
$\frac{1}{40}$	$1.50e-05$	1.92	$1.50e-05$	1.92	$1.50e-05$	1.92	$1.50e-05$	1.92	$1.49e-05$	1.93	$6.50e-05$	2.00
$\frac{1}{80}$	$3.85e-06$	1.96	$3.85e-06$	1.96	$3.84e-06$	1.97	$3.84e-06$	1.97	$3.83e-06$	1.96	$1.63e-05$	2.00
$\frac{1}{160}$	$9.75e-07$	1.98	$9.74e-06$	1.98	$9.73e-07$	1.98	$9.72e-07$	1.98	$9.70e-07$	1.98	$4.06e-06$	2.01
$\frac{1}{320}$	$2.45e-07$	1.99	$2.45e-07$	1.99	$2.45e-07$	1.99	$2.44e-07$	1.99	$2.44e-07$	1.99	$1.02e-06$	1.99
h	PCS $\bar{\alpha} = 1/16$ $\bar{\beta} = 7/16$		PCS $\bar{\alpha} = 1/14$ $\bar{\beta} = 3/7$		PCS $\bar{\alpha} = 1/12$ $\bar{\beta} = 5/12$		PCS $\bar{\alpha} = 1/10$ $\bar{\beta} = 2/5$		PCS $\bar{\alpha} = 1/8$ $\bar{\beta} = 3/8$			
	$\ E\ _\infty$	order	$\ E\ _\infty$	order	$\ E\ _\infty$	order	$\ E\ _\infty$	order	$\ E\ _\infty$	order		
$\frac{1}{20}$	$1.01e-04$		$1.01e-04$		$1.01e-04$		$1.01e-04$		$1.01e-04$			
$\frac{1}{40}$	$2.83e-05$	1.84	$2.83e-05$	1.84	$2.84e-05$	1.83	$2.84e-05$	1.83	$2.84e-05$	1.83		
$\frac{1}{80}$	$7.48e-06$	1.92	$7.48e-06$	1.93	$7.49e-06$	1.92	$7.49e-06$	1.92	$7.50e-06$	1.92		
$\frac{1}{160}$	$1.92e-06$	1.96	$1.92e-06$	1.97	$1.92e-06$	1.96	$1.92e-06$	1.96	$1.92e-06$	1.97		
$\frac{1}{320}$	$4.86e-07$	1.98	$4.86e-07$	1.98	$4.86e-07$	1.99	$4.87e-07$	1.98	$4.87e-07$	1.98		

In Figure 3.5, we illustrate the effect of $\bar{\alpha}$ on the maximum absolute error. It is observed that the minimum $\|E\|_\infty$ is achieved at about $\bar{\alpha} = \frac{1}{8}$, which is a different value from Example 3.2 but is about the same value as in Example 3.1.

FIGURE 3.5: (Example 3.3) Maximum absolute error for different $\bar{\alpha}$ when $h = \frac{1}{80}$

Remark 3.5. In Theorem 3.1, the condition $K = \frac{1}{8} [(b-a)^2 + h^2] \hat{g} < 1$ is proposed so that the numerical scheme has a unique solution and is convergent. If this condition is not satisfied, we cannot guarantee the unique solvability and convergence of our scheme. Example 3.1 and Example 3.2 both do not satisfy this condition. However, our method still gives second order convergence, this shows that the condition $K = \frac{1}{8} [(b-a)^2 + h^2] \hat{g} < 1$ is sufficient but not necessary.

3.4 Summary

In this chapter, we have developed a numerical scheme for a system of second-order boundary value problems, which arises from second-order obstacle problem. Our

scheme is obtained by using cubic non-polynomial spline at mid-knots to avoid the breakup points $\bar{a}$ and $\bar{b}$. We have proved the unique solvability and established convergence order of our scheme. To demonstrate the numerical efficiency and to compare with other methods in the literature, three examples are presented. The numerical results illustrate that our method gives the smallest errors in all the cases.

Chapter 4

Fractional Bagley-Torvik Equation

In this chapter, we consider the fractional Bagley-Torvik equation, which is one of the most important equations used to describe the motion of viscoelastically damped structures and the motion of fluids [14, 15, 38, 39, 46, 113, 120, 129]. The equation is first discussed by Bagley and Torvik [14, 15] who have used fractional derivatives to propose some viscoelastic models. It is found that the memory property of fractional derivatives is consistent with the physical principles of elastic materials. Further, the Bagley-Torvik equation is a particular case of the equation governing the motion of fluid through the MEMS instrument, an instrument that is specially designed to measure fluid viscosity in the oil exploration industry [46].

In this chapter, we consider the following fractional Bagley-Torvik equation

$$\begin{aligned} u''(x) + \theta \left[{}^C D_x^\gamma u(x) \right] + \sigma u(x) &= f(x), \quad x \in [0, 1], \\ u(0) &= 0, \quad u(1) = \hat{b}, \end{aligned} \tag{4.1}$$

where $0 < \gamma < 2$, the operator ${}^C D_x^\gamma$ denotes the Caputo fractional derivative of order γ , θ and γ are constants and the function $f(x)$ is continuous on the interval $[0, 1]$.

The existence and uniqueness of solution of the fractional Bagley-Torvik equation have been established in [119] using the nonlinear Leray-Schauder alternative.

There are some analytical methods for solving the fractional Bagley-Torvik equation, we list a few as follows: Adomian decomposition method [108]; differential transform method [11]; enhanced homotopy perturbation method [151]; fractional iteration method [91]; a method using expansion formula for fractional derivatives [12]. Nonetheless, it is still difficult to find the exact solution by these analytical methods. Numerical methods are therefore more practical and efficient in most situations. We mention some numerical methods for solving the fractional Bagley-Torvik equation as follows: an alternative scheme based on Adams-type predictor-corrector pairs with convergence order of $\frac{3}{2}$ [40]; a mathematical model of equation (4.1) is established using artificial neural network and the training of the network is done by evolutionary computational intelligence with a stochastic technique [105]; the Haar wavelet operational matrix method [107]; a collocation method based on the first kind Bessel functions [140]; hybridizable discontinuous Galerkin method [62]; a high order operational Tau method based on the Chebyshev polynomials as basis functions [95]; cubic polynomial spline [141, 142] and discrete cubic spline [143] have been used to obtain approximate solutions of the fractional Bagley-Torvik equation.

Motivated by the above research, we aim to develop a higher order numerical scheme for (4.1). We shall employ two tools – the first is a **new** fourth order approximation for the Caputo fractional derivative based on the *weighted shifted Grünwald-Letnikov difference (WSGD)* operator; the second is a *discrete cubic spline* operator which arises from the approximation of the second order derivative. Indeed, the new fourth order approximation will be first derived for the Riemann-Liouville fractional derivative and then extended to the Caputo fractional derivative. Meanwhile, the discrete spline used will involve central differences instead of derivatives (as in continuous spline), hence it is more suitable to approximate functions whose derivatives may not be defined at some points. Discrete spline was first introduced by Mangasarian and Schumaker [88] in 1971, and subsequent development can be found in the work of Lyche [86, 87] and Chen and Wong [27–31]. Recently, Zahra and Van Daele [143] have used discrete cubic spline to approximate the second order derivative and a third order approximation for the fractional derivative. The convergence order of their method is shown to be 3, which is the *best accuracy to date*. We shall prove that the convergence order of our method can achieve 4, hence *improves* the best result to date.

The chapter is organized as follows. In Section 4.1, we derive a new fourth order WSGD approximation for the Riemann-Liouville fractional derivative, extend it to the Caputo fractional derivative and apply the discrete cubic spline relation (2.4). A numerical scheme is then developed for the fractional Bagley-Torvik equation in Section 4.2. In Section 4.3, the unique solvability and convergence of the numerical scheme are proved by matrix analysis method. In section 4.4, we present four numerical examples to verify the theoretical results as well as to compare with other methods in the literature. Finally, a conclusion is given in section 4.5.

4.1 WSGD Approximation

The first result below **extends** Lemma 2.1 of [57] to a general γ . Note that the result in [57] is the special case when $\gamma \in (0, 1)$.

Lemma 4.1. *Let j be a positive integer. If $y(x) \in \{y(x) \in C^{(\lceil \gamma \rceil + j + 1)}(\mathcal{R}) \mid y, y', \dots, y^{(\lceil \gamma \rceil + j + 1)} \in L^1(\mathcal{R})\}$, then we have $y(x) \in \mathcal{C}^{\gamma+j}(\mathcal{R})$, where*

$$\mathcal{C}^{\gamma+j}(\mathcal{R}) = \left\{ y(x) \left| \int_{-\infty}^{\infty} (1 + |\varpi|)^{\gamma+j} |\tilde{y}(\varpi)| d\varpi < \infty \right. \right\},$$

and $\tilde{y}(\varpi) = \int_{-\infty}^{\infty} y(x) e^{-ix\varpi} dx$ is the Fourier transform of $y(x)$.

Proof. From Riemann-Lebesgue lemma, the assumption on $y(x)$ implies that for some positive constant $\bar{C}$, we have for all $\varpi \in \mathcal{R}$,

$$|\tilde{y}(\varpi)| \leq \frac{\bar{C}}{(1 + |\varpi|)^{(\lceil \gamma \rceil + j + 1)}}.$$

It follows that

$$\begin{aligned} \int_{-\infty}^{\infty} (1 + |\varpi|)^{\gamma+j} |\tilde{y}(\varpi)| d\varpi &\leq \int_{-\infty}^{\infty} (1 + |\varpi|)^{\gamma+j} \left| \frac{\bar{C}}{(1 + |\varpi|)^{(\lceil \gamma \rceil + j + 1)}} \right| d\varpi \\ &= \bar{C} \int_{-\infty}^{\infty} \frac{1}{(1 + |\varpi|)^{(\lceil \gamma \rceil - \gamma + 1)}} d\varpi = \bar{C} \frac{2}{\lceil \gamma \rceil - \gamma} < \infty, \end{aligned}$$

where we have used $\lceil \gamma \rceil - \gamma > 0$ in the last equality. Hence, $y(x) \in \mathcal{C}^{\gamma+j}(\mathcal{R})$. ■

The next lemma from [55, 124] gives a method to approximate the Riemann-Liouville fractional derivative ${}_{-\infty}^{RL}D_x^\gamma y(x)$.

Lemma 4.2. [55, 124] *Let γ be a positive number and $y(x) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+4}(\mathcal{R})$. Then, we have*

$$J_{h,l}' y(x) = {}^{RL}D_x^\gamma y(x) + \sum_{j=1}^3 \rho_j^{\gamma,l} [{}^{RL}D_x^{\gamma+j} y(x)] h^j + O(h^4), \quad (4.2)$$

uniformly for $x \in \mathcal{R}$, where l is an integer, h is the step size, $J_{h,l}' y(x)$ is the shifted Grünwald-Letnikov operator defined in (2.28) and

$$\begin{cases} \rho_1^{\gamma,l} = l - \frac{\gamma}{2}, \\ \rho_2^{\gamma,l} = \frac{l^2}{2} - \frac{\gamma l}{2} + \frac{\gamma(3\gamma+1)}{24}, \\ \rho_3^{\gamma,l} = \frac{l^3}{6} - \frac{\gamma l^2}{4} + \frac{\gamma(3\gamma+1)l}{24} - \frac{\gamma^2(\gamma+1)}{48}. \end{cases} \quad (4.3)$$

Inspired by Lemma 4.2, we shall derive a fourth order approximation for the Riemann-Liouville fractional derivative in the next result.

Theorem 4.1. (4-WSGD approximation) *Let γ be a positive number and $y(x) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+4}(\mathcal{R})$. Define the weighted shifted Grünwald-Letnikov operator G_h^γ by*

$$G_h^\gamma y(x) = \lambda_0 J_{h,0}' y(x) + \lambda_{-1} J_{h,-1}' y(x) + \lambda_{-2} J_{h,-2}' y(x) + \lambda_{-3} J_{h,-3}' y(x), \quad (4.4)$$

where h is the step size, $J_{h,l}'$ ($l = 0, -1, -2, -3$) is defined in (2.28) and

$$\begin{aligned} \lambda_0 &= \frac{\gamma^3 + 11\gamma^2 + 40\gamma + 48}{48}, & \lambda_{-1} &= \frac{-3\gamma^3 - 27\gamma^2 - 62\gamma}{48}, \\ \lambda_{-2} &= \frac{3\gamma^3 + 21\gamma^2 + 28\gamma}{48}, & \lambda_{-3} &= \frac{-\gamma^3 - 5\gamma^2 - 6\gamma}{48}. \end{aligned} \quad (4.5)$$

Then, we have

$${}^{RL}D_x^\gamma y(x) = G_h^\gamma y(x) + O(h^4), \quad (4.6)$$

uniformly for $x \in \mathcal{R}$.

Proof. Letting $l = 0, -1, -2, -3$ in (4.2), we find

$$\begin{aligned}
G_h^\gamma y(x) &= \lambda_0 J_{h,0}^\gamma y(x) + \lambda_{-1} J_{h,-1}^\gamma y(x) + \lambda_{-2} J_{h,-2}^\gamma y(x) + \lambda_{-3} J_{h,-3}^\gamma y(x) \\
&= (\lambda_0 + \lambda_{-1} + \lambda_{-2} + \lambda_{-3}) {}^{RL}D_x^\gamma y(x) \\
&\quad + (\lambda_0 \rho_1^{\gamma,0} + \lambda_{-1} \rho_1^{\gamma,-1} + \lambda_{-2} \rho_1^{\gamma,-2} + \lambda_{-3} \rho_1^{\gamma,-3}) h [{}^{RL}D_x^{\gamma+1} y(x)] \\
&\quad + (\lambda_0 \rho_2^{\gamma,0} + \lambda_{-1} \rho_2^{\gamma,-1} + \lambda_{-2} \rho_2^{\gamma,-2} + \lambda_{-3} \rho_2^{\gamma,-3}) h^2 [{}^{RL}D_x^{\gamma+2} y(x)] \\
&\quad + (\lambda_0 \rho_3^{\gamma,0} + \lambda_{-1} \rho_3^{\gamma,-1} + \lambda_{-2} \rho_3^{\gamma,-2} + \lambda_{-3} \rho_3^{\gamma,-3}) h^3 [{}^{RL}D_x^{\gamma+3} y(x)] + O(h^4).
\end{aligned} \tag{4.7}$$

Next, let the coefficients $\lambda_0, \lambda_{-1}, \lambda_{-2}$ and λ_{-3} satisfy the following equations:

$$\begin{cases} \lambda_0 + \lambda_{-1} + \lambda_{-2} + \lambda_{-3} = 1, \\ \lambda_0 \rho_1^{\gamma,0} + \lambda_{-1} \rho_1^{\gamma,-1} + \lambda_{-2} \rho_1^{\gamma,-2} + \lambda_{-3} \rho_1^{\gamma,-3} = 0, \\ \lambda_0 \rho_2^{\gamma,0} + \lambda_{-1} \rho_2^{\gamma,-1} + \lambda_{-2} \rho_2^{\gamma,-2} + \lambda_{-3} \rho_2^{\gamma,-3} = 0, \\ \lambda_0 \rho_3^{\gamma,0} + \lambda_{-1} \rho_3^{\gamma,-1} + \lambda_{-2} \rho_3^{\gamma,-2} + \lambda_{-3} \rho_3^{\gamma,-3} = 0. \end{cases} \tag{4.8}$$

The solution of the above is simply (4.3). Combining (4.8) and (4.7) leads to (4.5) immediately. ■

Remark 4.1. In order to apply Theorem 4.1 to a function $y(x)$ defined on the finite interval $[0, 1]$ (the interval of interest in (4.1)), we need to extend $y(x)$ to $\mathcal{R}$ as follows:

$$y_e(x) = \begin{cases} 0, & x < 0, \\ y(x), & 0 \leq x \leq 1, \\ \psi(x), & x > 1, \end{cases} \tag{4.9}$$

where $\psi(x)$ is a smooth function.

The next result presents a fourth order approximation for the *Caputo* fractional derivative ${}_0^C D_x^\gamma y(x)$ where $y(x)$ is defined on the interval $[0, 1]$. We consider the mesh P in (2.1).

Theorem 4.2. (4-WSGD approximation) Let $0 < \gamma < 2$. Suppose $y(x)$ is defined on the interval $[0, 1]$ with $y_e(x) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+4}(\mathcal{R})$ and $y^{(k)}(0) = 0$, $k =$

0, 1. Then, we have

$${}_0^C D_x^\gamma y(x_m) = \frac{1}{h^\gamma} \sum_{k=0}^m c_k^\gamma y_{m-k} + O(h^4), \quad 0 \leq m \leq M, \quad (4.10)$$

where

$$\begin{cases} c_0^\gamma = \lambda_0 g_0^\gamma, \\ c_1^\gamma = \lambda_0 g_1^\gamma + \lambda_{-1} g_0^\gamma, \\ c_2^\gamma = \lambda_0 g_2^\gamma + \lambda_{-1} g_1^\gamma + \lambda_{-2} g_0^\gamma, \\ c_k^\gamma = \lambda_0 g_k^\gamma + \lambda_{-1} g_{k-1}^\gamma + \lambda_{-2} g_{k-2}^\gamma + \lambda_{-3} g_{k-3}^\gamma, \quad k \geq 3. \end{cases} \quad (4.11)$$

Proof. Since $y_e(x) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+4}(\mathcal{R})$, we can apply Theorem 4.1 to $y_e(x)$ to get

$$\begin{aligned} {}_{-\infty}^{RL} D_x^\gamma y_e(x) &= G_h^\gamma y_e(x) + O(h^4) \\ &= \lambda_0 J_{h,0}^\gamma y_e(x) + \lambda_{-1} J_{h,-1}^\gamma y_e(x) + \lambda_{-2} J_{h,-2}^\gamma y_e(x) \\ &\quad + \lambda_{-3} J_{h,-3}^\gamma y_e(x) + O(h^4). \end{aligned} \quad (4.12)$$

For $x \in [0, 1]$, we have $y_e(x) = y(x)$ and so ${}_{-\infty}^{RL} D_x^\gamma y_e(x) = {}_0^{RL} D_x^\gamma y(x)$. Further, for $x \in [0, 1]$ and $l = 0, -1, -2, -3$,

$$J_{h,l}^\gamma y_e(x) = \frac{1}{h^\gamma} \sum_{k=0}^{\infty} g_k^\gamma y(x - (k-l)h) = \frac{1}{h^\gamma} \sum_{k=0}^{[\frac{x}{h}] + l} g_k^\gamma y(x - (k-l)h) \equiv \mathcal{J}_{h,l}^\gamma y(x). \quad (4.13)$$

It follows that at the grid point $x_m = mh$, we have

$$\mathcal{J}_{h,l}^\gamma y(x_m) = \frac{1}{h^\gamma} \sum_{k=0}^{m+l} g_k^\gamma y(x_m - (k-l)h) = \frac{1}{h^\gamma} \sum_{k=0}^{m+l} g_k^\gamma y(x_{m-k+l}). \quad (4.14)$$

Concluding from (4.12) and (4.13), we have for $x \in [0, 1]$,

$$\begin{aligned} {}_0^{RL} D_x^\gamma y(x) &= {}_{-\infty}^{RL} D_x^\gamma y_e(x) = \lambda_0 \mathcal{J}_{h,0}^\gamma y(x) + \lambda_{-1} \mathcal{J}_{h,-1}^\gamma y(x) + \lambda_{-2} \mathcal{J}_{h,-2}^\gamma y(x) \\ &\quad + \lambda_{-3} \mathcal{J}_{h,-3}^\gamma y(x) + O(h^4). \end{aligned} \quad (4.15)$$

Next, noting $y^{(k)}(0) = 0$, $k = 0, 1$ and Remark 2.5, we see that ${}_0^C D_x^\gamma y(x) = {}_0^{RL} D_x^\gamma y(x)$. Hence, from (4.14) and (4.15) we can obtain (4.10) finally. ■

We shall approximate the solution of (4.1) by the discrete cubic spline $S(x, h, h_c)$. Let $u(x)$ denote the exact solution of (4.1). Then, the truncation error T_m in the relation (2.4) satisfies

$$u_{m-1} - 2u_m + u_{m+1} = \alpha u_{m-1}'' + \beta u_m'' + \alpha u_{m+1}'' + T_m, \quad 1 \leq m \leq M-1. \quad (4.16)$$

By Taylor expansion, we obtain the following result which is also noted in (3.8) of [28].

Lemma 4.3. *Let $u(x) \in C^{(6)}[0, 1]$. Then, the local truncation error T_m , $1 \leq m \leq M-1$ associated with the spline relation (4.16) is given by*

$$T_m = -\frac{h^2}{12}(h^2 - 2h_c^2)u_m^{(4)} - \frac{h^4}{360}(4h^2 - 5h_c^2)u_m^{(6)} + O(h^8), \quad 1 \leq m \leq M-1. \quad (4.17)$$

Remark 4.2. From (4.17), it is clear that $T_m = O(h^6)$ if $h_c = \frac{1}{\sqrt{2}}h$. Thus, we shall fix $h_c = \frac{1}{\sqrt{2}}h$ for the rest of this chapter. It then follows from (2.5) that $\alpha = \frac{1}{12}h^2$ and $\beta = \frac{5}{6}h^2$.

For notational simplicity, we introduce the following operator which will be used in Section 4.2.

Definition 4.1. The averaging difference operator $\mathcal{K}$ applying to a function $Y(x)$ is defined by the following

$$\mathcal{K}Y(x) = \alpha Y(x-h) + \beta Y(x) + \alpha Y(x+h), \quad (4.18)$$

where α and β are given in (2.5).

Remark 4.3. Noting that a function $y(x)$ that is approximated by the discrete cubic spline $S(x, h, h_c)$ will naturally have $y(x_m)$ and $y''(x_m)$ approximated by S_m and W_m respectively, the spline relation (4.17) and Remark 4.2 lead to

$$\mathcal{K}y''(x) = y(x-h) - 2y(x) + y(x+h) + O(h^6). \quad (4.19)$$

4.2 Numerical Scheme

In this section, using the tools developed in Section 4.1 we shall derive the numerical scheme. To begin, consider the discretized form of the equation (4.1) over the uniform mesh P

$$u''(x_m) + \theta \left[{}_0^C D_x^\gamma u(x_m) \right] + \sigma u(x_m) = f(x_m). \quad (4.20)$$

First, we apply the 4-WSGD approximation (4.10) to the fractional term in (4.20), giving

$$u_m'' + h^{-\gamma} \theta \sum_{k=0}^m c_k^\gamma u_{m-k} + \sigma u_m = f_m + O(h^4). \quad (4.21)$$

Next, we apply the operator $\mathcal{K}$ to both sides of (4.21) to get

$$\mathcal{K}u_m'' + h^{-\gamma} \theta \mathcal{K} \sum_{k=0}^m c_k^\gamma u_{m-k} + \sigma \mathcal{K}u_m = \mathcal{K}f_m + O(h^6). \quad (4.22)$$

In view of (4.19), it follows from (4.22) that

$$u_{m-1} - 2u_m + u_{m+1} + h^{-\gamma} \theta \mathcal{K} \sum_{k=0}^m c_k^\gamma u_{m-k} + \sigma \mathcal{K}u_m = \mathcal{K}f_m + O(h^6), \quad 1 \leq m \leq M-1. \quad (4.23)$$

The numerical scheme is thus the system (4.23) with the exact solution u_m replaced by the approximate solution S_m and the error terms omitted, i.e.,

$$S_{m-1} - 2S_m + S_{m+1} + h^{-\gamma} \theta \mathcal{K} \sum_{k=0}^m c_k^\gamma S_{m-k} + \sigma \mathcal{K}S_m = \mathcal{K}f_m, \quad 1 \leq m \leq M-1. \quad (4.24)$$

Remark 4.4. The numerical scheme (4.24) employs the spline operator $\mathcal{K}$ and the 4-WSGD approximation (4.10). In comparison, the best performing method in [143] uses discrete cubic spline and a third order approximation (3-WSGD approximation). Hence, we expect the numerical scheme (4.24) to have a better convergence and this will be proven in the next section.

4.3 Unique Solvability and Convergence

In this section, we shall analyze the convergence of numerical scheme (4.24) by matrix analysis method.

Recall from Remark 4.2 that we fix $h_c = \frac{1}{\sqrt{2}}h$ so that the local truncation error associated with the spline relation (4.19) is $O(h^6)$.

Let $U = [u_m]$, $S = [S_m]$, $\bar{F} = [\bar{F}_m]$, $T = [T_m]$ and $E = U - S = [e_m]$, $1 \leq m \leq M - 1$ be $(M - 1) \times 1$ vectors. The vector U denotes the exact solution of (4.1), S denotes the solution obtained from (4.24), T is the local truncation error, and $E = U - S$ is the error. Then, it is clear that the scheme (4.24) can be written in matrix form as

$$\begin{cases} \bar{A}U = \bar{F} + T, \\ \bar{A}S = \bar{F}, \\ \bar{A}E = T, \end{cases} \quad (4.25)$$

where

$$\begin{cases} \bar{A} = A_1 + h^{-\gamma}\theta B_1 \hat{G} + \sigma B_2, \\ \bar{F} = B_2 Q_1 + Q_2, \\ T_m = O(h^6), \quad 1 \leq m \leq M - 1. \end{cases} \quad (4.26)$$

The matrices A_1 and B_2 are $(M - 1) \times (M - 1)$ matrices given by

$$A_1 = \begin{pmatrix} -2 & 1 & & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{pmatrix}, \quad B_2 = \begin{pmatrix} \beta & \alpha & & & \\ \alpha & \beta & \alpha & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha & \beta & \alpha \\ & & & \alpha & \beta \end{pmatrix}, \quad (4.27)$$

B_1 is a $(M-1) \times (M+1)$ matrix and $\hat{G}$ is a $(M+1) \times (M-1)$ matrix given by

$$B_1 = \begin{pmatrix} \alpha & \beta & \alpha & & & \\ & \alpha & \beta & \alpha & & \\ & & \ddots & \ddots & \ddots & \\ & & & \alpha & \beta & \alpha \\ & & & & \alpha & \beta & \alpha \end{pmatrix}, \quad \hat{G} = \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 \\ c_0^\gamma & 0 & \cdots & 0 & 0 \\ c_1^\gamma & c_0^\gamma & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ c_{M-3}^\gamma & \cdots & c_1^\gamma & c_0^\gamma & 0 \\ c_{M-2}^\gamma & \cdots & c_2^\gamma & c_1^\gamma & c_0^\gamma \\ c_{M-1}^\gamma & \cdots & c_3^\gamma & c_2^\gamma & c_1^\gamma \end{pmatrix}, \quad (4.28)$$

and Q_1 and Q_2 are $(M-1) \times 1$ vectors given by

$$Q_1 = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_{M-2} \\ f_{M-1} \end{pmatrix}, \quad Q_2 = \begin{pmatrix} \alpha f_0 - u_0 - \sigma \alpha u_0 - h^{-\gamma} \theta (\alpha c_0^\gamma + \beta c_1^\gamma + \alpha c_2^\gamma) u_0 \\ 0 \\ \vdots \\ 0 \\ \alpha f_M - u_M - \sigma \gamma u_M - h^{-\gamma} \theta \alpha c_0^\gamma u_M \end{pmatrix}. \quad (4.29)$$

Lemma 4.4. [127] *The inverse of A_1 , namely $A_1^{-1} = [\bar{a}_{mj}]$, is given by $\bar{a}_{mj} = \frac{\min\{m,j\}}{M} (M - \max\{m,j\})$. Moreover, we have*

$$\|A_1^{-1}\| \leq \frac{M^2}{8} = \frac{1}{8h^2}.$$

The next two results (Lemmas 4.5 and 4.6) give an upper bound for the Grünwald-Letnikov weight $|g_k^\gamma|$ and its sum. These results are essential in proving the unique solvability and convergence of (4.24). We remark that Lemmas 4.5 and 4.6 are more general than Lemmas 3 and 4 of [143] which are for $\gamma \in (0, 1)$.

Lemma 4.5. *Let j be an integer such that $1 \leq j \leq k$. The following holds for $\gamma \leq (1.27846454276107)j - 1$,*

$$|g_k^\gamma| \leq \left(\frac{j}{k+1}\right)^{\gamma+1} |g_{j-1}^\gamma|. \quad (4.30)$$

Proof. By direct computation, we have the inequality

$$|1 - x| \leq \exp(-x), \quad x \in [0, 1.27846454276107]. \quad (4.31)$$

Using (4.31) and the recursive formula (2.29) of g_k^γ , we find

$$|g_k^\gamma| = \left|1 - \frac{\gamma+1}{k}\right| \cdot |g_{k-1}^\gamma| \leq \exp\left(-\frac{\gamma+1}{k}\right) |g_{k-1}^\gamma| \quad (4.32)$$

for $\gamma \leq (1.27846454276107)k - 1$. Applying (4.32) repeatedly yields

$$|g_k^\gamma| \leq \exp\left(-\frac{\gamma+1}{k} - \frac{\gamma+1}{k-1} - \cdots - \frac{\gamma+1}{j}\right) |g_{j-1}^\gamma| = \exp\left[-(\gamma+1) \sum_{n=j}^k \frac{1}{n}\right] |g_{j-1}^\gamma| \quad (4.33)$$

for $\gamma \leq (1.27846454276107)j - 1$.

Using the inequality $\sum_{n=j}^k \frac{1}{n} > \int_j^{k+1} \frac{1}{x} dx = \ln \frac{k+1}{j}$ in (4.33), we get

$$|g_k^\gamma| \leq \exp\left[-(\gamma+1) \ln \frac{k+1}{j}\right] |g_{j-1}^\gamma| = \left(\frac{j}{k+1}\right)^{\gamma+1} |g_{j-1}^\gamma|$$

for $\gamma \leq (1.27846454276107)j - 1$. This completes the proof. ■

An application of Lemma 4.5 gives the next result.

Lemma 4.6. *Let j and ℓ be integers such that $1 \leq j \leq \ell$. The following holds for $\gamma \leq (1.27846454276107)j - 1$,*

$$\sum_{k=0}^{\ell} |g_k^\gamma| \leq \sum_{k=0}^{j-1} |g_k^\gamma| + \frac{j^{\gamma+1}}{\gamma} \left[\frac{1}{j^\gamma} - \frac{1}{(2\ell)^\gamma}\right] |g_{j-1}^\gamma|. \quad (4.34)$$

Proof. First, we sum the inequality (4.30) (Lemma 4.5) over k from j to ℓ , giving

$$\sum_{k=j}^{\ell} |g_k^\gamma| \leq \sum_{k=j}^{\ell} \left(\frac{j}{k+1}\right)^{\gamma+1} |g_{j-1}^\gamma|. \quad (4.35)$$

Next, we note that the following inequality holds for $1 \leq j \leq \ell$,

$$\sum_{k=j}^{\ell} \frac{1}{(k+1)^{\gamma}} < \int_j^{\ell+1} \frac{1}{x^{\gamma+1}} dx = \frac{1}{\gamma} \left[\frac{1}{j^{\gamma}} - \frac{1}{(\ell+1)^{\gamma}} \right] \leq \frac{1}{\gamma} \left[\frac{1}{j^{\gamma}} - \frac{1}{(2\ell)^{\gamma}} \right]. \quad (4.36)$$

Upon using (4.36) in (4.35), we get

$$\sum_{k=0}^{\ell} |g_k^{\gamma}| = \sum_{k=0}^{j-1} |g_k^{\gamma}| + \sum_{k=j}^{\ell} |g_k^{\gamma}| \leq \sum_{k=0}^{j-1} |g_k^{\gamma}| + \frac{j^{\gamma+1}}{\gamma} \left[\frac{1}{j^{\gamma}} - \frac{1}{(2\ell)^{\gamma}} \right] |g_{j-1}^{\gamma}|$$

which completes the proof. ■

Theorem 4.3. (Solvability) *Let $0 < \gamma < 2$. The scheme (4.24) is uniquely solvable if*

$$\frac{1}{8} \left\{ h^{-\gamma} |\theta| \left[\kappa \sum_{k=0}^2 |g_k^{\gamma}| + \frac{3\kappa}{\gamma} \left(1 - \frac{3^{\gamma}}{2^{\gamma}} h^{\gamma} \right) |g_2^{\gamma}| \right] + |\sigma| \right\} < 1, \quad (4.37)$$

where $\kappa = |\lambda_0| + |\lambda_{-1}| + |\lambda_{-2}| + |\lambda_{-3}|$, $g_0^{\gamma} = 1$, $|g_1^{\gamma}| = \gamma$ and $|g_2^{\gamma}| = \frac{1}{2}\gamma|1 - \gamma|$.

Proof. From (4.25), we see that (4.24) in matrix form is written as $\bar{A}S = \bar{F}$. Hence, the numerical scheme has a unique solution if and only if the matrix $\bar{A}$ is invertible. Noting (4.26) and the fact that A_1 is invertible (Lemma 4.4), we write

$$\bar{A} = A_1 + h^{-\gamma} \theta B_1 \hat{G} + \sigma B_2 = A_1 (I + A_1^{-1} V), \quad (4.38)$$

where

$$V = h^{-\gamma} \theta B_1 \hat{G} + \sigma B_2. \quad (4.39)$$

It follows that $\bar{A}^{-1} = (I + A_1^{-1} V)^{-1} A_1^{-1}$ provided that $(I + A_1^{-1} V)$ is invertible. In view of Lemma 3.2, the matrix $(I + A_1^{-1} V)$ is invertible if

$$\|A_1^{-1} V\|_{\infty} < 1. \quad (4.40)$$

It is then clear that the scheme (4.24) is uniquely solvable if the condition (4.37) holds.

From the definitions of the matrices B_1 , B_2 and $\hat{G}$, it is obvious that

$$\|B_1\|_{\infty} = h^2, \quad \|B_2\|_{\infty} = h^2, \quad (4.41)$$

and

$$\begin{aligned}
\|\hat{G}\|_\infty &= \max \left\{ \sum_{k=0}^{M-2} |c_k^\gamma|, \sum_{k=1}^{M-1} |c_k^\gamma| \right\} \\
&\leq \sum_{k=0}^{M-1} |c_k^\gamma| \\
&\leq \sum_{k=0}^{M-1} |\lambda_0 g_k^\gamma| + \sum_{k=0}^{M-2} |\lambda_{-1} g_k^\gamma| + \sum_{k=0}^{M-3} |\lambda_{-2} g_k^\gamma| + \sum_{k=0}^{M-4} |\lambda_{-3} g_k^\gamma| \\
&\leq (|\lambda_0| + |\lambda_{-1}| + |\lambda_{-2}| + |\lambda_{-3}|) \sum_{k=0}^{M-1} |g_k^\gamma| = \kappa \sum_{k=0}^{M-1} |g_k^\gamma|.
\end{aligned} \tag{4.42}$$

Hence, we have

$$\|B_1 \hat{G}\|_\infty \leq \|B_1\|_\infty \cdot \|\hat{G}\|_\infty \leq \kappa h^2 \sum_{k=0}^{M-1} |g_k^\gamma| \leq \kappa h^2 \sum_{k=0}^M |g_k^\gamma|. \tag{4.43}$$

Let $j = 3$ and $\ell = M$ in Lemma 4.6. Then, for $\gamma \leq (1.27846454276107)(3) - 1 = 2.8354 \dots$, the inequality (4.34) becomes

$$\sum_{k=0}^M |g_k^\gamma| \leq \sum_{k=0}^2 |g_k^\gamma| + \frac{3^{\gamma+1}}{\gamma} \left[\frac{1}{3^\gamma} - \frac{1}{(2M)^\gamma} \right] |g_2^\gamma| = \sum_{k=0}^2 |g_k^\gamma| + \frac{3}{\gamma} \left(1 - \frac{3^\gamma}{2^\gamma} h^\gamma \right) |g_2^\gamma|, \tag{4.44}$$

where it is known (see (2.29)) that $g_0^\gamma = 1$, $|g_1^\gamma| = \gamma$, and $|g_2^\gamma| = \frac{1}{2}\gamma|1 - \gamma|$.

Since we have $\gamma \in (0, 2)$ in this theorem, the inequality (4.44) can be used here, in particular in (4.43). Noting (4.41), (4.43), (4.44) and Lemma 4.4, we find

$$\begin{aligned}
\|\bar{A}^{-1}V\|_\infty &\leq \|\bar{A}^{-1}\|_\infty \cdot \|V\|_\infty \\
&\leq \|\bar{A}^{-1}\|_\infty \left(h^{-\gamma} |\theta| \cdot \|B_1 \hat{G}\|_\infty + |\sigma| \cdot \|B_2\|_\infty \right) \\
&\leq \frac{1}{8h^2} \left\{ h^{-\gamma} |\theta| \left[\kappa h^2 \left(\sum_{k=0}^2 |g_k^\gamma| + \frac{3}{\gamma} \left(1 - \frac{3^\gamma}{2^\gamma} h^\gamma \right) |g_2^\gamma| \right) \right] + |\sigma| h^2 \right\} \\
&= \frac{1}{8} \left\{ h^{-\gamma} |\theta| \left[\kappa \sum_{k=0}^2 |g_k^\gamma| + \frac{3\kappa}{\gamma} \left(1 - \frac{3^\gamma}{2^\gamma} h^\gamma \right) |g_2^\gamma| \right] + |\sigma| \right\} \equiv \text{RHS}_{(4.45)}
\end{aligned} \tag{4.45}$$

Hence, the condition (4.37) immediately implies (4.26) which guarantees the unique solvability of (4.40). ■

Theorem 4.4. (Convergence) *Let $0 < \gamma < 2$ and (4.37) hold. Suppose $U(x) \in C^{(6)}[0, 1]$, $U_e(x) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+4}(\mathcal{R})$ and $U^{(k)}(0) = 0$, $k = 0, 1$. Then, the error $E = U - S$, where U is the exact solution of (4.1) and S is the solution obtained from (4.24), satisfies*

$$\|E\|_\infty \leq C_1 h^4,$$

where C_1 is a constant.

Proof. From Theorem 4.3, we know that the matrix $\bar{A}$ is invertible and so it follows from (4.25) that $E = \bar{A}^{-1}T$.

Next, noting (4.38), we have $\bar{A}^{-1} = (I + A_1^{-1}V)^{-1}A_1^{-1}$. Then, using Lemma 3.2, (4.40) and (4.45), we find

$$\|\bar{A}^{-1}\|_\infty \leq \|(I + A_1^{-1}V)^{-1}\|_\infty \cdot \|A_1^{-1}\|_\infty \leq \frac{\|A_1^{-1}\|_\infty}{1 - \|A_1^{-1}V\|_\infty} \leq \frac{\|A_1^{-1}\|_\infty}{1 - \text{RHS}_{(4.45)}}.$$

Using the above inequality, the fact that $\|T\|_\infty = O(h^6)$ and $\|A_1^{-1}\|_\infty = O(h^{-2})$ (Lemma 4.4), it is clear that

$$\|E\|_\infty \leq \|\bar{A}^{-1}\|_\infty \cdot \|T\|_\infty \leq \frac{\|A_1^{-1}\|_\infty \cdot \|T\|_\infty}{1 - \text{RHS}_{(4.45)}} = O(h^4).$$

This completes the proof. ■

Remark 4.5. Theorem 4.4 shows that (4.24) can achieve convergence order of at least 4 for $\gamma \in (0, 2)$. The result improves/extends several numerical methods for Bagley-Torvik equation in the literature, listed as follows.

- (a) The numerical method in [143] combines discrete cubic spline with 3 different kinds of approximation for the Caputo fractional derivative, namely, 3-WSGD, nonstandard Grünwald-Letnikov derivative (*NSGD*) and Grünwald-Letnikov derivative (*GD*). The convergence analysis is carried out for the 3-WSGD case only and for $\gamma \in (0, 1)$ – it is shown that the convergence order is 3, and this is the best theoretically proven result to date until the current work.

- (b) In [141], cubic polynomial spline and Grünwald-Letnikov derivative (*CSGD*) are used to solve the Bagley-Torvik equation. It is shown that the convergence order is 2.
- (c) In [142], cubic polynomial spline combined with shooting (*CSS*) method is used, and the fractional derivative is transformed into a system of ordinary differential equations. The convergence order of the method is shown to be 2.

4.4 Experiment

In this section, we shall present four examples to illustrate the efficiency of the numerical scheme (4.24) and to compare with other methods in the literature.

Example 4.1. [141–143] Consider the Bagley-Torvik equation (4.1) with $\hat{b} = 0$ and

$$f(x) = (\lambda - 1)(\lambda x - \lambda + 2)x^{\lambda-3} + \theta \frac{(\lambda - 1)!}{\Gamma(\lambda - \gamma)} \left(\frac{\lambda x}{\lambda - \gamma} - 1 \right) x^{\lambda-\gamma-1} + \sigma x^{\lambda-1}(x - 1).$$

The exact solution is $u(x) = x^{\lambda-1}(x - 1)$.

Let $\lambda = 5$ be fixed. For different sets of (θ, σ, γ) , we shall apply the scheme (4.24) with $h_c = \frac{1}{\sqrt{2}}h$. The maximum absolute errors $\|E\|_\infty$, convergence orders and absolute errors at grid points are computed, and comparisons are made with several methods in the literature.

A brief description of the numerical simulation in Tables 4.1–4.4 and Figures 4.1–4.2:

- (i) In Table 4.1, we fix $(\theta, \sigma) = (0.0001, 0.1)$. For various values of γ , we present the maximum absolute errors $\|E\|_\infty$ and convergence orders obtained from (4.24). The numerical results indicate that (4.24) is at least a fourth order method, thus confirming the theoretical result in Theorems 4.4.
- (ii) We shall investigate the effects of θ and σ on the maximum absolute error $\|E\|_\infty$ obtained from applying the numerical scheme (4.24). Consider $\gamma = 0.1$.

First, we keep $\sigma = 0.1$ fixed and vary θ from 0.0001 to 100000. In Figure 4.1, we plot $-\log_2 \|E\|_\infty$ vs $-\log_2 h$. The gradients of the lines give the order of the scheme (4.24) and we observe that the gradients are around 4. This indicates that the scheme (4.24) is of order 4 for different θ 's. Similarly, in Figure 4.2, we keep $\theta = 1$ fixed and vary σ from 0.1 to 100. Once again the gradients of the lines are around 4, which means the scheme (4.24) is of order 4 for different σ 's. The observations from Figures 4.1 and 4.2 further illustrate the theoretical convergence (Theorem 4.4).

- (iii) In Table 4.2, we fix $(\theta, \sigma) = (0.5, 1)$. Here, we compare with 3-WSGD method and NSGD method in [143] (see Remark 4.5(a)). Clearly, (4.24) outperforms as it attains the smallest $\|E\|_\infty$ and the fastest convergence in all cases. Note that the theoretical convergence order of 3-WSGD method is 3, while that of (4.24) is 4.
- (iv) In Table 4.3, we fix $(\theta, \sigma) = (0.5, 1)$. A comparison is made with CSGD method [141] (see Remark 4.5(b)). Clearly, in terms of the size of $\|E\|_\infty$ and convergence order, (4.24) is the best performer in all cases.
- (v) In Table 4.4, we fix $(\theta, \sigma, \gamma) = (0.5, 1, 0.3)$. For $M = 8$, we present the absolute errors computed by several methods, including NSGD method [143], GD method [143], CSS method [142] (see Remark 4.5(c)) and CSGD method [141]. We observe that (4.24) has good agreement with the exact solution and attains the smallest absolute errors at almost all grid points.

TABLE 4.1: (Example 4.1) Maximum absolute error $\|E\|_\infty$ and convergence order of scheme (4.24)

M	$\gamma = 0.1$	order	$\gamma = 0.3$	order	$\gamma = 0.6$	order	$\gamma = 0.9$	order
2^3	$7.71e - 10$		$3.76e - 09$		$1.48e - 08$		$4.08e - 08$	
2^4	$6.43e - 11$	3.58	$3.07e - 10$	3.61	$1.17e - 09$	3.66	$3.12e - 09$	3.71
2^5	$4.55e - 12$	3.82	$2.16e - 11$	3.83	$8.06e - 11$	3.86	$2.10e - 10$	3.89
2^6	$2.98e - 13$	3.93	$1.42e - 12$	3.93	$5.26e - 12$	3.94	$1.35e - 11$	3.96
2^7	$5.63e - 15$	5.73	$9.65e - 14$	3.88	$3.51e - 13$	3.91	$8.67e - 13$	3.96
M	$\gamma = 1.1$	order	$\gamma = 1.3$	order	$\gamma = 1.6$	order	$\gamma = 1.9$	order
2^3	$7.31e - 08$		$1.25e - 07$		$2.53e - 07$		$4.86e - 07$	
2^4	$5.39e - 09$	3.76	$8.69e - 09$	3.85	$1.62e - 08$	3.97	$2.85e - 08$	4.09
2^5	$3.55e - 10$	3.92	$5.58e - 10$	3.96	$9.75e - 10$	4.05	$1.58e - 09$	4.17
2^6	$2.26e - 11$	3.97	$3.50e - 11$	3.99	$5.93e - 11$	4.04	$9.07e - 11$	4.12
2^7	$1.43e - 12$	3.98	$2.20e - 12$	3.99	$3.64e - 12$	4.03	$5.39e - 12$	4.07

FIGURE 4.1: (Example 4.1) Maximum absolute error $\|E\|_\infty$ for different θ 's FIGURE 4.2: (Example 4.1) Maximum absolute error $\|E\|_\infty$ for different σ 's

TABLE 4.2: (Example 4.1) Comparison with 3-WSGD and NSGD methods

γ	M	Scheme (4.24)	order	3-WSGD [143]	order	NSGD [143]	order
0.1	2^3	$4.44e-06$		$9.2e-06$		$6.2e-05$	
	2^4	$3.71e-07$	3.58	$1.2e-06$	2.94	$1.5e-05$	2.05
	2^5	$2.63e-08$	3.82	$1.5e-07$	3.00	$9.6e-06$	0.64
	2^6	$1.75e-09$	3.91	$1.9e-08$	2.98	$5.0e-06$	0.94
	2^7	$1.13e-10$	3.95	$2.4e-09$	2.98	$2.5e-06$	1.00
0.9	2^3	$2.29e-04$		$2.9e-04$		$1.6e-03$	
	2^4	$1.76e-05$	3.70	$4.0e-05$	2.86	$7.7e-04$	1.06
	2^5	$1.18e-06$	3.90	$5.3e-06$	2.92	$4.2e-04$	0.87
	2^6	$7.61e-08$	3.95	$6.7e-07$	2.98	$2.2e-04$	0.93
	2^7	$4.83e-09$	3.98	$8.5e-08$	2.98	$1.1e-04$	1.00

TABLE 4.3: (Example 4.1) Comparison with CSGD method

γ	M	Scheme (4.24)	order	CSGD [141]	order
0.3	2^3	$2.18e-05$		$6.85e-03$	
	2^4	$1.78e-06$	3.61	$1.93e-03$	1.83
	2^5	$1.26e-07$	3.82	$5.38e-04$	1.84
	2^6	$8.31e-09$	3.92	$1.52e-04$	1.82
	2^7	$5.34e-10$	3.96	$4.23e-05$	1.83
0.5	2^3	$5.73e-05$		$6.39e-03$	
	2^4	$4.62e-06$	3.63	$1.73e-03$	1.89
	2^5	$3.21e-07$	3.85	$4.95e-04$	1.81
	2^6	$2.11e-08$	3.93	$1.37e-04$	1.85
	2^7	$1.35e-09$	3.97	$3.69e-05$	1.89

TABLE 4.4: (Example 4.1) Absolute error at grid point

x	Scheme (4.24)	NSGD [143]	GD [143]	CSS [142]	CSGD [141]
0.125	$4.50e-06$	$3.05e-05$	$8.36e-05$	$1.73e-04$	$2.00e-03$
0.250	$9.64e-06$	$5.80e-05$	$1.59e-04$	$5.35e-04$	$4.08e-03$
0.375	$1.54e-05$	$7.31e-05$	$2.09e-04$	$7.98e-04$	$5.83e-03$
0.500	$2.00e-05$	$6.24e-05$	$2.01e-04$	$6.74e-04$	$6.85e-03$
0.625	$2.18e-05$	$1.60e-05$	$1.34e-04$	$9.50e-05$	$6.81e-03$
0.750	$1.97e-05$	$6.18e-05$	$1.12e-05$	$1.78e-03$	$5.57e-03$
0.875	$1.26e-05$	$1.51e-04$	$7.81e-05$	$3.42e-03$	$3.26e-03$

Example 4.2. [109, 143] Consider the Bagley-Torvik equation

$$u''(x) + \theta \left[{}^C_0 D_x^\gamma u(x) \right] = -1 - e^{x-1}$$

with $u(0) = 0 = u(1)$. The exact solution is not known for general values of γ , but for $\theta = -1$ and $\gamma = 1$ the exact solution is known to be $u(x) = x(1 - e^{x-1})$.

Let $h_c = \frac{1}{\sqrt{2}}h$ and $M = 64$. We apply (4.24) to compute the solutions for $\gamma = 0.1, 0.3, \dots, 1.9$. The solution plots for different values of γ given in Figure 4.3 show that as $\gamma \rightarrow 1$, the solutions of the γ order fractional differential equations approach to the exact solution for $\gamma = 1$. This observation matches the general expectation and hence serves as an assurance of the efficacy of the numerical scheme (4.24).

FIGURE 4.3: (Example 4.2) Numerical solutions by (4.24) for different values of γ

Example 4.3. [143] Consider the Bagley-Torvik equation

$$u''(x) + {}^C_0D_x^\gamma u(x) = g(x) + x^{1-\gamma}p(x),$$

with $u(0) = 0 = u(1)$, where $g(x) = 20x^3 - \frac{174}{5}x^2 + \frac{456}{25}x - \frac{339}{125}$ and $p(x) = \frac{120}{\Gamma(6-\gamma)}x^4 - \frac{348}{5\Gamma(5-\gamma)}x^3 + \frac{456}{25\Gamma(4-\gamma)}x^2 - \frac{339}{125\Gamma(3-\gamma)}x + \frac{27}{125\Gamma(2-\gamma)}$. The exact solution is $u(x) = x^5 - \frac{29}{10}x^4 + \frac{76}{25}x^3 - \frac{339}{250}x^2 + \frac{27}{125}x$.

Here, we fix $h_c = \frac{1}{\sqrt{2}}h$ and $M = 10$. In Table 4.5, we present the absolute errors computed by (4.24) and NSGD method [143] for the case $\gamma = 0.5$. It is observed that the scheme (4.24) gives smaller absolute errors at all grid points.

For visualization, in Figure 4.4 we plot the numerical solutions obtained from (4.24) (with $M = 64$) and the exact solution for the case $\gamma = 0.5$. The plots indicate good approximation of the exact solution at grid points.

TABLE 4.5: (Example 4.3) Absolute error at grid point

x	Scheme (4.24)	NSGD [143]
0.1	$1.05e-05$	$2.00e-03$
0.2	$3.21e-05$	$1.74e-03$
0.3	$6.79e-05$	$1.53e-03$
0.4	$7.17e-05$	$1.32e-03$
0.5	$6.19e-05$	$1.11e-03$
0.6	$4.75e-05$	$8.92e-04$
0.7	$3.21e-05$	$6.53e-04$
0.8	$1.81e-05$	$4.19e-04$
0.9	$7.01e-06$	$2.02e-04$

FIGURE 4.4: (Example 4.3) Numerical solution by (4.24) and exact solution when $\gamma = 0.5$

Example 4.4. [109] Consider the following Bagley-Torvik equation

$$u''(x) + \frac{8}{17} [{}_0^C D_x^{1.5} u(x)] + \frac{13}{51} u(x) = \frac{x^{-\frac{1}{2}}}{89250\sqrt{\pi}} [48p(x) + 7\sqrt{x}q(x)]$$

with $u(0) = 0 = u(1)$, where $p(x) = 16000x^4 - 32480x^3 + 21280x^2 - 4746x + 189$ and $q(x) = 3250x^5 - 9425x^4 + 264880x^3 - 448107x^2 + 233262x - 34578$. The exact solution is $u(x) = x^5 - \frac{29}{10}x^4 + \frac{76}{25}x^3 - \frac{339}{250}x^2 + \frac{27}{125}x$.

Here, we fix $h_c = \frac{1}{\sqrt{2}}h$ and $M = 10$. In Table 4.6, we present the absolute errors obtained by the scheme (4.24) and the method in [109]. Note that the method in [109] is based on the Haar wavelet operational matrices of integration and m^*

is the number of Haar wavelets used. The accuracy of this method has not been theoretically established in [109]. We observe that (4.24) attains smaller absolute errors at more than half of the grid points.

TABLE 4.6: (Example 4.4) Absolute error at grid point

x	Scheme (4.24)	Method [109] ($m^* = 8$)
0.1	$3.15e - 03$	$3.59e - 03$
0.2	$4.04e - 03$	$1.58e - 03$
0.3	$4.12e - 04$	$1.79e - 03$
0.4	$1.30e - 04$	$1.63e - 03$
0.5	$1.37e - 03$	$1.16e - 03$
0.6	$1.59e - 04$	$5.84e - 04$
0.7	$2.52e - 05$	$1.27e - 04$
0.8	$5.67e - 04$	$1.19e - 04$
0.9	$3.58e - 04$	$5.54e - 04$

Remark 4.6. In Theorem 4.4, the condition (4.37) is proposed so that the numerical scheme has a unique solution and is convergent. If this condition is not satisfied, we cannot guarantee the unique solvability and convergence of our scheme. The condition $U(x) \in C^{(6)}[0, 1]$ arises from spline method, while the conditions $U_e(x) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+4}(\mathcal{R})$ and $U^{(k)}(0) = 0$, $k = 0, 1$ arise from approximation of fractional derivative. If any of these conditions are not satisfied, the convergence order may be influenced and reduced.

- Cases (ii)-(v) of Example 4.1 do not satisfy the condition (4.37). But our method can still give unique numerical solution with small maximum absolute errors.
- The condition (4.37) is not satisfied by Example 4.2. From Figure 4.3, we observe that our scheme can be solved uniquely for fractional orders $\gamma = 0.1, 0.3, \dots, 1.9$; moreover as $\gamma \rightarrow 1$, the solutions of the γ order fractional differential equations approach the exact solution for $\gamma = 1$.
- Example 4.3 and Example 4.4 both do not satisfy the condition $U^{(1)}(0) = 0$. However, from Table 4.5 and Table 4.6, the maximum absolute errors of our numerical scheme are still smaller than existing methods. This indicates that our method can still give a good approximation even when the theoretical conditions are not entirely satisfied.

4.5 Summary

In this chapter, we consider the numerical treatment of the fractional Bagley-Torvik equation with fractional order $\gamma \in (0, 2)$. In our discussion, we derive a new 4-WSGD approximation for the Riemann-Liouville fractional derivative and extend the formula to the Caputo fractional derivative. Coupling with the discrete cubic spline operator, we derive at the numerical scheme (4.24). In tackling the convergence analysis, we generalize some previous work and obtain upper bounds for the Grünwald-Letnikov weight and its sum. Our scheme (4.24) is proved to be a fourth order method. Four numerical examples are presented to illustrate the efficiency of the scheme and to compare with other methods in the literature.

Part II

Partial Differential Equation

Chapter 5

New Generalized Fractional Diffusion Equation I

As we all know, there are different types of fractional derivatives in the literature, the most famous of them are the Riemann-Liouville and the Caputo fractional derivatives [38]. To unify the various types of fractional derivatives, Agrawal [4] has proposed a new *generalized fractional derivative*. The new generalization features a *scale function* $\mathcal{Z}(t)$ and a *weight function* $\mathcal{W}(t)$. By choosing specific scale and weight functions, the generalized fractional derivative will reduce to known fractional derivatives in the literature – as an example when $\mathcal{Z}(t) = t$ and $\mathcal{W}(t) = 1$, the generalized fractional derivative is simply the Caputo fractional derivative. Besides the purpose of unification, the scale function and the weight function have practical applications. The scale function $\mathcal{Z}(t)$ can stretch or contract the time domain, this helps to capture the phenomena over a desired range of time, which could be within micro/nano-seconds, or over several decades. Meanwhile, the weight function $\mathcal{W}(t)$ allows an event to be weighed differently at different time points, for example in the modelling of the memory of a person, a child may require a heavy weight at current time point, whereas a senior may require more weight on the past.

As one would expect, it is difficult to obtain analytical solutions of equations involving generalized fractional derivatives, and numerical treatment is more appropriate for such problems. In [132–134], Xu et al. have proposed numerical schemes for the generalized fractional Burgers equation, the generalized fractional diffusion equation and the generalized fractional advection-diffusion equation respectively. They

have used a simple quadrature formula to approximate the generalized Caputo fractional derivative, and the approximation is observed to have a order of $(2 - \gamma)$ through numerical experiments ($0 < \gamma < 1$ is the fractional order). In this chapter, we aim to derive a more accurate approximation of *order 3* for the generalized fractional derivative. As an application, we will apply the new approximation in the numerical treatment of a generalized fractional diffusion problem. The stability and convergence of the proposed numerical scheme will be proved rigorously using energy method and further demonstrated through numerical experiments.

We draw our inspiration from the Grünwald-Letnikov formula which is an efficient approach to approximate the classical Riemann-Liouville fractional derivative. In fact, Yuste and Acedo [138, 139] have applied a first order weighted Grünwald-Letnikov formula to approximate the fractional derivative and solve some fractional diffusion equations. In [35, 36], once again the first order weighted Grünwald-Letnikov formula, coupled with compact finite difference method, has been used to solve one-dimensional and two-dimensional fractional diffusion equations. Later, Tian et al. [125] have presented a second order weighted shifted Grünwald-Letnikov formula, while Ji and Sun [57] have presented a third order formula.

Upon getting the new approximation for the generalized fractional derivative, we shall apply it to obtain an efficient numerical scheme for the following generalized fractional diffusion problem which has also been considered in [133],

$$\begin{cases} {}^C_0D_{t;[\mathcal{Z}(t),\mathcal{W}(t)]}^\gamma V(x,t) = d \frac{\partial^2 V(x,t)}{\partial x^2} + g(x,t), & (x,t) \in [a,b] \times [0,T], \\ V(x,0) = V_0(x), & x \in [a,b], \\ V(a,t) = \zeta_1(t), \quad V(b,t) = \zeta_2(t), & t \in [0,T], \end{cases} \quad (5.1)$$

where $0 < \gamma < 1$ is the fractional order, $d > 0$ is the diffusion coefficient, $g(x,t)$, $V_0(x)$, $\zeta_1(t)$ and $\zeta_2(t)$ are continuous functions, and the *generalized Caputo fractional derivative* ${}^C_0D_{t;[\mathcal{Z}(t),\mathcal{W}(t)]}^\gamma V(x,t)$ with scale function $\mathcal{Z}(t)$ and weight function $\mathcal{W}(t)$ is defined in (2.26)

$${}^C_0D_{t;[\mathcal{Z}(t),\mathcal{W}(t)]}^\gamma V(x,t) = \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(1-\gamma)} \int_0^t \frac{1}{[\mathcal{Z}(t) - \mathcal{Z}(s)]^\gamma} \frac{\partial [\mathcal{W}(s)V(x,s)]}{\partial s} ds. \quad (5.2)$$

Let $u(x, t) = \mathcal{W}(t)V(x, t) - \mathcal{W}(0)V_0(x)$. It is easy to see that (5.1) can be transformed into the following equivalent problem, which has the same scale function $\mathcal{Z}(t)$ and unity weight function

$$\begin{cases} {}^C_0D_{t;[\mathcal{Z}(t),1]}^\gamma u(x, t) = d \frac{\partial^2 u(x, t)}{\partial x^2} + f(x, t), & (x, t) \in [a, b] \times [0, T], \\ u(x, 0) = 0, & x \in [a, b], \\ u(a, t) = \phi_1(t), \quad u(b, t) = \phi_2(t), & t \in [0, T], \end{cases} \quad (5.3)$$

where $\phi_1(t) = \mathcal{W}(t)\zeta_1(t) - \mathcal{W}(0)V_0(a)$, $\phi_2(t) = \mathcal{W}(t)\zeta_2(t) - \mathcal{W}(0)V_0(b)$ and $f(x, t) = d\mathcal{W}(0)V_0''(x) + \mathcal{W}(t)g(x, t)$. Our numerical scheme will be developed for the equivalent problem (5.3). The numerical solution of the original problem (5.1) can easily be computed from the relation $u(x, t) = \mathcal{W}(t)V(x, t) - \mathcal{W}(0)V_0(x)$.

The plan of this chapter is as follows. In Section 5.1, we derive a new approximation for the generalized fractional derivative and develop a numerical scheme for the equivalent problem (5.3). The stability and convergence of the numerical scheme is proved by energy method in Section 5.2. In Section 5.3, we present three numerical examples to verify our theoretical results. Finally, a conclusion is given in Section 5.4.

5.1 Numerical Scheme

In this section, we shall develop a numerical scheme for the equivalent problem (5.3). The discussion has 3 parts: (i) the derivation of a new approximation for the generalized fractional derivative; (ii) the consideration at the first time point; (iii) the final formulation of the numerical scheme.

Throughout, the scale function $\mathcal{Z}(t)$ is assumed to be strictly increasing. Let $\mathcal{Z} : t \rightarrow \mathcal{Z}(t)$ be a mapping from $[0, T]$ to $[\mathcal{Z}(0), \mathcal{Z}(T)]$.

Let P be a uniform partition of the spatial interval $[a, b]$ defined in (2.1) and let

$$P' : 0 = t_0 < t_1 < \cdots < t_N = T$$

be a mesh of the temporal interval $[0, T]$ such that $\tau_z \equiv \mathcal{Z}(t_n) - \mathcal{Z}(t_{n-1})$, $1 \leq n \leq N$ is a constant. Obviously, $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{N}$.

For any given function $y(x, t)$, we denote $y(x_m, t_n)$ by y_m^n and $y(x_m, t)$ by y_m for fixed t . Let $C^{(\ell, r)}([a, b] \times [0, T])$ be a space of functions $\{y(x, t)\}$ such that the derivatives $D_x^i D_t^j y(x, t)$, $i = 0, 1, \dots, \ell$, $j = 0, 1, \dots, r$ are continuous in $[a, b] \times [0, T]$. Moreover, denote $\mathcal{U}_P = \{y = (y_0, y_1, \dots, y_M) \mid y_0 = y_M = 0\}$. For any $y, \hat{y} \in \mathcal{U}_P$, we define

$$\delta_x y_{m+\frac{1}{2}} = \frac{1}{h} (y_{m+1} - y_m), \quad \delta_x^2 y_m = \frac{1}{h} \left(\delta_x y_{m+\frac{1}{2}} - \delta_x y_{m-\frac{1}{2}} \right), \quad (5.4)$$

and

$$(y, \hat{y}) = h \sum_{m=1}^{M-1} y_m \hat{y}_m, \quad (y, \hat{y})_1 = h \sum_{m=0}^{M-1} \left(\delta_x y_{m+\frac{1}{2}} \right) \left(\delta_x \hat{y}_{m+\frac{1}{2}} \right) \quad (5.5)$$

$$\|y\| = \sqrt{(y, y)}, \quad |y|_1 = \sqrt{(y, y)_1}, \quad \|y\|_\infty = \max_{1 \leq m \leq M-1} |y_m|. \quad (5.6)$$

Motivated by Lemma 2.4, we shall now develop a third order approximation for the *generalized Riemann-Liouville fractional derivative*. For this purpose, we write

$$u(x, t) = u(x, \mathcal{Z}^{-1}(z)) \equiv \tilde{u}(x, z), \quad \mathcal{W}(t) = \mathcal{W}(\mathcal{Z}^{-1}(z)) \equiv \tilde{\mathcal{W}}(z), \quad (5.7)$$

and extend the function $\tilde{u}$ as follows:

$$\tilde{u}_e(x, z) = \begin{cases} 0, & z < \mathcal{Z}(0), \\ \tilde{u}(x, z), & \mathcal{Z}(0) \leq z \leq \mathcal{Z}(T), \\ \psi(z), & \mathcal{Z}(T) < z \leq 2\mathcal{Z}(T), \\ 0, & z > 2\mathcal{Z}(T), \end{cases} \quad (5.8)$$

where $\psi(z)$ is a smooth function that can be determined later. The third order approximation for the *generalized Riemann-Liouville fractional derivative* is given in the next result.

Theorem 5.1. *Let $0 < \gamma < 1$. Suppose that $u(\cdot, \mathcal{Z}^{-1}(z)) \equiv \tilde{u}(\cdot, z) \in C^{(5)}[\mathcal{Z}(0), \mathcal{Z}(T)]$ and $\left. \frac{\partial^k}{\partial z^k} \tilde{u} \right|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1, 2, 3, 4, 5$. Define the generalized weighted shifted*

Grünwald-Letnikov difference (*gWSGD*) operator $\mathcal{G}_{\tau_z}^\gamma$ by

$$\mathcal{G}_{\tau_z}^\gamma u(x_m, t_n) = \mathfrak{S}_1 \mathcal{J}_{\tau_z, l}^\gamma u_m^n + \mathfrak{S}_2 \mathcal{J}_{\tau_z, \bar{l}}^\gamma u_m^n + \mathfrak{S}_3 \mathcal{J}_{\tau_z, \hat{l}}^\gamma u_m^n, \quad (5.9)$$

where $l, \bar{l}, \hat{l}$ are integers, $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{N}$ is the step size, $\mathfrak{S}_1, \mathfrak{S}_2, \mathfrak{S}_3$ are given in (2.32), and

$$\mathcal{J}_{\tau_z, l}^\gamma u_m^n = \frac{1}{\tau_z^\gamma} \sum_{k=0}^{n+l} g_k^\gamma u_m^{n-k+l} \quad (5.10)$$

(similar definitions for $\mathcal{J}_{\tau_z, \bar{l}}^\gamma u_m^n$ and $\mathcal{J}_{\tau_z, \hat{l}}^\gamma u_m^n$). Then, the generalized Riemann-Liouville fractional derivative with unity weight function has the following approximation:

$${}^{RL}_0 D_{t; [z(t), 1]}^\gamma u(x_m, t_n) = \mathcal{G}_{\tau_z}^\gamma u(x_m, t_n) + O(\tau_z^3). \quad (5.11)$$

Proof. In view of the assumptions, we can choose a function $\psi(z)$ such that $\tilde{u}_e(\cdot, z) \in C^{(5)}(\mathcal{R})$. In fact, we can apply Hermite interpolation to get a $\psi(z)$ that ensures the continuity at $z = \mathcal{Z}(T)$ and $z = 2\mathcal{Z}(T)$. Using Lemma 4.1, we have $\tilde{u}_e(\cdot, z) \in \mathcal{C}^{\gamma+3}(\mathcal{R})$. Also, it is obvious that $\tilde{u}_e(\cdot, z) \in L^1(\mathcal{R})$. Thus, $\tilde{u}_e(\cdot, z) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+3}(\mathcal{R})$.

Denote $\mathcal{Z}(t_n)$ by z_n . Clearly,

$$P'' : \mathcal{Z}(0) = z_0 < z_1 < \cdots < z_N = \mathcal{Z}(T) \quad (5.12)$$

is the uniform partition of $[\mathcal{Z}(0), \mathcal{Z}(T)]$ with step size $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{N}$. Hence, we can apply Lemma 2.4 to get

$$\begin{aligned} & {}^{RL}_{-\infty} D_z^\gamma \tilde{u}_e(x_m, z_n) \\ &= \mathfrak{S}_1 \mathcal{J}_{\tau_z, l}^\gamma \tilde{u}_e(x_m, z_n) + \mathfrak{S}_2 \mathcal{J}_{\tau_z, \bar{l}}^\gamma \tilde{u}_e(x_m, z_n) + \mathfrak{S}_3 \mathcal{J}_{\tau_z, \hat{l}}^\gamma \tilde{u}_e(x_m, z_n) + O(\tau_z^3), \end{aligned} \quad (5.13)$$

where

$$\mathcal{J}_{\tau_z, l}^\gamma \tilde{u}_e(x_m, z_n) = \frac{1}{\tau_z^\gamma} \sum_{k=0}^{n+l} g_k^\gamma \tilde{u}(x_m, z_{n-k+l}) = \frac{1}{\tau_z^\gamma} \sum_{k=0}^{n+l} g_k^\gamma u(x_m, t_{n-k+l}) = \mathcal{J}_{\tau_z, l}^\gamma u_m^n. \quad (5.14)$$

It follows from (5.13) and (5.14) that

$$\begin{aligned} {}^{RL}_{-\infty}D_z^\gamma \tilde{u}_e(x_m, z_n) &= \mathfrak{S}_1 \mathcal{J}_{\tau_z, l}^\gamma u_m^n + \mathfrak{S}_2 \mathcal{J}_{\tau_z, \hat{l}}^\gamma u_m^n + \mathfrak{S}_3 \mathcal{J}_{\tau_z, \bar{l}}^\gamma u_m^n + O(\tau_z^3) \\ &= \mathcal{G}_{\tau_z}^\gamma u(x_m, t_n) + O(\tau_z^3). \end{aligned} \quad (5.15)$$

Next, we shall show that ${}^{RL}_{-\infty}D_z^\gamma \tilde{u}_e(x_m, z_n) = {}^{RL}_0D_{t;[\mathcal{Z}(t), 1]}^\gamma u(x_m, t_n)$. Since $\tilde{u}_e(x, z) = 0$ for $z < \mathcal{Z}(0)$, we have for $z \geq \mathcal{Z}(0)$, noting Definition 2.6,

$${}^{RL}_{-\infty}D_z^\gamma \tilde{u}_e(x_m, z) = {}^{RL}_{z_0}D_z^\gamma \tilde{u}(x_m, z) = \frac{1}{\Gamma(1-\gamma)} \frac{d}{dz} \left[\int_{z_0}^z \frac{\tilde{u}(x_m, y)}{(z-y)^\gamma} dy \right]. \quad (5.16)$$

Using the transformation $y = \mathcal{Z}(s)$ and noting that $z = \mathcal{Z}(t)$ and $\tilde{u}(x, \mathcal{Z}(t)) = u(x, t)$, we further get

$$\begin{aligned} {}^{RL}_{z_0}D_z^\gamma \tilde{u}(x_m, z) &= \frac{1}{\Gamma(1-\gamma)} \frac{d}{dt} \left[\int_{z_0}^{\mathcal{Z}(t)} \frac{\tilde{u}(x_m, \mathcal{Z}(s))}{[\mathcal{Z}(t) - \mathcal{Z}(s)]^\gamma} d\mathcal{Z}(s) \right] \frac{dt}{d\mathcal{Z}(t)} \\ &= \frac{1}{\Gamma(1-\gamma)} \frac{d}{dt} \left[\int_0^t \frac{u(x_m, s)}{[\mathcal{Z}(t) - \mathcal{Z}(s)]^\gamma} \mathcal{Z}'(s) ds \right] \frac{1}{\mathcal{Z}'(t)} \\ &= \frac{1}{\Gamma(1-\gamma)} \frac{1}{\mathcal{Z}'(t)} \frac{d}{dt} \left[\int_0^t \frac{u(x_m, s)}{[\mathcal{Z}(t) - \mathcal{Z}(s)]^\gamma} \mathcal{Z}'(s) ds \right] \\ &= {}^{RL}_0D_{t;[\mathcal{Z}(t), 1]}^\gamma u(x_m, t), \end{aligned} \quad (5.17)$$

where we have used Definition 2.8 in the last equality. It follows from (5.16) and (5.17) that

$${}^{RL}_{-\infty}D_z^\gamma \tilde{u}_e(x_m, z_n) = {}^{RL}_0D_{t;[\mathcal{Z}(t), 1]}^\gamma u(x_m, t_n). \quad (5.18)$$

Hence, in view of (5.18) and (5.15), we immediately obtain the approximation (5.11). ■

Remark 5.1. The conditions in Theorem 5.1, namely, $u(\cdot, \mathcal{Z}^{-1}(z)) \equiv \tilde{u}(\cdot, z) \in C^{(5)}[\mathcal{Z}(0), \mathcal{Z}(T)]$ and $\frac{\partial^k}{\partial z^k} \tilde{u} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1, 2, 3, 4, 5$, can be replaced by the weaker condition $\tilde{u}_e(\cdot, z) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+3}(\mathcal{R})$, which is needed for us to apply Lemma 2.4.

Remark 5.2. Due to the symmetry of l , $\bar{l}$ and $\hat{l}$, we can assume that $l > \hat{l} > \bar{l}$. To compute u in consecutive time steps $t_1, t_2, \dots$, it is necessary to take $(l, \hat{l}, \bar{l}) = (0, -1, -2)$ in Theorem 5.1. We notice from the expression (5.10) that for $\mathcal{J}_{\tau_z, -2}^\gamma u_m^n$

to make sense, we require $n \geq 2$. The gWSGD operator (5.9) can then be written as

$$\mathcal{G}_{\tau_z}^\gamma u(x_m, t_n) = \frac{1}{\tau_z^\gamma} \sum_{k=0}^n \omega_k^\gamma u_m^{n-k}, \quad n \geq 2, \quad (5.19)$$

where

$$\begin{cases} \omega_0^\gamma = \mathfrak{S}_1 g_0^\gamma, \\ \omega_1^\gamma = \mathfrak{S}_1 g_1^\gamma + \mathfrak{S}_2 g_0^\gamma, \\ \omega_k^\gamma = \mathfrak{S}_1 g_k^\gamma + \mathfrak{S}_2 g_{k-1}^\gamma + \mathfrak{S}_3 g_{k-2}^\gamma, \quad k \geq 2. \end{cases} \quad (5.20)$$

Next, we shall derive the relation between the generalized Caputo fractional derivative (2.21) and the generalized Riemann-Liouville fractional derivative (2.22).

Theorem 5.2. *Let $0 < \gamma < 1$. Suppose $u(x, t)$ is sufficiently smooth as a function of t . We have the relation*

$${}^{RL}_0 D_{t;[\mathcal{Z}(t), \mathcal{W}(t)]}^\gamma u(x, t) = \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(1-\gamma)} \frac{\mathcal{W}(0)u(x, 0)}{[\mathcal{Z}(t) - \mathcal{Z}(0)]^\gamma} + {}^C_0 D_{t;[\mathcal{Z}(t), \mathcal{W}(t)]}^\gamma u(x, t). \quad (5.21)$$

Proof. Using Definition 2.8, we write

$$\begin{aligned} & {}^{RL}_0 D_{t;[\mathcal{Z}(t), \mathcal{W}(t)]}^\gamma u(x, t) \\ &= \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(1-\gamma)} \frac{1}{\mathcal{Z}'(t)} \frac{\partial}{\partial t} \left[\int_0^t \frac{\mathcal{W}(s) \mathcal{Z}'(s) u(x, s)}{[\mathcal{Z}(t) - \mathcal{Z}(s)]^\gamma} ds \right] \\ &= \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(1-\gamma)} \frac{1}{\mathcal{Z}'(t)} \frac{\partial}{\partial t} \left[- \int_0^t \mathcal{W}(s) u(x, s) d \left(\frac{[\mathcal{Z}(t) - \mathcal{Z}(s)]^{1-\gamma}}{1-\gamma} \right) \right]. \end{aligned} \quad (5.22)$$

Applying integration by parts, we have

$$\begin{aligned} & - \int_0^t \mathcal{W}(s) u(x, s) d \left(\frac{[\mathcal{Z}(t) - \mathcal{Z}(s)]^{1-\gamma}}{1-\gamma} \right) \\ &= - \mathcal{W}(s) u(x, s) \frac{[\mathcal{Z}(t) - \mathcal{Z}(s)]^{1-\gamma}}{1-\gamma} \Big|_0^t + \int_0^t \frac{\partial(\mathcal{W}(s) u(x, s))}{\partial s} \frac{[\mathcal{Z}(t) - \mathcal{Z}(s)]^{1-\gamma}}{1-\gamma} ds \\ &= \mathcal{W}(0) u(x, 0) \frac{[\mathcal{Z}(t) - \mathcal{Z}(0)]^{1-\gamma}}{1-\gamma} + \int_0^t \frac{\partial(\mathcal{W}(s) u(x, s))}{\partial s} \frac{[\mathcal{Z}(t) - \mathcal{Z}(s)]^{1-\gamma}}{1-\gamma} ds, \end{aligned}$$

which, upon differentiating with respect to t , yields

$$\begin{aligned} & \frac{\partial}{\partial t} \left[- \int_0^t \mathcal{W}(s) u(x, s) d \left(\frac{[\mathcal{Z}(t) - \mathcal{Z}(s)]^{1-\gamma}}{1-\gamma} \right) \right] \\ &= \frac{\mathcal{W}(0) u(x, 0)}{[\mathcal{Z}(t) - \mathcal{Z}(0)]^\gamma} \mathcal{Z}'(t) + \mathcal{Z}'(t) \int_0^t \frac{1}{[\mathcal{Z}(t) - \mathcal{Z}(s)]^\gamma} \frac{\partial(\mathcal{W}(s) u(x, s))}{\partial s} ds. \end{aligned} \quad (5.23)$$

Now, substituting (5.23) into (5.22) and noting the definition of the generalized Caputo fractional derivative (2.26), we obtain the relation (5.21) immediately. ■

Remark 5.3. If $u(x, 0) = 0$, then Theorem 5.2 leads to the *equality* of the generalized Riemann-Liouville and the generalized Caputo fractional derivatives.

Noting $u(x, 0) = u(x, \mathcal{Z}(0))$, we see that the conditions of Theorem 5.1 actually include the condition $u(x, 0) = 0$. Hence, by Remark 5.3, the approximation (5.11) is also applicable to the generalized *Caputo* fractional derivative. In view of (5.19), we have the following corollary.

Corollary 5.1. (Third order approximation) Let $0 < \gamma < 1$. Suppose that $u(\cdot, \mathcal{Z}^{-1}(z)) \equiv \tilde{u}(\cdot, z) \in C^{(5)}[\mathcal{Z}(0), \mathcal{Z}(T)]$ and $\frac{\partial^k}{\partial z^k} \tilde{u} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1, 2, 3, 4, 5$. Then, the generalized Caputo fractional derivative with unity weight function has the following approximation:

$${}_0^C D_{t; [\mathcal{Z}(t), 1]}^\gamma u(x_m, t_n) = \frac{1}{\tau_z^\gamma} \sum_{k=0}^n \omega_k^\gamma u_m^{n-k} + O(\tau_z^3), \quad n \geq 2, \quad (5.24)$$

where ω_k^γ is given in (5.20).

Remark 5.4. In view of Remarks 5.1 and 5.3, the conditions in Corollary 5.1 can be replaced by the *weaker* conditions $u(x, 0) = 0$ and $\tilde{u}_e(\cdot, z) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+3}(\mathcal{R})$.

It is obvious that the approximation (5.24) is applicable for $n \geq 2$. To handle the generalized Caputo fractional derivative at $t = t_1$, we shall make use of the *generalized Riemann-Liouville fractional integral*.

Lemma 5.1. [57] Let $0 < \gamma < 1$ and $x \in (a, b)$ be fixed. If $u(x, 0) = 0$, then we have

$${}^{RL}_0 I_t^\gamma [{}_0^C D_t^\gamma u(x, t)] = u(x, t). \quad (5.25)$$

We shall now establish the relationship between the generalized Caputo fractional derivative and the generalized Riemann-Liouville fractional integral. This result is a ‘generalized’ analog of Lemma 5.1.

Theorem 5.3. *Let $0 < \gamma < 1$ and $x \in (a, b)$ be fixed. If $u(x, 0) = 0$, then we have*

$${}^{RL}I_{t;[\mathcal{Z}(t), \mathcal{W}(t)]}^\gamma \left[{}^CD_{t;[\mathcal{Z}(t), \mathcal{W}(t)]}^\gamma u(x, t) \right] = u(x, t). \quad (5.26)$$

Proof. Recall from (5.7) that $u(x, t) \equiv \tilde{u}(x, \mathcal{Z}(t))$ and $\mathcal{W}(t) \equiv \mathcal{W}(\mathcal{Z}(t))$. We find, using the Definition 2.9 and Definition 2.8,

$$\begin{aligned} & {}^CD_{t;[\mathcal{Z}(t), \mathcal{W}(t)]}^\gamma u(x, t) \\ &= \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(1-\gamma)} \int_0^t \frac{1}{[\mathcal{Z}(t) - \mathcal{Z}(s)]^\gamma} \frac{\partial[\mathcal{W}(s)u(x, s)]}{\partial s} ds \\ &= \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(1-\gamma)} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t)} \frac{1}{[\mathcal{Z}(t) - \mathcal{Z}(s)]^\gamma} \frac{\partial[\mathcal{W}(\mathcal{Z}(s))\tilde{u}(x, \mathcal{Z}(s))]}{\partial s} \frac{d\mathcal{Z}(s)}{\mathcal{Z}'(s)} \\ &= \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(1-\gamma)} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t)} \frac{1}{[\mathcal{Z}(t) - \mathcal{Z}(s)]^\gamma} \frac{\partial[\mathcal{W}(\mathcal{Z}(s))\tilde{u}(x, \mathcal{Z}(s))]}{\partial z} d\mathcal{Z}(s). \\ &= [\mathcal{W}(t)]^{-1} {}^CD_{z_0}^\gamma [\mathcal{W}(\mathcal{Z}(t))\tilde{u}(x, \mathcal{Z}(t))]. \end{aligned} \quad (5.27)$$

It now follows from (5.27) and Definitions 2.4 and 2.5 that

$$\begin{aligned} & {}^{RL}I_{t;[\mathcal{Z}(t), \mathcal{W}(t)]}^\gamma \left[{}^CD_{t;[\mathcal{Z}(t), \mathcal{W}(t)]}^\gamma u(x, t) \right] \\ &= {}^{RL}I_{t;[\mathcal{Z}(t), \mathcal{W}(t)]}^\gamma \left\{ [\mathcal{W}(t)]^{-1} {}^CD_{z_0}^\gamma [\mathcal{W}(\mathcal{Z}(t))\tilde{u}(x, \mathcal{Z}(t))] \right\} \\ &= \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(\gamma)} \int_0^t \frac{\mathcal{Z}'(s) \left\{ {}^CD_{z_0}^\gamma [\mathcal{W}(\mathcal{Z}(s))\tilde{u}(x, \mathcal{Z}(s))] \right\}}{[\mathcal{Z}(t) - \mathcal{Z}(s)]^{1-\gamma}} ds \\ &= \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(\gamma)} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t)} \frac{{}^CD_{z_0}^\gamma [\mathcal{W}(\mathcal{Z}(s))\tilde{u}(x, \mathcal{Z}(s))]}{[\mathcal{Z}(t) - \mathcal{Z}(s)]^{1-\gamma}} d\mathcal{Z}(s) \\ &= [\mathcal{W}(t)]^{-1} {}^{RL}I_{z_0}^\gamma \left\{ {}^CD_{z_0}^\gamma [\mathcal{W}(\mathcal{Z}(t))\tilde{u}(x, \mathcal{Z}(t))] \right\}. \end{aligned} \quad (5.28)$$

Since $u(x, 0) = \tilde{u}(x, z_0) = 0$, we have $\mathcal{W}(z_0)\tilde{u}(x, z_0) = 0$. Hence, it is immediate from Lemma 5.1 that

$${}^{RL}I_{z_0}^\gamma \left\{ {}^CD_{z_0}^\gamma [\mathcal{W}(\mathcal{Z}(t))\tilde{u}(x, \mathcal{Z}(t))] \right\} = \mathcal{W}(\mathcal{Z}(t))\tilde{u}(x, \mathcal{Z}(t)) = \mathcal{W}(t)u(x, t). \quad (5.29)$$

Now, substituting (5.29) in (5.28) gives the relation (5.26) immediately. ■

The next result gives an approximation for the generalized Riemann-Liouville fractional integral of u_{xx} at $t = t_1$.

Theorem 5.4. *Let $0 < \gamma < 1$. Suppose that $\tilde{u}(x, z) \in C^{(2,3)}([a, b] \times [\mathcal{Z}(0), \mathcal{Z}(t_1)])$ and $\frac{\partial^k}{\partial z^k} \tilde{u} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1$. Then, we have*

$$\left| {}^{RL}_0 I_{t;[\mathcal{Z}(t),1]}^\gamma u_{xx}(x, t_1) - \frac{2}{\Gamma(\gamma+3)} \tau_z^\gamma u_{xx}(x, t_1) \right| \leq \frac{2C_2}{81\Gamma(\gamma+1)} \tau_z^{3+\gamma} = O(\tau_z^{3+\gamma}), \quad (5.30)$$

where $C_2 = \max_{(x,z) \in [a,b] \times [\mathcal{Z}(0), \mathcal{Z}(t_1)]} |\tilde{u}_{xxzzz}(x, z)|$.

Proof. By Definition 2.5, we have

$$\begin{aligned} {}^{RL}_0 I_{t;[\mathcal{Z}(t),1]}^\gamma u_{xx}(x, t_1) &= \frac{1}{\Gamma(\gamma)} \int_0^{t_1} \frac{u_{xx}(x, s) \mathcal{Z}'(s)}{[\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{1-\gamma}} ds \\ &= \frac{1}{\Gamma(\gamma)} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t_1)} \frac{\tilde{u}_{xx}(x, \mathcal{Z}(s))}{[\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{1-\gamma}} d\mathcal{Z}(s). \end{aligned} \quad (5.31)$$

To approximate $\tilde{u}_{xx}(x, z)$ over the interval $[\mathcal{Z}(0), \mathcal{Z}(t_1)]$, we shall use the Hermite interpolate, $H(x, z)$, of $\tilde{u}_{xx}(x, z)$ with interpolating conditions at $\tilde{u}_{xx}(x, \mathcal{Z}(0))$, $\tilde{u}_{xxz}(x, \mathcal{Z}(0))$ and $\tilde{u}_{xx}(x, \mathcal{Z}(t_1))$. In fact, the Hermite interpolate $H(x, z)$ can be expressed as

$$\begin{aligned} H(x, \mathcal{Z}(s)) &= \tilde{u}_{xx}(x, \mathcal{Z}(0)) + \tilde{u}_{xxz}(x, \mathcal{Z}(0))[\mathcal{Z}(s) - \mathcal{Z}(0)] \\ &\quad + \frac{1}{\tau_z^2} [\tilde{u}_{xx}(x, \mathcal{Z}(t_1)) - \tilde{u}_{xx}(x, \mathcal{Z}(0)) - \tau_z \tilde{u}_{xxz}(x, \mathcal{Z}(0))] [\mathcal{Z}(s) - \mathcal{Z}(0)]^2. \end{aligned} \quad (5.32)$$

The error function $\mathcal{R}(s)$ of the Hermite interpolation is given by [53]

$$\mathcal{R}(s) \equiv \tilde{u}_{xx}(x, \mathcal{Z}(s)) - H(x, \mathcal{Z}(s)) = \frac{1}{6} \tilde{u}_{xxzzz}(x, z(\eta)) [\mathcal{Z}(s) - \mathcal{Z}(0)]^2 [\mathcal{Z}(s) - \mathcal{Z}(t_1)] \quad (5.33)$$

where $\eta \in [0, t_1]$. Using $\tilde{u}(x, \mathcal{Z}(0)) = 0$, we get

$$\tilde{u}_x(x, \mathcal{Z}(0)) = \lim_{h \rightarrow 0} \frac{\tilde{u}(x+h, \mathcal{Z}(0)) - \tilde{u}(x, \mathcal{Z}(0))}{h} = 0,$$

and similarly $\tilde{u}_{xx}(x, \mathcal{Z}(0)) = 0$. Likewise, $\tilde{u}_z(x, \mathcal{Z}(0)) = 0$ leads to $\tilde{u}_{zx}(x, \mathcal{Z}(0)) = \tilde{u}_{zxx}(x, \mathcal{Z}(0)) = \tilde{u}_{xxz}(x, \mathcal{Z}(0)) = 0$. Therefore, noting (5.32) we have

$$\tilde{u}_{xx}(x, \mathcal{Z}(s)) \approx H(x, \mathcal{Z}(s)) = \frac{\tilde{u}_{xx}(x, \mathcal{Z}(t_1))}{\tau_z^2} [\mathcal{Z}(s) - \mathcal{Z}(0)]^2. \quad (5.34)$$

Upon substituting (5.34) into (5.31), we find, using the transformation $y = \frac{\mathcal{Z}(s) - \mathcal{Z}(0)}{\tau_z}$,

$$\begin{aligned} & {}^{RL}I_{t;[\mathcal{Z}(t),1]}^\gamma u_{xx}(x, t_1) \\ & \approx \frac{1}{\Gamma(\gamma)} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t_1)} \frac{H(x, \mathcal{Z}(s))}{[\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{1-\gamma}} d\mathcal{Z}(s) \\ & = \frac{1}{\Gamma(\gamma)} \frac{\tilde{u}_{xx}(x, \mathcal{Z}(t_1))}{\tau_z^2} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t_1)} [\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{\gamma-1} [\mathcal{Z}(s) - \mathcal{Z}(0)]^2 d\mathcal{Z}(s) \\ & = \frac{1}{\Gamma(\gamma)} \frac{\tilde{u}_{xx}(x, \mathcal{Z}(t_1))}{\tau_z^2} \int_0^1 (\tau_z - y\tau_z)^{\gamma-1} (y\tau_z)^2 \tau_z dy \\ & = \frac{\tilde{u}_{xx}(x, \mathcal{Z}(t_1)) \tau_z^\gamma}{\Gamma(\gamma)} \int_0^1 (1-y)^{\gamma-1} y^2 dy \\ & = \frac{2\tilde{u}_{xx}(x, \mathcal{Z}(t_1)) \tau_z^\gamma}{\Gamma(\gamma+3)} \\ & = \frac{2u_{xx}(x, t_1) \tau_z^\gamma}{\Gamma(\gamma+3)}. \end{aligned} \quad (5.35)$$

To compute the approximation error in (5.35), noting (5.33) we get

$$\begin{aligned} & \left| {}^{RL}I_{t;[\mathcal{Z}(t),1]}^\gamma u_{xx}(x, t_1) - \frac{2u_{xx}(x, t_1) \tau_z^\gamma}{\Gamma(\gamma+3)} \right| \\ & = \left| \frac{1}{\Gamma(\gamma)} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t_1)} \frac{\mathcal{R}(s)}{[\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{1-\gamma}} d\mathcal{Z}(s) \right| \\ & \leq \frac{C_2}{6\Gamma(\gamma)} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t_1)} [\mathcal{Z}(s) - \mathcal{Z}(0)]^2 [\mathcal{Z}(t_1) - \mathcal{Z}(s)] [\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{\gamma-1} d\mathcal{Z}(s) \\ & \leq \frac{2C_2 \tau_z^3}{81\Gamma(\gamma)} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t_1)} [\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{\gamma-1} d\mathcal{Z}(s) \\ & = \frac{2C_2 \tau_z^{3+\gamma}}{81\Gamma(\gamma+1)}, \end{aligned} \quad (5.36)$$

where we have used the facts $C_2 = \max_{(x,z) \in [a,b] \times [\mathcal{Z}(0), \mathcal{Z}(t_1)]} |\tilde{u}_{xxxx}(x, z)|$ and $[\mathcal{Z}(s) - \mathcal{Z}(0)]^2 [\mathcal{Z}(t_1) - \mathcal{Z}(s)] \leq \frac{4}{27} \tau_z^3$ in the above computation. This completes the proof. ■

So far we have established the third order approximation for the generalized Riemann-Liouville and the generalized Caputo fractional derivatives (Theorem 5.1 and Corollary 5.1), as well as the approximation for the generalized Riemann-Liouville fractional integral at $t = t_1$ (Theorem 5.4). The next lemma gives the approximation for the second order derivative by finite difference method. The proof is done by Taylor expansion.

Lemma 5.2. *For a fixed t_n , if $u(x, t_n) \in C^{(4)}[a, b]$, then we have*

$$\frac{\partial^2 u(x_m, t_n)}{\partial x^2} = \frac{u(x_{m-1}, t_n) - 2u(x_m, t_n) + u(x_{m+1}, t_n)}{h^2} + O(h^2) = \delta_x^2 u_m^n + O(h^2) \quad (5.37)$$

where $1 \leq m \leq M - 1$.

We have now gathered the necessary approximations to derive a numerical scheme for the equivalent problem (5.3). To begin, we discretize (5.3) at (x_m, t_n) to get

$${}_0^C D_{t; [\mathcal{Z}(t), 1]}^\gamma u(x_m, t_n) = du_{xx}(x_m, t_n) + f(x_m, t_n). \quad (5.38)$$

First, we deal with (5.38) at $t = t_1$ (as the gWSGD approximation (5.24) is applicable for $n \geq 2$), i.e.,

$${}_0^C D_{t; [\mathcal{Z}(t), 1]}^\gamma u(x_m, t_1) = du_{xx}(x_m, t_1) + f(x_m, t_1). \quad (5.39)$$

Applying the generalized Riemann-Liouville fractional integral operator on (5.39) and then using Theorems 5.3 and 5.4, we get

$$u(x_m, t_1) = \frac{2d}{\Gamma(\gamma + 3)} \tau_z^\gamma u_{xx}(x_m, t_1) + F(x_m, t_1) + O(\tau_z^{\gamma+3}), \quad (5.40)$$

where

$$F(x_m, t_1) = {}_0^{RL} I_{t; [\mathcal{Z}(t), 1]}^\gamma f(x_m, t_1). \quad (5.41)$$

Now, using Lemma 5.2 to approximate the second order derivative in (5.40) and then dividing by τ_z^γ , we obtain

$$\frac{1}{\tau_z^\gamma} u(x_m, t_1) = \frac{2d}{\Gamma(\gamma + 3)} \delta_x^2 u_m^1 + \frac{1}{\tau_z^\gamma} F(x_m, t_1) + O(\tau_z^3 + h^2). \quad (5.42)$$

Next, for the discretized equation (5.38) where $n \geq 2$, we use the gWSGD approximation (5.24) for the generalized Caputo fractional derivative and Lemma 5.2 for the second order derivative, giving

$$\frac{1}{\tau_z^\gamma} \sum_{k=0}^n \omega_k^\gamma u_m^{n-k} = d \delta_x^2 u_m^n + f_m^n + O(\tau_z^3 + h^2), \quad n \geq 2. \quad (5.43)$$

Omitting the truncation errors in (5.42) and (5.43), we finally get the following numerical scheme:

$$\left\{ \begin{array}{ll} \frac{1}{\tau_z^\gamma} u_m^1 = \frac{2d}{\Gamma(\gamma + 3)} \delta_x^2 u_m^1 + \frac{1}{\tau_z^\gamma} F(x_m, t_1), & 1 \leq m \leq M-1, \quad n=1, \\ \frac{1}{\tau_z^\gamma} \sum_{k=0}^n \omega_k^\gamma u_m^{n-k} = d \delta_x^2 u_m^n + f_m^n, & 1 \leq m \leq M-1, \quad 2 \leq n \leq N, \\ u_m^0 = 0, & 0 \leq m \leq M, \\ u_0^n = \phi_1^n, \quad u_M^n = \phi_2^n, & 1 \leq n \leq N, \end{array} \right. \quad (5.44)$$

where $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{N}$, ω_k^γ and $F(x_m, t_1)$ are given in (2.17) and (5.41) respectively.

The proposed numerical scheme (5.44) has a *unique solution* at each time level $t = t_n$, $1 \leq n \leq N$ since the coefficient matrix is easily seen to be strictly diagonally dominant. To implement the numerical scheme (5.44), we first solve for u_m^1 , $1 \leq m \leq M-1$; thereafter, we can get u_m^2 , $1 \leq m \leq M-1$. Continuing in this manner, we can obtain the numerical solution u_m^n , $1 \leq m \leq M-1$, $1 \leq n \leq N$ of the problem (5.3). The numerical solution $\{V_m^n\}$ of the original problem (5.1) is then computed from the relation $u(x, t) = \mathcal{W}(t)V(x, t) - \mathcal{W}(0)V_0(x)$.

5.2 Stability and Convergence

In this section, the stability and convergence of the numerical scheme (5.44) will be analyzed via energy method. We recall the definitions of $\|y\| = \sqrt{(y, y)}$, $|y|_1 = \sqrt{(y, y)_1}$ and $\|y\|_\infty = \max_{1 \leq m \leq M-1} |y_m|$ for $y \in \mathcal{U}_P$ (see (5.6)).

Lemma 5.3. [122] *Let $u \in \mathcal{U}_P$. Then, we have*

$$\|u\|_\infty \leq \frac{\sqrt{b-a}}{2} |u|_1, \quad \|u\| \leq \frac{b-a}{\sqrt{6}} |u|_1.$$

Lemma 5.4. [57] *Let $\gamma^* = 0.9569347$. If $\gamma \in (0, \gamma^*]$, then for any positive integer N and real vector $(u^0, u^1, \dots, u^N) \in \mathcal{R}^{N+1}$, we have*

$$\sum_{n=0}^N \left(\sum_{k=0}^n \omega_k^\gamma u^{n-k} \right) u^n \geq 0,$$

where ω_k^γ is defined in (2.17).

Lemma 5.5. [57] *Let $0 < \gamma < 1$. Then, we have*

$$10\omega_0^\gamma - 3\Gamma(\gamma + 3) > \frac{1}{3},$$

where $\omega_0^\gamma = \frac{24+17\gamma+3\gamma^2}{24}$.

We are now ready to show the stability of the numerical scheme (5.44) with respect to the initial value and the nonlinear term f .

Lemma 5.6. *Let $\{u_m^n\}$ be the solution of the following difference scheme:*

$$\left\{ \begin{array}{ll} \frac{1}{\tau_z^\gamma} \sum_{k=0}^n \omega_k^\gamma u_m^{n-k} = d\delta_x^2 u_m^n + f_m^n, & 1 \leq m \leq M-1, \quad 2 \leq n \leq N, \\ \frac{1}{\tau_z^\gamma} u_m^1 = \frac{2d}{\Gamma(\gamma+3)} \delta_x^2 u_m^1 + \frac{1}{\tau_z^\gamma} F_m^1, & 1 \leq m \leq M-1, \\ u_m^0 = \eta_m, & 0 \leq m \leq M, \\ u_0^n = 0, \quad u_M^n = 0, & 1 \leq n \leq N. \end{array} \right. \quad (5.45)$$

Suppose $\gamma \in (0, \gamma^*]$. For $1 \leq n \leq N$, we have

$$\begin{aligned} \sum_{i=1}^n |u^i|_1^2 &\leq \frac{(b-a)^2}{4d} \sum_{i=2}^n \|f^i\|^2 + \frac{1}{[\Gamma(\gamma+1)]^2} \left[\frac{\omega_0^\gamma}{2\varepsilon d} + \frac{(b-a)^2}{4d^2} \right] \|\hat{f}^1\|^2 \\ &\quad + \left[\frac{6|\omega_1^\gamma|}{\Gamma(\gamma+3)\omega_0^\gamma} + \frac{2|\omega_1^\gamma|^2}{3} \right] |u^0|_1^2, \end{aligned} \quad (5.46)$$

where $\varepsilon = \frac{d[10\omega_0^\gamma - 3\Gamma(3+\gamma)]}{\omega_0^\gamma(b-a)^2\Gamma(3+\gamma)}$ and $\hat{f}_m^1 = \max_{0 < t < t_1} |f(x_m, t)|$.

Proof. Multiplying the first equation of (5.45) by $\frac{hu_m^n}{d}$ and summing m from 1 to $(M-1)$, we obtain

$$\frac{1}{d\tau_z^\gamma} \sum_{k=0}^n \omega_k^\gamma(u^n, u^{n-k}) - (u^n, \delta_x^2 u^n) = \frac{1}{d}(u^n, f^n). \quad (5.47)$$

For the second term on the left side of equation (5.47), we have

$$-(u^n, \delta_x^2 u^n) = |u^n|_1^2. \quad (5.48)$$

For the term on the right side of equation (5.47), using the inequality $xy \leq \frac{1}{2}(x^2 + y^2)$ and Lemma 5.3, we find

$$\begin{aligned} \frac{1}{d}(u^n, f^n) &\leq \frac{1}{d} \left[\frac{2d}{(b-a)^2} \|u^n\|^2 + \frac{(b-a)^2}{8d} \|f^n\|^2 \right] \\ &\leq \frac{1}{3} |u^n|_1^2 + \frac{(b-a)^2}{8d^2} \|f^n\|^2. \end{aligned} \quad (5.49)$$

Upon substituting (5.48) and (5.49) into (5.47), we get

$$\frac{1}{d\tau_z^\gamma} \sum_{k=0}^n \omega_k^\gamma(u^n, u^{n-k}) + \frac{2}{3} |u^n|_1^2 \leq \frac{(b-a)^2}{8d^2} \|f^n\|^2. \quad (5.50)$$

Now, in (5.50) we replace n by i and sum i from 2 to n to give

$$\frac{1}{d\tau_z^\gamma} \sum_{i=2}^n \sum_{k=0}^i \omega_k^\gamma(u^i, u^{i-k}) + \frac{2}{3} \sum_{i=2}^n |u^i|_1^2 \leq \frac{(b-a)^2}{8d^2} \sum_{i=2}^n \|f^i\|^2. \quad (5.51)$$

Next, turning the attention to the second equation of (5.45), we multiply it by $\frac{hu_m^1\omega_0^\gamma}{d}$ and sum m from 1 to $(M-1)$ to get

$$\frac{1}{d\tau_z^\gamma}\omega_0^\gamma(u^1, u^1) - \frac{2\omega_0^\gamma}{\Gamma(\gamma+3)}(u^1, \delta_x^2 u^1) = \frac{\omega_0^\gamma}{d\tau_z^\gamma}(u^1, F^1). \quad (5.52)$$

For the second term on the left side of (5.52), we have

$$-\frac{2\omega_0^\gamma}{\Gamma(\gamma+3)}(u^1, \delta_x^2 u^1) = \frac{2\omega_0^\gamma}{\Gamma(\gamma+3)}|u^1|_1^2. \quad (5.53)$$

For the right side of (5.52), using the inequality $xy \leq \frac{1}{2}(x^2 + y^2)$ and Lemma 5.3, we find

$$\begin{aligned} \frac{\omega_0^\gamma}{d\tau_z^\gamma}(u^1, F^1) &\leq \frac{\omega_0^\gamma}{d} \left(\varepsilon \|u^1\|^2 + \frac{1}{4\varepsilon\tau_z^{2\gamma}} \|F^1\|^2 \right) \\ &\leq \frac{\varepsilon(b-a)^2\omega_0^\gamma}{6d} |u^1|_1^2 + \frac{\omega_0^\gamma}{4\varepsilon d\tau_z^{2\gamma}} \|F^1\|^2, \end{aligned} \quad (5.54)$$

where $\varepsilon = \frac{d[10\omega_0^\gamma - 3\Gamma(3+\gamma)]}{\omega_0^\gamma(b-a)^2\Gamma(3+\gamma)} > 0$ by Lemma 5.5. Upon substituting (5.53) and (5.54) into (5.52), we obtain

$$\frac{1}{d\tau_z^\gamma}\omega_0^\gamma(u^1, u^1) + \left[\frac{2\omega_0^\gamma}{\Gamma(\gamma+3)} - \frac{\varepsilon(b-a)^2\omega_0^\gamma}{6d} \right] |u^1|_1^2 \leq \frac{\omega_0^\gamma}{4\varepsilon d\tau_z^{2\gamma}} \|F^1\|^2. \quad (5.55)$$

Next, multiplying the second equation of (5.45) by $\frac{hu_m^0\omega_1^\gamma}{d}$ and summing m from 1 to $(M-1)$, we get

$$\frac{\omega_1^\gamma}{d\tau_z^\gamma}(u^0, u^1) - \frac{2\omega_1^\gamma}{\Gamma(\gamma+3)}(u^0, \delta_x^2 u^1) = \frac{\omega_1^\gamma}{d\tau_z^\gamma}(u^0, F^1). \quad (5.56)$$

For the second term on the left side of (5.56), using the inequality $xy \geq -\frac{1}{2}(x^2 + y^2)$, we find

$$\begin{aligned} -\frac{2\omega_1^\gamma}{\Gamma(\gamma+3)}(u^0, \delta_x^2 u^1) &= \frac{2\omega_1^\gamma}{\Gamma(\gamma+3)}(u^0, u^1)_1 \\ &\geq -\frac{|\omega_0^\gamma|}{\Gamma(\gamma+3)} \left[\frac{1}{3}|u^1|_1^2 + 3 \left(\frac{\omega_1^\gamma}{\omega_0^\gamma} \right)^2 |u^0|_1^2 \right]. \end{aligned} \quad (5.57)$$

For the term on the right side of (5.56), using the inequality $xy \leq \frac{1}{2}(x^2 + y^2)$ and Lemma 5.3, we get

$$\begin{aligned} \frac{\omega_1^\gamma}{d\tau_z^\gamma}(u^0, F^1) &\leq \frac{2|\omega_1^\gamma|^2}{(b-a)^2} \|u^0\|^2 + \frac{(b-a)^2}{8d^2\tau_z^{2\gamma}} \|F^1\|^2 \\ &\leq \frac{|\omega_1^\gamma|^2}{3} |u^0|_1^2 + \frac{(b-a)^2}{8d^2\tau_z^{2\gamma}} \|F^1\|^2. \end{aligned} \quad (5.58)$$

Upon substituting (5.57) and (5.58) into (5.56), we obtain

$$\frac{\omega_1^\gamma}{d\tau_z^\gamma}(u^0, u^1) - \frac{\omega_0^\gamma}{3\Gamma(\gamma+3)} |u^1|_1^2 \leq \left[\frac{3|\omega_1^\gamma|^2}{\Gamma(\gamma+3)\omega_0^\gamma} + \frac{|\omega_1^\gamma|^2}{3} \right] |u^0|_1^2 + \frac{(b-a)^2}{8d^2\tau_z^{2\gamma}} \|F^1\|^2. \quad (5.59)$$

Now, adding (5.51), (5.55) and (5.59) together yields

$$\begin{aligned} &\frac{1}{d\tau_z^\gamma} \sum_{i=0}^n \sum_{k=0}^i \omega_k^\gamma(u^i, u^{i-k}) + \frac{2}{3} \sum_{i=2}^n |u^i|_1^2 + \frac{1}{2} |u^1|_1^2 \\ &\leq \frac{(b-a)^2}{8d} \sum_{i=2}^n \|f^i\|^2 + \left[\frac{\omega_0^\gamma}{4\varepsilon d\tau_z^{2\gamma}} + \frac{(b-a)^2}{8d^2\tau_z^{2\gamma}} \right] \|F^1\|^2 + \left[\frac{3|\omega_1^\gamma|}{\Gamma(\gamma+3)\omega_0^\gamma} + \frac{|\omega_1^\gamma|^2}{3} \right] |u^0|_1^2. \end{aligned} \quad (5.60)$$

From Lemma 5.4, we know that $\sum_{i=0}^n \sum_{k=0}^i \omega_k^\gamma(u^i, u^{i-k}) \geq 0$. Thus, it follows from (5.60) that

$$\begin{aligned} &\frac{2}{3} \sum_{i=2}^n |u^i|_1^2 + \frac{1}{2} |u^1|_1^2 \\ &\leq \frac{(b-a)^2}{8d} \sum_{i=2}^n \|f^i\|^2 + \left[\frac{\omega_0^\gamma}{4\varepsilon d\tau_z^{2\gamma}} + \frac{(b-a)^2}{8d^2\tau_z^{2\gamma}} \right] \|F^1\|^2 + \left[\frac{3|\omega_1^\gamma|}{\Gamma(\gamma+3)\omega_0^\gamma} + \frac{|\omega_1^\gamma|^2}{3} \right] |u^0|_1^2. \end{aligned} \quad (5.61)$$

Using the inequality $\frac{1}{2} \sum_{i=1}^n |u^i|_1^2 \leq \frac{2}{3} \sum_{i=2}^n |u^i|_1^2 + \frac{1}{2} |u^1|_1^2$ in (5.61), we get

$$\begin{aligned} \sum_{i=1}^n |u^i|_1^2 &\leq \frac{(b-a)^2}{4d} \sum_{i=2}^n \|f^i\|^2 + \left[\frac{\omega_0^\gamma}{2\varepsilon d\tau_z^{2\gamma}} + \frac{(b-a)^2}{4d^2\tau_z^{2\gamma}} \right] \|F^1\|^2 \\ &\quad + \left[\frac{6|\omega_1^\gamma|}{\Gamma(\gamma+3)\omega_0^\gamma} + \frac{2|\omega_1^\gamma|^2}{3} \right] |u^0|_1^2. \end{aligned} \quad (5.62)$$

Further, from the definition of F_m^1 in (5.41), we find

$$\begin{aligned}
\|F^1\|^2 &= h \sum_{m=1}^{M-1} (F_m^1)^2 = h \sum_{m=1}^{M-1} \left\{ \frac{1}{\Gamma(\gamma)} \int_0^{t_1} \frac{\mathcal{Z}'(s)f(x_m, s)}{[\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{1-\gamma}} ds \right\}^2 \\
&\leq h \sum_{m=1}^{M-1} \left\{ \frac{\hat{f}_m^1}{\Gamma(\gamma)} \int_0^{t_1} \frac{\mathcal{Z}'(s)}{[\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{1-\gamma}} ds \right\}^2 \\
&= \frac{\tau_z^{2\gamma}}{[\Gamma(\gamma + 1)]^2} \|\hat{f}^1\|^2,
\end{aligned} \tag{5.63}$$

where $\hat{f}_m^1 = \max_{0 < t < t_1} |f(x_m, t)|$.

Finally, we substitute (5.63) into (5.62) to give the inequality (5.46) immediately. ■

From the above lemma, we can deduce the following stability result.

Theorem 5.5. (Stability) *The numerical scheme (5.44) is unconditionally stable with respect to the initial value and the nonlinear term f for all $\gamma \in (0, \gamma^*]$.*

Proof. From Lemma 5.3 and (5.46), we have for $1 \leq n \leq N$,

$$\begin{aligned}
\frac{4}{b-a} \sum_{i=1}^n \|u^i\|_\infty^2 &\leq \frac{(b-a)^2}{4d} \sum_{i=2}^n \|f^i\|^2 + \frac{1}{[\Gamma(\gamma + 1)]^2} \left[\frac{\omega_0^\gamma}{2\varepsilon d} + \frac{(b-a)^2}{4d^2} \right] \|\hat{f}^1\|^2 \\
&\quad + \left[\frac{6|\omega_1^\gamma|}{\Gamma(\gamma + 3)\omega_0^\gamma} + \frac{2|\omega_1^\gamma|^2}{3} \right] |u^0|_1^2.
\end{aligned}$$

Hence, it is obvious that the numerical scheme (5.44) is stable with respect to the initial value and the nonlinear term f . ■

Theorem 5.6. (Convergence) *Let $U(x, t)$ be the exact solution of (5.3) and $\{u_m^n\}$ be the solution of the numerical scheme (5.44). Let $e_m^n = U(x_m, t_n) - u_m^n$ be the error at (x_m, t_n) , $0 \leq m \leq M$, $0 \leq n \leq N$. Let $\gamma \in (0, \gamma^*]$. Suppose that $U(x, \mathcal{Z}^{-1}(z)) = \tilde{U}(x, z) \in C^{(4,5)}([a, b] \times [\mathcal{Z}(0), \mathcal{Z}(T)])$ and $\frac{\partial^k}{\partial z^k} \tilde{U} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1, 2, 3, 4, 5$. Then, we have for $1 \leq n \leq N$,*

$$\tau_z \sum_{i=1}^n \|e^i\|_\infty \leq \frac{b-a}{2} [\mathcal{Z}(T) - \mathcal{Z}(0)] \sqrt{\bar{C}(\bar{C}_1^2 + \bar{C}_2^2)} (\tau_z^3 + h^2) = O(\tau_z^3 + h^2), \tag{5.64}$$

where $\bar{C}$, $\bar{C}_1$ and $\bar{C}_2$ are positive finite constants.

Proof. Subtracting (5.44) from (5.42) and (5.43), we obtain the following

$$\left\{ \begin{array}{ll} \frac{1}{\tau_z^\gamma} \sum_{k=0}^n \omega_k^\gamma e_m^{n-k} = d\delta_x^2 e_m^n + T_m^n, & 1 \leq m \leq M-1, \quad 2 \leq n \leq N, \\ \frac{1}{\tau_z^\gamma} e_m^1 = \frac{2d}{\Gamma(\gamma+3)} \delta_x^2 e_m^1 + T_m^1, & 1 \leq m \leq M-1, \\ e_m^0 = 0, & 0 \leq m \leq M, \\ e_0^n = 0, \quad e_M^n = 0, & 1 \leq n \leq N. \end{array} \right. \quad (5.65)$$

where T_m^n , $1 \leq n \leq N$ are truncation errors and

$$|T_m^1| \leq \bar{C}_1(\tau_z^3 + h^2), \quad |T_m^n| \leq \bar{C}_2(\tau_z^3 + h^2), \quad n \geq 2, \quad (5.66)$$

for some positive constants $\bar{C}_1$ and $\bar{C}_2$.

Analogous to (5.62), we have for $1 \leq n \leq N$,

$$\begin{aligned} \tau_z \sum_{i=1}^n |e^i|_1^2 &\leq \tau_z \left\{ \frac{(b-a)^2}{4d} \sum_{i=2}^n \|T^i\|^2 + \left[\frac{\omega_0^\gamma}{2\varepsilon d \tau_z^{2\gamma}} + \frac{(b-a)^2}{4d^2 \tau_z^{2\gamma}} \right] \|\tau_z^\gamma T^1\|^2 \right\} \\ &= \tau_z \left\{ \frac{(b-a)^2}{4d} \sum_{i=2}^n \|T^i\|^2 + \left[\frac{\omega_0^\gamma}{2\varepsilon d} + \frac{(b-a)^2}{4d^2} \right] \|T^1\|^2 \right\} \\ &\leq \bar{C} \tau_z \sum_{i=1}^n \|T^i\|^2, \end{aligned} \quad (5.67)$$

where $\bar{C} = \max \left\{ \frac{(b-a)^2}{4d}, \frac{\omega_0^\gamma}{2\varepsilon d} + \frac{(b-a)^2}{4d^2} \right\}$.

Next, from (5.66) we find

$$\begin{aligned} \bar{C} \tau_z \sum_{i=1}^n \|T^i\|^2 &\leq \bar{C} \tau_z \left[(b-a) \bar{C}_1^2 (\tau_z^3 + h^2)^2 + N(b-a) \bar{C}_2^2 (\tau_z^3 + h^2)^2 \right] \\ &= \bar{C} (b-a) (\tau_z^3 + h^2)^2 \left\{ \tau_z \bar{C}_1^2 + [\mathcal{Z}(T) - \mathcal{Z}(0)] \bar{C}_2^2 \right\} \\ &\leq \bar{C} (b-a) [\mathcal{Z}(T) - \mathcal{Z}(0)] (\bar{C}_1^2 + \bar{C}_2^2) (\tau_z^3 + h^2)^2. \end{aligned} \quad (5.68)$$

Now, from Lemma 5.3 and (5.67), we get, noting (5.68), for $1 \leq n \leq N$,

$$\frac{4}{b-a} \tau_z \sum_{i=1}^n \|e^i\|_\infty^2 \leq \tau_z \sum_{i=1}^n |e^i|_1^2 \leq \bar{C}(b-a)[\mathcal{Z}(T) - \mathcal{Z}(0)](\bar{C}_1^2 + \bar{C}_2^2)(\tau_z^3 + h^2)^2. \quad (5.69)$$

Finally, using Cauchy-Schwarz inequality and (5.69), we obtain, for $1 \leq n \leq N$

$$\begin{aligned} \left(\tau_z \sum_{i=1}^n \|e^i\|_\infty \right)^2 &\leq \left(\tau_z \sum_{i=1}^n 1^2 \right) \left(\tau_z \sum_{i=1}^n \|e^i\|_\infty^2 \right) \\ &\leq \frac{1}{4} \bar{C}(b-a)^2 [\mathcal{Z}(T) - \mathcal{Z}(0)]^2 (\bar{C}_1^2 + \bar{C}_2^2) (\tau_z^3 + h^2)^2. \end{aligned} \quad (5.70)$$

Then, taking square root of (5.70) leads to the inequality (5.64) immediately. ■

Remark 5.5. When $n = N$, the relation (5.64) establishes the convergence of the numerical scheme (5.44) in ‘average norm’ as

$$\frac{1}{N} \sum_{i=1}^N \|e^i\|_\infty = O(\tau_z^3 + h^2). \quad (5.71)$$

This is clear since $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{N}$.

Remark 5.6. The relations (5.64) and (5.71) indicate third order convergence $O(\tau_z^3)$ with respect to the uniform mesh of $[\mathcal{Z}(0), \mathcal{Z}(T)]$. We shall investigate the convergence with respect to the mesh of $[0, T]$. Let $\tau = \max_{1 \leq n \leq N} |t_n - t_{n-1}|$, the maximum step size of $[0, T]$. Suppose $0 \leq \mathcal{Z}'(t) \leq C_3$ for $t \in [0, T]$. By mean value theorem, we have

$$\tau_z = \mathcal{Z}(t_n) - \mathcal{Z}(t_{n-1}) = \mathcal{Z}'(\xi)(t_n - t_{n-1}),$$

for some $\xi \in (t_{n-1}, t_n)$. It follows that

$$\tau_z \leq C_3 |t_n - t_{n-1}| \leq C_3 \tau.$$

Hence, the relations (5.64) and (5.71) now yield

$$\tau_z \sum_{i=1}^n \|e^i\|_\infty = O(\tau^3 + h^2), \quad 1 \leq n \leq N \quad (5.72)$$

and

$$\frac{1}{N} \sum_{i=1}^N \|e^i\|_{\infty} = O(\tau^3 + h^2). \quad (5.73)$$

respectively. In particular, the relation (5.73) establishes the convergence of the numerical scheme (5.44) in ‘average norm’ with respect to the maximum step size τ of the time interval $[0, T]$.

Remark 5.7.

- (a) We claim that the *third order temporal convergence* obtained in (5.64) (or (5.71)) *improves* the work of [133] where the temporal convergence order is observed to be $(2 - \gamma)$ from numerical experiments. Indeed, this improvement will be illustrated in Example 5.2 where we compute the maximum absolute error at $t = t_N$.
- (b) In [133], the authors establish the convergence of their method by using the Lax-Richtmyer Theorem, which states that if the numerical scheme is well-posed and consistent, then the scheme is convergent if and only if it is stable. Also, the convergence order is not proved explicitly but is observed numerically to be $(2 - \gamma)$. In comparison, our proof of convergence is more straightforward and the convergence order is explicitly given in (5.64) (or (5.71)).

Remark 5.8. In view of Remark 5.4, Theorem 5.4 and Lemma 5.2, the conditions of Theorem 5.6, namely, $U(x, \mathcal{Z}^{-1}(z)) = \tilde{U}(x, z) \in C^{(4,5)}([a, b] \times [\mathcal{Z}(0), \mathcal{Z}(T)])$ and $\frac{\partial^k}{\partial z^k} \tilde{U} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1, 2, 3, 4, 5$, can be replaced by the *weaker* conditions $\tilde{U}(x, z) \in C^{(4,3)}([a, b] \times [\mathcal{Z}(0), \mathcal{Z}(t_1)])$ and $\frac{\partial^k}{\partial z^k} \tilde{U} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1$ and $\tilde{U}_e(\cdot, z) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+3}(\mathcal{R})$.

5.3 Experiment

In this section, we shall demonstrate the efficiency of our numerical scheme (5.44) and confirm the theoretical convergence in (5.71) (which is immediate from Theorem 5.6). Moreover, some numerical experiments are conducted when the conditions of Theorem 5.6 are *not* entirely satisfied, just to observe the influence of the theoretical conditions on the actual convergence of the numerical scheme. Note

that the convergence indicated in (5.71) is in terms of average norm, nonetheless it would also be interesting to see the convergence in terms of maximum norm.

Let $\{U_m^n\}$ be the exact solution of the diffusion problem and $\{u_m^n\}$ be the numerical solution. In the following examples, we shall compute the average norm and maximum norm errors as follows:

$$E_{av}(h, N) = \tau_z \sum_{n=1}^N \max_{1 \leq m \leq M-1} |U_m^n - u_m^n|, \quad E_\infty(h, N) = \max_{1 \leq m \leq M-1} |U_m^N - u_m^N|. \quad (5.74)$$

Further, the convergence orders in the temporal and spacial dimensions with respect to the *average norm* are computed as

$$T_{av} = \log_2 \left[\frac{E_{av}(h, N)}{E_{av}(h, 2N)} \right], \quad S_{av} = \log_2 \left[\frac{E_{av}(2h, N)}{E_{av}(h, N)} \right]. \quad (5.75)$$

The temporal and spatial convergence orders with respect to the *maximum norm*, T_∞ and S_∞ , can be similarly computed.

Example 5.1. Consider the generalized fractional diffusion problem

$$\begin{cases} {}^C_0 D_{t;[\mathcal{Z}(t),1]}^\gamma u(x, t) = \frac{\partial^2 u(x, t)}{\partial x^2} + f(x, t), & (x, t) \in [0, 1] \times [0, 1], \\ u(x, 0) = 0, & x \in [0, 1], \\ u(0, t) = 0, \quad u(1, t) = t^{\beta_1}(\sin 1), & t \in [0, 1], \end{cases} \quad (5.76)$$

where $0 < \gamma < \gamma^*$, $\beta_1 \geq \gamma r > 0$ and $\mathcal{Z}(t) = t^r$ is the scale function.

$$f(x, t) = t^{\beta_1}(\sin x) \left[\frac{\Gamma(\frac{\beta_1}{r} + 1)}{\Gamma(\frac{\beta_1}{r} + 1 - \gamma)} t^{-\gamma r} + 1 \right]. \quad (5.77)$$

The exact solution of this problem is

$$U(x, t) = t^{\beta_1}(\sin x).$$

We shall apply the numerical scheme (5.44) to solve the problem for two different sets of (β_1, r) . It is easy to verify that the conditions of Theorem 5.6 are satisfied by the first set of (β_1, r) but not entirely satisfied by the second set. The purpose

is to observe the influence of the theoretical conditions on the actual convergence of the numerical scheme.

Case 1. Let $\beta_1 = 5$ and $r = \frac{1}{2}$. Here, the exact solution of the problem is

$$U(x, t) = t^5(\sin x).$$

Clearly, we have $\tilde{U}(x, z) = z^{10}(\sin x)$ and the conditions of Theorem 5.6 are satisfied.

To illustrate the convergence in the temporal dimension, we fix $h = \frac{1}{1000}$ and let N vary. In Table 5.1, we present the maximum norm error $E_\infty(h, N)$, average norm error $E_{av}(h, N)$ and the respective temporal convergence orders. It is observed that our method is third order in the temporal dimension, thus confirming the theoretical result (Theorem 5.6).

Next, to illustrate the convergence in the spatial dimension, we fix $N = 1000$ and let M vary. The errors and spatial convergence orders are presented in Table 5.2. Clearly, our method is second order convergent in the spacial dimension, thus confirming the theoretical result (Theorem 5.6).

TABLE 5.1: (Example 5.1) Case 1: Errors and temporal convergence orders

N	$\gamma = 0.1$		$\gamma = 0.3$		$\gamma = 0.5$		$\gamma = 0.8$	
	E_∞	T_∞	E_∞	T_∞	E_∞	T_∞	E_∞	T_∞
20	5.966e-05		2.894e-04		7.549e-04		2.210e-03	
40	8.625e-06	2.792	4.225e-05	2.776	1.113e-04	2.762	3.309e-04	2.740
80	1.163e-06	2.893	5.712e-06	2.887	1.511e-05	2.881	4.529e-05	2.869
160	1.547e-07	2.904	7.460e-07	2.937	1.972e-06	2.938	5.926e-06	2.934
N	$\gamma = 0.1$		$\gamma = 0.3$		$\gamma = 0.5$		$\gamma = 0.8$	
	E_{av}	T_{av}	E_{av}	T_{av}	E_{av}	T_{av}	E_{av}	T_{av}
20	8.402e-06		4.132e-05		1.090e-04		3.224e-04	
40	1.150e-06	2.869	5.731e-06	2.850	1.531e-05	2.832	4.617e-05	2.804
80	1.509e-07	2.930	7.555e-07	2.923	2.032e-06	2.914	6.187e-06	2.900
160	1.966e-08	2.940	9.732e-08	2.957	2.620e-07	2.955	8.012e-07	2.949

Case 2. Let $\beta_1 = 1$ and $r = \frac{1}{2}$. Here, the exact solution of the problem is

$$U(x, t) = t(\sin x).$$

Clearly, we have $\tilde{U}(x, z) = z^2(\sin x)$ and the conditions of Theorem 5.6 are not entirely satisfied.

To investigate the temporal convergence, we fix $h = \frac{1}{1000}$ and vary N . From Table 5.3, where the errors and temporal convergence orders are presented, we observe

TABLE 5.2: (Example 5.1) Case 1: Errors and spatial convergence orders

M	$\gamma = 0.1$		$\gamma = 0.3$		$\gamma = 0.5$		$\gamma = 0.8$	
	E_∞	S_∞	E_∞	S_∞	E_∞	S_∞	E_∞	S_∞
20	$1.107e-05$		$1.038e-05$		$9.457e-06$		$7.611e-06$	
40	$2.774e-06$	1.997	$2.602e-06$	1.996	$2.371e-06$	1.996	$1.923e-06$	1.985
80	$6.939e-07$	1.999	$6.523e-07$	1.996	$5.995e-07$	1.984	$4.966e-07$	1.953
160	$1.740e-07$	1.996	$1.656e-07$	1.978	$1.561e-07$	1.941	$1.438e-07$	1.788
	E_{av}	S_{av}	E_{av}	S_{av}	E_{av}	S_{av}	E_{av}	S_{av}
20	$1.001e-06$		$9.441e-07$		$8.543e-07$		$6.760e-07$	
40	$2.531e-07$	1.984	$2.366e-07$	1.997	$2.145e-07$	1.994	$1.716e-07$	1.978
80	$6.333e-08$	1.999	$5.947e-08$	1.992	$5.447e-08$	1.977	$4.545e-08$	1.917
160	$1.589e-08$	1.995	$1.517e-08$	1.971	$1.444e-08$	1.915	$1.390e-08$	1.709

that the temporal convergence order is indeed reduced to below 3 (theoretical convergence order). However, our method still gives a good approximation of the exact solution as the errors are small.

TABLE 5.3: (Example 5.1) Case 2: Temporal convergence when theoretical conditions are not satisfied

N	$\gamma = 0.1$		$\gamma = 0.3$		$\gamma = 0.5$		$\gamma = 0.8$	
	E_∞	T_∞	E_∞	T_∞	E_∞	T_∞	E_∞	T_∞
20	$3.927e-07$		$6.711e-06$		$3.022e-05$		$1.232e-04$	
40	$1.043e-07$	1.913	$1.962e-06$	1.774	$9.251e-06$	1.708	$4.078e-05$	1.595
80	$2.768e-08$	1.914	$5.687e-07$	1.787	$2.755e-06$	1.748	$1.278e-05$	1.674
160	$7.341e-09$	1.915	$1.634e-07$	1.799	$7.987e-07$	1.786	$3.748e-06$	1.770
	E_{av}	T_{av}	E_{av}	T_{av}	E_{av}	T_{av}	E_{av}	T_{av}
20	$6.239e-08$		$9.224e-07$		$4.011e-06$		$2.008e-05$	
40	$9.254e-09$	2.753	$1.590e-07$	2.536	$7.659e-07$	2.389	$4.561e-06$	2.138
80	$2.360e-09$	1.971	$2.556e-08$	2.637	$1.411e-07$	2.440	$1.017e-06$	2.165
160	$1.591e-09$	0.569	$4.888e-09$	2.387	$2.532e-08$	2.478	$2.236e-07$	2.185

The next example is from [133] where the authors only conducted numerical experiment for $\mathcal{Z}(t) = t$ and $\mathcal{W}(t) = 1$ (classical Caputo fractional derivative). To demonstrate the improvement of the temporal convergence order in our method, we shall perform the numerical simulation for different $\mathcal{Z}(t)$ and $\mathcal{W}(t)$, including the classical case of $\mathcal{Z}(t) = t$ and $\mathcal{W}(t) = 1$. Since the exact solution is not known for general $\mathcal{Z}(t)$ and $\mathcal{W}(t)$, we shall compute the ‘exact’ solution by using our numerical scheme with sufficiently small spatial step size $h = \frac{1}{1000}$ and sufficiently large $N = 10000$.

Example 5.2. [133] Consider the generalized fractional diffusion problem

$$\begin{cases} {}^C_0D_{t;[\mathcal{Z}(t),\mathcal{W}(t)]}^{0.85}u(x,t) = \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), & (x,t) \in [0,1] \times [0,1], \\ u(x,0) = \sin(\pi x), & x \in [0,1], \\ u(0,t) = 0, \quad u(1,t) = 0, & t \in [0,1], \end{cases} \quad (5.78)$$

where

$$f(x,t) = \frac{2}{\Gamma(2.15)}(x^2 - x)t^{1.15} + \pi^2 \sin(\pi x) - 2t^2. \quad (5.79)$$

When $\mathcal{Z}(t) = t$ and $\mathcal{W}(t) = 1$, the exact solution is $U(x,t) = \sin(\pi x) + x(x-1)t^2$.

Let $h = \frac{1}{1000}$ be fixed. In Table 5.4, we present the errors $E_\infty(h, N)$, $E_{av}(h, N)$ and the temporal convergence orders T_∞ , T_{av} for four sets of $\mathcal{W}(t)$ and $\mathcal{Z}(t)$. Note that the numerical scheme (5.44) is applied directly when $\mathcal{W}(t) = 1$. If $\mathcal{W}(t) \neq 1$, we shall first convert the original problem to the equivalent form (5.3) before applying the scheme (5.44). The numerical solution of the original problem is then obtained via a relation that relates the solutions of (5.1) and (5.3). From Table 5.4, we observe that the temporal convergence orders T_∞ , T_{av} are below 3 for the classical case $\mathcal{Z}(t) = t$ and $\mathcal{W}(t) = 1$. This could due to the exact solution in this case does not satisfy the conditions of Theorem 5.6. For other cases where the theoretical solutions are not known, the temporal convergence is mostly 3.

Next, we shall compare our numerical scheme (5.44) with the method in [133]. With $h = \frac{1}{1000}$ fixed, in Table 5.5 we present the maximum absolute error at $t = t_N$, $E_\infty(h, N)$, and the temporal convergence order T_∞ . It is observed that the proposed scheme (5.44) achieves third order accuracy in temporal dimension (except the classical case) as well as smaller errors for all cases.

In the next example, we shall illustrate the effects of scale function $\mathcal{Z}(t)$, weight function $\mathcal{W}(t)$ and diffusion constant d on the solution.

TABLE 5.4: (Example 5.2) Errors and temporal convergence orders

	N	E_∞	T_∞	E_{av}	T_{av}
$\mathcal{W}(t) = 1, \quad \mathcal{Z}(t) = t$	50	$5.1823e-08$		$1.6379e-06$	
	100	$9.5802e-09$	2.4355	$3.6704e-07$	2.1578
	200	$1.9180e-09$	2.3205	$8.2480e-08$	2.1538
$\mathcal{W}(t) = 1, \quad \mathcal{Z}(t) = t^{0.5}$	50	$9.4544e-07$		$6.4600e-07$	
	100	$1.1888e-07$	2.9915	$8.1858e-08$	2.9803
	200	$1.4904e-08$	2.9957	$1.0383e-08$	2.9789
$\mathcal{W}(t) = \exp(t), \quad \mathcal{Z}(t) = t$	50	$5.8703e-07$		$2.9835e-06$	
	100	$7.3243e-08$	3.0027	$6.0462e-07$	2.2810
	200	$8.8274e-09$	3.0526	$1.3006e-07$	2.2175
$\mathcal{W}(t) = \exp(t), \quad \mathcal{Z}(t) = t^{0.5}$	50	$1.3673e-05$		$3.2578e-06$	
	100	$1.9014e-06$	2.8462	$4.3841e-07$	2.8935
	200	$2.5079e-07$	2.9225	$5.6950e-08$	2.9445

TABLE 5.5: (Example 5.2) Comparison between our scheme and scheme in [133]

	N	Our scheme	T_∞	Scheme in [133]	T_∞
$\mathcal{W}(t) = 1, \quad \mathcal{Z}(t) = t$	50	$5.1823e-08$		$2.2467e-04$	
	100	$9.5802e-09$	2.4355	$9.7243e-05$	1.2081
	200	$1.9180e-09$	2.3205	$3.9765e-05$	1.2901
$\mathcal{W}(t) = 1, \quad \mathcal{Z}(t) = t^{0.5}$	50	$9.4544e-07$		$7.2103e-06$	
	100	$1.1888e-07$	2.9915	$3.1380e-06$	1.2002
	200	$1.4904e-08$	2.9957	$1.2866e-06$	1.2863
$\mathcal{W}(t) = \exp(t), \quad \mathcal{Z}(t) = t$	50	$5.8703e-07$		$2.5599e-04$	
	100	$7.3243e-08$	3.0027	$1.1217e-04$	1.1903
	200	$8.8274e-09$	3.0526	$4.6173e-05$	1.2806
$\mathcal{W}(t) = \exp(t), \quad \mathcal{Z}(t) = t^{0.5}$	50	$1.3673e-05$		$2.6804e-04$	
	100	$1.9014e-06$	2.8462	$1.1626e-04$	1.2051
	200	$2.5079e-07$	2.9225	$4.7601e-05$	1.2883

Example 5.3. Consider the generalized fractional diffusion problem

$$\begin{cases} {}^C_0D_{t;[\mathcal{Z}(t),\mathcal{W}(t)]}^{0.45}u(x,t) = d\frac{\partial^2 u(x,t)}{\partial x^2} + \frac{(x-1)(t-1)}{2+\sin(xt)}, & (x,t) \in [0,1] \times [0,1], \\ u(x,0) = x^2 - x^3, & x \in [0,1], \\ u(0,t) = 0, \quad u(1,t) = 0, & t \in [0,1], \end{cases} \quad (5.80)$$

where $d > 0$ is the diffusion constant.

To visualize the effects of scale function $\mathcal{Z}(t)$, weight function $\mathcal{W}(t)$ and diffusion constant d on the solution of the diffusion problem, we shall apply the numerical scheme (5.44) to four sets of $(\mathcal{Z}(t), \mathcal{W}(t), d)$ and plot the numerical solutions in Figure 5.1. Let $h = \frac{1}{100}$ and $N = 500$ be fixed in the computation.

From Figure 5.1, the following observations can be made:

- (1) Figure 5.1(a): Base case $(\mathcal{Z}(t), \mathcal{W}(t), d) = (t, 1, 1)$. We observe that the numerical solution depicts the zero boundary conditions.
- (2) Figure 5.1(b): Change $\mathcal{Z}(t) - (\mathcal{Z}(t), \mathcal{W}(t), d) = (t^{\frac{1}{7}}, 1, 1)$. We observe that the scale function $\mathcal{Z}(t)$ is compressing the time domain which results in a finer mesh compared to Figure 5.1(a).
- (3) Figure 5.1(c): Change $\mathcal{W}(t) - (\mathcal{Z}(t), \mathcal{W}(t), d) = (t, \exp(t), 1)$. Typically, the solution tends to be smaller with larger weights. We observe that the numerical solution is indeed smaller compared to Figure 5.1(a).
- (4) Figure 5.1(d): Change $d - (\mathcal{Z}(t), \mathcal{W}(t), d) = (t, 1, 0.5)$. We observe that the diffusion process becomes slower than that in Figure 5.1(a) because the diffusion constant d reduces to 0.5.

FIGURE 5.1: (Example 5.3) The diffusion behavior of generalized fractional diffusion equation: (a) $(\mathcal{Z}(t), \mathcal{W}(t), d) = (t, 1, 1)$; (b) $(\mathcal{Z}(t), \mathcal{W}(t), d) = (t^{\frac{1}{7}}, 1, 1)$; (c) $(\mathcal{Z}(t), \mathcal{W}(t), d) = (t, \exp(t), 1)$; (d) $(\mathcal{Z}(t), \mathcal{W}(t), d) = (t, 1, 0.5)$.

It is noted in [4] that the scale function $\mathcal{Z}(t)$ can stretch or contract the domain, the weight function $\mathcal{W}(t)$ can weigh differently at different time points, and the diffusion constant d measures the rate of the diffusion process. From the above observations (2)–(4), we conclude that the numerical solutions computed from the scheme (5.44) indeed illustrate correctly the effects of the scale function $\mathcal{Z}(t)$, the weight function $\mathcal{W}(t)$ and the diffusion constant d .

Remark 5.9. In Theorem 5.6, the condition $\gamma \in (0, \gamma^*]$ arises from the proofs of the stability and convergence of the numerical scheme. If this condition is not satisfied, our scheme may not be stable or convergent. The condition $U(x, \mathcal{Z}^{-1}(z)) = \tilde{U}(x, z) \in C^{(4)}[a, b]$ arises from finite difference method, while the conditions $U(x, \mathcal{Z}^{-1}(z)) = \tilde{U}(x, z) \in C^{(5)}[\mathcal{Z}(0), \mathcal{Z}(T)]$ and $\frac{\partial^k}{\partial z^k} \tilde{U} \Big|_{z=\mathcal{Z}(0)} = 0, k = 0, 1, 2, 3, 4, 5$ arise from approximation of fractional derivative. If any of these conditions are not satisfied, the convergence order may be influenced and reduced.

- Case 2 of Example 5.1 does not satisfy the condition $\frac{\partial^k}{\partial z^k} \tilde{U} \Big|_{z=\mathcal{Z}(0)} = 0, k = 2, 3, 4, 5$. We observe from Table 5.3 that the convergence order is reduced to below three. However, the numerical solution still approximates quite well with small maximum absolute errors.
- The general solution of Example 5.2 is not known. From Table 5.4, we observe that the temporal convergence orders are below three for some $\mathcal{Z}(t)$ and $\mathcal{W}(t)$. This could be due to the exact solutions in these cases do not satisfy the theoretical conditions.

5.4 Summary

We consider the numerical treatment of a diffusion problem involving *generalized* fractional derivative which is characterized by a scale function $\mathcal{Z}(t)$ and a weight function $\mathcal{W}(t)$. A new approximation of order 3 is developed for the generalized fractional derivative. This is the most accurate approximation to date. Applying the new approximation and finite difference method, we construct a numerical scheme for the generalized fractional diffusion problem and prove the stability and convergence of the scheme by energy method. The convergence is shown to be third order in temporal dimension and second order in spacial dimension, and is verified by several numerical experiments.

Chapter 6

New Generalized Fractional Diffusion Equation II

In this chapter, we aim to improve the result of Chapter 5 and derive a new *fourth order* approximation for the generalized fractional derivative. We shall apply it in the treatment of a generalized time-fractional diffusion problem (5.1). It is noted that the classical fractional diffusion equation is a special case of the generalized fractional diffusion equation (5.1) with $z(t) = t$. Therefore, our numerical scheme is also applicable to the classical equation. Many numerical methods have been developed for classical fractional diffusion equations [35, 49, 57, 77, 138, 139, 145, 150], among them Ji and Sun [57] give the best result of *order 3* in the temporal convergence. Since our numerical scheme can achieve *order 4* in the temporal convergence, hence we also *improve* the numerical methods for classical fractional diffusion equations in the literature. In this chapter, we shall present a fourth order approximation combining with compact finite difference to solve the equivalent problem (5.3). The numerical solution of the original problem (5.1) can easily be computed from the relation $u(x, t) = \mathcal{W}(t)V(x, t) - \mathcal{W}(0)V_0(x)$. The convergence order of our scheme is *order 4* in both of time and space direction. Thus, we also make an improvement for classical fractional diffusion equation.

This chapter is organized as follows. In Section 6.1, we derive a fourth order approximation for the generalized fractional derivative and develop a numerical scheme to solve (5.3). In Section 6.2, we present an a priori estimate of the numerical solution, which is then used in Section 6.3 to prove the stability and convergence

of the numerical scheme. In Section 6.4, three numerical examples are presented to verify our theoretical results and to compare with other methods in the literature. Finally, we give a conclusion in Section 6.5.

6.1 Numerical Scheme

In this section, we shall develop a numerical scheme for the equivalent problem (5.3). The discussion has 3 parts: (i) the derivation of a fourth order approximation for the generalized fractional derivative; (ii) the consideration at the first and second time points; (iii) the final formulation of the numerical scheme.

Throughout, the scale function $\mathcal{Z}(t)$ is assumed to be strictly increasing. Let $\mathcal{X} : t \rightarrow \mathcal{Z}(t)$ be a mapping from $[0, T]$ to $[\mathcal{Z}(0), \mathcal{Z}(T)]$.

Recall we have defined

$$P : a = x_0 < x_1 < \cdots < x_M = b$$

to be a uniform partition of the spatial interval $[a, b]$ with step size $h = \frac{b-a}{M}$, and let

$$P' : 0 = t_0 < t_1 < \cdots < t_N = T$$

be a mesh of the temporal interval $[0, T]$ such that $\tau_z \equiv \mathcal{Z}(t_n) - \mathcal{Z}(t_{n-1})$, $1 \leq n \leq N$ is a constant. Obviously, $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{N}$.

Motivated by Theorem 4.1, we shall now develop a fourth order approximation for the *generalized Riemann-Liouville fractional derivative*. We will use the extend function $\tilde{u}_e(x, z)$ in (5.8).

Theorem 6.1. (Fourth order approximation) *Let $0 < \gamma < 1$. Suppose that $u(\cdot, \mathcal{Z}^{-1}(z)) \equiv \tilde{u}(\cdot, z) \in C^{(6)}[\mathcal{Z}(0), \mathcal{Z}(T)]$ and $\frac{\partial^k}{\partial z^k} \tilde{u} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1, 2, 3, 4, 5, 6$. Define the generalized weighted shifted Grünwald-Letnikov difference (gWSGD) operator $\hat{\mathcal{G}}_{\tau_z}^\gamma$ by*

$$\hat{\mathcal{G}}_{\tau_z}^\gamma u(x_m, t_n) = \lambda_0 \mathcal{J}_{\tau_z, 0}^\gamma u_m^n + \lambda_{-1} \mathcal{J}_{\tau_z, -1}^\gamma u_m^n + \lambda_{-2} \mathcal{J}_{\tau_z, -2}^\gamma u_m^n + \lambda_{-3} \mathcal{J}_{\tau_z, -3}^\gamma u_m^n, \quad (6.1)$$

where $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{N}$ is the step size, $\lambda_0, \lambda_{-1}, \lambda_{-2}, \lambda_{-3}$ are given in (4.5), and $\mathcal{J}_{\tau_z, l}^\gamma u_m^n$ are given in (5.10). Then, the generalized Riemann-Liouville fractional

derivative with unity weight function has the following approximation:

$${}^{RL}_0 D_{t;[\mathcal{Z}(t),1]}^\gamma u(x_m, t_n) = \hat{\mathcal{G}}_{\tau_z}^\gamma u(x_m, t_n) + O(\tau_z^4). \quad (6.2)$$

Proof. In view of the assumptions, we can choose a function $\psi(z)$ such that $\tilde{u}_e(\cdot, z) \in C^{(6)}(\mathcal{R})$. In fact, we can apply Hermite interpolation to get a $\psi(z)$ that ensures the continuity at $z = \mathcal{Z}(T)$ and $z = 2\mathcal{Z}(T)$. Using Lemma 4.1, we have $\tilde{u}_e(\cdot, z) \in \mathcal{C}^{\gamma+4}(\mathcal{R})$. Also, it is obvious that $\tilde{u}_e(\cdot, z) \in L^1(\mathcal{R})$. Thus, $\tilde{u}_e(\cdot, z) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+4}(\mathcal{R})$.

Denote $\mathcal{Z}(t_n)$ by z_n . Clearly, $P'' : \mathcal{Z}(0) = z_0 < z_1 < \cdots < z_N = \mathcal{Z}(T)$ is the uniform partition of $[\mathcal{Z}(0), \mathcal{Z}(T)]$ with step size $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{N}$. Hence, we can apply Theorem 4.1 to get

$$\begin{aligned} {}^{RL}_{-\infty} D_z^\gamma \tilde{u}_e(x_m, z_n) &= G_{\tau_z}^\gamma \tilde{u}_e(x_m, z_n) + O(\tau_z^4) \\ &= \lambda_0 J_{\tau_z,0}^\gamma \tilde{u}_e(x_m, z_n) + \lambda_{-1} J_{\tau_z,-1}^\gamma \tilde{u}_e(x_m, z_n) \\ &\quad + \lambda_{-2} J_{\tau_z,-2}^\gamma \tilde{u}_e(x_m, z_n) + \lambda_{-3} J_{\tau_z,-3}^\gamma \tilde{u}_e(x_m, z_n) + O(\tau_z^4). \end{aligned} \quad (6.3)$$

Noting (5.14), we have

$$\begin{aligned} {}^{RL}_{-\infty} D_z^\gamma \tilde{u}_e(x_m, z_n) &= \lambda_0 \mathcal{J}_{\tau_z,0}^\gamma u_m^n + \lambda_{-1} \mathcal{J}_{\tau_z,-1}^\gamma u_m^n + \lambda_{-2} \mathcal{J}_{\tau_z,-2}^\gamma u_m^n \\ &\quad + \lambda_{-3} \mathcal{J}_{\tau_z,-3}^\gamma u_m^n + O(\tau_z^4) \\ &= \hat{\mathcal{G}}_{\tau_z}^\gamma u(x_m, t_n) + O(\tau_z^4). \end{aligned} \quad (6.4)$$

Hence, in view of (5.18) and (6.4), we immediately obtain the approximation (2.10). $\blacksquare$

Remark 6.1. The conditions in Theorem 6.1, namely, $u(\cdot, \mathcal{Z}^{-1}(z)) \equiv \tilde{u}(\cdot, z) \in C^{(6)}[\mathcal{Z}(0), \mathcal{Z}(T)]$ and $\frac{\partial^k}{\partial z^k} \tilde{u} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1, 2, 3, 4, 5, 6$, can be replaced by the weaker condition $\tilde{u}_e(\cdot, z) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+4}(\mathcal{R})$, which is needed for us to apply Theorem 4.1.

Remark 6.2. We notice from the expression (5.10) that for $\mathcal{J}_{\tau_z,-3}^\gamma u_m^n$ to make sense, we require $n \geq 3$. From (4.11), the gWSGD operator (6.1) can then be written as

$$\hat{\mathcal{G}}_{\tau_z}^\gamma u(x_m, t_n) = \frac{1}{\tau_z^\gamma} \sum_{k=0}^n c_k^\gamma u_m^{n-k}, \quad n \geq 3. \quad (6.5)$$

Corollary 6.1. (Fourth order approximation) Let $0 < \gamma < 1$. Suppose that $u(\cdot, \mathcal{Z}^{-1}(z)) \equiv \tilde{u}(\cdot, z) \in C^{(6)}[\mathcal{Z}(0), \mathcal{Z}(T)]$ and $\frac{\partial^k}{\partial z^k} \tilde{u} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1, 2, 3, 4, 5, 6$. Then, the generalized Caputo fractional derivative with unity weight function has the following approximation

$${}_0^C D_{t;[\mathcal{Z}(t),1]}^\gamma u(x_m, t_n) = \frac{1}{\tau_z^\gamma} \sum_{k=0}^n c_k^\gamma u_m^{n-k} + O(\tau_z^4), \quad n \geq 3, \quad (6.6)$$

where c_k^γ is given in (4.11).

Remark 6.3. In view of Remarks 6.1 and 5.3, the conditions in Corollary 6.1 can be replaced by the *weaker* conditions $u(x, 0) = 0$ and $\tilde{u}_e(\cdot, z) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+4}(\mathcal{R})$.

It is obvious that the approximation (6.6) is applicable for $n \geq 3$. To handle the generalized Caputo fractional derivative at $t = t_1$ and $t = t_2$, we shall make use of the *generalized Riemann-Liouville fractional integral*. The next result gives an approximation for the generalized Riemann-Liouville fractional integral of u_{xx} at $t = t_1$.

Theorem 6.2. Let $0 < \gamma < 1$. Suppose that $\tilde{u}(x, z) \in C^{(2,4)}([a, b] \times [\mathcal{Z}(0), \mathcal{Z}(t_1)])$ and $\frac{\partial^k}{\partial z^k} \tilde{u} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1, 2$. Then, we have

$$\left| {}_0^{RL} I_{t;[\mathcal{Z}(t),1]}^\gamma u_{xx}(x, t_1) - \frac{6\tau_z^\gamma}{\Gamma(\gamma+4)} u_{xx}(x, t_1) \right| \leq \frac{9C_4\tau_z^{4+\gamma}}{2048\Gamma(\gamma+1)} = O(\tau_z^{4+\gamma}), \quad (6.7)$$

where $C_4 = \max_{(x,z) \in [a,b] \times [\mathcal{Z}(0), \mathcal{Z}(t_1)]} |\tilde{u}_{xxxxzz}(x, z)|$.

Proof. From (5.31), we have

$${}_0^{RL} I_{t;[\mathcal{Z}(t),1]}^\gamma u_{xx}(x, t_1) = \frac{1}{\Gamma(\gamma)} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t_1)} \frac{\tilde{u}_{xx}(x, \mathcal{Z}(s))}{[\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{1-\gamma}} d\mathcal{Z}(s). \quad (6.8)$$

To approximate $\tilde{u}_{xx}(x, z)$ over the interval $[\mathcal{Z}(0), \mathcal{Z}(t_1)]$, we shall use the Hermite interpolate, $\overline{H}(x, z)$, of $\tilde{u}_{xx}(x, z)$ with interpolating conditions at $\tilde{u}_{xx}(x, \mathcal{Z}(0))$, $\tilde{u}_{xxz}(x, \mathcal{Z}(0))$, $\tilde{u}_{xxzz}(x, \mathcal{Z}(0))$ and $\tilde{u}_{xx}(x, \mathcal{Z}(t_1))$. In fact, the Hermite interpolate

$\overline{H}(x, z)$ can be expressed as

$$\begin{aligned}
& \overline{H}(x, \mathcal{Z}(s)) \\
&= \tilde{u}_{xx}(x, \mathcal{Z}(0)) + \tilde{u}_{xxz}(x, \mathcal{Z}(0))[\mathcal{Z}(s) - \mathcal{Z}(0)] + \frac{1}{2}\tilde{u}_{xxzz}(x, \mathcal{Z}(0))[\mathcal{Z}(s) - \mathcal{Z}(0)]^2 \\
&\quad + \frac{\tilde{u}_{xx}(x, \mathcal{Z}(t_1)) - \tilde{u}_{xx}(x, \mathcal{Z}(0))}{\tau_z^3}[\mathcal{Z}(s) - \mathcal{Z}(0)]^3. \\
&\quad + \frac{-\tilde{u}_{xxz}(x, \mathcal{Z}(0))\tau_z - \frac{1}{2}\tilde{u}_{xxzz}(x, \mathcal{Z}(0))\tau_z^2}{\tau_z^3}[\mathcal{Z}(s) - \mathcal{Z}(0)]^3.
\end{aligned} \tag{6.9}$$

The error function $R(s)$ of the Hermite interpolation is given by [54]

$$\begin{aligned}
R(s) : &= \tilde{u}_{xx}(x, \mathcal{Z}(s)) - \overline{H}(x, \mathcal{Z}(s)) \\
&= \frac{1}{24}\tilde{u}_{xxxxz}(x, \mathcal{Z}(\eta))[\mathcal{Z}(s) - \mathcal{Z}(0)]^3[\mathcal{Z}(s) - \mathcal{Z}(t_1)], \quad \eta \in [0, t_1].
\end{aligned} \tag{6.10}$$

Using $\tilde{u}(x, \mathcal{Z}(0)) = 0$, we get

$$\tilde{u}_x(x, \mathcal{Z}(0)) = \lim_{h \rightarrow 0} \frac{\tilde{u}(x+h, \mathcal{Z}(0)) - \tilde{u}(x, \mathcal{Z}(0))}{h} = 0,$$

and similarly $\tilde{u}_{xx}(x, \mathcal{Z}(0)) = 0$. Likewise, $\tilde{u}_z(x, \mathcal{Z}(0)) = 0$ leads to $\tilde{u}_{zx}(x, \mathcal{Z}(0)) = \tilde{u}_{zxx}(x, \mathcal{Z}(0)) = \tilde{u}_{xxz}(x, \mathcal{Z}(0)) = 0$; while $\tilde{u}_{zz}(x, \mathcal{Z}(0)) = 0$ leads to $\tilde{u}_{zzx}(x, \mathcal{Z}(0)) = \tilde{u}_{zzxx}(x, \mathcal{Z}(0)) = \tilde{u}_{xxzz}(x, \mathcal{Z}(0)) = 0$. Therefore, noting (6.9) we have

$$\tilde{u}_{xx}(x, \mathcal{Z}(s)) \approx \overline{H}(x, \mathcal{Z}(s)) = \frac{\tilde{u}_{xx}(x, \mathcal{Z}(t_1))}{\tau_z^3}[\mathcal{Z}(s) - \mathcal{Z}(0)]^3. \tag{6.11}$$

Upon substituting (6.11) into (6.8), we find, using the transformation $y = \frac{\mathcal{Z}(s) - \mathcal{Z}(0)}{\tau_z}$,

$$\begin{aligned}
& {}^{RL}I_{t;[\mathcal{Z}(t),1]}^\gamma u_{xx}(x, t_1) \\
& \approx \frac{1}{\Gamma(\gamma)} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t_1)} \frac{\overline{H}(x, \mathcal{Z}(s))}{[\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{1-\gamma}} d\mathcal{Z}(s) \\
& = \frac{1}{\Gamma(\gamma)} \frac{\tilde{u}_{xx}(x, \mathcal{Z}(t_1))}{\tau_z^3} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t_1)} [\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{\gamma-1} [\mathcal{Z}(s) - \mathcal{Z}(0)]^3 d\mathcal{Z}(s) \\
& = \frac{1}{\Gamma(\gamma)} \frac{\tilde{u}_{xx}(x, \mathcal{Z}(t_1))}{\tau_z^3} \int_0^1 (\tau_z - y\tau_z)^{\gamma-1} (y\tau_z)^3 \tau_z dy \\
& = \frac{\tilde{u}_{xx}(x, \mathcal{Z}(t_1)) \tau_z^\gamma}{\Gamma(\gamma)} \int_0^1 (1-y)^{\gamma-1} y^3 dy \\
& = \frac{6\tau_z^\gamma}{\Gamma(\gamma+4)} \tilde{u}_{xx}(x, \mathcal{Z}(t_1)).
\end{aligned} \tag{6.12}$$

To compute the approximation error in (6.12), noting (6.10) we get

$$\begin{aligned}
& \left| {}^{RL}I_{t;[\mathcal{Z}(t),1]}^\gamma u_{xx}(x, t_1) - \frac{6\tau_z^\gamma u_{xx}(x, t_1)}{\Gamma(\gamma+4)} \right| \\
& = \left| \frac{1}{\Gamma(\gamma)} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t_1)} \frac{R(s)}{[\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{1-\gamma}} d\mathcal{Z}(s) \right| \\
& \leq \frac{C_4}{24\Gamma(\gamma)} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t_1)} [\mathcal{Z}(s) - \mathcal{Z}(0)]^3 [\mathcal{Z}(t_1) - \mathcal{Z}(s)] [\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{\gamma-1} d\mathcal{Z}(s) \tag{6.13} \\
& \leq \frac{9C_4\tau_z^4}{2048\Gamma(\gamma)} \int_{\mathcal{Z}(0)}^{\mathcal{Z}(t_1)} [\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{\gamma-1} d\mathcal{Z}(s) \\
& \leq \frac{9C_4\tau_z^{4+\gamma}}{2048\Gamma(\gamma+1)},
\end{aligned}$$

where we have used the facts $C_4 = \max_{(x,z) \in [a,b] \times [\mathcal{Z}(0), \mathcal{Z}(t_1)]} |\tilde{u}_{xxxxx}(x, z)|$ and $[\mathcal{Z}(s) - \mathcal{Z}(0)]^3 [\mathcal{Z}(t_1) - \mathcal{Z}(s)] \leq \frac{27}{256} \tau_z^4$ in the above computation. This completes the proof.

■

Theorem 6.3. Let $0 < \gamma < 1$. Suppose that $\tilde{u}(x, z) \in C^{(2,4)}([a, b] \times [\mathcal{Z}(0), \mathcal{Z}(t_2)])$ and $\frac{\partial^k}{\partial z^k} \tilde{u} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1, 2$. Then, we have

$$\left| {}^{RL}_0 I_{t;[\mathcal{Z}(t),1]}^\gamma u_{xx}(x, t_2) - \frac{6(2\tau_z)^\gamma}{\Gamma(\gamma+4)} u_{xx}(x, t_2) \right| = O(\tau_z^{4+\gamma}). \quad (6.14)$$

Proof. The proof of Theorem 6.3 is similar with Theorem 6.2. ■

So far we have established the fourth order approximation for the generalized Riemann-Liouville fractional derivatives and the generalized Caputo fractional derivatives (Theorem 6.1 and Corollary 6.1), as well as the approximation for the generalized Riemann-Liouville fractional integral at $t = t_1$ and $t = t_2$ (Theorem 6.2 and 6.3). The next lemma will give the approximation for the second order derivative by compact finite difference method. For this, we introduce some notations as follows.

For any $y \in \mathcal{U}_P$, we define the *average operator* $\mathcal{H}$ by

$$\mathcal{H}y_m = \begin{cases} \frac{1}{12}(y_{m-1} + 10y_m + y_{m+1}) = \left(I + \frac{h^2}{12}\delta_x^2\right)y_m, & 1 \leq m \leq M-1, \\ y_m, & m = 0, M. \end{cases} \quad (6.15)$$

Lemma 6.1. [85] For a fixed t_n , if $u(x, t_n) \in C^{(6)}[a, b]$, then for $1 \leq m \leq M-1$, we have

$$\mathcal{H} \frac{\partial^2 u(x_m, t_n)}{\partial x^2} = \frac{u(x_{m-1}, t_n) - 2u(x_m, t_n) + u(x_{m+1}, t_n)}{h^2} + O(h^4) = \delta_x^2 u_m^n + O(h^4). \quad (6.16)$$

We are now ready to derive a numerical scheme for the equivalent problem (5.3). To begin, we discretize (5.3) at (x_m, t_n) to get

$${}_0^C D_{t;[\mathcal{Z}(t),1]}^\gamma u(x_m, t_n) = d \frac{\partial^2 u(x_m, t_n)}{\partial x^2} + f(x_m, t_n), \quad (6.17)$$

Since the gWSGD approximation (6.6) is applicable for $n \geq 3$, we first deal with (6.17) at $t = t_1$ and $t = t_2$, i.e.,

$${}_0^C D_{t;[\mathcal{Z}(t),1]}^\gamma u(x_m, t_1) = d \frac{\partial^2 u(x_m, t_1)}{\partial x^2} + f(x_m, t_1). \quad (6.18)$$

$${}_0^C D_{t;[\mathcal{Z}(t),1]}^\gamma u(x_m, t_2) = d \frac{\partial^2 u(x_m, t_2)}{\partial x^2} + f(x_m, t_2). \quad (6.19)$$

Applying the generalized Riemann-Liouville fractional integral operator on both sides of (6.18) and (6.19) and then using Theorem 5.3 and Theorems 6.2–6.3, we obtain

$$u(x_m, t_1) = \frac{6d\tau_z^\gamma}{\Gamma(\gamma+4)} u_{xx}(x_m, t_1) + F(x_m, t_1) + O(\tau_z^{4+\gamma}), \quad (6.20)$$

$$u(x_m, t_2) = \frac{6d(2\tau_z)^\gamma}{\Gamma(\gamma+4)} u_{xx}(x_m, t_2) + F(x_m, t_2) + O(\tau_z^{4+\gamma}), \quad (6.21)$$

where

$$F(x_m, t_1) = {}_0^{RL} I_{t;[\mathcal{Z}(t),1]}^\gamma f(x_m, t_1), \quad F(x_m, t_2) = {}_0^{RL} I_{t;[\mathcal{Z}(t),1]}^\gamma f(x_m, t_2). \quad (6.22)$$

Now, applying the average operator $\mathcal{H}$ to (6.20) and (6.21), and then dividing the equations by τ_z^α and $(2\tau_z)^{2\alpha}$ respectively, we get, in view of 6.1,

$$\frac{1}{\tau_z^\gamma} \mathcal{H} u_m^1 = \frac{6d}{\Gamma(\gamma+4)} \delta_x^2 u_m^1 + \frac{1}{\tau_z^\gamma} \mathcal{H} F_m^1 + O(\tau_z^4 + h^4), \quad (6.23)$$

$$\frac{1}{(2\tau_z)^\gamma} \mathcal{H} u_m^2 = \frac{6d}{\Gamma(\gamma+4)} \delta_x^2 u_m^2 + \frac{1}{(2\tau_z)^\gamma} \mathcal{H} F_m^2 + O(\tau_z^4 + h^4), \quad (6.24)$$

Next, for the discretized equation (6.17) where $n \geq 3$, we first use the gWSGD approximation (6.6) for the generalized Caputo fractional derivative, and then apply the average operator $\mathcal{H}$ throughout. Noting Lemma 6.1, this leads to

$$\frac{1}{\tau_z^\gamma} \sum_{k=0}^n c_k^\gamma \mathcal{H} u_m^{n-k} = d \delta_x^2 u_m^n + \mathcal{H} f_m^n + O(\tau_z^4 + h^4), \quad n \geq 3. \quad (6.25)$$

Omitting the truncation errors in (6.23)-(6.25), we finally get the following numerical scheme:

$$\left\{ \begin{array}{ll} \frac{1}{\tau_z^\gamma} \mathcal{H}u_m^1 = \frac{6d}{\Gamma(\gamma+4)} \delta_x^2 u_m^1 + \frac{1}{\tau_z^\gamma} \mathcal{H}F_m^1, & 1 \leq m \leq M-1, \quad n=1, \\ \frac{1}{(2\tau_z)^\gamma} \mathcal{H}u_m^2 = \frac{6d}{\Gamma(\gamma+4)} \delta_x^2 u_m^2 + \frac{1}{(2\tau_z)^\gamma} \mathcal{H}F_m^2, & 1 \leq m \leq M-1, \quad n=2, \\ \frac{1}{\tau_z^\gamma} \sum_{k=0}^n c_k^\gamma \mathcal{H}u_m^{n-k} = d\delta_x^2 u_m^n + \mathcal{H}f_m^n, & 1 \leq m \leq M-1, \quad n \geq 3, \\ u_m^0 = 0, & 1 \leq m \leq M-1, \\ u_0^n = g_1^n, \quad u_M^n = g_2^n, & 0 \leq n \leq N, \end{array} \right. \quad (6.26)$$

where $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{N}$, c_k^γ is given in (4.11) and $F(x_m, t_1), F(x_m, t_2)$ are given in (6.22).

The proposed numerical scheme (6.26) has a *unique solution* at each time level $t = t_n$, $1 \leq n \leq N$ since the coefficient matrix is easily seen to be strictly diagonally dominant. To implement the numerical scheme (6.26), we first solve for u_m^1 , $1 \leq m \leq M-1$; thereafter, we can get u_m^2 , $1 \leq m \leq M-1$. Continuing in this manner, we can obtain the numerical solution u_m^n , $1 \leq m \leq M-1$, $1 \leq n \leq N$ of the problem (5.3). The numerical solution $\{V_m^n\}$ of the original problem (5.1) is then computed from the relation $u(x, t) = \mathcal{W}(t)V(x, t) - \mathcal{W}(0)V_0(x)$.

6.2 A Priori Estimate

In this section, we shall establish an a priori estimate for the solution of a related numerical scheme of (6.26). This result will be used in the stability and convergence analysis in the next section. For any $y, \hat{y} \in \mathcal{U}_P$, we define

$$(y, \hat{y})_H = (\mathcal{H}y, \hat{y}), \quad (6.27)$$

where the average operator $\mathcal{H}$ is given in (6.15). Obviously, $(\cdot, \cdot)_H$ is an inner product, so let $\|y\|_H = \sqrt{(y, y)_H}$ denote the induced norm.

We shall now present 3 lemmas which will be used to establish the a priori estimate in Theorem 6.4.

Lemma 6.2. [49] *Let $u \in \mathcal{U}_P$. Then we have*

$$\frac{2}{3}\|u\|^2 \leq (\mathcal{H}u, u) \leq \|u\|^2, \quad \|\delta_x^2 u\| \leq \frac{2}{h}|u|_1. \quad (6.28)$$

Lemma 6.3. *Let $\gamma^{**} = 0.83273597$. If $\gamma \in (0, \gamma^{**}]$, then for any positive integer N and real vector $(u^0, u^1, \dots, u^N) \in \mathcal{R}^{N+1}$, it holds that*

$$\sum_{n=0}^N \left(\sum_{k=0}^n c_k^\gamma u^{n-k} \right) u^n \geq 0, \quad (6.29)$$

where $\{c_k^\gamma\}_{k=0}^\infty$ be defined as in (4.11).

Proof. For notational simplicity, we denote $c_k = c_k^\gamma$. As in [57, 125], it suffices to prove that the following symmetric Toeplitz matrix W_1 is positive semi-definite

$$W_1 = \begin{pmatrix} c_0 & \frac{c_1}{2} & \frac{c_2}{2} & \dots & \frac{c_{N-1}}{2} & \frac{c_N}{2} \\ \frac{c_1}{2} & c_0 & \frac{c_1}{2} & \dots & \frac{c_{N-2}}{2} & \frac{c_{N-1}}{2} \\ \frac{c_2}{2} & \frac{c_1}{2} & c_0 & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \frac{c_1}{2} & \frac{c_2}{2} \\ \frac{c_{N-1}}{2} & \frac{c_{N-2}}{2} & \dots & \frac{c_1}{2} & c_0 & \frac{c_1}{2} \\ \frac{c_N}{2} & \frac{c_{N-1}}{2} & \dots & \frac{c_2}{2} & \frac{c_1}{2} & c_0 \end{pmatrix}. \quad (6.30)$$

The generating function [57, 125] of W_1 is given by [57, 125]

$$\begin{aligned}
y(x, \gamma) &= c_0 + \frac{1}{2} \sum_{k=1}^{\infty} c_k e^{ikx} + \frac{1}{2} \sum_{k=1}^{\infty} c_k e^{-ikx} \\
&= \lambda_0 g_0^\gamma + \frac{1}{2} (\lambda_0 g_1^\gamma + \lambda_{-1} g_0^\gamma) e^{ix} + \frac{1}{2} (\lambda_0 g_2^\gamma + \lambda_{-1} g_1^\gamma + \lambda_{-2} g_0^\gamma) e^{i2x} \\
&\quad + \frac{1}{2} \sum_{k=3}^{\infty} (\lambda_0 g_k^\gamma + \lambda_{-1} g_{k-1}^\gamma + \lambda_{-2} g_{k-2}^\gamma + \lambda_{-3} g_{k-3}^\gamma) e^{ikx} \\
&\quad + \frac{1}{2} (\lambda_0 g_1^\gamma + \lambda_{-1} g_0^\gamma) e^{-ix} + \frac{1}{2} (\lambda_0 g_2^\gamma + \lambda_{-1} g_1^\gamma + \lambda_{-2} g_0^\gamma) e^{-i2x} \\
&\quad + \frac{1}{2} \sum_{k=3}^{\infty} (\lambda_0 g_k^\gamma + \lambda_{-1} g_{k-1}^\gamma + \lambda_{-2} g_{k-2}^\gamma + \lambda_{-3} g_{k-3}^\gamma) e^{-ikx} \\
&= \frac{1}{2} (\lambda_0 + \lambda_{-1} e^{ix} + \lambda_{-2} e^{i2x} + \lambda_{-3} e^{i3x}) \sum_{k=0}^{\infty} g_k^\gamma e^{ikx} \\
&\quad + \frac{1}{2} (\lambda_0 + \lambda_{-1} e^{-ix} + \lambda_{-2} e^{-i2x} + \lambda_{-3} e^{-i3x}) \sum_{k=0}^{\infty} g_k^\gamma e^{-ikx}.
\end{aligned} \tag{6.31}$$

Obviously, $y(x, \gamma)$ is a real-valued and even function of x on $[-\pi, \pi]$, so we just consider its principle value on $[0, \pi]$. Applying the formula

$$(1 - e^{\pm ix})^\gamma = \left(2 \sin \frac{x}{2}\right)^\gamma e^{\pm i\gamma(\frac{x}{2} - \frac{\pi}{2})}, \tag{6.32}$$

it follows from (6.31) that

$$\begin{aligned}
y(x, \gamma) &= \left(2 \sin \frac{x}{2}\right)^\gamma \left[\lambda_0 \cos \left(\frac{x\gamma}{2} - \frac{\pi\gamma}{2} \right) + \lambda_{-1} \cos \left(x + \frac{x\gamma}{2} - \frac{\pi\gamma}{2} \right) \right. \\
&\quad \left. + \lambda_{-2} \cos \left(2x + \frac{x\gamma}{2} - \frac{\pi\gamma}{2} \right) + \lambda_{-3} \cos \left(3x + \frac{x\gamma}{2} - \frac{\pi\gamma}{2} \right) \right].
\end{aligned} \tag{6.33}$$

Since it is difficult to analyze the property of $y(x, \gamma)$ analytically, we shall analyze it numerically. Figure 6.1 shows that $y(x, \gamma) \leq 0$ on a very small domain. To depict the values of $y(x, \gamma)$ clearly, we draw the contours of the function $y(x, \gamma)$ in Figure 6.2. Let γ^{**} be such that $y(x, \gamma) \geq 0$ for $\gamma \in (0, \gamma^{**}]$ and $x \in [0, \pi]$. So, we consider the tangent line parallel to the x -axis of the curve $y(x, \gamma)$ and solve the

system

$$y(x, \gamma) = 0, \quad y_x(x, \gamma) = 0.$$

By Newton iteration method, we obtain the solution $(x^*, \gamma^{**}) = (1.44368825, 0.83273597)$, which is the tangent point in Figure 6.2. Thus, $y(x, \gamma) \geq 0$ for $\gamma \in (0, \gamma^{**}]$. The lemma follows as a result of the Grenander-Szegö Theorem [20]. ■

FIGURE 6.1: The generating function $y(x, \gamma)$

FIGURE 6.2: Contours of the generating function $y(x, \gamma)$ for $\gamma \in (0, 1)$ and $x \in [0, \pi]$

Lemma 6.4. *Let $0 < \gamma < 1$. We have*

$$\frac{c_0^\gamma}{\Gamma(\gamma+4)} > \frac{1}{15}, \quad 2c_0^\gamma - |c_1^\gamma| > 0, \quad (6.34)$$

where c_0^γ and c_1^γ are defined in (4.11).

Proof. From (2.29), (4.5) and (4.11), we have

$$c_0^\gamma = \frac{1}{48}(\gamma^3 + 11\gamma^2 + 40\gamma + 48), \quad c_1^\gamma = \frac{1}{48}(-\gamma^4 - 14\gamma^3 - 67\gamma^2 - 110\gamma). \quad (6.35)$$

First, using an inequality of the Gamma function [53]

$$n^{1-\gamma} < \frac{\Gamma(n+1)}{\Gamma(n+\gamma)} < (n+1)^{1-\gamma}, \quad 0 < \gamma < 1, \quad n = 1, 2, \dots$$

with $n = 4$, we get $4^{1-\gamma} < \frac{\Gamma(5)}{\Gamma(\gamma+4)} < 5^{1-\gamma}$, or

$$\frac{1}{6 \cdot 4^\gamma} < \frac{1}{\Gamma(\gamma+4)} < \frac{5}{24 \cdot 5^\gamma}.$$

Hence,

$$\frac{5c_0^\gamma}{\Gamma(\gamma+4)} > \frac{5c_0^\gamma}{6 \cdot 4^\gamma}. \quad (6.36)$$

Let

$$y(\gamma) = 5c_0^\gamma - 2 \cdot 4^\gamma = \frac{5}{48}(\gamma^3 + 11\gamma^2 + 40\gamma + 48) - 2 \cdot 4^\gamma.$$

It is easy to check that the function $y(\gamma)$ is monotonely increasing for $\gamma \in (0, \gamma_0)$ and monotonely decreasing for $\gamma \in (\gamma_0, 1)$, for some $\gamma_0 \in (0, 1)$. Noting that $y(0) = 3$ and $y(1) = \frac{29}{12}$, we see that $y(\gamma) > y(1) = \frac{29}{12} > 0$ for $\gamma \in (0, 1)$. Using this, it then follows from (6.36) that

$$\frac{5c_0^\gamma}{\Gamma(\gamma+4)} > \frac{2 \cdot 4^\gamma}{6 \cdot 4^\gamma} = \frac{1}{3},$$

which yields the first inequality in (6.35). Next, let

$$\hat{y}(\gamma) = 2c_0^\gamma - |c_1^\gamma| = \frac{1}{48}(-\gamma^4 - 12\gamma^3 - 45\gamma^2 - 30\gamma + 96).$$

It is easy to check that $\hat{y}(\gamma)$ is monotonely decreasing for $\gamma \in (0, 1)$. Hence, we have

$$\hat{y}(\gamma) \geq \hat{y}(1) = \frac{1}{6} > 0,$$

which is the second inequality in (6.35). ■

We are now ready to obtain an a priori estimate for the solution of a related scheme of (6.26). Our proof is accomplished by the energy method.

Theorem 6.4. (A priori estimate) *Let u_m^n denote the solution of the following scheme:*

$$\left\{ \begin{array}{ll} \frac{1}{\tau_z^\gamma} \mathcal{H}u_m^1 = \frac{6d}{\Gamma(\gamma+4)} \delta_x^2 u_m^1 + \bar{f}_m^1, & 1 \leq m \leq M-1, \quad n=1, \\ \frac{1}{(2\tau_z)^\gamma} \mathcal{H}u_m^2 = \frac{6d}{\Gamma(\gamma+4)} \delta_x^2 u_m^2 + \bar{f}_m^2, & 1 \leq m \leq M-1, \quad n=2, \\ \frac{1}{\tau_z^\gamma} \sum_{k=0}^n c_k^\gamma \mathcal{H}u_m^{n-k} = d\delta_x^2 u_m^n + \bar{f}_m^n, & 1 \leq m \leq M-1, \quad n \geq 3, \\ u_m^0 = \eta_m, & 1 \leq m \leq M-1, \\ u_0^n = 0, \quad u_M^n = 0, & 1 \leq n \leq N. \end{array} \right. \quad (6.37)$$

Suppose $\gamma \in (0, \gamma^{**}]$. For $1 \leq n \leq N$, we have

$$\sum_{i=1}^n |u^i|_1^2 \leq C_5 \sum_{i=1}^n \|\bar{f}^i\|^2 + C_6 |u^0|_1^2, \quad (6.38)$$

where C_5 and C_6 are positive constants.

Proof. First, we need to obtain 6 inequalities in a series of steps.

Step 1. Multiplying the third equation of (6.37) by $\frac{h}{d} \mathcal{H}u_m^n$ and summing m from 1 to $M-1$, we obtain

$$\frac{1}{d\tau_z^\gamma} \sum_{k=0}^n c_k^\gamma (\mathcal{H}u^n, \mathcal{H}u^{n-k}) - (u^n, \delta_x^2 u^n)_H = \frac{1}{d} (u^n, \bar{f}^n)_H. \quad (6.39)$$

For the second term on the left side of (6.39), using Lemma 6.2 we find

$$\begin{aligned}
-(u^n, \delta_x^2 u^n)_H &= -(u^n, \delta_x^2 u^n) - \frac{h^2}{12} (\delta_x^2 u^n, \delta_x^2 u^n) \\
&= |u^n|_1^2 - \frac{h^2}{12} \|\delta_x^2 u^n\|^2 \\
&\geq |u^n|_1^2 - \frac{h^2}{12} \left(\frac{2}{h} |u^n|_1 \right)^2 \\
&= \frac{2}{3} |u^n|_1^2.
\end{aligned} \tag{6.40}$$

For the term on the right side of (6.39), applying the inequality $xy \leq \frac{1}{2}(x^2 + y^2)$ and Lemma 5.3 and 6.2, we get

$$\begin{aligned}
\frac{1}{d} (u^n, \bar{f}^n)_H &\leq \frac{1}{d} \|u^n\|_H \cdot \|\bar{f}^n\|_H \\
&\leq \frac{1}{d} \left[\frac{2d}{(b-a)^2} \|u^n\|_H^2 + \frac{(b-a)^2}{8d} \|\bar{f}^n\|_H^2 \right] \\
&\leq \frac{1}{d} \left[\frac{2d}{(b-a)^2} \|u^n\|^2 + \frac{(b-a)^2}{8d} \|\bar{f}^n\|^2 \right] \\
&\leq \frac{1}{3} |u^n|_1^2 + \frac{(b-a)^2}{8d^2} \|\bar{f}^n\|^2.
\end{aligned} \tag{6.41}$$

Substituting (6.40) and (6.41) into (6.39) gives

$$\frac{1}{d\tau_z^\gamma} \sum_{k=0}^n c_k^\gamma (\mathcal{H}u^n, \mathcal{H}u^{n-k}) + \frac{1}{3} |u^n|_1^2 \leq \frac{(b-a)^2}{8d^2} \|\bar{f}^n\|^2. \tag{6.42}$$

Now, replacing n by i in (6.42) and then summing i from 3 to n , we obtain

$$\frac{1}{d\tau_z^\gamma} \sum_{i=3}^n \sum_{k=0}^i c_k^\gamma (\mathcal{H}u^i, \mathcal{H}u^{i-k}) + \frac{1}{3} \sum_{i=3}^n |u^i|_1^2 \leq \frac{(b-a)^2}{8d} \sum_{i=3}^n \|\bar{f}^i\|^2. \tag{6.43}$$

Step 2. Multiplying the first equation of (6.37) by $\frac{hc_0^\gamma}{d} \mathcal{H}u_m^1$ and summing m from 1 to $M-1$, we obtain

$$\frac{1}{d\tau_z^\gamma} c_0^\gamma (\mathcal{H}u^1, \mathcal{H}u^1) - \frac{6c_0^\gamma}{\Gamma(\gamma+4)} (u^1, \delta_x^2 u^1)_H = \frac{c_0^\gamma}{d} (u^1, \bar{f}^1)_H. \tag{6.44}$$

For the second term on the left side of (6.44), similar to (6.40), we get

$$-\frac{6c_0^\gamma}{\Gamma(\gamma+4)}(u^1, \delta_x^2 u^1)_H \geq \frac{4c_0^\gamma}{\Gamma(\gamma+4)}|u^1|_1^2. \quad (6.45)$$

Consider the term on the right side of (6.44). For $\sigma_1 > 0$, we find, together with the use of Lemmas 5.3 and 6.2,

$$\begin{aligned} \frac{c_0^\gamma}{d}(u^1, \bar{f}^1)_H &\leq \frac{c_0^\gamma}{d}\|u^1\|_H \cdot \|\bar{f}^1\|_H \\ &\leq \frac{c_0^\gamma}{d} \left(\sigma_1 \|u^1\|_H^2 + \frac{1}{4\sigma_1} \|\bar{f}^1\|_H^2 \right) \\ &\leq \frac{c_0^\gamma}{d} \left(\sigma_1 \|u^1\|^2 + \frac{1}{4\sigma_1} \|\bar{f}^1\|^2 \right) \\ &\leq \frac{\sigma_1(b-a)^2 c_0^\gamma}{6d} |u^1|_1^2 + \frac{c_0^\gamma}{4\sigma_1 d} \|\bar{f}^1\|^2, \end{aligned} \quad (6.46)$$

Substituting (6.45) and (6.46) into (6.44), and taking $\sigma_1 = \frac{6d}{(b-a)^2 \Gamma(\gamma+4)}$, we get

$$\frac{1}{d\tau_z^\gamma} c_0^\gamma(\mathcal{H}u^1, \mathcal{H}u^1) + \frac{3c_0^\gamma}{\Gamma(\gamma+4)} |u^1|_1^2 \leq \frac{c_0^\gamma(b-a)^2 \Gamma(\gamma+4)}{24d^2} \|\bar{f}^1\|^2. \quad (6.47)$$

Multiplying $(13 \cdot 2^\gamma)$ on both sides of (6.47) gives

$$\frac{13 \cdot 2^\gamma}{d\tau_z^\gamma} c_0^\gamma(\mathcal{H}u^1, \mathcal{H}u^1) + \frac{39 \cdot 2^\gamma c_0^\gamma}{\Gamma(\gamma+4)} |u^1|_1^2 \leq \frac{13 \cdot 2^\gamma c_0^\gamma(b-a)^2 \Gamma(\gamma+4)}{24d^2} \|\bar{f}^1\|^2. \quad (6.48)$$

Since $\frac{13 \cdot 2^\gamma}{d\tau_z^\gamma} c_0^\gamma(\mathcal{H}u^1, \mathcal{H}u^1) \geq \frac{1}{d\tau_z^\gamma} c_0^\gamma(\mathcal{H}u^1, \mathcal{H}u^1) \geq 0$, it follows from (6.48) that

$$\frac{1}{d\tau_z^\gamma} c_0^\gamma(\mathcal{H}u^1, \mathcal{H}u^1) + \frac{39 \cdot 2^\gamma c_0^\gamma}{\Gamma(\gamma+4)} |u^1|_1^2 \leq \frac{13 \cdot 2^\gamma c_0^\gamma(b-a)^2 \Gamma(\gamma+4)}{24d^2} \|\bar{f}^1\|^2. \quad (6.49)$$

Step 3. Multiplying the first equation of (6.37) by $\frac{hc_1^\gamma}{d} \mathcal{H}u_m^0$ and summing m from 1 to $M-1$, we obtain

$$\frac{1}{d\tau_z^\gamma} c_1^\gamma(\mathcal{H}u^0, \mathcal{H}u^1) - \frac{6c_1^\gamma}{\Gamma(\gamma+4)}(u^0, \delta_x^2 u^1)_H = \frac{c_1^\gamma}{d}(u^0, \bar{f}^1)_H. \quad (6.50)$$

For the second term on the left hand of (6.50), using Lemma 6.2 then we have

$$\begin{aligned}
-\frac{6c_1^\gamma}{\Gamma(\gamma+4)}(u^0, \delta_x^2 u^1)_H &= -\frac{6c_1^\gamma}{\Gamma(\gamma+4)} \left[(u^0, \delta_x^2 u^1) + \frac{h^2}{12} (\delta_x^2 u^0, \delta_x^2 u^1) \right] \\
&\geq -\frac{6c_1^\gamma}{\Gamma(\gamma+4)} \left[-(\delta_x u^0, \delta_x u^1) + \frac{h^2}{12} \|\delta_x^2 u^0\| \cdot \|\delta_x^2 u^1\| \right] \\
&\geq -\frac{6c_1^\gamma}{\Gamma(\gamma+4)} \left(|u^0|_1 \cdot |u^1|_1 + \frac{h^2}{12} \cdot \frac{2}{h} |u^0|_1 \cdot \frac{2}{h} |u^1|_1 \right) \\
&\geq -\frac{4|c_1^\gamma|}{\Gamma(\gamma+4)} \left(\sigma_2 |u^1|_1^2 + \frac{1}{\sigma_2} |u^0|_1^2 \right),
\end{aligned} \tag{6.51}$$

where $\sigma_2 > 0$. For the term on the right side of (6.50), similar to (6.41), we obtain

$$\frac{c_1^\gamma}{d}(u^0, \bar{f}^1)_H \leq \frac{|c_1^\gamma|^2}{3} |u^0|_1^2 + \frac{(b-a)^2}{8d^2} \|\bar{f}^1\|^2. \tag{6.52}$$

Now, substituting (6.51) and (6.52) into (6.50), and taking $\sigma_2 = \frac{2^\gamma}{4}$, we obtain

$$\frac{1}{d\tau_z^\gamma} c_1^\gamma (\mathcal{H}u^0, \mathcal{H}u^1) - \frac{2^\gamma |c_1^\gamma|}{\Gamma(\gamma+4)} |u^1|_1^2 \leq \left[\frac{2^{4-\gamma} |c_1^\gamma|}{\Gamma(\gamma+4)} + \frac{|c_1^\gamma|^2}{3} \right] |u^0|_1^2 + \frac{(b-a)^2}{8d^2} \|\bar{f}^1\|^2. \tag{6.53}$$

Step 4. Multiplying the second equation of (6.37) by $\frac{2^\gamma h c_0^\gamma}{d} \mathcal{H}u_m^2$ and summing m from 1 to $M-1$, we obtain

$$\frac{1}{d\tau_z^\gamma} c_0^\gamma (\mathcal{H}u^2, \mathcal{H}u^2) - \frac{2^\gamma 6c_0^\gamma}{\Gamma(\gamma+4)} (u^2, \delta_x^2 u^2)_H = \frac{2^\gamma c_0^\gamma}{d} (u^2, \bar{f}^2)_H. \tag{6.54}$$

For the second term on the left hand of (6.54), similar to (6.40), we get

$$-\frac{2^\gamma 6c_0^\gamma}{\Gamma(\gamma+4)} (u^2, \delta_x^2 u^2)_H \geq \frac{2^\gamma 4c_0^\gamma}{\Gamma(\gamma+4)} |u^2|_1^2. \tag{6.55}$$

Consider the term on the right hand of (6.54). For $\sigma_3 > 0$, similar to (6.46), we find

$$\frac{2^\gamma c_0^\gamma}{d} (u^2, \bar{f}^2)_H \leq \frac{2^\gamma c_0^\gamma (b-a)^2 \sigma_3}{12d} |u^2|_1^2 + \frac{2^\gamma c_0^\gamma}{2d\sigma_3} \|\bar{f}^2\|^2. \tag{6.56}$$

Substituting (6.55) and (6.56) into (6.54), and taking $\sigma_3 = \frac{6 \cdot d}{(b-a)^2 \Gamma(\gamma+4)}$, we obtain

$$\frac{1}{d\tau_z^\gamma} c_0^\gamma (\mathcal{H}u^2, \mathcal{H}u^2) + \left[\frac{4 \cdot 2^\gamma c_0^\gamma}{\Gamma(\gamma+4)} - \frac{2^\gamma c_0^\gamma}{2\Gamma(\gamma+4)} \right] |u^2|_1^2 \leq \frac{2^\gamma c_0^\gamma (b-a)^2 \Gamma(\gamma+4)}{12d^2} \|\bar{f}^2\|^2. \tag{6.57}$$

Step 5. Multiplying the second equation of (6.37) by $\frac{2^\gamma hc_1^\gamma}{d} \mathcal{H}u_m^1$ and summing m from 1 to $M - 1$, we obtain

$$\frac{1}{d\tau_z^\gamma} c_1^\gamma (\mathcal{H}u^1, \mathcal{H}u^2) - \frac{2^\gamma 6c_1^\gamma}{\Gamma(\gamma + 4)} (u^1, \delta_x^2 u^2)_H = \frac{2^\gamma c_1^\gamma}{d} (u^1, \bar{f}^2)_H. \quad (6.58)$$

For the second term on the left side of (6.58), similar to (6.51), we find $\sigma_4 > 0$,

$$-\frac{2^\gamma 6c_1^\gamma}{\Gamma(\gamma + 4)} (u^1, \delta_x^2 u^2)_H \geq -\frac{2^\gamma 4|c_1^\gamma| \sigma_4}{\Gamma(\gamma + 4)} |u^1|_1^2 - \frac{2^\gamma 4|c_1^\gamma|}{\Gamma(\gamma + 4) \sigma_4} |u^2|_1^2. \quad (6.59)$$

For the term on the right side of (6.58), similar to (6.46), we get for $\sigma_5 > 0$,

$$\frac{2^\gamma c_1^\gamma}{d} (u^1, \bar{f}^2)_H \leq \frac{2^\gamma |c_1^\gamma| \sigma_5 (b - a)^2}{12d} |u^1|_1^2 + \frac{2^\gamma |c_1^\gamma|}{2\sigma_5 d} \|\bar{f}^2\|^2. \quad (6.60)$$

Substituting (6.59) and (6.60) into (6.58), and taking $\sigma_4 = 4, \sigma_5 = \frac{12 \cdot d}{(b-a)^2 \Gamma(\gamma+4)}$ yields

$$\begin{aligned} & \frac{1}{d\tau_z^\gamma} c_1^\gamma (\mathcal{H}u^1, \mathcal{H}u^2) + \left[-\frac{16 \cdot 2^\gamma |c_1^\gamma|}{\Gamma(\gamma + 4)} - \frac{2^\gamma |c_1^\gamma|}{\Gamma(\gamma + 4)} \right] |u^1|_1^2 - \frac{2^\gamma |c_1^\gamma|}{\Gamma(\gamma + 4)} |u^2|_1^2 \\ & \leq \frac{2^\gamma |c_1^\gamma| (b - a)^2 \Gamma(\gamma + 4)}{24d^2} \|\bar{f}^2\|^2. \end{aligned} \quad (6.61)$$

Step 6. Multiplying the second equation of (6.37) by $\frac{2^\gamma hc_2^\gamma}{d} \mathcal{H}u_m^0$ and summing m from 1 to $M - 1$, we obtain

$$\frac{1}{d\tau_z^\gamma} c_2^\gamma (\mathcal{H}u^0, \mathcal{H}u^2) - \frac{2^\gamma 6c_2^\gamma}{\Gamma(\gamma + 4)} (u^0, \delta_x^2 u^2)_H = \frac{2^\gamma c_2^\gamma}{d} (u^0, \bar{f}^2)_H. \quad (6.62)$$

For the second term on the left side of (6.62), similar to (6.51), we get for $\sigma_6 > 0$,

$$-\frac{2^\gamma 6c_2^\gamma}{\Gamma(\gamma + 4)} (u^0, \delta_x^2 u^2)_H \geq -\frac{2^\gamma 4|c_2^\gamma| \sigma_6}{\Gamma(\gamma + 4)} |u^0|_1^2 - \frac{2^\gamma 4|c_2^\gamma|}{\Gamma(\gamma + 4) \sigma_6} |u^2|_1^2. \quad (6.63)$$

For the term on the right side of (6.62), similar to (6.46), we obtain

$$\frac{2^\gamma c_2^\gamma}{d} (u^0, \bar{f}^2)_H \leq \frac{2^\gamma |c_2^\gamma| (b - a)^2}{12d} |u^0|_1^2 + \frac{2^\gamma |c_2^\gamma|}{2d} \|\bar{f}^2\|^2. \quad (6.64)$$

Substituting (6.63) and (6.64) into (6.62), and taking $\sigma_6 = \frac{8|c_2^\gamma|}{c_0^\gamma}$, we get

$$\frac{1}{d\tau_z^\gamma} c_2^\gamma (\mathcal{H}u^0, \mathcal{H}u^2) - \frac{2^\gamma c_0^\gamma}{2\Gamma(\gamma+4)} |u^2|_1^2 \leq \left[\frac{|c_2^\gamma|(b-a)^2}{12d} + \frac{2^{5+\gamma}|c_2^\gamma|^2}{\Gamma(\gamma+4)c_0^\gamma} \right] |u^0|_1^2 + \frac{2^\gamma |c_2^\gamma|}{2d} \|\bar{f}^2\|^2. \quad (6.65)$$

Next, we sum the 6 inequalities obtained in Steps 1–6, viz., (6.43), (6.49), (6.53), (6.57), (6.61) and (6.65), to get

$$\begin{aligned} & \frac{1}{d\tau_z^\gamma} \sum_{i=0}^n \sum_{k=0}^i c_k^\gamma (\mathcal{H}u^i, \mathcal{H}u^{i-k}) + \frac{1}{3} \sum_{i=3}^n |u^i|_1^2 + \left[\frac{39 \cdot 2^\gamma c_0^\gamma}{\Gamma(\gamma+4)} - \frac{18 \cdot 2^\gamma |c_1^\gamma|}{\Gamma(\gamma+4)} \right] |u^1|_1^2 \\ & + \left[\frac{5 \cdot 2^\gamma c_0^\gamma}{2\Gamma(\gamma+4)} - \frac{2^\gamma |c_1^\gamma|}{\Gamma(\gamma+4)} \right] |u^2|_1^2 \\ & \leq \frac{(b-a)^2}{8d} \sum_{i=3}^n \|\bar{f}^i\|^2 + \left[\frac{13 \cdot 2^\gamma c_0^\gamma (b-a)^2 \Gamma(\gamma+4)}{24d^2} + \frac{(b-a)^2}{8d^2} \right] \|\bar{f}^1\|^2 \\ & + \left[\frac{2^\gamma c_0^\gamma (b-a)^2 \Gamma(\gamma+4)}{12K_\gamma^2} + \frac{2^\gamma |c_1^\gamma| (b-a)^2 \Gamma(\gamma+4)}{24d^2} + \frac{2^\gamma |c_2^\gamma|}{2d} \right] \|\bar{f}^2\|^2 \\ & + \left[\frac{2^{4-\gamma} |c_1^\gamma|}{\Gamma(\gamma+4)} + \frac{|c_1^\gamma|^2}{3} + \frac{|c_2^\gamma|(b-a)^2}{12d} + \frac{2^{5+\gamma} |c_2^\gamma|}{c_0^\gamma \Gamma(\gamma+4)} \right] |u^0|_1^2. \end{aligned} \quad (6.66)$$

In view of Lemma 6.3, we have

$$\sum_{i=0}^n \sum_{k=0}^i c_k^\gamma (\mathcal{H}u^i, \mathcal{H}u^{i-k}) \geq 0. \quad (6.67)$$

Moreover, using Lemma 6.4, we find

$$\begin{aligned} & \left[\frac{39 \cdot 2^\gamma c_0^\gamma}{\Gamma(\gamma+4)} - \frac{18 \cdot 2^\gamma |c_1^\gamma|}{\Gamma(\gamma+4)} \right] |u^1|_1^2 + \left[\frac{5 \cdot 2^\gamma c_0^\gamma}{2\Gamma(\gamma+4)} - \frac{2^\gamma |c_1^\gamma|}{\Gamma(\gamma+4)} \right] |u^2|_1^2 \\ & = \left[\frac{18 \cdot 2^\gamma (2c_0^\gamma - |c_1^\gamma|) + 3 \cdot 2^\gamma c_0^\gamma}{\Gamma(\gamma+4)} \right] |u^1|_1^2 + \left[\frac{2^\gamma (2c_0^\gamma - |c_1^\gamma|)}{\Gamma(\gamma+4)} + \frac{2^\gamma c_0^\gamma}{2\Gamma(\gamma+4)} \right] |u^2|_1^2 \\ & \geq \frac{1}{5} |u^1|_1^2 + \frac{1}{30} |u^2|_1^2. \end{aligned} \quad (6.68)$$

Finally, using (6.67) and (6.68) in (6.66), it follows that

$$\begin{aligned}
& \sum_{i=1}^n |u^i|_1^2 \\
& \leq \frac{15(b-a)^2}{4d} \sum_{i=3}^n \|\bar{f}^i\|^2 + \left[\frac{195c_0^\gamma(b-a)^2\Gamma(\gamma+4)}{2^{3-\gamma}d^2} + \frac{15(b-a)^2}{4d^2} \right] \|\bar{f}^1\|^2 \\
& \quad + \left[\frac{5 \cdot 2^\gamma c_0^\gamma(b-a)^2\Gamma(\gamma+4)}{2K_\gamma^2} + \frac{5 \cdot 2^\gamma |c_1^\gamma|(b-a)^2\Gamma(\gamma+4)}{4d^2} + \frac{15 \cdot 2^\gamma |c_2^\gamma|}{d} \right] \|\bar{f}^2\|^2 \\
& \quad + \left[\frac{15 \cdot 2^{5-\gamma} |c_1^\gamma|}{\Gamma(\gamma+4)} + 10|c_1^\gamma|^2 + \frac{5|c_2^\gamma|(b-a)^2}{2d} + \frac{15 \cdot 2^{6+\gamma} |c_2^\gamma|}{c_0^\gamma\Gamma(\gamma+4)} \right] |u^0|_1^2 \\
& \leq C_5 \sum_{i=1}^n \|\bar{f}^i\|^2 + C_6 |u^0|_1^2,
\end{aligned} \tag{6.69}$$

where

$$\begin{aligned}
C_5 &= \max \left\{ \frac{15(b-a)^2}{4d}, \frac{195c_0^\gamma(b-a)^2\Gamma(\gamma+4)}{2^{3-\gamma}d^2} + \frac{15(b-a)^2}{4d^2}, \right. \\
& \quad \left. \frac{5 \cdot 2^\gamma c_0^\gamma(b-a)^2\Gamma(\gamma+4)}{2K_\gamma^2} + \frac{5 \cdot 2^\gamma |c_1^\gamma|(b-a)^2\Gamma(\gamma+4)}{4d^2} + \frac{15 \cdot 2^\gamma |c_2^\gamma|}{d} \right\}, \\
C_6 &= \frac{15 \cdot 2^{5-\gamma} |c_1^\gamma|}{\Gamma(\gamma+4)} + 10|c_1^\gamma|^2 + \frac{5|c_2^\gamma|(b-a)^2}{2d} + \frac{15 \cdot 2^{6+\gamma} |c_2^\gamma|}{c_0^\gamma\Gamma(\gamma+4)}.
\end{aligned} \tag{6.70}$$

This completes the proof. ■

6.3 Stability and Convergence

Using the a priori estimate established in Section 6.2, we shall analyze the stability and convergence of the numerical scheme (6.26) rigorously in this section.

Theorem 6.5. (Stability) *The numerical scheme (6.26) is unconditionally stable with respect to the initial value and the non-homogeneous term f for all $\gamma \in (0, \gamma^{**}]$.*

Proof. Using Lemma 5.3 in (6.38), we have for $1 \leq n \leq N$,

$$\frac{4}{b-a} \sum_{i=1}^n \|u^i\|_\infty^2 \leq C_5 \sum_{i=1}^n \|\bar{f}^i\|^2 + C_6 |u^0|_1^2, \quad (6.71)$$

where

$$\begin{cases} \bar{f}_m^1 = \frac{1}{\tau_z^\gamma} \mathcal{H}F_m^1, & 1 \leq m \leq M-1, \\ \bar{f}_m^2 = \frac{1}{(2\tau_z)^\gamma} \mathcal{H}F_m^2, & 1 \leq m \leq M-1, \\ \bar{f}_m^n = \mathcal{H}f_m^n, & 1 \leq m \leq M-1, \quad 3 \leq n \leq N. \end{cases} \quad (6.72)$$

From (6.22), we find

$$\begin{aligned} F_m^1 &= \frac{1}{\Gamma(\gamma)} \int_0^{t_1} \frac{\mathcal{Z}'(s) f(x_m, s)}{[\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{1-\gamma}} ds \\ &\leq \frac{\hat{f}_m^1}{\Gamma(\gamma)} \int_0^{t_1} \frac{\mathcal{Z}'(s)}{[\mathcal{Z}(t_1) - \mathcal{Z}(s)]^{1-\gamma}} ds \\ &= \frac{\tau_z^\gamma}{\Gamma(\gamma+1)} \hat{f}_m^1, \end{aligned} \quad (6.73)$$

where $\hat{f}_m^1 = \max_{0 \leq t \leq t_1} |f(x_m, t)|$. Similarly, we can get

$$F_m^2 \leq \frac{(2\tau_z)^\gamma}{\Gamma(\gamma+1)} \hat{f}_m^2, \quad (6.74)$$

where $\hat{f}_m^2 = \max_{0 \leq t \leq t_2} |f(x_m, t)|$. Using (6.73) and (6.74) in (6.72), it then follows from (6.71) that

$$\frac{4}{b-a} \sum_{i=1}^n \|u^i\|_\infty^2 \leq C_5 \left[\frac{1}{(\Gamma(\gamma+1))^2} (\|\mathcal{H}\hat{f}^1\|^2 + \|\mathcal{H}\hat{f}^2\|^2) + \sum_{i=3}^n \|\mathcal{H}f^i\|^2 \right] + C_6 |u^0|_1^2. \quad (6.75)$$

The relation (6.75) indicates that the numerical scheme (6.26) is stable with respect to the initial value and the nonlinear term f . ■

Theorem 6.6. (Convergence) Let $U(x, t)$ be the exact solution of (5.3) and $\{u_m^n\}$ be the solution of the numerical scheme (6.26). Let $e_m^n = U(x_m, t_n) - u_m^n$ be the error at (x_m, t_n) , $0 \leq m \leq M$, $0 \leq n \leq N$. Let $\gamma \in (0, \gamma^{**}]$. Suppose that $U(x, \mathcal{Z}^{-1}(z)) = \tilde{U}(x, z) \in C^{(6,6)}([a, b] \times [\mathcal{Z}(0), \mathcal{Z}(T)])$ and $\frac{\partial^k}{\partial z^k} \tilde{U} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1, 2, 3, 4, 6$. Then

we have for $1 \leq n \leq N$,

$$\tau_z \sum_{i=1}^n \|e^i\|_\infty \leq \frac{1}{2} \overline{C}_5 \sqrt{C_5} [\mathcal{Z}(T) - \mathcal{Z}(0)](b-a)(\tau_z^4 + h^4), \quad (6.76)$$

where C_5 and $\overline{C}_5$ are positive finite constants.

Proof. Subtracting (6.26) from (6.23)-(6.25), we obtain

$$\left\{ \begin{array}{ll} \frac{1}{\tau_z^\gamma} \mathcal{H}e_m^1 = \frac{6d}{\Gamma(\gamma+4)} \delta_x^2 e_m^1 + T_m^1, & 1 \leq m \leq M-1, \quad n=1, \\ \frac{1}{(2\tau_z)^\gamma} \mathcal{H}e_m^2 = \frac{6d}{\Gamma(\gamma+4)} \delta_x^2 e_m^2 + T_m^2, & 1 \leq m \leq M-1, \quad n=2, \\ \frac{1}{\tau_z^\gamma} \sum_{k=0}^n c_k^\gamma \mathcal{H}e_m^{n-k} = d \delta_x^2 e_m^n + T_m^n, & 1 \leq m \leq M-1, \quad n \geq 3, \\ e_m^0 = 0, & 1 \leq m \leq M-1, \\ e_0^n = 0, \quad e_M^n = 0, & 0 \leq n \leq N, \end{array} \right. \quad (6.77)$$

where $T_m^n, 1 \leq n \leq N$ are truncation errors and

$$|T_m^n| \leq \overline{C}_5 (\tau_z^4 + h^4) \quad (6.78)$$

for some positive finite constant $\overline{C}_5$.

Applying Theorem 6.4 to the system (6.77) and noting Lemma 5.3 and (6.78), we find for $1 \leq n \leq N$,

$$\begin{aligned} \frac{4\tau_z}{b-a} \sum_{i=1}^n \|e^i\|_\infty^2 &\leq C_5 \tau_z \sum_{i=1}^n \|T^i\|^2 \leq C_5 \tau_z \left[N(b-a) \overline{C}_5^2 (\tau_z^4 + h^4)^2 \right] \\ &\leq C_5 \overline{C}_5^2 [\mathcal{Z}(T) - \mathcal{Z}(0)](b-a)(\tau_z^4 + h^4)^2, \end{aligned} \quad (6.79)$$

Now, using Cauchy-Schwarz inequality and (6.79), we get for $1 \leq n \leq N$,

$$\begin{aligned} \left(\tau_z \sum_{i=1}^n \|e^i\|_\infty \right)^2 &\leq \left(\tau_z \sum_{i=1}^n 1^2 \right) \left(\tau_z \sum_{i=1}^n \|e^i\|_\infty^2 \right) \\ &\leq \frac{1}{4} C_5 \overline{C}_5^2 [\mathcal{Z}(T) - \mathcal{Z}(0)]^2 (b-a)^2 (\tau_z^4 + h^4)^2, \end{aligned} \quad (6.80)$$

which leads to (6.76) immediately. Then, taking square root of (6.80) leads to the inequality immediately. ■

Remark 6.4. When $n = N$, the relation (6.76) establishes the convergence of the numerical scheme (6.26) in ‘average norm’ as

$$\frac{1}{N} \sum_{i=1}^N \|e^i\|_\infty = O(\tau_z^4 + h^4). \quad (6.81)$$

This is clear since $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{N}$.

Remark 6.5. The relations (6.76) and (6.81) indicate fourth order convergence $O(\tau_z^4)$ with respect to the uniform mesh of $[\mathcal{Z}(0), \mathcal{Z}(T)]$. We shall investigate the convergence with respect to the mesh of $[0, T]$. Let $\tau = \max_{1 \leq n \leq N} |t_n - t_{n-1}|$, the maximum step size of $[0, T]$. Suppose $0 \leq z'(t) \leq C_3$ for $t \in [0, T]$. By mean value theorem, we have

$$\tau_z = \mathcal{Z}(t_n) - \mathcal{Z}(t_{n-1}) = z'(\xi)(t_n - t_{n-1}),$$

for some $\xi \in (t_{n-1}, t_n)$. It follows that

$$\tau_z \leq C_3 |t_n - t_{n-1}| \leq C_3 \tau.$$

Hence, the relations (6.76) and (6.81) now yield

$$\tau_z \sum_{i=1}^n \|e^i\|_\infty = O(\tau^4 + h^4), \quad 1 \leq n \leq N \quad (6.82)$$

and

$$\frac{1}{N} \sum_{i=1}^N \|e^i\|_\infty = O(\tau^4 + h^4). \quad (6.83)$$

respectively. In particular, the relation (6.83) establishes the convergence of the numerical scheme (6.26) in ‘average norm’ with respect to the maximum step size τ of the time interval $[0, T]$.

Remark 6.6.

- (a) We claim that the *fourth order temporal convergence* obtained in (6.76) (or (6.81)) *improves* the work of [133] where the temporal convergence order is observed to be $(2 - \gamma)$ from numerical experiments.
- (b) In [133], the authors establish the convergence of their method by using the Lax-Richtmyer Theorem, which states that if the numerical scheme is well-posed and consistent, then the scheme is convergent if and only if it is stable. Also, the convergence order is not proved explicitly but is observed numerically to be $(2 - \gamma)$. In comparison, our proof of convergence is more straightforward and the convergence order is explicitly given in (6.76) (or (6.81)).
- (c) For the classical fractional diffusion problem (5.1) $|_{z(t)=t}$, the *best* temporal convergence order achieved so far is 3, and this is achieved by the third order weighted and shifted Grünwald-Letnikov compact finite difference scheme developed in [57]. Hence, our proven temporal convergence order of 4 also *improves* the best result for the classical case.

Remark 6.7. In view of Remark 6.3, Theorem 6.2 and 6.3 and Lemma 6.1, the conditions in Theorem 6.6, namely, $U(x, \mathcal{Z}^{-1}(z)) = \tilde{U}(x, z) \in C^{(6,6)}([a, b] \times [\mathcal{Z}(0), \mathcal{Z}(T)])$ and $\frac{\partial^k}{\partial z^k} \tilde{U} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1, 2, 3, 4, 5, 6$, can be replaced by the *weaker* conditions $\tilde{U}(x, z) \in C^{(6,4)}([a, b] \times [\mathcal{Z}(0), \mathcal{Z}(t_2)])$, $\frac{\partial^k}{\partial z^k} \tilde{U} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 0, 1, 2$ and $\tilde{U}_e(\cdot, z) \in L^1(\mathcal{R}) \cap \mathcal{C}^{\gamma+4}(\mathcal{R})$.

6.4 Experiment

In this section, we shall demonstrate the efficiency of our numerical scheme (6.26) and confirm the theoretical convergence in Theorem 6.6. Moreover, some numerical experiments are conducted when the conditions of Theorem 6.6 are *not* entirely satisfied, just to observe the influence of the theoretical conditions on the actual

convergence of the numerical scheme. Note that the convergence indicated in (6.81) is in terms of average norm, nonetheless it would also be interesting to see the convergence in terms of maximum norm.

Let $\{U_m^n\}$ be the exact solution of the diffusion problem and $\{u_m^n\}$ be the numerical solution obtained from the scheme (6.26).

Example 6.1. Consider the generalized fractional diffusion problem

$$\begin{cases} {}^C_0D_{t;[\mathcal{Z}(t),1]}^\gamma u(x,t) = \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), & (x,t) \in [0,1] \times [0,1], \\ u(x,0) = 0, & x \in [0,1], \\ u(0,t) = 0, \quad u(1,t) = t^{\beta_1}(\sin 1), & t \in [0,1], \end{cases} \quad (6.84)$$

where $0 < \gamma < \gamma^{**}$, $\beta_1 \geq \gamma r > 0$ and $\mathcal{Z}(t) = t^r$ is the scale function.

$$f(x,t) = t^{\beta_1}(\sin x) \left[\frac{\Gamma(\frac{\beta_1}{r} + 1)}{\Gamma(\frac{\beta_1}{r} + 1 - \gamma)} t^{-\gamma r} + 1 \right]. \quad (6.85)$$

The exact solution of this problem is

$$U(x,t) = t^{\beta_1}(\sin x).$$

We shall apply the numerical scheme (6.26) to solve the problem for three different sets of (β_1, r) . It is easy to verify that the conditions of Theorem 6.6 are satisfied by the first set of (β_1, r) but not entirely satisfied by the second and third sets. The purpose is to observe the influence of the theoretical conditions on the actual convergence of the numerical scheme.

Case 1. Let $(\beta_1, r) = (4, \frac{1}{2})$. The exact solution of the problem is $U(x,t) = t^4(\sin x)$. Clearly, we have $\tilde{U}(x,z) = z^8(\sin x)$ and the conditions of Theorem 6.6 are satisfied.

To illustrate the convergence in the temporal dimension, we fix $h = \frac{1}{1000}$ and let N vary. In Table 6.1, we present the maximum norm error $E_\infty(h, N)$, average norm error $E_{av}(h, N)$ and the respective temporal convergence orders of the scheme (6.26). It is observed that our method is of fourth order in the temporal dimension, thus verifying the theoretical result in Theorem 6.6.

Next, to illustrate the convergence in the spatial dimension, we fix $N = 1000$ and let M vary. The errors and spatial convergence orders of the scheme (6.26) are presented in Table 6.2. Clearly, our method is also fourth order convergent in the spatial dimension, thus confirming the theoretical result in Theorem 6.6.

TABLE 6.1: (Example 6.1) Case 1: Errors and temporal convergence orders

N	$\gamma = 0.1$		$\gamma = 0.3$		$\gamma = 0.5$		$\gamma = 0.8$	
	E_∞	T_∞	E_∞	T_∞	E_∞	T_∞	E_∞	T_∞
20	$4.861e - 06$		$2.252e - 05$		$5.659e - 05$		$1.607e - 04$	
40	$3.458e - 07$	3.813	$1.607e - 06$	3.809	$4.049e - 06$	3.805	$1.155e - 05$	3.798
80	$2.303e - 08$	3.908	$1.072e - 07$	3.906	$2.705e - 07$	3.904	$7.728e - 07$	3.902
160	$1.486e - 09$	3.954	$6.927e - 09$	3.952	$1.747e - 08$	3.953	$4.996e - 08$	3.951
	E_{av}	T_{av}	E_{av}	T_{av}	E_{av}	T_{av}	E_{av}	T_{av}
20	$1.004e - 06$		$4.777e - 06$		$1.230e - 05$		$3.596e - 05$	
40	$7.081e - 08$	3.826	$3.394e - 07$	3.815	$8.797e - 07$	3.806	$2.599e - 06$	3.790
80	$4.701e - 09$	3.913	$2.262e - 08$	3.907	$5.882e - 08$	3.903	$1.746e - 07$	3.896
160	$3.029e - 10$	3.956	$1.460e - 09$	3.954	$3.802e - 09$	3.952	$1.132e - 08$	3.947

TABLE 6.2: (Example 6.1) Case 1: Errors and spatial convergence orders

M	$\gamma = 0.1$		$\gamma = 0.3$		$\gamma = 0.5$		$\gamma = 0.8$	
	E_∞	S_∞	E_∞	S_∞	E_∞	S_∞	E_∞	S_∞
3	$2.658e - 06$		$2.531e - 06$		$2.363e - 06$		$2.031e - 06$	
6	$1.676e - 07$	3.987	$1.587e - 07$	3.995	$1.472e - 07$	4.005	$1.265e - 07$	4.005
12	$1.074e - 08$	3.964	$1.020e - 08$	3.960	$9.492e - 09$	3.955	$8.091e - 09$	3.967
24	$6.717e - 10$	3.999	$6.394e - 10$	3.996	$5.981e - 10$	3.988	$5.189e - 10$	3.962
	E_{av}	S_{av}	E_{av}	S_{av}	E_{av}	S_{av}	E_{av}	S_{av}
3	$3.329e - 07$		$3.155e - 07$		$2.925e - 07$		$2.464e - 07$	
6	$2.098e - 08$	3.988	$1.978e - 08$	3.996	$1.822e - 08$	4.005	$1.535e - 08$	4.005
12	$1.345e - 09$	3.963	$1.272e - 09$	3.959	$1.175e - 09$	3.955	$9.819e - 10$	3.967
24	$8.416e - 11$	3.998	$8.001e - 11$	3.991	$7.477e - 11$	3.974	$6.531e - 11$	3.910

Case 2. Let $(\beta_1, r) = (5, 1)$. Here the exact solution of this problem is $U(x, t) = t^5(\sin x)$, so the conditions of Theorem 6.6 are not entirely satisfied.

Moreover, since $\mathcal{W}(t) = 1$ and $\mathcal{Z}(t) = t$, the generalized fractional diffusion equation reduces to the classical problem in [57], where the authors have proposed the third order weighted shifted Grünwald-Letnikov compact finite difference (3-WSGD-CFD) scheme to solve such problems.

Let $h = \frac{1}{1000}$ be fixed. In Table 6.3, we present the maximum norm error $E_\infty(h, N)$ and temporal convergence order of both the scheme (6.26) and 3-WSGD-CFD [57]. It is observed that the temporal convergence order of the numerical scheme (6.26) is still fourth order and clearly *outperforms* 3-WSGD-CFD [57] (which has a theoretical temporal convergence order of 3). We remark that the conditions in Theorem 6.6 are just *sufficient conditions*, so the temporal convergence could still be good even when the sufficient conditions are not entirely satisfied.

TABLE 6.3: (Example 6.1) Case 2: Comparison with the scheme in [57]

γ	N	Our scheme	T_∞	3-WSGD-CFD [57]	T_∞
0.1	20	$3.824e-07$		$5.547e-06$	
	40	$2.465e-08$	3.955	$7.227e-07$	2.940
	80	$1.556e-09$	3.986	$9.218e-08$	2.971
	160	$9.840e-11$	3.983	$1.163e-08$	2.987
0.5	20	$3.036e-06$		$5.015e-05$	
	40	$1.938e-07$	3.970	$6.528e-06$	2.941
	80	$1.224e-08$	3.985	$8.325e-07$	2.971
	160	$7.709e-10$	3.989	$1.051e-07$	2.986
0.9	20	$7.640e-06$		$1.509e-04$	
	40	$4.803e-07$	3.992	$1.957e-05$	2.947
	80	$3.011e-08$	3.996	$2.491e-06$	2.974
	160	$1.883e-09$	3.999	$3.141e-07$	2.987
0.95	20	$8.316e-06$		$1.692e-04$	
	40	$5.214e-07$	3.995	$2.192e-05$	2.948
	80	$3.264e-08$	3.998	$2.788e-06$	2.975
	160	$2.037e-09$	4.002	$3.516e-07$	2.987

Case 3. Let $(\beta_1, r) = (1, \frac{1}{2})$. Here the exact solution of the problem is $U(x, t) = t(\sin x)$, so the conditions of Theorem 6.6 are *not* entirely satisfied. To investigate the temporal convergence, let $h = \frac{1}{1000}$ be fixed. In Table 6.4, we present the errors $E_\infty(h, N)$, $E_{av}(h, N)$ and the respective temporal convergence orders of the scheme (6.26). It is obvious that the temporal convergence order is reduced to below 4. Hence, in this case, the partial-fulfillment of the sufficient conditions in Theorem 6.6 does affect the convergence. However, the errors are small and the scheme (6.26) still gives a good approximation of the exact solution.

TABLE 6.4: (Example 6.6) Case 3: Errors and temporal convergence orders

N	$\gamma = 0.1$		$\gamma = 0.3$		$\gamma = 0.5$		$\gamma = 0.8$	
	E_∞	T_∞	E_∞	T_∞	E_∞	T_∞	E_∞	T_∞
20	$1.749e-05$		$4.636e-05$		$6.218e-05$		$1.266e-04$	
40	$4.335e-06$	2.012	$1.102e-05$	2.073	$1.347e-05$	2.207	$3.422e-05$	1.887
80	$1.073e-06$	2.014	$2.596e-06$	2.086	$2.877e-06$	2.227	$1.003e-05$	1.771
160	$2.657e-07$	2.014	$6.064e-07$	2.098	$7.461e-07$	1.947	$2.784e-06$	1.849
	E_{av}	T_{av}	E_{av}	T_{av}	E_{av}	T_{av}	E_{av}	T_{av}
20	$1.099e-06$		$3.497e-06$		$6.772e-06$		$1.938e-05$	
40	$1.410e-07$	2.962	$4.555e-07$	2.941	$9.453e-07$	2.841	$3.593e-06$	2.431
80	$1.786e-08$	2.981	$5.878e-08$	2.954	$1.339e-07$	2.820	$7.028e-07$	2.354
160	$2.249e-09$	2.989	$7.573e-09$	2.956	$1.945e-08$	2.783	$1.430e-07$	2.297

The next example is from [50] where the authors only consider the classical fractional diffusion equation. We shall illustrate the efficiency of our numerical scheme on the classical problem.

Example 6.2. [50] *Considering the classical fractional diffusion problem*

$$\left\{ \begin{array}{l} {}^C_0D_{t;[\mathcal{Z}(t)=t, \mathcal{W}(t)=1]}^\gamma u(x, t) = \frac{\partial^2 u(x, t)}{\partial x^2} + f(x, t), \quad (x, t) \in [0, 1] \times [0, 1], \\ u(x, 0) = 0, \quad x \in [0, 1], \\ u(0, t) = t^{4+\gamma}, \quad u(1, t) = et^{4+\gamma}, \quad t \in [0, 1], \end{array} \right. \quad (6.86)$$

where $0 < \gamma < 1$ and

$$f(x, t) = e^x t^4 \left[\frac{\Gamma(5 + \gamma)}{24} - t^\gamma \right].$$

The exact solution is $U(x, t) = e^x t^{4+\gamma}$.

It is clear that the conditions of Theorem 6.6 are not entirely satisfied. We shall compare the performance of our scheme (6.26) with the $L1$ central finite difference ($L1$ -CF) scheme in [123] and the $L1$ -2 central finite difference ($L1$ -2-CF) scheme in [50]. Note that the theoretical temporal convergence order of $L1$ -CF is $(2 - \gamma)$ while that of $L1$ -2-CF is $(3 - \gamma)$.

Let $h = \frac{1}{20000}$ be fixed. In Table 6.5, we present the maximum norm error $E_\infty(h, N)$ and temporal convergence order of our scheme (6.26), $L1$ -CF [123] and $L1$ -2-CF [50]. It is observed that our method is of about fourth order and *outperforms* $L1$ -CF and $L1$ -2-CF in terms of error size and convergence.

To visualize the performance of the scheme (6.26), in Figure 6.3 we plot the absolute errors for the case $\gamma = 0.3$, $h = \frac{1}{100}$ and $N = 20$. The graph shows that the errors become smaller as time passes.

TABLE 6.5: (Example 6.2) Comparison with the schemes in [50, 123]

γ	N	Our scheme	T_∞	$L1$ -CF [123]	T_∞	$L1$ -2-CF [50]	T_∞
0.1	10	$1.760e-04$		$9.660e-04$		$1.191e-04$	
	20	$1.298e-05$	3.76	$3.015e-04$	1.68	$1.845e-05$	2.69
	40	$9.238e-07$	3.81	$9.111e-05$	1.73	$2.753e-06$	2.74
	80	$6.411e-08$	3.85	$2.695e-05$	1.76	$3.977e-07$	2.79
	160	$4.365e-09$	3.88	$7.849e-06$	1.78	$5.203e-08$	2.93
0.5	10	$7.136e-04$		$1.652e-02$		$2.494e-03$	
	20	$4.263e-05$	4.07	$6.348e-03$	1.38	$4.837e-04$	2.37
	40	$2.412e-06$	4.14	$2.366e-03$	1.42	$9.015e-05$	2.42
	80	$1.303e-07$	4.21	$8.657e-04$	1.45	$1.644e-05$	2.45
	160	$6.759e-09$	4.27	$3.131e-04$	1.47	$2.973e-06$	2.47
0.9	10	$8.697e-04$		$9.883e-02$		$1.860e-02$	
	20	$4.252e-05$	4.35	$4.832e-02$	1.03	$4.723e-03$	1.98
	40	$1.884e-06$	4.50	$2.310e-02$	1.06	$1.149e-03$	2.04
	80	$8.634e-08$	4.45	$1.092e-02$	1.08	$2.737e-04$	2.07
	160	$5.396e-09$	4.00	$5.130e-03$	1.09	$6.452e-05$	2.08

FIGURE 6.3: (Example 6.2) Absolute error of scheme (6.26)

The next example is from [133] where the authors only conducted numerical experiment for $\mathcal{Z}(t) = t$ and $\mathcal{W}(t) = 1$ (classical Caputo fractional derivative). To demonstrate the improvement of the temporal convergence order in our method,

we shall perform the numerical simulation for different $\mathcal{Z}(t)$ and $\mathcal{W}(t)$, including the classical case of $\mathcal{Z}(t) = t$ and $\mathcal{W}(t) = 1$. Since the exact solution is not known for general $\mathcal{Z}(t)$ and $\mathcal{W}(t)$, we shall compute the ‘exact’ solution by using our numerical scheme with sufficiently small spatial step size $h = \frac{1}{1000}$ and sufficiently large $N = 10000$.

Example 6.3. [133] *Consider the generalized fractional diffusion problem*

$$\begin{cases} {}^C D_{t;[\mathcal{Z}(t), \mathcal{W}(t)]}^{0.85} u(x, t) = \frac{\partial^2 u(x, t)}{\partial x^2} + f(x, t), & (x, t) \in [0, 1] \times [0, 1], \\ u(x, 0) = \sin(\pi x), & x \in [0, 1], \\ u(0, t) = 0, \quad u(1, t) = 0, & t \in [0, 1], \end{cases} \quad (6.87)$$

where

$$f(x, t) = \frac{2}{\Gamma(2.15)}(x^2 - x)t^{1.15} + \pi^2 \sin(\pi x) - 2t^2. \quad (6.88)$$

When $\mathcal{Z}(t) = t$ and $\mathcal{W}(t) = 1$, the exact solution is $U(x, t) = \sin(\pi x) + x(x - 1)t^2$.

Let $h = \frac{1}{1000}$ be fixed. In Table 6.6, we present the errors $E_\infty(h, N)$, $E_{av}(h, N)$ and the respective temporal convergence orders of the scheme (6.26) for four sets of $\mathcal{W}(t)$ and $\mathcal{Z}(t)$. Note that the numerical scheme (6.26) is applied directly when $\mathcal{W}(t) = 1$. If $\mathcal{W}(t) \neq 1$, we shall first convert the original problem to the equivalent form (5.3) before applying the scheme (6.26). The numerical solution of the original problem is then obtained via a relation between the solutions of (5.1) and (5.3). From Table 6.6, we observe that the temporal convergence orders T_∞ and T_{av} are below 4. This could due to the exact solution does not satisfy the conditions of Theorem 6.6.

Next, we shall compare our numerical scheme (6.26) with the method in [133]. With $h = \frac{1}{1000}$ fixed, in Table 6.7 we present the maximum absolute error $E_\infty(h, N)$, and the temporal convergence order. It is observed that the proposed scheme (6.26) achieves higher order accuracy in the temporal dimension as well as smaller errors for all cases.

TABLE 6.6: (Example 6.3) Errors and temporal convergence orders

	N	E_∞	T_∞	E_{av}	T_{av}
$\mathcal{W}(t) = 1, \quad \mathcal{Z}(t) = t$	50	$9.8581e-08$		$4.5157e-06$	
	100	$1.7920e-08$	2.4597	$8.5932e-07$	2.3937
	200	$3.4839e-09$	2.3628	$1.7097e-07$	2.3295
$\mathcal{W}(t) = \exp(t/2), \quad \mathcal{Z}(t) = t^{0.4}$	50	$1.1204e-06$		$3.4099e-07$	
	100	$7.9789e-08$	3.8117	$2.3485e-08$	3.8599
	200	$5.3184e-09$	3.9071	$1.5565e-09$	3.9154
$\mathcal{W}(t) = t + 1, \quad \mathcal{Z}(t) = t^{0.25}$	50	$1.4018e-05$		$1.8901e-06$	
	100	$1.0620e-06$	3.7224	$1.3838e-07$	3.7718
	200	$7.2908e-08$	3.8646	$9.3432e-09$	3.8886
$\mathcal{W}(t) = \log(t + 10), \quad \mathcal{Z}(t) = t^{0.2}$	50	$6.2129e-06$		$9.1543e-07$	
	100	$4.6126e-07$	3.7516	$6.6104e-08$	3.7916
	200	$3.1353e-08$	3.8789	$4.4323e-09$	3.8986

TABLE 6.7: (Example 6.3) Comparison with the scheme in [133]

	N	Our scheme	T_∞	Scheme in [133]	T_∞
$\mathcal{W}(t) = 1, \quad \mathcal{Z}(t) = t$	50	$9.8581e-08$		$2.2467e-04$	
	100	$1.7920e-08$	2.4597	$9.7243e-05$	1.2081
	200	$3.4839e-09$	2.3628	$3.9765e-05$	1.2901
$\mathcal{W}(t) = \exp(t/2), \quad \mathcal{Z}(t) = t^{0.4}$	50	$1.1204e-06$		$4.0231e-04$	
	100	$7.9789e-08$	3.8117	$1.7966e-04$	1.1630
	200	$5.3184e-09$	3.9071	$7.4622e-05$	1.2676
$\mathcal{W}(t) = t + 1, \quad \mathcal{Z}(t) = t^{0.25}$	50	$1.4018e-05$		$4.2337e-04$	
	100	$1.0620e-06$	3.7224	$1.9248e-04$	1.1372
	200	$7.2908e-08$	3.8646	$8.0639e-05$	1.2552
$\mathcal{W}(t) = \log(t + 10), \quad \mathcal{Z}(t) = t^{0.2}$	50	$6.2129e-06$		$7.9278e-04$	
	100	$4.6126e-07$	3.7516	$3.4586e-04$	1.1967
	200	$3.1353e-08$	3.8789	$1.4198e-04$	1.2845

Remark 6.8. In Theorem 6.6 (p. 115), the condition $\gamma \in (0, \gamma^{**}]$ arises from the proofs of the stability and convergence of numerical scheme. If this condition is not satisfied, our scheme may not be stable and convergent. The condition $U(x, \mathcal{Z}^{-1}(z)) = \tilde{U}(x, z) \in C^{(6)}[a, b]$ arises from finite difference method, while the conditions $U(x, \mathcal{Z}^{-1}(z)) = \tilde{U}(x, z) \in C^{(6)}[\mathcal{Z}(0), \mathcal{Z}(T)]$ and $\frac{\partial^k}{\partial z^k} \tilde{U} \Big|_{z=\mathcal{Z}(0)} = 0, k = 0, 1, 2, 3, 4, 5, 6$ arise from approximation of fractional derivative. If any of these conditions are not satisfied, the convergence order may be influenced and reduced.

- Case 2 of Example 6.1 does not satisfy the condition $\frac{\partial^k}{\partial z^k} \tilde{U} \Big|_{z=\mathcal{Z}(0)} = 0, k = 5, 6$. However, we observe from Table 6.3 that the temporal convergence order is still four. This confirms that $\frac{\partial^k}{\partial z^k} \tilde{U} \Big|_{z=\mathcal{Z}(0)} = 0, k = 5, 6$ is a sufficient but not necessary condition.

- Case 3 of Example 6.1 does not satisfy the condition $\frac{\partial^k}{\partial z^k} \tilde{U} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 2, 3, 4, 5, 6$. From Table 6.4, we observe that the temporal convergence order is reduced to below four. However, we note that the maximum absolute errors are still very small, indicating good approximation to the exact solution.
- Example 6.2 does not satisfy the condition $\frac{\partial^k}{\partial z^k} \tilde{U} \Big|_{z=\mathcal{Z}(0)} = 0$, $k = 5, 6$. However, the temporal convergence order is still four.
- The general solution of Example 6.3 is not known. From Table 6.6, we observe that the temporal convergence orders are below four for some $\mathcal{Z}(t)$ and $\mathcal{W}(t)$. This could be due to the exact solutions in these cases do not satisfy the conditions.

6.5 Summary

A new approximation of order 4 is developed for the generalized fractional derivatives – this is the most accurate approximation to date. Applying the new approximation and compact finite difference method, we construct a numerical scheme for the generalized diffusion problem and prove the stability and convergence of the scheme by energy method. The convergence order of the numerical scheme is shown to be four in both temporal and spacial dimensions, and this is confirmed by numerical experiments.

Chapter 7

Fractional Nonlinear Schrödinger Equation

The Schrödinger equation was first proposed by Austrian physicist Erwin Schrödinger in 1926 [114] – it is a fundamental equation in quantum physics that describes the evolution of the position-space wave function of a particle. In fact, the nonlinear Schrödinger equations describe a wide class of physical phenomena such as models of protein dynamics, self-focusing in laser pulses and nonlinear fibre optics [4, 37, 47, 121]. In the past few decades, fractional differential equations have gained much importance due to their usefulness in modelling physical phenomena in various areas such as physics, engineering, finance, biology and chemistry [38, 70, 90, 104]. As such, the Schrödinger equation has also been generalized to fractional differential equations. In 2000, Laskin [72] generalized the non-fractional Schrödinger equation to a space-fractional Schrödinger equation by using the Feynman path integrals over the Lévy trajectories and replacing the quantum Riesz derivative with the Laplace operator. Later, in 2004 Naber [98] proposed a different generalization by changing the first order time-derivative to a Caputo fractional derivative – this time-fractional Schrödinger equation has been used to describe fractional quantum mechanical behavior.

Many researchers pay attention to the numerical treatment of fractional Schrödinger equations. For *space-fractional* Schrödinger equation: a linear implicit conservative difference scheme of order $O(\tau^2 + h^2)$ has been proposed in [128] for the coupled nonlinear Schrödinger equation, where τ is the temporal step size and

h is the spacial step size; Zhao et al. [148] have used a compact operator to approximate the Riesz derivative, and the proposed linearized difference scheme for a two-dimensional nonlinear space-fractional Schrödinger equation can achieve $O(\tau^2 + \bar{h}^4)$, where $\bar{h} = \max\{h_1, h_2\}$, h_1 and h_2 are the spacial step sizes in the x and y dimensions respectively; Wang and Huang [131] have presented a conservative linearized difference scheme, which can achieve the order of $O(\tau^2 + h^2)$; a collocation method has been applied to a multi-dimensional space-time variable-order fractional Schrödinger equation in [18]; a fourth-order implicit time-discretization scheme based on the exponential time differencing approach together with a fourth-order compact scheme in space have been proposed in [64], the method is of order $O(\tau^4 + h^4)$; Li et al. [77] have used a fast linearized conservative finite element method to solve the coupled type equation; Wang and Xiao [130] have proposed an efficient conservative scheme for the fractional Klein-Gordon-Schrödinger equation with central difference and Crank-Nicolson scheme, their method can achieve $O(\tau^2 + h^2)$.

For *time-fractional* Schrödinger equation: Khan et al. [68] have applied the homotopy analysis method; Mohebbi et al. [94] have used the Kansa approach to approximate the spatial derivative and $L1$ discretization to approximate the Caputo time-fractional derivative; a Krylov projection method has been developed in [51]; a Jacobi spectral collocation method has been applied to a multi-dimensional time-fractional Schrödinger equation in [17]; a quadratic B-spline Galerkin method combined with $L1$ discretization scheme has been proposed in [45]; a linearized $L1$ -Galerkin finite element method has been used in [80] for a multi-dimensional nonlinear time-fractional Schrödinger equation; a cubic non-polynomial spline method combined with $L1$ discretization has been proposed in [76] and the stability has been shown by Fourier method, the convergence order is not proved but is observed from numerical experiments to be $O(\tau^{2-\gamma} + h^4)$.

Motivated by the above research, in this chapter we consider the following time-fractional nonlinear Schrödinger equation

$$\begin{cases} i {}^C_0D_t^\gamma u(x, t) + \frac{\partial^2 u(x, t)}{\partial x^2} + \lambda |u(x, t)|^2 u(x, t) = f(x, t), & (x, t) \in [0, L] \times [0, T], \\ u(x, 0) = \bar{A}_0(x), & x \in [0, L], \\ u(0, t) = \bar{A}_1(t), \quad u(L, t) = \bar{A}_2(t), & t \in [0, T], \end{cases} \quad (7.1)$$

where λ is a real constant, $f(x, t)$, $\bar{A}_0(x)$, $\bar{A}_1(t)$, $\bar{A}_2(t)$ are continuous functions with $\bar{A}_0(0) = \bar{A}_1(0)$ and $\bar{A}_0(L) = \bar{A}_2(0)$, and ${}^C_0D_t^\gamma u(x, t)$ is the Caputo fractional derivative of order $\gamma \in (0, 1)$.

We shall employ a quintic non-polynomial spline together with $L1$ discretization to solve (7.1). The stability, unique solvability and convergence of our numerical scheme are then proved by Fourier method. It is shown that our method is of order $O(\tau^{2-\gamma} + h^6)$ – this *improves* the *spatial convergence* achieved by other methods for time-fractional Schrödinger equation. It is worthwhile to mention that non-polynomial spline usually exhibits a better approximation than polynomial spline because of its parameter, as seen in the applications of non-polynomial spline in different problems [41, 44, 79–84, 106, 118]; while $L1$ discretization is a stable and widely used approximation for the Caputo fractional derivative [44, 49, 59, 79].

The organization of this chapter is as follows. We derive the numerical scheme in Section 7.1. The stability, unique solvability and convergence are established by Fourier method in Sections 7.2, 7.3 and 7.4 respectively. In Section 7.5, we present three examples to verify the efficiency of our numerical scheme and to compare with other methods in the literature. Finally, a conclusion is given in Section 7.6.

7.1 Numerical Scheme

In this section, we shall develop a numerical scheme for problem (7.1) by using quintic non-polynomial spline and $L1$ discretization.

Let

$$P : 0 = x_0 < x_1 < \cdots < x_M = L \quad \text{and} \quad P' : 0 = t_0 < t_1 < \cdots < t_N = T \quad (7.2)$$

be uniform meshes of the spatial interval $[0, L]$ with step size $h = \frac{L}{M}$ and the temporal interval $[0, T]$ with step size $\tau = \frac{T}{N}$, respectively.

Let $U(x, t)$ denote the exact solution of (7.1) and u_m^n denote the numerical approximation of u_m^n . We shall set u_m^n to be the value of the quintic non-polynomial spline at (x_m, t_n) .

Noting that spline relation (7.10), for $2 \leq m \leq M - 2$, we obtain

$$\begin{aligned} & p\hat{W}_{m+2}^n + q\hat{W}_{m+1}^n + s\hat{W}_m^n + q\hat{W}_{m-1}^n + p\hat{W}_{m-2}^n \\ &= \frac{1}{h^2} \left[\hat{\alpha}u_{m+2}^n + 2(\hat{\beta} - \hat{\alpha})u_{m+1}^n + 2(\hat{\alpha} - 2\hat{\beta})u_m^n + 2(\hat{\beta} - \hat{\alpha})u_{m-1}^n + \hat{\alpha}u_{m-2}^n \right], \end{aligned} \quad (7.3)$$

where p , q and s are defined in (2.17).

Using the quintic non-polynomial spline to approximate the exact solution $U(x, t)$ of (7.1), the spline relation (7.3) leads to

$$\begin{aligned} & p\frac{\partial^2 U_{m+2}^n}{\partial x^2} + q\frac{\partial^2 U_{m+1}^n}{\partial x^2} + s\frac{\partial^2 U_m^n}{\partial x^2} + q\frac{\partial^2 U_{m-1}^n}{\partial x^2} + p\frac{\partial^2 U_{m-2}^n}{\partial x^2} \\ &= \frac{1}{h^2} \left[\hat{\alpha}U_{m+2}^n + 2(\hat{\beta} - \hat{\alpha})U_{m+1}^n + 2(\hat{\alpha} - 2\hat{\beta})U_m^n + 2(\hat{\beta} - \hat{\alpha})U_{m-1}^n + \hat{\alpha}U_{m-2}^n \right] + \Upsilon_m^n, \end{aligned} \quad (7.4)$$

where Υ_m^n is the local truncation error in the spatial dimension. The next lemma gives a result on this error.

Lemma 7.1. *For any fixed $t = t_n$, $1 \leq n \leq N$, let $U(x, t_n) \in C^{(8)}[0, L]$. If*

$$p = \frac{1}{12}\hat{\alpha} - \frac{1}{240}, \quad q = \frac{2}{3}\hat{\alpha} + \frac{1}{10}, \quad s = -\frac{3}{2}\hat{\alpha} + \frac{97}{120}, \quad (7.5)$$

then the local truncation error Υ_m^n associated with the spline relation (7.4) satisfies

$$\Upsilon_m^n = O(h^6), \quad 2 \leq m \leq M - 2. \quad (7.6)$$

Proof. We carry out the Taylor expansion at $x = x_m$ in (7.4), this gives

$$\Upsilon_m^n = Z_1 \frac{\partial^2 U_m^n}{\partial x^2} + Z_2 h^2 \frac{\partial^4 U_m^n}{\partial x^4} + Z_3 h^4 \frac{\partial^6 U_m^n}{\partial x^6} + O(h^6),$$

where

$$Z_1 = 2(\hat{\alpha} + \hat{\beta}) - 2p - 2q - s, \quad Z_2 = \frac{1}{6}(7\hat{\alpha} + \hat{\beta}) - 4p - q, \quad Z_3 = \frac{1}{180}(31\hat{\alpha} + \hat{\beta}) - \frac{4}{3}p - \frac{1}{12}q.$$

To achieve the highest order of $O(h^6)$, we set $Z_1 = Z_2 = Z_3 = 0$, which together with the consistency relation $2(\hat{\alpha} + \hat{\beta}) = 1$, gives (7.5) and (7.6). ■

A similar result as Lemma 7.1 has also been obtained in [79].

Remark 7.1. In order to compute the numerical solution u_m^n , $1 \leq j \leq M - 1$, we need another two equations besides (7.3) or (7.4). We consider the following equations which incorporate the boundary conditions in (7.1),

$$\begin{aligned} (a) \quad & b_0 \frac{\partial^2 U_0^n}{\partial x^2} + b_1 \frac{\partial^2 U_1^n}{\partial x^2} + b_2 \frac{\partial^2 U_2^n}{\partial x^2} + b_3 \frac{\partial^2 U_3^n}{\partial x^2} + b_4 \frac{\partial^2 U_4^n}{\partial x^2} \\ &= \frac{1}{h^2} (a_0 U_0^n + a_1 U_1^n + a_2 U_2^n + a_3 U_3^n + a_4 U_4^n) + \Upsilon_1^n, \\ (b) \quad & b_{M-4} \frac{\partial^2 U_{M-4}^n}{\partial x^2} + b_{M-3} \frac{\partial^2 U_{M-3}^n}{\partial x^2} + b_{M-2} \frac{\partial^2 U_{M-2}^n}{\partial x^2} + b_{M-1} \frac{\partial^2 U_{M-1}^n}{\partial x^2} + b_M \frac{\partial^2 U_M^n}{\partial x^2} \\ &= \frac{1}{h^2} (a_{M-4} U_{M-4}^n + a_{M-3} U_{M-3}^n + a_{M-2} U_{M-2}^n + a_{M-1} U_{M-1}^n + a_M U_M^n) + \Upsilon_{M-1}^n, \end{aligned} \quad (7.7)$$

where Υ_1^n and Υ_{M-1}^n are local truncation errors in the spatial dimension, and the constants a_i 's and b_i 's have to be computed such that

$$\Upsilon_m^n = O(h^6), \quad m = 1, M - 1. \quad (7.8)$$

By carrying out Taylor expansion at $x = x_2$ and $x = x_{M-2}$ in (7.7)(a) and (7.7)(b) respectively, we get the following which satisfies (7.8),

$$(a_0, a_1, a_2, a_3, a_4) = (a_M, a_{M-1}, a_{M-2}, a_{M-3}, a_{M-4}) = \left(\frac{1}{10}, \frac{3}{5}, -\frac{7}{5}, \frac{3}{5}, \frac{1}{10} \right), \quad (7.9)$$

$$(b_0, b_1, b_2, b_3, b_4) = (b_M, b_{M-1}, b_{M-2}, b_{M-3}, b_{M-4}) = \left(\frac{1}{240}, \frac{1}{6}, \frac{79}{120}, \frac{1}{6}, \frac{1}{240} \right). \quad (7.10)$$

Remark 7.2. If we let the spline parameter $\hat{\alpha} = \frac{1}{10}$ in (7.4), then $(7.4)|_{m=2}$ and $(7.4)|_{m=M-2}$ are simply the same as (7.7)(a) and (7.7)(b) respectively. Therefore, we should have $\hat{\alpha} \neq \frac{1}{10}$.

To simplify the notations of the spline relations (7.4) and (7.7), we introduce the following definition.

Definition 7.1. For $y = (y_1, \dots, y_{M-1})$, we define the operators $\wedge$ and $\wedge_1$ by

$$\wedge y_m = \begin{cases} b_0 y_0 + b_1 y_1 + b_2 y_2 + b_3 y_3 + b_4 y_4, & m = 1, \\ p y_{m-2} + q y_{m-1} + s y_m + q y_{m+1} + p y_{m+2}, & 2 \leq m \leq M-2, \\ b_{M-4} y_{M-4} + b_{M-3} y_{M-3} + b_{M-2} y_{M-2} + b_{M-1} y_{M-1} + b_M y_M, & m = M-1, \end{cases}$$

and

$$\wedge_1 y_m = \begin{cases} \frac{1}{h^2} (a_0 y_0 + a_1 y_1 + a_2 y_2 + a_3 y_3 + a_4 y_4), & m = 1, \\ \frac{1}{h^2} [\hat{\alpha} y_{m-2} + 2(\hat{\beta} - \hat{\alpha}) y_{m-1} + 2(\hat{\alpha} - 2\hat{\beta}) y_m + 2(\hat{\beta} - \hat{\alpha}) y_{m+1} + \hat{\alpha} y_{m+2}], & 2 \leq m \leq M-2, \\ \frac{1}{h^2} (a_{M-4} y_{M-4} + a_{M-3} y_{M-3} + a_{M-2} y_{M-2} + a_{M-1} y_{M-1} + a_M y_M), & m = M-1. \end{cases}$$

Remark 7.3. In view of Definition 7.1, (7.6) and (7.8), the spline relations (7.4) and (7.7) can be presented as

$$\wedge \frac{\partial^2 U_m^n}{\partial x^2} = \wedge_1 U_m^n + O(h^6), \quad 1 \leq m \leq M-1. \quad (7.11)$$

Lemma 7.2. [32, 49] For $R_{n,k}^\gamma$ defined in Lemma 2.2, we have

$$\begin{aligned} (a) \quad & 1 = R_{n,n-1}^\gamma > R_{n,n-2}^\gamma > \dots > R_{n,k}^\gamma > \dots > R_{n,1}^\gamma > R_{n,0}^\gamma > 0, \\ (b) \quad & R_{n,k}^\gamma > \frac{1-\gamma}{(n-k)^\gamma}, \quad 0 \leq k \leq n-1. \end{aligned} \quad (7.12)$$

We are now ready to derive the numerical scheme for (7.1). To begin, we discretize (7.1) at (x_m, t_n) to get

$$i {}^C_0 D_t^\gamma U(x_m, t_n) + \frac{\partial^2 U(x_m, t_n)}{\partial x^2} + \lambda |U(x_m, t_n)|^2 U(x_m, t_n) = f(x_m, t_n). \quad (7.13)$$

Using the $L1$ discretization (2.27) in (7.13), we obtain

$$\frac{\partial^2 U(x_m, t_n)}{\partial x^2} = -i\mu \sum_{k=0}^{n-1} R_{n,k}^\gamma (U_m^{k+1} - U_m^k) - \lambda |U_m^n|^2 U_m^n + f_m^n + O(\tau^{2-\gamma}). \quad (7.14)$$

Next, applying the operator $\wedge$ to (7.14) yields

$$\wedge \frac{\partial^2 U(x_m, t_n)}{\partial x^2} = -i\mu \sum_{k=0}^{n-1} R_{n,k}^\gamma (\wedge U_m^{k+1} - \wedge U_m^k) - \lambda \wedge (|U_m^n|^2 U_m^n) + \wedge f_m^n + O(\tau^{2-\gamma}).$$

Noting (7.11), it follows that

$$\wedge_1 U_m^n = -i\mu \sum_{k=0}^{n-1} R_{n,k}^\gamma (\wedge U_m^{k+1} - \wedge U_m^k) - \lambda \wedge (|U_m^n|^2 U_m^n) + \wedge f_m^n + O(h^6 + \tau^{2-\gamma}).$$

Upon rearranging the above relation, we have

$$\begin{aligned} \wedge_1 U_m^n + i\mu \wedge U_m^n + \lambda \wedge (|U_m^n|^2 U_m^n) &= i\mu \wedge U_m^{n-1} - i\mu \sum_{k=0}^{n-2} R_{n,k}^\gamma (\wedge U_m^{k+1} - \wedge U_m^k) \\ &\quad + \wedge f_m^n + O(h^6 + \tau^{2-\gamma}). \end{aligned} \quad (7.15)$$

After omitting the error and replacing the exact solution U with the numerical solution u , we get the numerical scheme

$$\begin{aligned} &\wedge_1 u_m^n + i\mu \wedge u_m^n + \lambda \wedge (|u_m^n|^2 u_m^n) \\ &= i\mu \wedge u_m^{n-1} - i\mu \sum_{k=0}^{n-2} R_{n,k}^\gamma (\wedge u_m^{k+1} - \wedge u_m^k) + \wedge f_m^n, \quad 1 \leq m \leq M-1, \quad 1 \leq n \leq N, \end{aligned} \quad (7.16)$$

with

$$\begin{cases} u_m^0 = \bar{A}_0(x_m), & 0 \leq m \leq M, \\ u_0^n = \bar{A}_1(t_n), & u_M^n = \bar{A}_2(t_n), \quad 1 \leq n \leq N. \end{cases} \quad (7.17)$$

Remark 7.4. It is obvious that our scheme (7.16) is a nonlinear scheme. To linearize (7.16), following [78] we shall use the iterative algorithm

$$\begin{aligned} & \wedge_1 u_m^{n(r+1)} + i\mu \wedge u_m^{n(r+1)} + \lambda \wedge (|u_m^{n(r)}|^2 u_m^{n(r+1)}) \\ &= i\mu \wedge u_m^{n-1} - i\mu \sum_{k=0}^{n-2} R_{n,k}^\gamma (\wedge u_m^{k+1} - \wedge u_m^k) + \wedge f_m^n, \quad 1 \leq m \leq M-1, \quad 1 \leq n \leq N, \end{aligned} \quad (7.18)$$

where $u_m^{n(r)}$ is the r -th iterate of u_m^n , and

$$u_m^{n(0)} = \begin{cases} u_m^{n-1}, & n = 1, \\ 2u_m^{n-1} - u_m^{n-2}, & 2 \leq n \leq N. \end{cases} \quad (7.19)$$

Note that the scheme (7.18) is linear in $u^{n(r+1)}$. Hence, instead of (7.16)–(7.17), in practice we shall employ the linearized iterative scheme (7.18) with

$$\begin{cases} u_m^{0(r+1)} = \bar{A}_0(x_m), & 0 \leq m \leq M, \\ u_0^{n(r+1)} = \bar{A}_1(t_n), & u_M^{n(r+1)} = \bar{A}_2(t_n), \quad 1 \leq n \leq N. \end{cases} \quad (7.20)$$

For practical purpose, we would certainly need a stopping criterion to get $u_m^{n(r+1)}$ to a desired accuracy. An example of such a stopping criterion is

$$\frac{|u_m^{n(r+1)} - u_m^{n(r)}|}{|u_m^{n(r)}|} \leq \text{a small constant}. \quad (7.21)$$

In fact, we shall use the above stopping criterion with the small constant as 1×10^{-6} for our numerical simulations in Section 7.5.

7.2 Stability

In this section, we shall analyze the stability of the scheme (7.16)–(7.17) via Fourier method [24, 35]. Noting from Remark 7.4 that in practice we employ the linearized scheme (7.18)–(7.20) instead, effectively this means that in (7.16) we linearize the nonlinear term $|u|^2 u$ by replacing $|u|^2$ with a local constant ϱ . Note that a similar linearization technique has also been used in [43, 44]. With the linearization, we

can rewrite (7.16)–(7.17) as

$$\left\{ \begin{array}{l} \wedge_1 u_m^n + i\mu \wedge u_m^n + \lambda \varrho \wedge u_m^n = i\mu \wedge u_m^{n-1} - i\mu \sum_{k=0}^{n-2} R_{n,k}^\gamma (\wedge u_m^{k+1} - \wedge u_m^k) + \wedge f_m^n, \\ \\ u_m^0 = \bar{A}_0(x_m), \quad 0 \leq m \leq M, \\ u_0^n = \bar{A}_1(t_n), \quad u_M^n = \bar{A}_2(t_n), \quad 1 \leq n \leq N. \end{array} \right. \quad 1 \leq m \leq M-1, \quad (7.22)$$

Consider the perturbed system of (7.22) with perturbation in the initial values

$$\left\{ \begin{array}{l} \wedge_1 \hat{u}_m^n + i\mu \wedge \hat{u}_m^n + \lambda \varrho \wedge \hat{u}_m^n = i\mu \wedge \hat{u}_m^{n-1} - i\mu \sum_{k=0}^{n-2} R_{n,k}^\gamma (\wedge \hat{u}_m^{k+1} - \wedge \hat{u}_m^k) + \wedge f_m^n, \\ \\ \hat{u}_m^0 = \hat{A}_0(x_m), \quad 0 \leq m \leq M, \\ \hat{u}_0^n = \bar{A}_1(t_n), \quad \hat{u}_M^n = \bar{A}_2(t_n), \quad 1 \leq n \leq N. \end{array} \right. \quad 1 \leq m \leq M-1, \quad (7.23)$$

Let u_m^n be the solution of (7.22) and let $\hat{u}_m^n$ be the solution of the perturbed system (7.23). Let $\chi_m^n = u_m^n - \hat{u}_m^n$, $0 \leq j \leq M$, $0 \leq n \leq N$. It follows from (7.22) and (7.23) that

$$\left\{ \begin{array}{l} \wedge_1 \chi_m^n + i\mu \wedge \chi_m^n + \lambda \varrho \wedge \chi_m^n = i\mu \wedge \chi_m^{n-1} - i\mu \sum_{k=0}^{n-2} R_{n,k}^\gamma (\wedge \chi_m^{k+1} - \wedge \chi_m^k), \\ \\ \chi_m^0 = \bar{A}_0(x_m) - \hat{A}_0(x_m), \quad 0 \leq m \leq M, \\ \chi_0^n = 0, \quad \chi_M^n = 0, \quad 1 \leq n \leq N. \end{array} \right. \quad 1 \leq m \leq M-1, \quad (7.24)$$

Denote $\chi^n = [\chi_0^n, \chi_1^n, \dots, \chi_M^n]$, $0 \leq n \leq N$. Since $\chi_0^n = \chi_M^n = 0$, we define the L^2 norm of χ^n by

$$\|\chi^n\| = \left(\sum_{m=1}^{M-1} h |\chi_m^n|^2 \right)^{\frac{1}{2}}. \quad (7.25)$$

To apply the Fourier method, we expand χ^n to a piecewise constant function $\chi^n(x)$, where

$$\chi^n(x) = \begin{cases} \chi_m^n, & x \in \left(x_m - \frac{h}{2}, x_m + \frac{h}{2}\right], \quad 1 \leq m \leq M-1, \\ 0, & x \in \left[0, \frac{h}{2}\right] \cup \left[L - \frac{h}{2}, L\right]. \end{cases} \quad (7.26)$$

Then, $\chi^n(x)$ can be expanded as a Fourier series

$$\chi^n(x) = \sum_{\iota=-\infty}^{\infty} d_n(\iota) e^{i2\pi\iota x/L}, \quad 0 \leq n \leq N, \quad (7.27)$$

where

$$d_n(\iota) = \frac{1}{L} \int_0^L \chi^n(x) e^{-i2\pi\iota x/L} dx. \quad (7.28)$$

To carry out the Fourier stability analysis, it is sufficient to consider an individual harmonic of the form [21]

$$\chi_m^n(\iota) = d_n(\iota) e^{i2\pi\iota m h/L}.$$

Lemma 7.3. *Suppose the solution of (7.24) has the following form*

$$\chi_m^n(\iota) = d_n(\iota) e^{i\theta m h}, \quad (7.29)$$

where $\theta = 2\pi\iota/L$ and ι is the wave number. Then, the following inequality holds

$$|d_n(\iota)| \leq |d_0(\iota)|, \quad 1 \leq n \leq N. \quad (7.30)$$

Proof. For notational simplicity, let $d_n \equiv d_n(\iota)$ for a fixed wave number ι . We shall use mathematical induction to complete the proof. First, we consider $n = 1$. Upon substituting (7.29) into (7.24), we obtain

$$\wedge_1 d_1 e^{i\theta m h} + i\mu \wedge d_1 e^{i\theta m h} + \lambda \varrho \wedge d_1 e^{i\theta m h} = i\mu \wedge d_0 e^{i\theta m h}. \quad (7.31)$$

After a series of computations, (7.31) leads to

$$d_1 = \Omega d_0, \quad (7.32)$$

where

$$\Omega = \frac{i\bar{\eta}_m}{\bar{\phi}_m + i\bar{\eta}_m}, \quad (7.33)$$

$$\bar{\eta}_m = \begin{cases} 2b_0\mu \cos(2\theta h) + 2b_1\mu \cos(\theta h) + b_2\mu, & m = 1, M-1, \\ 2p\mu \cos(2\theta h) + 2q\mu \cos(\theta h) + s\mu, & 2 \leq m \leq M-2, \end{cases} \quad (7.34)$$

and

$$\bar{\phi}_m = \begin{cases} \left[\frac{2a_0}{h^2} + 2b_0\lambda\varrho \right] \cos(2\theta h) + \left[\frac{2a_1}{h^2} + 2b_1\lambda\varrho \right] \cos(\theta h) + \frac{a_2}{h^2} + b_2\lambda\varrho, & m = 1, M-1, \\ \left[\frac{2\hat{\alpha}}{h^2} + 2p\lambda\varrho \right] \cos(2\theta h) + \left[\frac{4(\hat{\beta} - \hat{\alpha})}{h^2} + 2q\lambda\varrho \right] \cos(\theta h) + \frac{2\hat{\alpha} - 4\hat{\beta}}{h^2} + s\lambda\varrho, & 2 \leq m \leq M-2. \end{cases} \quad (7.35)$$

It is obvious that $|\Omega| \leq 1$, therefore from (7.32) we have

$$|d_1| \leq |d_0|. \quad (7.36)$$

Next, assume that $|d_\ell| \leq |d_0|$, $1 \leq \ell \leq n-1$. We shall show that $|d_n| \leq |d_0|$. For any $n \geq 2$, we substitute (7.29) into (7.24) to get

$$\begin{aligned} \wedge_1 d_n e^{i\theta m h} + i\mu \wedge d_n e^{i\theta m h} + \lambda\varrho \wedge d_n e^{i\theta m h} &= -i\mu \sum_{k=0}^{n-2} R_{n,k}^\gamma (\wedge d_{k+1} e^{i\theta m h} - \wedge d_k e^{i\theta m h}) \\ &\quad + i\mu \wedge d_{n-1} e^{i\theta m h}. \end{aligned} \quad (7.37)$$

After a series of computations, (7.37) yields

$$d_n = \Omega d_{n-1} - \Omega \sum_{k=0}^{n-2} R_{n,k}^\gamma (d_{k+1} - d_k),$$

or equivalently

$$d_n = \Omega \left[(1 - R_{n,n-2}^\gamma) d_{n-1} + \sum_{k=1}^{n-2} (R_{n,k}^\gamma - R_{n,k-1}^\gamma) d_k + R_{n,0}^\gamma d_0 \right]. \quad (7.38)$$

Using Lemma 7.2, $|d_\ell| \leq |d_0|$ for $1 \leq \ell \leq n-1$, and $|\Omega| \leq 1$, it follows from (7.38) that

$$\begin{aligned}
|d_n| &= |\Omega| \left| (1 - R_{n,n-2}^\gamma) d_{n-1} + \sum_{k=1}^{n-2} (R_{n,k}^\gamma - R_{n,k-1}^\gamma) d_k + R_{n,0}^\gamma d_0 \right| \\
&\leq |\Omega| \left[|(1 - R_{n,n-2}^\gamma)| |d_{n-1}| + \sum_{k=1}^{n-2} |(R_{n,k}^\gamma - R_{n,k-1}^\gamma)| |d_k| + |R_{n,0}^\gamma| |d_0| \right] \\
&\leq |\Omega| \left[(1 - R_{n,n-2}^\gamma) |d_0| + \sum_{k=1}^{n-2} (R_{n,k}^\gamma - R_{n,k-1}^\gamma) |d_0| + R_{n,0}^\gamma |d_0| \right] \\
&= |\Omega| |d_0| \left[(1 - R_{n,n-2}^\gamma) + \sum_{k=1}^{n-2} (R_{n,k}^\gamma - R_{n,k-1}^\gamma) + R_{n,0}^\gamma \right] \\
&= |\Omega| |d_0| \leq |d_0|.
\end{aligned} \tag{7.39}$$

Hence, we have completed the proof of (7.30). ■

Theorem 7.1. (Stability) *The numerical scheme (7.18)–(7.20) or equivalently (7.22) is unconditionally stable with respect to the initial data.*

Proof. From the definition of the $L2$ norm (7.25) and (7.26), we find

$$\begin{aligned}
\|\chi^n\| &= \left(\sum_{m=1}^{M-1} h |\chi_m^n|^2 \right)^{\frac{1}{2}} \\
&= \left[\int_0^{h/2} |\chi^n(x)|^2 dx + \sum_{m=1}^{M-1} \int_{x_m-h/2}^{x_m+h/2} |\chi^n(x)|^2 dx + \int_{L-h/2}^L |\chi^n(x)|^2 dx \right]^{\frac{1}{2}} \\
&= \left[\int_0^L |\chi^n(x)|^2 dx \right]^{\frac{1}{2}}.
\end{aligned} \tag{7.40}$$

Noting the Parseval equality [24, 35]

$$\int_0^L |\chi^n(x)|^2 dx = \sum_{\iota=-\infty}^{\infty} |d_n(\iota)|^2, \tag{7.41}$$

7.4 Convergence

In this section, we shall establish the convergence of the numerical scheme (7.18)–(7.20) or equivalently (7.22). Recall that $U(x, t)$ is the exact solution of (7.1) and u_m^n is the numerical approximation of U_m^n obtained from (7.22). Let the error E_m^n at (x_m, t_n) be $E_m^n = U_m^n - u_m^n$, $0 \leq m \leq M$, $0 \leq n \leq N$.

Clearly, from (7.22) we obtain the error equation

$$\begin{aligned} \wedge_1 E_m^n + i\mu \wedge E_m^n + \lambda \varrho \wedge E_m^n &= i\mu \wedge E_m^{n-1} - i\mu \sum_{k=0}^{n-2} R_{n,k}^\gamma (\wedge E_m^{k+1} - \wedge E_m^k) + T_m^n, \\ 1 \leq m \leq M-1, \quad 1 \leq n \leq N, \end{aligned} \quad (7.45)$$

where T_m^n is the local truncation error,

$$E_m^n = 0, \quad 0 \leq j \leq M \quad \text{and} \quad E_0^n = E_M^n = 0, \quad 1 \leq n \leq N.$$

Denote $E^n = [E_0^n, E_1^n, \dots, E_M^n]$, $0 \leq n \leq N$. Since $E_0^n = E_M^n = 0$, we define the $L2$ norm of E^n by

$$\|E^n\| = \left(\sum_{m=1}^{M-1} h |E_m^n|^2 \right)^{\frac{1}{2}}.$$

Likewise, denote $T^n = [T_1^n, T_2^n, \dots, T_{M-1}^n]$, $1 \leq n \leq N$ and the $L2$ norm of T^n is given by

$$\|T^n\| = \left(\sum_{m=1}^{M-1} h |T_m^n|^2 \right)^{\frac{1}{2}}.$$

In view of (7.11), (2.27) and (7.15), we see that $T_m^n = O(h^6 + \tau^{2-\gamma})$ and there is a constant C_7 such that

$$|T_m^n| \leq C_7(h^6 + \tau^{2-\gamma}), \quad 1 \leq m \leq M-1, \quad 1 \leq n \leq N.$$

It follows that

$$\|T^n\| = \left(\sum_{m=1}^{M-1} h |T_m^n|^2 \right)^{\frac{1}{2}} \leq C_7 \sqrt{L}(h^6 + \tau^{2-\gamma}). \quad (7.46)$$

Next, similar to (7.26)–(7.28), we define the piecewise constant functions $E^n(x)$ and $T^n(x)$ by

$$E^n(x) = \begin{cases} E_m^n, & x \in \left(x_m - \frac{h}{2}, x_m + \frac{h}{2}\right], \quad 1 \leq m \leq M-1, \\ 0, & x \in \left[0, \frac{h}{2}\right] \cup \left[L - \frac{h}{2}, L\right], \end{cases} \quad (7.47)$$

and

$$T^n(x) = \begin{cases} T_m^n, & x \in \left(x_m - \frac{h}{2}, x_m + \frac{h}{2}\right], \quad 1 \leq m \leq M-1, \\ 0, & x \in \left[0, \frac{h}{2}\right] \cup \left[L - \frac{h}{2}, L\right]. \end{cases} \quad (7.48)$$

Then, $E^n(x)$ and $T^n(x)$ have the Fourier series expansions

$$E^n(x) = \sum_{\iota=-\infty}^{\infty} \epsilon_n(\iota) e^{i2\pi\iota x/L}, \quad T^n(x) = \sum_{\iota=-\infty}^{\infty} \Psi_n(\iota) e^{i2\pi\iota x/L}, \quad (7.49)$$

where

$$\epsilon_n(\iota) = \frac{1}{L} \int_0^L E^n(x) e^{-i2\pi\iota x/L} dx, \quad \Psi_n(\iota) = \frac{1}{L} \int_0^L T^n(x) e^{-i2\pi\iota x/L} dx. \quad (7.50)$$

Similar to (7.40)–(7.42), by applying the Parseval identities we find

$$\|E^n\|^2 = \sum_{\iota=-\infty}^{\infty} |\epsilon_n(\iota)|^2, \quad \|T^n\|^2 = \sum_{\iota=-\infty}^{\infty} |\Psi_n(\iota)|^2. \quad (7.51)$$

Further, noting (7.46), we see that $\sum_{\iota=-\infty}^{\infty} |\Psi_n(\iota)|^2$ converges and there is a positive constant $C_8 \geq 1$ [25] such that

$$|\Psi_n(\iota)| \leq C_8 |\delta_1(\iota)|, \quad 1 \leq n \leq N. \quad (7.52)$$

As in Section 7.2, we shall consider individual harmonics $E_m^n(\iota)$ and $T_m^n(\iota)$ of the forms

$$E_m^n(\iota) = \epsilon_n(\iota) e^{i\theta_m h}, \quad T_m^n(\iota) = \Psi_n(\iota) e^{i\theta_m h}, \quad (7.53)$$

where $\theta = 2\pi\iota/L$. Denote $\epsilon_n \equiv \epsilon_n(\iota)$ and $\delta_n \equiv \Psi_n(\iota)$ for a fixed wave number ι . Upon substituting (7.53) into (7.45), we get

$$\begin{aligned} & \wedge_1 \epsilon_n e^{i\theta m h} + i\mu \wedge \epsilon_n e^{i\theta m h} + \lambda_Q \wedge \epsilon_n e^{i\theta m h} \\ &= i\mu \wedge \epsilon_{n-1} e^{i\theta m h} - i\mu \sum_{k=0}^{n-2} R_{n,k}^\gamma (\wedge \epsilon_{k+1} e^{i\theta m h} - \wedge \epsilon_k e^{i\theta m h}) + \delta_n e^{i\theta m h}, \end{aligned} \quad (7.54)$$

$$1 \leq m \leq M-1, \quad 1 \leq n \leq N.$$

Now, we shall present two lemmas which are essential in the proof of the convergence result.

Lemma 7.4. *Let $\hat{\alpha} \in (0, \frac{1}{10}) \cup (\frac{1}{10}, \frac{37}{180})$. Then, we have*

$$|s| - 2|p| - 2|q| > 0, \quad (7.55)$$

where p , q and s are defined in (7.5).

Proof. Recall from Remark 7.2 that $\hat{\alpha} \neq \frac{1}{10}$. For $\hat{\alpha} \in (0, \frac{1}{20})$, we have $p < 0$, $q > 0$ and $s > 0$, therefore

$$|s| - 2|p| - 2|q| = -\frac{3}{2}\hat{\alpha} + \frac{97}{120} - 2\left(\frac{1}{240} - \frac{1}{12}\hat{\alpha}\right) - 2\left(\frac{2}{3}\hat{\alpha} + \frac{1}{10}\right) = -\frac{8}{3}\hat{\alpha} + \frac{3}{5} > 0.$$

For $\hat{\alpha} \in [\frac{1}{20}, \frac{1}{10}) \cup (\frac{1}{10}, \frac{37}{180})$, we have $p \geq 0$, $q > 0$ and $s > 0$, therefore

$$|s| - 2|p| - 2|q| = -\frac{3}{2}\hat{\alpha} + \frac{97}{120} - 2\left(\frac{1}{12}\hat{\alpha} - \frac{1}{240}\right) - 2\left(\frac{2}{3}\hat{\alpha} + \frac{1}{10}\right) = -3\hat{\alpha} + \frac{37}{60} > 0.$$

The proof is complete. ■

Lemma 7.5. *Let $\hat{\alpha} \in (0, \frac{1}{10}) \cup (\frac{1}{10}, \frac{37}{180})$. Let ϵ_n , $1 \leq n \leq N$ be the solution of (7.54). Then, we have*

$$|\epsilon_n| \leq C_8 C_9 |\delta_1|, \quad 1 \leq n \leq N, \quad (7.56)$$

where $C_9 = T^\gamma \Gamma(1 - \gamma)/C_{10}$ and $C_{10} = \min \left\{ \frac{19}{60}, |s| - 2|p| - 2|q| \right\}$.

Proof. Since $E^0 = 0$, it is clear from (7.51) that

$$\epsilon_0(m) = \epsilon_0 = 0. \quad (7.57)$$

We shall first show that (7.56) is true for $n = 1$. Indeed, when $n = 1$, from (7.54) we get

$$\epsilon_1 = \frac{1}{\bar{\phi}_m + i\bar{\eta}_m} \delta_1, \quad (7.58)$$

where $\bar{\eta}_m$ and $\bar{\phi}_m$ are defined in (7.34) and (7.35) respectively.

Next, it is clear from Lemma 7.4 that $C_{10} > 0$. Moreover, we note that $|b_2| - 2|b_0| - 2|b_1| = \frac{19}{60}$, where b_0 , b_1 and b_2 are given in (7.10). Together with (7.34), we obtain

$$\begin{aligned} C_{10} &= \min \left\{ \frac{19}{60}, |s| - 2|p| - 2|q| \right\} \\ &= \min \{ |b_2| - 2|b_0| - 2|b_1|, |s| - 2|p| - 2|q| \} \\ &\leq \min \{ |b_2 + 2b_0 \cos(2\theta h) + 2b_1 \cos(\theta h)|, |s + 2p \cos(2\theta h) + 2q \cos(\theta h)| \} \\ &\leq \frac{1}{\mu} |\bar{\eta}_m|, \quad 1 \leq m \leq M-1. \end{aligned} \quad (7.59)$$

Using (7.59), the fact $|\Omega| = \left| \frac{i\bar{\eta}_m}{\bar{\phi}_m + i\bar{\eta}_m} \right| \leq 1$, the definition of μ (Lemma 2.2), Lemma 7.2 and $C_8 \geq 1$ (refer to (7.52)), we further find from (7.58)

$$\begin{aligned} |\epsilon_1| &= \frac{1}{|\bar{\phi}_m + i\bar{\eta}_m|} |\delta_1| \\ &= \frac{C_9 C_{10}}{T^\gamma \Gamma(1-\gamma)} \frac{1}{|\bar{\phi}_m + i\bar{\eta}_m|} |\delta_1| \\ &\leq \frac{C_9}{T^\gamma \Gamma(1-\gamma)} \frac{|\bar{\eta}_m|}{\mu} \frac{1}{|\bar{\phi}_m + i\bar{\eta}_m|} |\delta_1| \\ &= \frac{\tau^\gamma \Gamma(2-\gamma) C_9}{T^\gamma \Gamma(1-\gamma)} |\Omega| |\delta_1| \\ &= \frac{1-\gamma}{N^\gamma} C_9 |\Omega| |\delta_1| < R_{N,0}^\gamma C_9 |\Omega| |\delta_1| \leq C_8 C_9 |\delta_1|. \end{aligned} \quad (7.60)$$

Hence, we have proved (7.56) for $n = 1$.

Now, assume that for $n \geq 2$,

$$|\epsilon_\ell| \leq C_8 C_9 |\delta_1|, \quad 1 \leq \ell \leq n-1. \quad (7.61)$$

From (7.54), after a series of computations we get

$$\epsilon_n = \Omega \epsilon_{n-1} - \Omega \sum_{k=0}^{n-2} R_{n,k}^\gamma (\epsilon_{k+1} - \epsilon_k) + \frac{1}{\bar{\phi}_m + i\bar{\eta}_m} \delta_n,$$

or equivalently

$$\epsilon_n = \Omega \left[(1 - R_{n,n-2}^\gamma) \epsilon_{n-1} + \sum_{k=1}^{n-2} (R_{n,k}^\gamma - R_{n,k-1}^\gamma) \epsilon_k + R_{n,0}^\gamma \epsilon_0 \right] + \frac{1}{\bar{\phi}_m + i\bar{\eta}_m} \delta_n. \quad (7.62)$$

Using (7.57), a similar argument as in (7.60), (7.52), Lemma 7.2, (7.61) and $|\Omega| \leq 1$, it follows from (7.62) that

$$\begin{aligned} |\epsilon_n| &\leq |\Omega| \left| (1 - R_{n,n-2}^\gamma) \epsilon_{n-1} + \sum_{k=1}^{n-2} (R_{n,k}^\gamma - R_{n,k-1}^\gamma) \epsilon_k + R_{n,0}^\gamma \epsilon_0 \right| + \frac{1}{|\bar{\phi}_m + i\bar{\eta}_m|} |\delta_n| \\ &\leq |\Omega| \left[|(1 - R_{n,n-2}^\gamma) \epsilon_{n-1}| + \left| \sum_{k=1}^{n-2} (R_{n,k}^\gamma - R_{n,k-1}^\gamma) \epsilon_k \right| \right] + R_{n,0}^\gamma C_9 |\Omega| |\delta_n| \\ &\leq |\Omega| \left[|(1 - R_{n,n-2}^\gamma)| |\epsilon_{n-1}| + \sum_{k=1}^{n-2} |(R_{n,k}^\gamma - R_{n,k-1}^\gamma)| |\epsilon_k| + R_{n,0}^\gamma C_8 C_9 |\delta_1| \right] \\ &\leq C_8 C_9 |\Omega| |\delta_1| \left[(1 - R_{n,n-2}^\gamma) + \sum_{k=1}^{n-2} (R_{n,k}^\gamma - R_{n,k-1}^\gamma) + R_{n,0}^\gamma \right] \\ &\leq C_8 C_9 |\delta_1|. \end{aligned}$$

Hence, we have proved (7.56). ■

Theorem 7.3. (Convergence) Let $\hat{\alpha} \in (0, \frac{1}{10}) \cup (\frac{1}{10}, \frac{37}{180})$. Suppose $U(x, t)$ is the exact solution of (7.1) and $U(x, t) \in C^{(8,2)}([0, L] \times [0, T])$. Then, we have for $1 \leq n \leq N$,

$$\|E^n\| = O(h^6 + \tau^{2-\gamma}). \quad (7.63)$$

Hence, the numerical scheme (7.18)–(7.20) or equivalently (7.22) is convergent with order $O(h^6 + \tau^{2-\gamma})$.

Proof. Using (7.51), Lemma 7.5 and (7.46), we find for $1 \leq n \leq N$,

$$\begin{aligned}
 \|E^n\| &= \left(\sum_{\iota=-\infty}^{\infty} |\epsilon_n(\iota)|^2 \right)^{\frac{1}{2}} \\
 &\leq C_8 C_9 \left(\sum_{\iota=-\infty}^{\infty} |\delta_1(\iota)|^2 \right)^{\frac{1}{2}} \\
 &= C_8 C_9 \|T^1\| \\
 &\leq C_7 C_8 C_9 \sqrt{L} (h^6 + \tau^{2-\gamma}).
 \end{aligned}$$

The proof is complete. ■

Remark 7.5. As shown in Theorem 7.3, the numerical scheme (7.18)–(7.20) achieves sixth order convergence in the spatial dimension. This *improves* the work of [76] where the spatial convergence order is observed to be four through numerical experiment. Further, in [76] the authors have only proved the stability of their scheme; while we have proven the stability, unique solvability as well as convergence of our method by Fourier method.

7.5 Experiment

In this section, we shall present three numerical examples to verify the efficiency of the scheme (7.18)–(7.20) as well as to compare with other methods in the literature.

Note that our theoretical convergence result is in $L2$ norm, nonetheless it would also be interesting to see the convergence in maximum norm. In fact, for a fixed pair of (h, τ) , we shall compute the following accuracy indicators – maximum $L2$ norm error $E_2(h, \tau)$, maximum modulus error $E_\infty(h, \tau)$, maximum real part absolute error $E_\infty^{Re}(h, \tau)$ and maximum imaginary part absolute error $E_\infty^{Im}(h, \tau)$, defined by

$$E_2(h, \tau) = \max_{0 \leq n \leq N} \|E^n\| = \max_{0 \leq n \leq N} \left(\sum_{m=1}^{M-1} h |U_m^n - u_m^n|^2 \right)^{\frac{1}{2}}, \quad (7.64)$$

$$E_\infty(h, \tau) = \max_{0 \leq n \leq N} \max_{0 \leq m \leq M} |U_m^n - u_m^n|, \quad (7.65)$$

$$E_{\infty}^{Re}(h, \tau) = \max_{0 \leq n \leq N} \max_{0 \leq m \leq M} |Re(U_m^n - u_m^n)|, \quad E_{\infty}^{Im}(h, \tau) = \max_{0 \leq n \leq N} \max_{0 \leq m \leq M} |Im(U_m^n - u_m^n)|. \quad (7.66)$$

The convergence orders in temporal and spacial dimensions can be computed by

$$T_2 = \log_2 \left[\frac{E_2(h, 2\tau)}{E_2(h, \tau)} \right], \quad T_{\infty} = \log_2 \left[\frac{E_{\infty}(h, 2\tau)}{E_{\infty}(h, \tau)} \right], \quad (7.67)$$

$$S_2 = \log_2 \left[\frac{E_2(2h, \tau)}{E_2(h, \tau)} \right], \quad S_{\infty} = \log_2 \left[\frac{E_{\infty}(2h, \tau)}{E_{\infty}(h, \tau)} \right]. \quad (7.68)$$

Example 7.1. [45, 76, 94] Consider the time-fractional Schrödinger equation

$$\begin{cases} i {}^C_0 D_t^{\gamma} u(x, t) + \frac{\partial^2 u(x, t)}{\partial x^2} + |u(x, t)|^2 u(x, t) = f(x, t), & (x, t) \in [0, 1] \times [0, 1], \\ u(x, 0) = 0, & x \in [0, 1], \\ u(0, t) = it^2, \quad u(1, t) = it^2, & t \in [0, 1], \end{cases} \quad (7.69)$$

where $0 < \gamma < 1$ and

$$\begin{aligned} f(x, t) = & -\frac{2t^{2-\gamma}}{\Gamma(3-\gamma)} \cos(2\pi x) + (-4\pi^2 t^2 + t^6) \sin(2\pi x) \\ & + i \left[\frac{2t^{2-\gamma}}{\Gamma(3-\gamma)} \sin(2\pi x) + (-4\pi^2 t^2 + t^6) \cos(2\pi x) \right]. \end{aligned} \quad (7.70)$$

The exact solution is $u(x, t) = t^2[\sin(2\pi x) + i \cos(2\pi x)]$.

Let $\hat{\alpha} = 1/20$ be fixed. We shall apply the scheme (7.18)–(7.20) to compute the errors and convergence orders, and comparisons are made with other methods in the literature. A brief description of the numerical simulation in Tables 7.1–7.4 and Figures 7.1–7.3:

- (i) In Table 7.1, we fix $h = 1/1000$ and let τ vary. Applying (7.18)–(7.20), we compute $E_2(h, \tau)$, $E_{\infty}(h, \tau)$ and the respective temporal convergence orders. The numerical results indicate that our method is of order $(2-\gamma)$ in the temporal dimension, thus verifying the theoretical temporal convergence order in Theorem 7.3.
- (ii) In Table 7.2, we fix $\tau = 1/5000$ and let h vary. We present $E_2(h, \tau)$, $E_{\infty}(h, \tau)$ and the spatial convergence orders of our scheme (7.18)–(7.20) and those of

the cubic non-polynomial spline (CNS) method [76]. From Table 7.2, we see that our method can achieve at least $O(h^6)$, while CNS method is $O(h^4)$. Moreover, our method obtains smaller errors in all the cases. The observation also confirms the theoretical spacial convergence order in Theorem 7.3.

- (iii) Let $\tau = 1/512$ be fixed. In Table 7.3, we compare $E_\infty^{Re}(h, \tau)$ and $E_\infty^{Im}(h, \tau)$ of our scheme (7.18)–(7.20) with those of the meshless collocation (MC) method [94] and CNS method [76]. The numerical results indicate that our method gives the smallest errors in all the cases.
- (iv) In Table 7.4, we fix $(h, \tau) = (1/40, 1/200)$ and compare $E_\infty^{Re}(h, \tau)$ and $E_\infty^{Im}(h, \tau)$ of our scheme (7.18)–(7.20) with those of the quadratic B-spline Galerkin (QBG) method [45] and CNS method [76]. Once again, the numerical results show that our scheme outperforms these methods.
- (v) To visualize the efficiency of our scheme (7.18)–(7.20), we plot the real part (imaginary part) of the numerical solution and exact solution in Figure 7.1 (Figure 7.2) for $\gamma = 0.1$ and $(h, \tau) = (1/16, 1/200)$. From the figures, we observe that our method gives good approximation of the exact solution.
- (vi) In Figure 7.3, we plot the absolute modulus error $|U_m^n - u_m^n|$ obtained from the scheme (7.18)–(7.20) for $\gamma = 0.1$ and $(h, \tau) = (1/16, 1/200)$. We observe from Figure 7.3 that the error is very small.

TABLE 7.1: (Example 7.1) $E_2(h, \tau)$, $E_\infty(h, \tau)$ and temporal convergence orders

γ	τ	$E_2(h, \tau)$	T_2	$E_\infty(h, \tau)$	T_∞
0.2	1/20	$3.4967e - 05$		$5.0107e - 05$	
	1/40	$1.0627e - 05$	1.7183	$1.5231e - 05$	1.7180
	1/80	$3.2052e - 06$	1.7292	$4.5947e - 06$	1.7290
0.4	1/20	$1.2356e - 04$		$1.7701e - 04$	
	1/40	$4.1683e - 05$	1.5677	$5.9711e - 05$	1.5678
	1/80	$1.3977e - 05$	1.5764	$2.0021e - 05$	1.5765
0.6	1/20	$3.4186e - 04$		$4.8943e - 04$	
	1/40	$1.3047e - 04$	1.3897	$1.8678e - 04$	1.3898
	1/80	$4.9681e - 05$	1.3930	$7.1121e - 05$	1.3930

TABLE 7.2: (Example 7.1) $E_2(h, \tau)$, $E_\infty(h, \tau)$ and spatial convergence orders

γ	h	$E_2(h, \tau)$ Our method	S_2	$E_\infty(h, \tau)$ Our method	S_∞	$E_\infty(h, \tau)$ CNS [76]	S_∞
0.2	1/5	$1.0859e-02$		$1.5316e-02$		$2.6917e-02$	
	1/10	$5.7595e-05$	7.5587	$7.7591e-05$	7.6249	$1.6360e-03$	4.0403
	1/20	$7.4037e-07$	6.2816	$1.0556e-06$	6.1998	$1.0096e-04$	4.0183
0.4	1/5	$1.0799e-02$		$1.5303e-02$		$2.6888e-02$	
	1/10	$5.7073e-05$	7.5639	$7.6880e-05$	7.6370	$1.6188e-03$	4.0540
	1/20	$7.3276e-07$	6.2833	$1.0440e-06$	6.2024	$1.0048e-04$	4.0099
0.6	1/5	$1.0697e-02$		$1.5252e-02$		$2.6750e-02$	
	1/10	$5.6275e-05$	7.5705	$7.5741e-05$	7.6537	$1.5965e-03$	4.0666
	1/20	$7.2262e-07$	6.2831	$1.0382e-06$	6.1889	$9.9534e-05$	4.0036

TABLE 7.3: (Example 7.1) Compare $E_\infty^{Re}(h, \tau)$ and $E_\infty^{Im}(h, \tau)$ with other methods

γ	h	$E_\infty^{Re}(h, \tau)$ our method	$E_\infty^{Re}(h, \tau)$ MC [94]	$E_\infty^{Re}(h, \tau)$ CNS [76]	$E_\infty^{Im}(h, \tau)$ our method	$E_\infty^{Im}(h, \tau)$ MC [94]	$E_\infty^{Im}(h, \tau)$ CNS [76]
0.1	1/9	$1.2703e-04$	$7.0404e-02$	$1.2683e-03$	$1.2556e-04$	$7.6325e-02$	$2.4250e-03$
	1/14	$3.0566e-06$	$2.1873e-02$	$2.2077e-04$	$1.0443e-05$	$2.6090e-02$	$4.1972e-04$
	1/19	$4.1062e-07$	$1.0022e-02$	$6.5147e-05$	$1.4591e-06$	$1.2230e-02$	$1.2268e-04$
	1/24	$9.4755e-08$	$5.1958e-03$	$2.5400e-05$	$3.2571e-07$	$6.4207e-03$	$4.8343e-05$
	1/29	$6.5541e-08$	$2.8536e-03$	$1.1938e-05$	$1.0337e-07$	$ch7.26662e-03$	$2.2621e-05$
0.3	1/9	$1.2838e-04$	$7.0520e-02$	$1.3135e-03$	$1.2426e-04$	$ch7.26128e-02$	$2.3999e-03$
	1/14	$3.1059e-06$	$2.1979e-02$	$2.2990e-04$	$1.0361e-05$	$1.4733e-02$	$4.1516e-04$
	1/19	$4.0294e-07$	$1.0068e-02$	$6.7510e-05$	$1.5206e-06$	$7.1997e-03$	$1.2140e-04$
	1/24	$4.1570e-07$	$5.2146e-03$	$2.6167e-05$	$4.6692e-07$	$3.8478e-03$	$4.7855e-05$
	1/29	$4.3146e-07$	$2.8610e-03$	$1.2195e-05$	$2.9081e-07$	$2.1771e-03$	$2.2402e-05$

TABLE 7.4: (Example 7.1) Compare $E_\infty^{Re}(h, \tau)$ and $E_\infty^{Im}(h, \tau)$ with other methods

γ	$E_\infty^{Re}(h, \tau)$ our method	$E_\infty^{Re}(h, \tau)$ QBG [45]	$E_\infty^{Re}(h, \tau)$ CNS [76]	$E_\infty^{Im}(h, \tau)$ our method	$E_\infty^{Im}(h, \tau)$ QBG [45]	$E_\infty^{Im}(h, \tau)$ CNS [76]
0.10	$3.1730e-07$	$4.6850e-04$	$3.1153e-06$	$1.5460e-07$	$7.7635e-04$	$6.2728e-06$
0.30	$2.1533e-06$	$4.9949e-04$	$3.3537e-06$	$1.1104e-06$	$3.2833e-04$	$6.5370e-06$
0.70	$3.9262e-05$	$6.6590e-04$	$3.9311e-05$	$3.2046e-05$	$1.0614e-03$	$3.2046e-05$
0.90	$1.9926e-04$	$8.4460e-04$	$1.9971e-04$	$1.4957e-04$	$1.3150e-03$	$1.4957e-04$

FIGURE 7.1: (Example 7.1) Real part of numerical solution and exact solution

FIGURE 7.2: (Example 7.1) Imaginary part of numerical solution and exact solution

FIGURE 7.3: (Example 7.1) Absolute modulus error

Example 7.2. Consider the time-fractional Schrödinger equation

$$\begin{cases} i {}^C_0 D_t^\gamma u(x, t) + \frac{\partial^2 u(x, t)}{\partial x^2} + |u(x, t)|^2 u(x, t) = f(x, t), & (x, t) \in [0, 1] \times [0, 1], \\ u(x, 0) = 0, & x \in [0, 1], \\ u(0, t) = it^{\gamma+1}, \quad u(1, t) = it^{\gamma+1}, & t \in [0, 1], \end{cases} \quad (7.71)$$

where $0 < \gamma < 1$ and

$$f(x, t) = t\Gamma(\gamma + 2)[i \sin(2\pi x) - \cos(2\pi x)] + (t^{3\gamma+3} - 4\pi^2 t^{\gamma+1})[\sin(2\pi x) + i \cos(2\pi x)]. \quad (7.72)$$

The exact solution is $u(x, t) = t^{\gamma+1}[\sin(2\pi x) + i \cos(2\pi x)]$.

Let $\hat{\alpha} = 1/20$ in the implementation of the scheme (7.18)–(7.20). In Table 7.5, we fix $\tau = 1/5000$ and present the spatial convergence orders of our scheme and those of CNS method [76]. In Table 7.6, we fix $\tau = 1/512$ and compare the maximum real/imaginary part absolute errors of our numerical scheme with those of CNS method [76]. Further, in Figure 7.4 we plot the absolute modulus error $|U_m^n - u_m^n|$ obtained from our scheme for $\gamma = 0.3$ and $(h, \tau) = (1/20, 1/200)$.

From the numerical simulation and plot, once again we demonstrate that the theoretical spatial convergence order of our scheme is at least six (Theorem 7.3) and our scheme performs better than CNS method.

TABLE 7.5: (Example 7.2) $E_2(h, \tau)$, $E_\infty(h, \tau)$ and spatial convergence orders

γ	h	$E_2(h, \tau)$ Our method	S_2	$E_\infty(h, \tau)$ Our method	S_∞	$E_\infty(h, \tau)$ CNS [76]	S_∞
0.3	1/5	1.0859e-02		1.5317e-02		2.6918e-02	
	1/10	5.7585e-05	7.5590	7.7577e-05	7.6253	1.6327e-03	4.0432
	1/20	7.3933e-07	6.2833	1.0550e-06	6.2003	1.0095e-04	4.0155
0.5	1/5	1.0808e-02		1.5308e-02		2.6893e-02	
	1/10	5.7103e-05	7.5643	7.6944e-05	7.6363	1.6200e-03	4.0532
	1/20	7.3204e-07	6.2855	1.0429e-06	6.2051	1.0053e-04	4.0103
0.7	1/5	1.0698e-02		1.5253e-02		2.6736e-02	
	1/10	5.6084e-05	7.5755	7.5675e-05	7.6551	1.5956e-03	4.0666
	1/20	7.6999e-07	6.1866	1.2828e-06	5.8824	9.9461e-05	4.0038

TABLE 7.6: (Example 7.2) $E_{\infty}^{Re}(h, \tau)$ and $E_{\infty}^{Im}(h, \tau)$

γ	h	$E_{\infty}^{Re}(h, \tau)$ our method	$E_{\infty}^{Re}(h, \tau)$ CNS [76]	$E_{\infty}^{Im}(h, \tau)$ our method	$E_{\infty}^{Im}(h, \tau)$ CNS [76]
0.1	1/9	$1.2677e-04$	$1.2598e-03$	$1.2575e-04$	$2.4285e-03$
	1/14	$3.0465e-06$	$2.1903e-04$	$1.0459e-05$	$4.2040e-04$
	1/19	$6.4303e-07$	$6.4687e-05$	$1.4559e-06$	$1.2287e-04$
	1/24	$6.4494e-07$	$2.5240e-05$	$4.0624e-07$	$4.8414e-05$
	1/29	$6.4482e-07$	$1.1872e-05$	$4.0832e-07$	$2.2651e-05$
0.3	1/9	$1.2773e-04$	$1.2910e-03$	$1.2491e-04$	$2.4131e-03$
	1/14	$4.6524e-06$	$2.2543e-04$	$1.0386e-05$	$4.1757e-04$
	1/19	$4.6830e-06$	$6.6416e-05$	$5.1023e-06$	$1.2207e-04$
	1/24	$4.6805e-06$	$2.5865e-05$	$5.1264e-06$	$4.8095e-05$
	1/29	$4.6723e-06$	$1.2160e-05$	$5.1146e-06$	$2.2506e-05$

FIGURE 7.4: (Example 7.2) Absolute modulus error

In the next example, we shall investigate the effect of $\hat{\alpha}$ on the actual maximum $L2$ norm error $E_2(h, \tau)$.

Example 7.3. Consider the time-fractional Schrödinger equation

$$\begin{cases} i {}^C_0 D_t^\gamma u(x, t) + \frac{\partial^2 u(x, t)}{\partial x^2} + |u(x, t)|^2 u(x, t) = f(x, t), & (x, t) \in [0, 1] \times [0, 1], \\ u(x, 0) = 0, & x \in [0, 1], \\ u(0, t) = i(t^{\gamma+2} - t^2), \quad u(1, t) = i(t^{\gamma+2} - t^2), & t \in [0, 1], \end{cases} \quad (7.73)$$

where $0 < \gamma < 1$ and

$$\begin{aligned} f(x, t) = & \left[\frac{\Gamma(\gamma+3)}{\Gamma(3)} t^2 - \frac{\Gamma(3)}{\Gamma(3-\gamma)} t^{2-\gamma} \right] [i \sin(2\pi x) - \cos(2\pi x)] \\ & + [-4\pi^2(t^{\gamma+2} - t^2) + (t^{\gamma+2} - t^2)^3] [\sin(2\pi x) + i \cos(2\pi x)]. \end{aligned} \quad (7.74)$$

The exact solution is $u(x, t) = (t^{\gamma+2} - t^2)[\sin(2\pi x) + i \cos(2\pi x)]$.

First, we let $\hat{\alpha} = 1/20$ and $\tau = 1/5000$ and present the spatial convergence orders of our scheme (7.18)–(7.20) and those of CNS method [76] (Table 7.7). To visualize the efficiency of our method, in Figures 7.5–7.7 we plot the real/imaginary parts of the numerical and exact solutions as well as the absolute modulus error for $\gamma = 0.5$ and $(h, \tau) = (1/16, 1/200)$. We observe that the theoretical spatial convergence of our method is indeed at least $O(h^6)$ (Theorem 7.3) and our method gives a good approximation of the exact solution.

Next, we shall investigate the influence of $\hat{\alpha}$ on the error $E_2(h, \tau)$. Consider the case when $\gamma = 0.5$ and $(h, \tau) = (1/10, 1/5000)$. We apply our scheme (7.18)–(7.20) with different values of $\hat{\alpha} \in (0, \frac{1}{10}) \cup (\frac{1}{10}, \frac{37}{180})$ and plot the error $E_2(1/10, 1/5000)$ against $\hat{\alpha}$ in Figure 7.8. It is observed that the exponent of the error remains the same (10^{-6}) for all $\hat{\alpha} \in (0, \frac{1}{10}) \cup (\frac{1}{10}, \frac{37}{180})$. Noting Table 7.7, we see that *regardless* of the chosen value of $\hat{\alpha}$, our method (error $\sim 10^{-6}$) is better than CNS method (error $\sim 10^{-4}$) in this case.

TABLE 7.7: (Example 7.3) $E_2(h, \tau)$, $E_\infty(h, \tau)$ and spatial convergence orders

γ	h	$E_2(h, \tau)$		$E_\infty(h, \tau)$		$E_\infty(h, \tau)$	
		Our method		Our method		CNS [76]	
0.1	1/5	$1.6057e-04$		$2.4239e-04$		$3.8406e-04$	
	1/10	$8.4508e-07$	7.5699	$1.0992e-06$	7.7847	$2.3556e-05$	4.0272
	1/20	$1.0644e-08$	6.3110	$1.5054e-08$	6.1902	$1.4549e-06$	4.0171
0.3	1/5	$4.6080e-04$		$6.9537e-04$		$1.1029e-03$	
	1/10	$2.4213e-06$	7.5705	$ch7.3427e-06$	7.7850	$6.7549e-05$	4.0292
	1/20	$3.0459e-08$	6.3128	$4.3067e-08$	6.1939	$4.1711e-06$	4.0174
0.5	1/5	$7.4202e-04$		$1.1157e-03$		$1.7736e-03$	
	1/10	$3.8806e-06$	7.5790	$5.0736e-06$	7.7807	$1.0865e-04$	4.0289
	1/20	$5.3287e-08$	6.1864	$7.6384e-08$	6.0536	$6.6960e-06$	4.0202

FIGURE 7.5: (Example 7.3) Real part of numerical solution and exact solution

FIGURE 7.6: (Example 7.3) Imaginary part of numerical solution and exact solution

FIGURE 7.7: (Example 7.3) Absolute modulus error

FIGURE 7.8: (Example 7.3) Influence of $\hat{\alpha}$ on the error $E_2(h, \tau)$

Remark 7.6. In Theorem 7.3, the condition $\hat{\alpha} \in (0, \frac{1}{10}) \cup (\frac{1}{10}, \frac{37}{180})$ arises from the proofs of the uniquely solvability and convergence of the numerical scheme. If this condition is not satisfied, our scheme may not be uniquely solvable and convergent. The condition $U(x, t) \in C^{(8,2)}([0, L] \times [0, T])$ arises from $L1$ approximation method and spline method. If this condition is not satisfied, the convergence order of our scheme may be reduced. Example 7.2 does not satisfy the condition $U(\cdot, t) \in C^{(2)}[0, T]$. However, the convergence order is still the same as the theoretical one. This indicates that the condition $U(\cdot, t) \in C^{(2)}[0, T]$ is a sufficient but not necessary condition.

7.6 Summary

In this chapter, we derive a numerical scheme to solve the time-fractional nonlinear Schrödinger equation (7.1) of fractional order $\gamma \in (0, 1)$. Our tools include the quintic non-polynomial spline and $L1$ discretization. The unconditional stability, unique solvability and convergence are proved by Fourier method. It is shown that our method can achieve sixth order convergence in space and $(2 - \gamma)$ th order convergence in time. Three numerical examples are presented to verify the theoretical results and to compare with other methods in the literature.

Chapter 8

Conclusion and Future Research

8.1 Conclusion

It is well known that fractional and non-fractional differential equations are widely used to model various phenomena in a great variety of fields. However, it is really difficult to obtain the analytical solutions for most differential equations. Thus, the development of efficient and accurate numerical algorithms becomes necessary. In this thesis, we focus on proposing efficient numerical schemes for different differential equations. The contributions of our work can be described in two aspects.

In the first aspect, we apply suitable approximation methods to the second order derivative in space and prove the stability and convergence of our schemes. In Chapter 3, we apply a mid-knot cubic non-polynomial spline to a second order obstacle problem. The mid-knot mesh can avoid the two breakup points of the obstacle problem. We rigorously prove the convergence by matrix analysis method. From the numerical experiments, our scheme gives more accurate solutions than other methods. In Chapter 7, we apply a quintic non-polynomial spline method to approximate the second order derivative in a nonlinear time-fractional Schrödinger equation. To the best of our knowledge, this is the first work that employs quintic non-polynomial spline to solve a *nonlinear* fractional problem. We demonstrate the stability and convergence by Fourier method. The theoretical results indicate that our scheme is sixth order convergent in space, which is the best result to date.

The second aspect of our contribution is the development of new approximation methods for fractional derivatives. In Chapter 4, we derive a new fourth order approximation method, which is based on the WSGD operator, for the classical Riemann-Liouville fractional derivative. We also extend the approximation to the classical Caputo fractional derivative and apply it to solve the fractional Bagley-Torvik equation. Using matrix analysis method, we have proved that our scheme is fourth order convergent, which is the best result so far. In Chapter 5, we propose a third order approximation for the generalized fractional derivative based on the generalized WSGD operator. Then we apply it to solve a generalized fractional diffusion problem. It is rigorously proved that our method is more accurate than other methods in the literature. In Chapter 6, we aim to improve the result of Chapter 5. Indeed, we derive a fourth order approximation method for the generalized fractional derivative. By discrete energy method, we demonstrate that our scheme is fourth order accurate in both time and space directions. To the best of our knowledge, we achieve the best convergence result to date.

8.2 Future Research

In the future, we may conduct research on a few aspects that include but not limited to the following.

- In Chapter 5, we derive a third order approximation for the generalized fractional derivative and apply it to solve a generalized fractional diffusion problem. Using discrete energy method, our scheme is shown to be stable and convergent when the fractional order $\gamma \in (0, \gamma^*)$, where $\gamma^* = 0.9569347$. In fact, through numerical simulation we observe that our scheme is also useful for $\gamma \in (\gamma^*, 1)$ in several examples. In the future, we shall investigate other methods to analyze our scheme theoretically. For example, we will try to use Fourier method instead of discrete energy method to analyze the stability and convergence. Actually, we have used Fourier method to analyze the scheme in Chapter 7. Fourier method is a very useful analytical tool, which has been applied in lots of papers. Readers can obtain the details of this method in [24, 35, 43, 44].

- In Chapter 6, we derive a fourth order approximation for the generalized fractional derivative and apply it to solve a generalized fractional diffusion problem. Using discrete energy method, our scheme is shown to be stable and convergent when the fractional order $\gamma \in (0, \gamma^{**})$, where $\gamma^{**} = 0.83273597$. In fact, through numerical simulation we observe that our scheme is also useful for $\gamma \in (\gamma^{**}, 1)$ in several examples. In the future, we shall investigate other methods to analyze our scheme theoretically. For example, we will try to use Fourier method instead of discrete energy method to analyze the stability and convergence. Actually, we have used Fourier method to analyze the scheme in Chapter 7. Fourier method is a very useful analytical tool, which has been applied in lots of papers. Readers can obtain the details of this method in [24, 35, 43, 44].
- In Chapters 4, 5 and 6, we derive approximation methods for fractional derivatives based on WSGD method and achieve high order convergence. However, this type of methods relies on strong continuous conditions of the function. However, these conditions are just sufficient conditions. From the observation of numerical experiments, the approximation methods could keep the same convergence order even if the conditions are not entirely satisfied. In the future, we shall investigate other approximation methods that impose weaker conditions on the function. We use $L1$ discretization in Chapter 7. The condition of it is normally weaker than WSGD methods, while the approximation order of it is lower than WSGD ones. $L1$ discretization is a well-known approximation method of fractional derivative. There are many variants of it to derive higher order approximation methods. We shall derive different approximation methods based on the idea of $L1$ discretization. For different variants of $L1$, readers can refer to papers [10, 19, 49, 50, 56, 75, 79, 97, 123].
- In this thesis, we only discuss the approximation methods for Riemann-Liouville fractional derivative, Caputo fractional derivative, generalized Riemann-Liouville fractional derivative and generalized Caputo fractional derivative. The approximations of other types of fractional derivatives are also important, such as distributed order fractional derivative. Distributed order fractional derivative allows the fractional order to vary and is found to be more appropriate in modeling ultraslow diffusion [22, 23]. However, the numerical

treatment of this kind of fractional derivative is still limited. Therefore, we shall investigate the approximations for this type of fractional derivative.

- In this thesis, we have considered the ordinary and partial differential equations. However, we only consider one-dimensional problems. In the future, we shall consider the numerical solution of high-dimensional problems. Actually, the computation cost of high-dimensional problems is usually very large. Thus, it is more important to propose efficient algorithms for this kind of problems. There are some pioneer work on two-dimensional problem [1, 26, 58, 146]. In the future, we will study the decomposition of matrix or alternating direction techniques which convert the original problem into a series of sub problems that can be efficiently solved.

Author's Publications

Journal Articles

- **Qinxu Ding** and Patricia Jia Yiing Wong, “Mid-knot cubic non-polynomial spline for a system of second-order boundary value problems,” *Boundary Value Problems*, 2018, Paper No. 156, 16 pp.
- **Qinxu Ding** and Patricia Jia Yiing Wong, “A higher order numerical scheme for a generalized fractional diffusion equation,” submitted for publication.
- **Qinxu Ding** and Patricia Jia Yiing Wong, “A fourth order approximation for the generalized fractional derivatives and its applications,” submitted for publication.
- **Qinxu Ding** and Patricia Jia Yiing Wong, “A higher order numerical scheme for solving fractional Bagley-Torvik equation,” submitted for publication.
- **Qinxu Ding** and Patricia Jia Yiing Wong, “Quintic non-polynomial spline method for fractional nonlinear Schrödinger equation,” submitted for publication.

Conference Proceedings

- **Qinxu Ding** and Patricia Jia Yiing Wong, “Non-polynomial spline method for time-fractional nonlinear Schrödinger equation,” *Proceedings of the 15th International Conference on Control, Automation, Robotics and Vision, Singapore (2018)*.

- **Qinxu Ding** and Patricia Jia Yiing Wong, “Numerical treatment of a system of second-order boundary value problems via mid-knot cubic non-polynomial spline,” *Proceedings of the International Conference on Numerical Analysis and Applied Mathematics 2018 (ICNAAM-2018)*, *AIP Conference Proceedings* 2116, 240008 (2019); <https://doi.org/10.1063/1.5114239>.
- **Qinxu Ding** and Patricia Jia Yiing Wong, “An efficient numerical approach for a new generalized fractional diffusion equation,” *Proceedings of the International Conference on Numerical Analysis and Applied Mathematics 2018 (ICNAAM-2018)*, *AIP Conference Proceedings* 2116, 240009 (2019); <https://doi.org/10.1063/1.5114240>.
- **Qinxu Ding** and Patricia Jia Yiing Wong, “Numerical method for fractional Bagley-Torvik equation,” *Proceedings of the International Conference on Numerical Analysis and Applied Mathematics 2018 (ICNAAM-2018)*, *AIP Conference Proceedings* 2116, 240007 (2019); <https://doi.org/10.1063/1.5114238>.

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