Numerical methods for fractional differential equations

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Numerical Methods for Fractional Differential Equations

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Doctor of Philosophy

2018

Statement of Originality

I hereby certify that the intellectual content of this thesis is the product of my original research work and has not been submitted for a higher degree to any other University or Institution.

25/10/2018

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Date

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Xuhao Li

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“It is important to work hard, and work professionally. But it is also important to enjoy your work.”

—Tao, Terence

To my dear family

Abstract

Fractional differential equations have received much attention in recent decades likely due to its powerful ability in modeling ‘memory’ processes, which are mostly observed in real world. Fractional models have been widely investigated and applied in many fields such as physics, biochemistry, electrical engineering, continuum and statistical mechanics. It is shown by many researchers that fractional derivatives can provide more accurate models than integer order derivatives do. However, for most models involving fractional operators, it is very challenging if not impossible to get analytical solutions. This motivates us to propose numerical techniques, especially those that can obtain numerical approximations both efficiently and effectively.

In this thesis, we aim to construct high order accuracy numerical scheme for two categories: (i) four classes of typical fractional problems, and (ii) some classes of generalized fractional problems. In tackling the first category, we focus on the improvement of the theoretical spatial convergence order mainly using *parametric quintic spline*. The parametric spline method has been used in previous work and has been numerically shown to get satisfying performance. Unfortunately, no strict theoretical result is established and we note that the analysis is not trivial. Due to this reason, we are greatly motivated to further investigate this method and provide strict analysis which is extremely important for a numerical method. Our contributions for topics in the first category mainly lies in two aspects: 1) we develop new numerical methods for fractional problems that improve the spatial convergence order achieved so far in the literature; 2) we establish the solvability, stability and convergence results of the proposed methods that are not given in previous work relating to parametric spline method.

The other category is about numerical treatment on some classes of generalized fractional problems. As the name suggests, the generalized fractional problems include typical fractional problems as special cases and may represent even more:

both existing and potential new cases. In fact, it is shown that many integral equations can be solved in a much elegant way using generalized fractional operators and it can somehow blur the distinction between the differential and integral equations. For this topic, the numerical investigations are very scarce and the temporal convergence order of the existing work is not so satisfying and may not meet the demand in reality. Motivated by these two observations, we shall construct some new approximations of generalized fractional derivatives through generalizations of some typical techniques, e.g. $L2 - 1_\sigma$ method and weighted shifted Grünwald-Letnikov method to improve the temporal convergence order. This will help to solve this kind of problems more efficiently and effectively.

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Notations and Acronyms

Notations

P	uniform mesh of $[0, L]$ in (3.2)
P'	uniform mesh of $[0, L']$ in (4.2)
P''	uniform mesh of $[0, T]$ in (3.2)
h	grid step size in x dimension
ℓ	grid step size in y dimension
τ	grid step size in t dimension
$D_t^k \left(\frac{\partial^k}{\partial t^k} \right)$	k -th derivative w.r.t. t
$D_x^m \left(\frac{\partial^m}{\partial x^m} \right)$	m -th derivative w.r.t. x
$D_y^n \left(\frac{\partial^n}{\partial y^n} \right)$	n -th derivative w.r.t. y
v_t	first derivative of v w.r.t variable t
$v_{xx} \left(v_{xxxx} \right)$	second order (fourth order) derivative of v w.r.t. variable x
v_{yy}	second order derivative of v w.r.t. variable y
Ω	domain of interest
$\partial\Omega$	boundary of domain Ω
$\mathcal{R}$	set of real numbers
$\mathcal{R}^+$	set of positive real numbers
$\mathcal{N}$	set of positive integer numbers
$\mathcal{F}(\cdot)$	Fourier transform of a given function
$\phi^{(k)}(\cdot)$	k -th derivative of $\phi(\cdot)$
$\mathcal{C}^k(\cdot)$	$\{\phi(\cdot) \mid \phi^{(i)}(\cdot) \text{ is continuous, } 0 \leq i \leq k\}$
$\mathcal{C}^{m,k}(\cdot)$	$\{\phi(\cdot) \mid D_x^i D_t^j \phi \text{ is continuous, } 0 \leq i \leq m, 0 \leq j \leq k\}$
$\mathcal{C}^{m,n,k}(\cdot)$	$\{\phi(\cdot) \mid D_x^i D_y^l D_t^j \phi \text{ is continuous, } 0 \leq i \leq m, 0 \leq l \leq n, 0 \leq j \leq k\}$

$L_1(\mathcal{R})$	$\{\phi(t) \mid \int_{-\infty}^{\infty} \phi(s) ds < +\infty\}$
$\mathcal{C}^{\beta+m}(\mathcal{R})$	$\{\phi(t) \mid \int_{-\infty}^{\infty} (1 + \varpi ^{\beta+m}) \mathcal{F}(\phi)(\varpi) d \varpi < \infty\}$
$\mathcal{R}(\cdot)$	spectral radius of a given matrix
$\mathcal{U}_P$	$\{u \mid u = (u_0, u_1, \dots, u_M) \text{ and } u_0 = u_M = 0\}$
$\mathcal{U}_P^*$	$\{u \mid u \in \mathcal{U}_P, \delta_x^2 u_0 = \delta_x^2 u_M = 0\}$
$\mathcal{U}_{M,N}$	$\{u \mid u = \{u_{m,n}\}, 0 \leq m \leq M, 0 \leq n \leq N\}$
$\mathcal{U}_{M,N}^*$	$\{u \in \mathcal{U}_{M,N} \mid u_{m,n} = 0 \text{ for } (x_m, y_n) \in \partial\Omega\}$
δ_t	t dimension difference notations in (6.7)
δ_x^i	x dimension difference notations in (3.26) or (4.3)
δ_y^i	y dimension difference notations in (4.4)
$(\cdot, \cdot)_1$	semi-inner product in (3.27)
$(\cdot, \cdot)$	inner product in (3.27) or (4.5)
$\langle \cdot, \cdot \rangle$	new inner product in (5.13)
$ \cdot _1$	semi-norm in (3.28)
$\ \cdot\ $	l_2 norm in (3.28) or (4.6)
$\ \cdot\ _{\infty}$	l_{∞} norm in (3.28) or (4.6)
$\mathcal{O}_{\infty,x}$	spatial convergence order in terms of l_{∞} norm in (3.58) or (4.69)
$\mathcal{O}_{2,x}$	spatial convergence order in terms of l_2 norm in (4.69)
$\mathcal{O}_{\infty,t}$	temporal convergence order in terms of l_{∞} norm in (5.47)

Acronyms

PQS	Parametric Quintic Spline
CFD	Compact Finite Difference
GL	Grünwald-Letnikov
WSGL	Weighted Shifted Grünwald-Letnikov
RL	Riemann-Liouville
w.r.t.	with respect to

i.e.	id est (“ that is ”)
e.g.	exempli gratia (“ for example ”)

Chapter 1

Introduction

1.1 Background

Differential equations involving integer derivatives have been investigated since Newton and Leibniz invented calculus in 1671 (from Wikipedia). Since then, various models like ordinary differential equations, partial differential equations are successfully used to describe real world problems. It is well known that the integer derivative is a kind of local descriptor that is affected or determined merely by its neighbors. However, for most real world problems, especially those that require ‘memory’, these models may not be exact anymore due to its local nature. This motivates researchers to seek a different but more suitable tool replacing the integer derivative. This is what the fractional derivative does.

The fractional derivative is not a new concept. In fact, 24 years after the invention of calculus, it first appears in a letter from Gottfried Wilhelm Leibniz to Guillaume de l’Hôpital. It is actually a kind of generalization of the integer derivative. There are many fractional derivatives in the literature, such as Grünwald-Letnikov (GL) derivative [104], Riemann-Liouville (RL) fractional derivative [104], Caputo fractional derivative [30, 104], Katugampola derivative [64], local fractional operator [133, 144], Risez fractional derivative [137] and tempered fractional derivative [111]. Amongst all fractional derivatives, the most two widely used generalizations are RL and Caputo fractional derivatives which are powerful enough for modeling most memory processes. However, for ultraslow diffusion with the mean square displacement growing as a power of the logarithm of time [21, 22], a more general

distributed order fractional derivative which allows the fractional order to vary, is found to be more appropriate. The *distributed order* fractional derivative was first discussed by Caputo [19] in 1969, it is actually a continuous generalization of the single-order fractional derivative, in fact it reduces to the single-order fractional derivative when the distribution function $\mathcal{D}(\beta)$ in the integral takes the Dirac- δ function. Besides above mentioned fractional derivatives, Agrawal [6] recently did a survey on some generalizations of fractional operators [64, 71] and presented a new generalization involved with a scale function $\mathcal{Z}(t)$ that can stretch or contract the domain, and a weight function $\mathcal{W}(t)$ which is used to weight the function differently at different points. It is claimed that many equations can be unified in a much more elegant way using this newly generalized operator. Therefore, we shall get a more general framework which conveniently represents analytical solutions of various problems. From the kernel point of view, the above mentioned fractional derivative all involves with a singular kernel. As stated in [60, 61, 132], since the kernel of the generalization is singular, the solution may have a weak singularity in reality which may affect the non-local dynamics characteristic or the complete memory effect of the physical system exactly. Inspired by these observations, some new fractional derivatives with non-singular kernel such as Mittag-Leffler type kernel [12, 74, 116], Extended Mittag-Leffler type kernel [134], Exponential kernel and Stretched Exponential kernel [117], have been investigated and successfully applied in the real world. Though these fractional derivatives with non-singular kernels can be well applied in real world, it is argued by Tarasov [119] that these operators may not be fractional derivatives anymore. In this thesis, we do not discuss these new subjects but focus on the fractional derivative with a singular kernel.

Although the fractional derivative has a history more than 300 years, it did not catch much attention until recent decades. In fact, it is found that when modeling memory processes, the fractional model is much more accurate than the ordinary model due to its global nature. This observation encourages researchers to investigate fractional problems deeply. Till now, fractional models have been widely applied in various fields, such as Abel's integral equation, physics, mechanics (viscoelasticity), biochemistry, medicine, electrical engineering and control [30, 69, 102, 104, 110]. Generally speaking, the fractional model, in essence, is a kind of equation involving with a fractional derivative. The most simple and straightforward way to get a fractional model is to replace the integer derivative by a fractional derivative. Some rigorous explanations can be found in the excellent

works [28, 87–91, 95, 98, 99]. Here, we shall adopt continuous time random walk (CTRW) to derive the fractional sub-diffusion equation as in [95] and the fractional sub-diffusion models will be considered in Chapters 3-5. We shall begin with the discrete time random walk and then proceed to CTRW that leads to fractional models under some conditions. Let $u(x, t)$ denote the location of a test particle at x and at time t . In the discrete context, the uniform partitions of the x dimension with spatial lattice constant Δx (see Figure 1.1) and of the t dimension with temporal lattice constant Δt are considered. Assume that the test particle must jump to the adjacent locations and the probability of jumping to the left adjacent location is $\frac{1}{2}$. It is well known that the above process can be modelled by the

FIGURE 1.1: The discrete time random walk in one dimension. Here, the spatial lattice constant is Δx and j (or $x_j = j\Delta x$) denotes the node.

master equation below

$$u(x_j, t + \Delta t) = \frac{1}{2}u(x_{j-1}, t) + \frac{1}{2}u(x_{j+1}, t). \quad (1.1)$$

Applying Taylor expansion at $x = x_j$ and at time t , in the continuum limit $\Delta t \rightarrow 0$ and $\Delta x \rightarrow 0$, we get the diffusion equation

$$\frac{\partial u(x, t)}{\partial t} = K_1 \frac{\partial^2 u(x, t)}{\partial x^2}, \quad (1.2)$$

where $K_1 = \lim_{\Delta x \rightarrow 0, \Delta t \rightarrow 0} \frac{(\Delta x)^2}{\Delta t}$ is called the diffusion constant and is of the dimension $\text{cm}^2 \text{s}^{-1}$. We refer to [95] for detailed discussion on (1.2). Note that in discrete time random walk, the length of jump Δx and the waiting time between two successive jumps Δt are both assumed to be constant. On the contrary, the CTRW model assumes that these two components are drawn from a probability density function (pdf) $\mathbb{P}(x, t)$. Then the pdf of the jump length and the waiting

time are deduced from

$$\Upsilon(x) = \int_0^\infty \mathbb{P}(x, t) dt, \quad \Theta(t) = \int_{-\infty}^\infty \mathbb{P}(x, t) dx. \quad (1.3)$$

Using (1.3), the characteristic waiting time $\mathbb{T}$ and the jump length variance Σ^2 are given by

$$\mathbb{T} = \int_0^\infty t \Theta(t) dt, \quad \Sigma^2 = \int_{-\infty}^\infty x^2 \Upsilon(x) dx. \quad (1.4)$$

As stated in [95], the CTRW processes can be categorized by $\mathbb{T}$ and Σ^2 being finite or diverging as follows:

- If $\mathbb{T} < \infty$ and $\Sigma^2 < \infty$, the CTRW is a Brownian motion.
- If $\mathbb{T} = \infty$ and $\Sigma^2 < \infty$, the CTRW corresponds to a fractal time random walk that relates to the fractional sub-diffusion process. For example, for the waiting time pdf $\Theta(t) \sim A_\gamma (\tau/t)^{1+\gamma}$ with $0 < \gamma < 1$ [98, 99], the characteristic waiting time satisfies $\mathbb{T} = \infty$ which leads to the fractional equation:

$${}_0^{RL}D_t^\gamma u(x, t) = K_\gamma \frac{\partial^2 u(x, t)}{\partial x^2} + f(x, t), \quad (1.5)$$

where ${}_0^{RL}D_t^\gamma$ is the Riemann-Louville fractional derivative (see Definition 2.4 in Chapter 2) and K_γ is the generalized diffusion constant and is of the dimension $\text{cm}^2 \text{s}^{-\gamma}$. We shall focus on this type of fractional equations in subsequent chapters.

- If $\mathbb{T} < \infty$ and $\Sigma^2 = \infty$, the CTRW describes the Lévy flight [28] which corresponds to the fractal in spatial which is not considered in this thesis.
- The case $\mathbb{T} = \infty$ and $\Sigma^2 = \infty$ is still under exploration.

Having obtained various accurate fractional models at hand, one fundamental question is: whether the solution of the fractional equation exists and whether the solution is unique if it exists? In fact, this has been studied since 1832 by Louville, see [34]. For further discussions, one can refer to excellent books [30, 69, 102, 104, 110]. Another a very natural but important question is: can we solve it analytically? Unfortunately, the answer is no for most fractional problems. Therefore, numerical methods, especially effective and efficient ones, are very necessary and vital in reality. In this thesis, we aim to construct high accuracy numerical schemes for various

fractional differential equations, and demonstrate the efficiency and effectiveness both theoretically and numerically.

1.2 Major Contributions

The objective of the thesis is to propose new and efficient high order numerical methods for fractional differential equations that consist of two parts:

- (a) four classes of typical fractional problems;
- (b) one class of generalized fractional sub-diffusion equations.

In tackling the fractional problems in the first part, the *parametric quintic spline* is mainly used to improve the theoretical spatial convergence order to at least $O(h^{4.5})$. The parametric spline method has been used in solving ordinary equations [65–68] and fractional equations [35, 50] where parametric cubic spline is applied, and it is numerically shown that the performance of the proposed scheme is satisfying. Unfortunately, none of them provides strict analysis which is *not trivial*. Because of this, we are greatly motivated to further investigate parametric quintic spline method for the following fractional problems:

- (i) second-order one-dimensional and two-dimensional fractional sub-diffusion problems that are used to describe sub-diffusive phenomena with a non-homogeneous source term [95, 138];
- (ii) fourth-order fractional sub-diffusion problems that may be necessary in transverse vibration of beams [114] and groove formation on the surface of metal by a grain boundary [102];
- (iii) fourth-order fractional diffusion-wave model [52–54];
- (iv) distributed order fractional sub-diffusion equations that are applied to model the stress behavior of an elastic medium [39];

and provide strict analysis that is extremely important for a numerical method.

Our contributions for topics in the first part mainly lie in two aspects:

- 1) we develop numerical methods for fractional problems that improve the spatial convergence order till current work;
- 2) we establish the solvability, stability and convergence of the proposed methods that are not given in previous parametric spline method related works.

The second part is about two numerical treatments on a class of new generalized fractional sub-diffusion equations [130]. The usage of new generalized derivative can somehow blur the distinction between the differential and integral equations and many integral equations can then be solved in a much elegant way. Hence, it is meaningful to study numerical schemes for such problems. Our aim here is to improve temporal convergence order using non-uniform methods as the numerical investigations are very scarce and the result in the existing work is not so satisfying and may not meet the demand in reality.

1.3 Outline of the Thesis

The thesis is organized as follows. In Chapter 2, we shall introduce basic fractional calculus and review related work in the literature. Then, we present parametric quintic spline methods for various typical fractional problems in a series of chapters: second-order one-dimensional fractional sub-diffusion problems in Chapter 3, second-order two-dimensional fractional sub-diffusion problems in Chapter 4, fourth-order fractional sub-diffusion problems in Chapter 5, two numerical schemes for fourth-order fractional diffusion-wave model in Chapters 6 and 7 respectively, and distributed order fractional sub-diffusion equations in Chapter 8. After that, in Chapters 9 and 10, two efficient fully schemes are proposed for new generalized fractional sub-diffusion problems. Chapter 11 summarizes the work done so far and lists some potential future work.

Chapter 2

Literature Review

In this chapter, we start with the introduction of basic definitions of fractional integrals and derivatives and then give a brief review of approximation methods for fractional derivatives including RL fractional derivatives and Caputo fractional derivatives with order between 0 and 2, distributed order fractional derivatives and new generalized fractional derivatives. After that, we present existing methods used in space dimension for second-order and fourth-order fractional problems.

2.1 Fractional Integrals and Derivatives

In this section, we shall introduce some fundamental concepts of fractional integrals and derivatives of a given function $\Phi(t)$. We consider $t \in [0, T]$ without loss of generality and assume that the function $\Phi(t)$ are sufficiently smooth.

2.1.1 Fractional Integrals

The fractional integral has been discussed in some very good books [30, 102, 104]. It is actually a generalization of the following k -fold integral, i.e.

$$\int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{k-1}} \Phi(s_k) ds_k, \quad (2.1)$$

which, by simple calculation, is equal to

$$\frac{1}{\Gamma(k)} \int_0^t (t-s)^{k-1} \Phi(s) ds, \quad (2.2)$$

where $k \in \mathcal{N}$ and $\Gamma(k)$ is the gamma function defined as

$$\Gamma(k) = \int_0^\infty x^{k-1} e^{-x} dx.$$

By replacing k by a positive real number $\beta \in \mathcal{R}^+$, we extend the k -th integration of $\Phi(t)$ to β -th integration of $\Phi(t)$.

Definition 2.1. Given that $\beta \in \mathcal{R}^+ \setminus \mathcal{N}$ and $t > 0$, the fractional integral of $\Phi(t)$ with the fractional order β is defined by

$${}_0I_t^\beta \Phi(t) = \frac{1}{\Gamma(\beta)} \int_0^t (t-s)^{\beta-1} \Phi(s) ds. \quad (2.3)$$

Besides above typical fractional integral, there is a new generalized fractional integral that will be used later. In fact, it incorporates a weight function $\mathcal{W}(t)$ that weighs function $\Phi(t)$ differently at different time t , and a scale function $\mathcal{Z}(t)$ that allows to contract or stretch the interested domain. It was first proposed in 2012 by Agrawal [6]. Here, we only present the left weighted/scaled fractional integral and refer readers to [6] for complete discussions.

Definition 2.2. For a given scale function $\mathcal{Z}(t)$ and a weight function $\mathcal{W}(t)$, the left weighted/scaled fractional integral of order $\beta \in \mathcal{R}^+ \setminus \mathcal{N}$ of $\Phi(t)$ is defined as

$${}_0I_{t;[\mathcal{Z},\mathcal{W}]}^\beta \Phi(t) = \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(\beta)} \int_0^t [\mathcal{Z}(t) - \mathcal{Z}(s)]^{\beta-1} \mathcal{W}(s) \mathcal{Z}'(s) \Phi(s) ds. \quad (2.4)$$

Remark 2.1. Note that when $\mathcal{Z}(t) = t$, $\mathcal{W}(t) \equiv 1$, (2.4) reduces to the typical fractional integral (2.3).

2.1.2 Fractional Derivatives

Now, we shall introduce some fractional derivatives that used in this thesis, that is, GL fractional derivative, RL fractional derivative, Caputo fractional derivative,

distributed order fractional derivative and new generalized fractional derivative. We refer readers to [64, 70, 71, 111, 137] for other fractional derivatives.

Let us start with the GL fractional derivative. The basic idea of this approximation is to generalize the characteristic of the well known definition of the integer order derivative. As in [104], a direct generalization gives

Definition 2.3. For fixed $t > 0$, let τ be the step size, then the β -th order GL fractional derivative of $\Phi(t)$ is given by

$${}_0D_t^\beta \Phi(t) = \lim_{\tau \rightarrow 0} \tau^{-\beta} \sum_{k=0}^{\lceil \frac{t}{\tau} \rceil} (-1)^k \binom{\beta}{k} \Phi(t - k\tau), \quad (2.5)$$

where $\beta \in \mathcal{R}^+ \setminus \mathcal{N}$.

Remark 2.2. If $\Phi^{(j)}(0), 1 \leq j \leq k$ are continuous in the interval $[0, t]$ and $k - 1 < \beta < k$, then we have an equivalent formulation:

$${}_0D_t^\beta \Phi(t) = \sum_{j=0}^{k-1} \frac{\Phi^{(j)}(0)}{\Gamma(j+1-\beta)} t^{j-\beta} + \frac{1}{\Gamma(k-\beta)} \int_0^t (t-s)^{k-\beta-1} \Phi^{(k)}(s) ds. \quad (2.6)$$

Next, we come to the two widely used fractional derivatives in the literature: RL fractional derivative and Caputo fractional derivative. As one can see later, these two operators can be related to each other under proper assumptions. This property increases flexibility in deriving various numerical schemes that will be demonstrated in Chapters 8 and 9. The definition of these two fractional derivatives can be found in any fractional related books [30, 102, 104]. Here we just list what we need throughout the thesis and leave details for readers.

Definition 2.4. For a function $\Phi(t)$, the β -th order RL fractional derivative of $\Phi(t)$ is given by

$${}_0^{RL}D_t^\beta \Phi(t) = D_t^k ({}_0I_t^{k-\beta} \Phi(t)) = \frac{1}{\Gamma(k-\beta)} \frac{d^k}{dt^k} \int_0^t (t-s)^{k-\beta-1} \Phi(s) ds, \quad (2.7)$$

where $k - 1 < \beta < k$.

Remark 2.3. If $\Phi(t)$ is k times continuously differentiable, then

$${}_0^{RL}D_t^\beta \Phi(t) = {}_0D_t^\beta \Phi(t).$$

Definition 2.5. For a function $\Phi(t)$, the β -th order Caputo fractional derivative of $\Phi(t)$ is given by

$${}_0^C D_t^\beta \Phi(t) = {}_0 I_t^{k-\beta} (D_t^k \Phi(t)) = \frac{1}{\Gamma(k-\beta)} \int_0^t (t-s)^{k-\beta-1} \Phi^{(k)}(s) ds, \quad (2.8)$$

where $k-1 < \beta < k$.

According to the Definitions 2.4 and 2.5, it is possible to relate the RL fractional derivative to the Caputo fractional derivative using integration by parts. This is illustrated in the following lemma.

Lemma 2.1. [30] Let $\beta > 0$ and k be an integer such that $k-1 < \beta < k$, we have

$${}_0^C D_t^\beta \Phi(t) = {}_0^{RL} D_t^\beta \Phi(t) - \sum_{j=1}^{k-1} \frac{\Phi^{(j)}(0)}{\Gamma(j-\beta+1)} t^{j-\beta}. \quad (2.9)$$

Remark 2.4. From Lemma 2.1, it is obvious that ${}_0^C D_t^\beta \Phi(t) = {}_0^{RL} D_t^\beta \Phi(t)$ if and only if $\Phi^{(j)}(0) = 0$, $0 \leq j \leq k-1$.

Using the definition of the Caputo fractional derivative, we can further define the distributed order fractional derivative ${}_0^C D_t^{\mathcal{D}(\beta)} \Phi(t)$ that is used in Chapter 8.

Definition 2.6. For a proper defined function $\Phi(t)$, we have

$${}_0^C D_t^{\mathcal{D}(\beta)} \Phi(t) = \int_0^1 \mathcal{D}(\beta) {}_0^C D_t^\beta \Phi(t) d\beta. \quad (2.10)$$

Here, ${}_0^C D_t^\beta \Phi(t)$ is the Caputo fractional derivative as in Definition 2.4 and $\mathcal{D}(\beta)$ (≥ 0) is the distribution of the fractional order satisfying $\int_0^1 \mathcal{D}(\beta) d\beta > 0$.

Finally, we briefly introduce two new generalized fractional derivatives in [6] that will be used in Chapters 9 and 10. These two fractional derivatives can be regarded as generalizations of the typical fractional derivatives in Definitions 2.4 and 2.5 in the sense that they coincide when $\mathcal{Z}(t) = t$ and $\mathcal{W}(t) \equiv 1$. To better explain this, we need the following notation that denotes the left weighted/scaled m -th integer order derivative of a function $\Phi(t)$

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

where $\mathcal{Z}(t)$ and $\mathcal{W}(t)$ have the same meaning as before.

With this tool and (2.4) at hand, we can define the generalized RL fractional derivative and the generalized Caputo fractional derivative for $0 \leq k-1 < \beta < k$.

Definition 2.7. The β -th generalized RL fractional derivative is defined as

$${}_0^{RL}D_{t;[\mathcal{Z},\mathcal{W}]}^\beta \Phi(t) = D_{[\mathcal{Z},\mathcal{W}]}^k \left(I_{t;[\mathcal{Z},\mathcal{W}]}^{k-\beta} \Phi(t) \right). \quad (2.11)$$

Definition 2.8. The β -th generalized Caputo fractional derivative is given by

$${}_0^CD_{t;[\mathcal{Z},\mathcal{W}]}^\beta \Phi(t) = I_{t;[\mathcal{Z},\mathcal{W}]}^{k-\beta} \left(D_{[\mathcal{Z},\mathcal{W}]}^k \Phi(t) \right). \quad (2.12)$$

We note that a similar argument to Lemma 2.1 can be proved for general β . Here, we just prove a simple case when $0 < \beta < 1$ that will be used in Chapter 9.

Lemma 2.2. *If $\Phi(t)$ is sufficiently smooth, it holds that*

$${}_0^{RL}D_{t;[\mathcal{Z},\mathcal{W}]}^\beta \Phi(t) = \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(1-\alpha)} \frac{\mathcal{W}(0)\Phi(0)}{[\mathcal{Z}(t) - \mathcal{Z}(0)]^\beta} + {}_0^CD_{t;[\mathcal{Z},\mathcal{W}]}^\beta \Phi(t), \quad (2.13)$$

where $0 < \beta < 1$, $\mathcal{Z}(t)$ and $\mathcal{W}(t)$ are properly defined scale and weight functions respectively.

Proof. From (2.4) and (2.11), it is found that

$$\begin{aligned} {}_0^{RL}D_{t;[\mathcal{Z},\mathcal{W}]}^\beta \Phi(t) &= \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(1-\beta)} \frac{1}{\mathcal{Z}'(t)} D_t \left[\int_0^t \frac{\mathcal{W}(s)\mathcal{Z}'(s)\Phi(s)}{[\mathcal{Z}(t) - \mathcal{Z}(s)]^\beta} ds \right] \\ &= \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(1-\beta)} \frac{1}{\mathcal{Z}'(t)} D_t \left[- \int_0^t \mathcal{W}(s)\Phi(s) d \frac{[\mathcal{Z}(t) - \mathcal{Z}(s)]^{1-\beta}}{1-\beta} \right]. \end{aligned} \quad (2.14)$$

Applying integration by parts, we have

$$\begin{aligned} - \int_0^t \mathcal{W}(s)\Phi(s) d \frac{[\mathcal{Z}(t) - \mathcal{Z}(s)]^{1-\beta}}{1-\beta} &= - \mathcal{W}(s)\Phi(s) \frac{[\mathcal{Z}(t) - \mathcal{Z}(s)]^{1-\beta}}{1-\beta} \Big|_0^t \\ &\quad + \int_0^t \frac{d(\mathcal{W}(s)\Phi(s))}{ds} \frac{[\mathcal{Z}(t) - \mathcal{Z}(s)]^{1-\beta}}{1-\beta} ds. \end{aligned} \quad (2.15)$$

Then, differentiating both sides of (2.15) w.r.t. variable t yields

$$\begin{aligned} & D_t \left[- \int_0^t \mathcal{W}(s) \Phi(s) d \frac{[\mathcal{Z}(t) - \mathcal{Z}(s)]^{1-\beta}}{1-\beta} \right] \\ &= \frac{\mathcal{W}(0) \Phi(0) \mathcal{Z}'(t)}{[\mathcal{Z}(t) - \mathcal{Z}(0)]^\beta} + \mathcal{Z}'(t) \int_0^t \frac{(\mathcal{W}(s) \Phi(s))'}{[\mathcal{Z}(t) - \mathcal{Z}(s)]^\beta} ds. \end{aligned} \quad (2.16)$$

Using formula (2.16) in (2.14) and the definition of the generalized Caputo fractional derivative (2.12), we shall get (2.13) which ends the proof. $\square$

2.2 Discretization of Fractional Derivatives

The discretization methods for fractional derivatives in the literature are discussed in this section. For the sake of convenience, we first briefly introduce methods for $0 < \beta < 1$ that appears in fractional sub-diffusion problems quite often, and then approximations for $1 < \beta < 2$ that is used to solve fractional diffusion-wave problems. In the end, we mention some techniques applied to other fractional derivatives.

2.2.1 Fractional Order in (0,1)

There are many techniques on the discretization of the Caputo fractional derivative or the RL fractional derivative with order $\beta \in (0, 1)$, like $L1$ discretization [37, 38, 41, 43, 47, 50, 59, 60, 76, 78, 80–82, 101, 106, 118, 120, 122, 135, 142, 145, 146] or backward Euler [115] or quadrature formula [125], modified $L1$ [132], $L1$ on non-uniform mesh [143], $L1 - 2$ formula [42], a slightly different method based on Taylor expansion [79], $L1 - 3$ scheme [16], $L1 - r$ [77] ($r \geq 4$), $L2 - 1_\sigma$ method [7], GL [96, 121, 138], a modified GL method [40, 48], 2-WSGL [81, 121, 123], 3-WSGL [57, 58, 121], fractional Crank-Nicolson method [62], difference method for integral [97], convolution quadrature [61] and other methods in [32]. We are not trying to describe every method in details but presenting $L1$ discretization, $L2 - 1_\sigma$ method, GL approximation and WSGL approximation that may be used in subsequent chapters. It is noted that the former two methods are proposed for the Caputo fractional derivative while the rest two are for the RL fractional derivative.

To my best knowledge, $L1$ discretization is first proposed in [118] for a fractional sub-diffusion problem. The idea is based on finite difference and is rather simple to understand. Here, we try to derive $L1$ approximation from a different way, i.e. interpolation technique. We claim that many high order methods [16, 42, 77] can be conveniently constructed using this interpolation technique, see Remark 2.5. In (2.8), let $t = t_k$, we have

$${}_0^C D_t^\beta \Phi(t_k) = \frac{1}{\Gamma(1-\beta)} \int_0^{t_k} \frac{\Phi'(s)}{(t_k-s)^\beta} ds = \frac{1}{\Gamma(1-\beta)} \sum_{j=1}^k \int_{t_{j-1}}^{t_j} \frac{\Phi'(s)}{(t_k-s)^\beta} ds, \quad (2.17)$$

where $0 < \beta < 1$ and $t_j = j\tau$.

In each interval $[t_{j-1}, t_j]$, applying the linear interpolation of (t_{j-1}, Φ_{j-1}) , (t_j, Φ_j)

$$\mathcal{I}_{1,j}(t) = \frac{t - t_{j-1}}{t_j - t_{j-1}} \Phi_j + \frac{t - t_j}{t_{j-1} - t_j} \Phi_{j-1}, \quad (2.18)$$

to approximate $\Phi(t)|_{[t_{j-1}, t_j]}$ gives

$$\begin{aligned} \int_{t_{j-1}}^{t_j} \frac{\Phi'(s)}{(t_k-s)^\beta} ds &\approx \int_{t_{j-1}}^{t_j} (t_k-s)^{-\beta} \frac{\Phi_j - \Phi_{j-1}}{t_j - t_{j-1}} ds = \frac{\Phi_j - \Phi_{j-1}}{\tau} \int_{t_{j-1}}^{t_j} (t_k-s)^{-\beta} ds \\ &= \frac{(k-j)^{1-\beta} - (k-j-1)^{1-\beta}}{(1-\beta)\tau^\beta} (\Phi_j - \Phi_{j-1}). \end{aligned}$$

Substituting above result into a former formula (2.17), we can get the $L1$ discretization. The next lemma presents the accuracy of this scheme.

Lemma 2.3. [118] *If $\Phi(t) \in \mathcal{C}^2[0, t_k]$, then the $L1$ discretization has $O(\tau^{2-\beta})$ accuracy, i.e.,*

$${}_0^C D_t^\beta \Phi(t_k) = \mu \left[a_0 \Phi_k - \sum_{j=1}^{k-1} (a_{k-j-1} - a_{k-j}) \Phi_j - a_{k-1} \Phi_0 \right] + O(\tau^{2-\beta}), \quad (2.19)$$

where $\mu = \frac{1}{\Gamma(2-\beta)\tau^\beta}$ and $a_j = (j+1)^{1-\beta} - j^{1-\beta}$, $j \geq 0$.

Remark 2.5. Following the derivation of $L1$ scheme, it is possible to construct even high order accuracy method using quadratic interpolation ($O(\tau^{3-\beta})$) [42], cubic interpolation ($O(\tau^{4-\beta})$) [16] or even high order interpolation ($O(\tau^{r-\beta})$, $r \geq 4$) [77]. Note that these methods achieve high accuracy but bring great difficulties in applications.

Remark 2.6. If $\Phi(t)$ is non-smooth, $L1$ discretization method only achieves $O(\tau)$ as stated in [60]. Fortunately, with a slightly modification of $L1$ scheme [132], the accuracy can be kept. Using convolution quadrature [61], second-order accuracy is possible even if the data is non-smooth.

The next result is about $L2 - 1_\sigma$ scheme which improves the accuracy obtained by $L1$ discretization. Unlike other high order methods [16, 42, 77] that may be difficult to analyze the convergence of numerical schemes, the $L2 - 1_\sigma$ can be successfully used and analyzed in applications. As stated in [7], this approximation method is actually inspired by [42] where a $L1 - 2$ formula is proposed. Different from $L1 - 2$ formula, the approximation is considered at a non-integer node $t_{k-1+\sigma} = (k-1+\sigma)\tau$ where $\sigma = 1 - \frac{\gamma}{2}$. To be specific, we have

$$\begin{aligned} {}^C_0 D_t^\beta \Phi(t_{k-1+\sigma}) &= \frac{1}{\Gamma(1-\beta)} \int_0^{t_{k-1+\sigma}} (t_{k-1+\sigma} - s)^{-\beta} f'(s) ds \\ &= \frac{1}{\Gamma(1-\beta)} \left[\sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} \frac{\Phi'(s)}{(t_{k-1+\sigma} - s)^\gamma} ds + \int_{t_{k-1}}^{t_{k-1+\sigma}} \frac{\Phi'(s)}{(t_{k-1+\sigma} - s)^\beta} ds \right]. \end{aligned}$$

In each subinterval $[t_{j-1}, t_j]$ ($1 \leq j \leq k-1$), we shall apply the quadratic interpolation of points (t_{j-1}, Φ_{j-1}) , (t_j, Φ_j) and (t_{j+1}, Φ_{j+1}) as follows

$$\mathcal{I}_{2,j}(t) = \sum_{n=0}^2 \prod_{m=0, m \neq n}^2 \frac{t - t_{j-1+m}}{t_{j-1+n} - t_{j-1+m}} \Phi_{j-1+n}, \quad (2.20)$$

to replace $\Phi(t)$ in $[t_{j-1}, t_j]$ and the linear interpolation $\mathcal{I}_{1,k}$ in (2.18) of (t_{k-1}, Φ_{k-1}) and (t_k, Φ_k) in the last interval $[t_{k-1}, t_{k-1+\sigma}]$. After sufficient calculations and rigorous analysis, the complete formula of $L2 - 1_\sigma$ and its accuracy is illustrated by a lemma below.

Lemma 2.4. [7] Let $\Phi(t) \in \mathcal{C}^3[0, t_{k-1+\sigma}]$, μ be the same as in Lemma 2.3 and $\sigma = 1 - \frac{\beta}{2}$, we get

$${}^C_0 D_t^\beta \Phi(t_{k-1+\sigma}) = \mu \left[r_0 \Phi_k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \Phi_j - r_{k-1} \Phi_0 \right] + O(\tau^{3-\beta}), \quad (2.21)$$

where $r_0 = a_{\sigma,0}$ if $k = 1$ and when $k \geq 2$,

$$r_j = \begin{cases} a_{\sigma,0} + b_{\sigma,1}, & j = 0, \\ a_{\sigma,j} + b_{\sigma,j+1} - b_{\sigma,j}, & 1 \leq j \leq k-2, \\ a_{\sigma,k-1} - b_{\sigma,k-1}, & j = k-1. \end{cases} \quad (2.22)$$

Here, $a_{\sigma,0} = \sigma^{1-\beta}$, $a_{\sigma,j} = (j + \sigma)^{1-\beta} - (j - 1 + \sigma)^{1-\beta}$, $j \geq 1$ and $b_{\sigma,j}$ is given by

$$b_{\sigma,j} = \frac{1}{2-\beta} [(j + \sigma)^{2-\beta} - (j - 1 + \sigma)^{2-\beta}] - \frac{1}{2} [(j + \sigma)^{1-\beta} + (j - 1 + \sigma)^{1-\beta}].$$

Till now, we have introduced two fundamental approaches for the Caputo fractional derivative with order between 0 and 1. In what follows, we will demonstrate two methods for the RL fractional derivative: GL technique and WSGL method.

We begin with the GL approach. Considering Remark 2.3 and Definition 2.3, obviously we can approximate ${}_0^RL_t^\beta \Phi(t)$ using equation (2.5). However, this approximation is not used quite often in tackling fractional problems except in [24–27, 29] where the fractional derivative is in terms of space variable. Since we deal with the fractional derivative in time variable in applications, in reality, the most common applied method in the literature involves with an integer shift $l \geq 0$ of (2.5). To better illustrate this, we suppose that $\Phi(t)$ is a properly defined function over $\mathcal{R}$ for a while till the end of this part. Also, we need the shifted GL operator discussed in [94, 121], namely,

$$\mathcal{A}_{\tau,l}^\beta \Phi(t) = \frac{1}{\tau^\beta} \sum_{k=0}^{\infty} \omega_k^\beta \Phi(t - (k-l)\tau), \quad (2.23)$$

where ω_k^β are coefficients from the generating functions $\omega(z, \beta) = \sum_{k=0}^{\infty} \omega_k^\beta z^k$.

Remark 2.7. If $\omega(z, \beta) = (1 - z)^\beta$ and $l = 0$, then it is essentially the same as equation (2.5) which gives $O(\tau)$. High order approximation is possible for other options of the generating function $\omega(z, \beta)$ when $l = 0$, see [83, 104].

In this thesis, we shall focus on the case $\omega(z, \beta) = (1 - z)^\beta$ and $l \geq 0$. Hence, ω_k^β can be explicitly given by $\omega_k^\beta = (-1)^k \binom{\beta}{k}$. In [94], it is pointed out that under appropriate conditions, (2.23) approximates the RL fractional derivative ${}_{-\infty}^RL_t^\beta \Phi(t)$ (obtained by replacing 0 by $-\infty$ in (2.7) of Definition 2.4) uniformly for every $t \in \mathcal{R}$. To be specific,

Lemma 2.5. [94] If $\Phi(t) \in L_1(\mathcal{R}) \cap \mathcal{C}^{\beta+1}(\mathcal{R})$, then one has

$${}_{-\infty}^{RL}D_t^\beta \Phi(t) = \mathcal{A}_{\tau,l}^\beta \Phi(t) + O(\tau), \quad (2.24)$$

where $l \geq 0$ is an integer.

It is noted that GL method only achieves first order accuracy. To get higher order approximation method for the RL fractional derivative, a so-called WSGL approximation is developed in [121] and then used in [123] for a fractional sub-diffusion equation and [39] for a distributed order problem. This method is based on the shifted GL operator (2.23). The details are given in the following lemma.

Lemma 2.6. [39, 121, 123] Let $\Phi(t)$, ${}_{-\infty}^{RL}D_t^{\beta+2}\Phi(t)$ and $\mathcal{F}({}_{-\infty}^{RL}D_t^{\beta+2}\Phi(t)) \in L_1(\mathcal{R})$. For any given $t \in \mathcal{R}$, it is obtained that

$${}_{-\infty}^{RL}D_t^\beta \Phi(t) = \frac{\beta - 2l}{2(\hat{l} - l)} \mathcal{A}_{\tau,\hat{l}}^\beta + \frac{2k - \beta}{2(\hat{l} - l)} \mathcal{A}_{\tau,l}^\beta + O(\tau^2), \quad (2.25)$$

where $\hat{l}, l$ are integers and $\hat{l} \neq l$.

Remark 2.8. For the approximation of the RL fractional derivative of a given function, it is possible to pick $(\hat{l}, l)$ randomly. However, when it comes to solving fractional sud-diffusion differential equations, the pair $(\hat{l}, l)$ is not freely chosen since we need to solve it numerically iteratively. In reality, people take $(\hat{l}, l) = (0, -1)$ or $(-1, 0)$ which leads to an implicit numerical scheme. Also, for non-smooth data, one can refer to a modified WSGL in [141].

Lemma 2.6 is also called 2-WSGL. There is a 3-WSGL discussed in [57, 58].

Lemma 2.7. [57, 58] Let $\Phi(t)$, ${}_{-\infty}^{RL}D_t^{\beta+3}\Phi(t)$ and $\mathcal{F}({}_{-\infty}^{RL}D_t^{\beta+3}\Phi(t)) \in L_1(\mathcal{R})$. For any given $t \in \mathcal{R}$, it holds that

$${}_{-\infty}^{RL}D_t^\beta \Phi(t) = \mathfrak{S}_1 \mathcal{A}_{\tau,\hat{l}}^\beta + \mathfrak{S}_2 \mathcal{A}_{\tau,l}^\beta + \mathfrak{S}_3 \mathcal{A}_{\tau,m}^\beta + O(\tau^3), \quad (2.26)$$

where

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

and $\hat{l}$, l , m are integers.

Remark 2.9. The 3-WSGL result is established in [57, 58]. Then it is applied to solve one-dimensional and two-dimensional fractional sub-diffusion problems when $(\hat{l}, l, m) = (0, -1, -2)$. It is noted that the convergence and stability of the proposed scheme can be only proved for $\beta \in (0, \beta^*]$ where $\beta^* = 0.9569347$.

2.2.2 Fractional Order in (1,2)

In the literature, the fractional derivative with order $\beta \in (1, 2)$ is typically in the Caputo sense as the initial conditions required there are more natural and meaningful than the RL fractional derivative. The approximation methods for the fractional derivative with $1 < \beta < 2$ include both direct and indirect techniques. Direct methods consist of WSGL for the space fractional derivative [121], difference scheme [52–54, 118], forward finite difference [136], GL [94], fractional trapezoid rule [140], corrected WSGL [141], convolution quadrature with the generating function given by second-order backward difference method [61] and references [83–85] while indirect ones include GL for integral [55], WSGL for integral [123, 124]. Here, we only present the difference scheme that is used in subsequent chapters.

Lemma 2.8. [52–54, 118] Suppose $\Phi(t) \in \mathcal{C}^3[0, t_k]$. It is proved that

$${}_0^C D_t^\beta \Phi(t_{k-\frac{1}{2}}) = \tilde{\mu} \left[\tilde{a}_0 \delta_t \Phi^{k-\frac{1}{2}} - \sum_{j=1}^{k-1} (\tilde{a}_{k-j-1} - \tilde{a}_{k-j}) \delta_t \Phi^{j-\frac{1}{2}} - \tilde{a}_{k-1} \Phi'(0) \right] + O(\tau^{3-\beta}), \quad (2.27)$$

where $\tilde{\mu} = \frac{1}{\Gamma(3-\beta)\tau^{\beta-1}}$ and $\tilde{a}_j = (j+1)^{\beta-1} - j^{\beta-1}$, $j \geq 0$.

2.2.3 Other Fractional Derivatives

There are some other fractional derivatives such as distributed order fractional derivatives [19], Risez fractional derivatives [137] and new generalized fractional derivatives [6]. We are not going further on these topics but encouraging readers to the excellent papers [14, 31, 32, 39, 51, 63, 100, 128, 130, 131, 137] for approximation methods.

2.3 Approximation in Spatial Dimension

Another main ingredient in tackling the fractional problems numerically lies in the discretization in the spatial dimension. In this section, we shall introduce methods based on the fractional second-order and fourth-order equations which are the main problems studied in this thesis and other fractional equations.

2.3.1 Second-order Fractional Equations

Second-order fractional equations have been received sufficient attention and have been extensively investigated in recent decades. There are many useful methods proposed in tackling such equations efficiently. For one-dimensional cases, methods like finite difference [24, 38, 40, 41, 43, 51, 55, 57, 76, 100, 101, 118, 138, 140], compact finite difference [25, 29, 33, 37, 40, 96, 106, 123, 143, 146], a particular difference scheme [79], polynomial and non-polynomial method [50], Galerkin spectral method and Legendre collocation method [80], Galerkin finite element method [60–62], cubic trigonometric B-spline collocation [136] and box-type scheme [145, 146], have been developed and successfully applied in reality. Also, for two-dimensional problems, there are finite difference [26, 39, 142], compact finite difference [39, 58, 124], radial basis function (RBF) [97], orthogonal spline collocation [135] and Galerkin finite element method [60–62]. Three-dimensional problems are very challenging but they can still be solved using finite difference [23] with ADI technique and Galerkin finite element method [60–62].

2.3.2 Fourth-order Fractional Equations

Comparing to the second-order fractional problems, works on the fourth-order fractional equation are much less. To deal with one-dimensional problem, Homotopy perturbation method (HPM) [44], local discontinuous Galerkin [47, 125], compact finite difference [52, 54, 59, 122], finite difference [53], decomposition method [56], (mixed) finite element [81, 82], quintic B-spline collocation [115] and quintic spline [120] are constructed and well used in applications. For two-dimensional or even

higher dimension problems, methods such as compact finite difference [59] and homotopy perturbation method (HPM) based on Jumarie's derivative [45] can provide very good and satisfying results.

2.3.3 Other Fractional Equations

Besides second-order and fourth-order fractional models, there are some other fractional problems that are studied in literature, e.g. finite difference for fractional Fokker-Planck equations [27] and new generalized fractional sub-diffusion equations [130], parametric cubic spline for fractional Burger's equations [35], non-standard finite difference for fractional chaotic systems [48], fractional homotopy analysis transform method for fractional Lienard's equations and Fitzhugh-Nagumo equations [72, 73], difference scheme for fractional advection-dispersion flow equations [94], WSGL for space fractional diffusion equations [121] and fractional centered difference for Riesz space fractional problems [137]. We do not go further here but refer readers to related works for details.

Part I

Parametric Quintic Spline Method

Chapter 3

Second-order One-dimensional Fractional Sub-diffusion Problems

In this chapter, we shall tackle fractional sub-diffusion equation which is used to describe sub-diffusive phenomena with a non-homogeneous source term [95, 138]. The problem is formulated as

$$\left\{ \begin{array}{l} {}^C_0 D_t^\gamma u(x, t) - du_{xx}(x, t) = f(x, t), \quad (x, t) \in \Omega = [0, L] \times [0, T] \\ u(x, 0) = \psi(x), \quad x \in [0, L] \\ u(0, t) = \phi_1(t), \quad u(L, t) = \phi_2(t), \quad t \in [0, T]. \end{array} \right. \quad (3.1)$$

where $0 < \gamma < 1$, $d (> 0)$ is the generalized diffusion constant, $f(x, t)$, $\psi(x)$, $\phi_1(t)$, $\phi_2(t)$ are properly defined functions.

The problem (3.1) has been studied in [29, 37] using different methodologies of which the global convergence orders are $O(\tau + h^4)$ and $O(\tau^{2-\gamma} + h^4)$ respectively. Motivated by [29, 37], we shall propose a numerical scheme for problem (3.1) using parametric quintic spline in the spatial direction and $L1$ discretization of the Caputo derivative. We shall show that the convergence of the proposed scheme is at least $O(\tau^{2-\gamma} + h^{4.5})$ (see Theorem 3.2 and Remark 3.2) in maximum norm – this clearly improves the results of [29, 37] as well as other work on the numerical solution of (3.1) established to date. We are motivated to use a non-polynomial method as there are indications [35, 50, 65–67] that such methods are superior to polynomial methods. In fact, Khan et al. [65–67] have used parametric quintic spline

to solve third, fourth and sixth order boundary value problems of *integer order* differential equations. In fractional differential equations, parametric cubic spline method has been applied by El-Danaf and Hadhoud [35] to time fractional Burgers' equations. Also, Hosseini and Ghaffari [50] have used parametric cubic spline to solve a fractional sub-diffusion problem that is different from our consideration. In both [35, 50], Von Neumann method is used for stability analysis, the global convergence is *not* proved theoretically but numerical examples are presented to illustrate the efficiency of their methods. Different from the work of [35, 50], we shall apply *parametric quintic spline* and use *energy method* to prove the convergence and stability. To the best of our knowledge, this is the first exploration of using parametric quintic spline for fractional differential equations. Moreover, in using energy method we need to identify a suitable inner product and the corresponding norm, which are different from those in [37]. It is noted that this technique is very different from other related work [25, 33].

In what follows, we develop the numerical scheme based on parametric quintic spline in Section 3.1 and establish the solvability of the scheme in Section 3.2. The convergence and stability of the scheme are analyzed in Section 3.3. To demonstrate the accuracy and efficiency of the method, some numerical experiments are presented in Section 3.4. Finally, a brief conclusion is given in Section 3.5.

3.1 Parametric Quintic Spline Method

In this section, we shall develop a numerical scheme for problem (3.1) using parametric quintic spline. Consider uniform partitions P and P'' as follows:

$$P : 0 = x_0 < x_1 < \cdots < x_M = L \text{ and } P'' : 0 = t_0 < t_1 < \cdots < t_K = T \quad (3.2)$$

where $x_m = mh$ and $t_k = k\tau$ with $h = \frac{L}{M}$ and $\tau = \frac{T}{K}$. Let $U(x, t)$ denote the exact solution of problem (3.1). At each fixed $t = t_k$, $1 \leq k \leq K$, we shall approximate the solution $U(x, t_k)$ of (3.1) by the parametric quintic spline $\mathcal{S}_k(x; \xi)$ which is defined as follows.

Definition 3.1. Let $t = t_k$, $1 \leq k \leq K$ be fixed. We say $\mathcal{S}_k(x; \xi) \in \mathcal{C}^4[0, L]$ is the *parametric quintic spline with parameter* $\xi > 0$ (with respect to mesh P) if its

restriction $\mathcal{S}_{m,k}(x; \xi) \equiv \mathcal{S}_{m,k}(x)$ in $[x_{m-1}, x_m]$, $1 \leq m \leq M$ satisfies

$$\mathcal{S}_{m,k}(x_j) = u_j^k, \quad j = m-1, m \quad (3.3)$$

and

$$\mathcal{S}_{m,k}^{(4)}(x) + \xi^2 \mathcal{S}_{m,k}''(x) = (F_m^k + \xi^2 W_m^k) \frac{x - x_{m-1}}{h} + (F_{m-1}^k + \xi^2 W_{m-1}^k) \frac{x_m - x}{h}, \quad (3.4)$$

where

$$\mathcal{S}_{m,k}''(x_j) = W_j^k, \quad \mathcal{S}_{m,k}^{(4)}(x_j) = F_j^k, \quad j = m-1, m. \quad (3.5)$$

It is noted that parametric quintic spline is similarly defined in [35, 65–67]. Solving (3.4) for $\mathcal{S}_{m,k}(x)$, we get

$$\begin{aligned} \mathcal{S}_{m,k}(x) = & c_{1,k} + c_{2,k}x + c_{3,k} \cos(\xi x) + c_{4,k} \sin(\xi x) \\ & + \frac{1}{\xi^2} \left[(F_m^k + \xi^2 W_m^k) \frac{(x - x_{m-1})^3}{6h} + (F_{m-1}^k + \xi^2 W_{m-1}^k) \frac{(x_m - x)^3}{6h} \right] \end{aligned} \quad (3.6)$$

where $c_{i,k}$, $i = 1, 2, 3, 4$ are constants that can be determined by (3.3) and (3.5) in terms of u_j^k , W_j^k and F_j^k , $j = m-1, m$. Upon substituting the expressions of $c_{i,k}$'s into (3.6), we obtain

$$\begin{aligned} \mathcal{S}_{m,k}(x) = & \zeta u_m^k + \bar{\zeta} u_{m-1}^k + \frac{h^2}{6} [q_3(\zeta) W_m^k + q_3(\bar{\zeta}) W_{m-1}^k] \\ & + \left(\frac{h}{\nu}\right)^4 \left[\frac{\nu^2}{6} q_3(\zeta) - q_1(\zeta) \right] F_m^k + \left(\frac{h}{\nu}\right)^4 \left[\frac{\nu^2}{6} q_3(\bar{\zeta}) - q_1(\bar{\zeta}) \right] F_{m-1}^k \end{aligned} \quad (3.7)$$

where

$$\nu = \xi h, \quad \zeta = \frac{x - x_{m-1}}{h}, \quad \bar{\zeta} = 1 - \zeta, \quad q_3(\zeta) = \zeta^3 - \zeta, \quad q_1(\zeta) = \zeta - \frac{\sin \nu \zeta}{\sin \nu}.$$

Applying the continuity of the first and the third derivatives of the spline at $x = x_m$, i.e., $\mathcal{S}'_{m+1,k}(x_m) = \mathcal{S}'_{m,k}(x_m)$ and $\mathcal{S}'''_{m+1,k}(x_m) = \mathcal{S}'''_{m,k}(x_m)$, we obtain the relations

$$\begin{aligned} (a) \quad & W_{m+1}^k + 4W_m^k + W_{m-1}^k = 6\delta_x^2 u_m^k - 6h^2 (\kappa_1 F_{m+1}^k + 2\rho_1 F_m^k + \kappa_1 F_{m-1}^k); \\ (b) \quad & W_{m+1}^k - 2W_m^k + W_{m-1}^k = h^2 (\kappa F_{m+1}^k + 2\rho F_m^k + \kappa F_{m-1}^k) \end{aligned} \quad (3.8)$$

where

$$\begin{aligned}\kappa &= \frac{1}{\nu^2} \left(\frac{\nu}{\sin \nu} - 1 \right), & \rho &= \frac{1}{\nu^2} \left(3 - \frac{\nu \cos \nu}{\sin \nu} \right), \\ \kappa_1 &= \frac{1}{6\nu^2} + \frac{1}{\nu^4} - \frac{1}{\nu^3 \sin \nu}, & \rho_1 &= \frac{1}{3\nu^2} - 1 + \frac{\cos \nu}{\nu^3 \sin \nu}.\end{aligned}\tag{3.9}$$

Note that the consistency relation for (3.8)(b) will lead to $2\kappa + 2\rho = 1$ [35, 65–67]. Moreover, if $\xi \rightarrow 0$ (i.e., $\nu \rightarrow 0$), then $(\kappa, \rho, \kappa_1, \rho_1) \rightarrow (\frac{1}{6}, \frac{1}{3}, -\frac{7}{360}, -\frac{8}{360})$ and (3.8) will become the well known quintic spline relations. Using the two equations in (3.8), it is easy to derive

$$F_m^k = \frac{(\kappa + 6\kappa_1)W_{m+1}^k + 4(\kappa - 3\kappa_1)W_m^k + (\kappa + 6\kappa_1)W_{m-1}^k - 6\kappa\delta_x^2 u_m^k}{12h^2(\kappa_1\rho - \rho_1\kappa)}\tag{3.10}$$

The expressions of F_{m-1}^k and F_{m+1}^k can be deduced from that of F_m^k . Now, we substitute F_{m+1}^k , F_m^k and F_{m-1}^k in (3.8)(b) to get

$$\wedge W_m^k = \frac{1}{h^2} [\kappa u_{m+2}^k + 2(\rho - \kappa)u_{m+1}^k + 2(\kappa - 2\rho)u_m^k + 2(\rho - \kappa)u_{m-1}^k + \kappa u_{m-2}^k],\tag{3.11}$$

where $2 \leq m \leq M - 2$, $\wedge$ is an operator and $\wedge W_m^k$ is defined by

$$\wedge W_m^k = pW_{m+2}^k + qW_{m+1}^k + sW_m^k + qW_{m-1}^k + pW_{m-2}^k, \quad 2 \leq m \leq M - 2\tag{3.12}$$

where

$$p = \kappa_1 + \frac{\kappa}{6}, \quad q = 2 \left[\frac{2\kappa + \rho}{6} - (\kappa_1 - \rho_1) \right], \quad s = 2 \left[\frac{\kappa + 4\rho}{6} + (\kappa_1 - 2\rho_1) \right].$$

From (3.1), using $L1$ approximation (2.19) to discretize the Caputo fractional term, it is obvious that

$$u_{xx}(x_m, t_k) = \frac{\mu}{d} \sum_{j=0}^{k-1} a_j (u_m^{j+1} - u_m^j) - \frac{1}{d} f_m^k + O(\tau^{2-\gamma}).\tag{3.13}$$

Since the exact solution of (3.1) at $t = t_k$ is approximated by the parametric quintic spline $\mathcal{S}_k(x; \xi)$, it follows that $\mathcal{S}_{m,k}''(x_m) = W_m^k$ is an approximation to $u_{xx}(x_m, t_k)$,

so in view of (3.12) we set

$$W_m^k = \frac{\mu}{d} \sum_{k=0}^{n-1} a_k (u_m^{k+1} - u_m^k) - \frac{1}{d} f_m^k. \quad (3.14)$$

Hence, we have

$$W_m^k = u_{xx}(x_m, t_k) + O(\tau^{2-\gamma}). \quad (3.15)$$

Applying the operator $\wedge$ to (3.14) yields

$$\wedge W_m^k = \frac{\mu}{d} \sum_{k=0}^{n-1} a_k (\wedge u_m^{k+1} - \wedge u_m^k) - \frac{1}{d} \wedge f_m^k, \quad 2 \leq m \leq M-2.$$

Noting (3.11) and the definition of $\wedge$, we rearrange the above relation to get

$$A_1 (u_{m-2}^k + u_{m+2}^k) + A_2 (u_{m-1}^k + u_{m+1}^k) + A_3 u_m^k = \frac{\mu}{d} \sum_{j=0}^{k-1} a_j^\gamma (\wedge u_m^j) + \frac{1}{d} \wedge f_m^k, \quad (3.16)$$

where $2 \leq m \leq M-2$, $A_1 = \frac{\mu}{d}p - \frac{\kappa}{h^2}$, $A_2 = \frac{\mu}{d}q - \frac{2(\rho-\kappa)}{h^2}$, $A_3 = \frac{\mu}{d}s - \frac{2(\kappa-2\rho)}{h^2}$ and

$$a_0^\gamma = a_0, \quad a_j^\gamma = a_j - a_{j-1}, \quad 1 \leq m \leq k-1 \quad (3.17)$$

Note that the boundary conditions in (3.1) give $u_0^k = \phi_1(t_k)$ and $u_M^k = \phi_2(t_k)$. Hence, in order to compute the numerical solution u_m^k , $1 \leq m \leq M-1$, besides (3.16) we need two more equations. To this aim, we consider the following equations

$$\begin{aligned} \text{(a)} \quad & \frac{1}{h^2} (c_0 u_0^k + c_1 u_1^k + c_2 u_2^k) + b_0 W_0^k + b_1 W_1^k + b_2 W_2^k + T_1^k = 0; \\ \text{(b)} \quad & \frac{1}{h^2} (c_M u_M^k + c_{M-1} u_{M-1}^k + c_{M-2} u_{M-2}^k) + b_M W_M^k + b_{M-1} W_{M-1}^k + b_{M-2} W_{M-2}^k + T_{M-1}^k = 0 \end{aligned}$$

where the constants c_i and b_i , $i = 0, 1, 2, M-2, M-1, M$ are to be determined.

Using (3.15), we carry out Taylor expansion at $x = x_1$ in equation (a) and $x = x_{M-1}$ in equation (b). By setting the coefficients of $D_x^j u_m^k$, $0 \leq j \leq 5$, $m = 1, M-1$ to zero, we obtain

$$(c_0, c_1, c_2, b_0, b_1, b_2) = (c_M, c_{M-1}, c_{M-2}, b_M, b_{M-1}, b_{M-2}) = \left(-1, 2, -1, \frac{1}{12}, \frac{5}{6}, \frac{1}{12} \right) \quad (3.18)$$

and

$$T_m^k = -\frac{1}{240}h^4 D_x^6 u_m^k + O(h^6 + \tau^{2-\gamma}), \quad m = 1, M-1. \quad (3.19)$$

Omitting T_m^k , $m = 1, M-1$ in equations (a) and (b), substituting the constants and using (3.14), we get for $m = 1, M-1$ that

$$\begin{aligned} A_1^* u_{m-1}^k + A_2^* u_m^k + A_1^* u_{m+1}^k &= \frac{\mu}{12d} \sum_{j=0}^{k-1} a_j^\gamma (u_{m-1}^j + 10u_m^j + u_{m+1}^j) \\ &\quad + \frac{1}{12d} (f_{m-1}^k + 10f_m^k + f_{m+1}^k), \end{aligned} \quad (3.20)$$

where a_j^γ is defined in (3.17),

$$A_1^* = \frac{\mu}{12d} - \frac{1}{h^2}, \quad A_2^* = \frac{5\mu}{6d} + \frac{2}{h^2}. \quad (3.21)$$

We have now derived the numerical scheme comprising (3.16) and (3.20). In practice, since the initial condition in (3.4) gives $u_m^0 = \psi(x_m)$, $0 \leq m \leq M$, we just use (3.16), (3.20) to calculate the approximate solution at $t = t_1$, i.e., u_m^1 , $0 \leq m \leq M$, thereafter the approximate solution at the next time step $t = t_2$ can be computed. Continuing in this manner, the approximate solution u_m^k , $0 \leq m \leq M$ can be obtained for $1 \leq k \leq K$. Note that we will use this technique to obtain numerical solutions in Chapters 4-10 as well.

3.2 Local Truncation Error and Solvability

In this section, we shall analyze the local truncation error of the numerical scheme (3.16), (3.20), and then establish the solvability of the scheme.

Lemma 3.1. *Let T_m^k be the local truncation error of the m -th formula in the numerical scheme (3.16), (3.20). We have*

$$T_m^k = \begin{cases} -\frac{1}{240}h^4 D_x^6 u_m^k + O(h^6 + \tau^{2-\gamma}), & m = 1, M-1 \\ \sum_{l=1}^4 Z_l h^{2l-2} D_x^{2l} u_m^k + O(h^8 + \tau^{2-\gamma}), & 2 \leq m \leq M-2 \end{cases} \quad (3.22)$$

where the constants Z_l , $l = 1, 2, 3, 4$ are given by

$$\begin{aligned} Z_1 &= 2(\kappa + \rho) - 2p - 2q - s, & Z_2 &= \frac{1}{6}(7\kappa + \rho) - 4p - q, \\ Z_3 &= \frac{1}{180}(31\kappa + \rho) - \frac{4}{3}p - \frac{1}{12}q, & Z_4 &= \frac{1}{10080}(327\kappa + \rho) - \frac{8}{45}p - \frac{1}{360}q. \end{aligned} \quad (3.23)$$

From Lemma 3.1, we can easily see that for $2 \leq m \leq M - 2$, the order of h varies from 2 to 6 depending on whether the related coefficients are zero or not. In the present work, we shall consider the highest order of h , i.e., h^6 , which is achieved by setting

$$Z_1 = Z_2 = Z_3 = 0. \quad (3.24)$$

Together with the consistency relation $2(\kappa + \rho) = 1$, equation (3.24) yields

$$p = \frac{1}{12}\kappa - \frac{1}{240}, \quad q = \frac{2}{3}\kappa + \frac{1}{10}, \quad s = -\frac{3}{2}\kappa + \frac{97}{120}. \quad (3.25)$$

(Note that from $Z_1 = 0$, we also have the relation $2p + 2q + s = 1$.) In the next result, we shall investigate the solvability of system (3.16), (3.20) under (3.25) and the consistency relation $2(\kappa + \rho) = 1$.

Theorem 3.1. *If $0 < \kappa < \frac{37}{180}$, then system (3.16), (3.20) with (3.6) and the consistency relation $2(\kappa + \rho) = 1$ has a unique solution.*

Proof. It is sufficient to prove that the coefficient matrix of system (3.16), (3.20) given by

$$\begin{pmatrix} A_2^* & A_1^* & & & & & \\ A_2 & A_3 & A_2 & A_1 & & & \\ A_1 & A_2 & A_3 & A_2 & A_1 & & \\ & & & \ddots & & & \\ & & & & A_1 & A_2 & A_3 & A_2 & A_1 \\ & & & & & A_1 & A_2 & A_3 & A_2 \\ & & & & & & & A_1^* & A_2^* \end{pmatrix}$$

is strictly diagonally dominated.

In fact, for the first and the last rows of the matrix, it is easy to check that $|A_2^*| > |A_1^*|$.

For other rows of the matrix, by considering four cases (i) $A_2, A_1 < 0$, (ii) $A_2 > 0, A_1 < 0$, (iii) $A_2, A_1 > 0$ and (iv) $A_2 < 0, A_1 > 0$ individually, we shall get

$$\bar{\Delta} \equiv |A_3| - 2|A_2| - 2|A_1| > 0.$$

in all cases. Therefore, the coefficient matrix is strictly diagonally dominated which implies that the system (3.16), (3.20) has a unique solution. $\square$

3.3 Convergence and Stability

In this section, we shall establish the convergence and stability of the proposed numerical scheme in maximum norm. Our methodology, known as energy method, involves introducing a suitable inner product and the corresponding norm.

To begin, for $u, v \in \mathcal{U}_P$, define difference notations

$$\begin{aligned} \delta_x u_{m+\frac{1}{2}} &= \frac{u_{m+1} - u_m}{h}, & \delta_x^2 u_m &= \frac{\delta_x u_{m+\frac{1}{2}} - \delta_x u_{m-\frac{1}{2}}}{h}, \\ \delta_x^3 u_{m+\frac{1}{2}} &= \frac{\delta_x^2 u_{m+1} - \delta_x^2 u_m}{h}, & \delta_x^4 u_m &= \frac{\delta_x^3 u_{m+\frac{1}{2}} - \delta_x^3 u_{m-\frac{1}{2}}}{h}, \end{aligned} \quad (3.26)$$

and

$$(u, v)_1 = h \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2}} \right) \left(\delta_x v_{m+\frac{1}{2}} \right), \quad (u, v) = h \sum_{m=1}^{M-1} u_m v_m \quad (3.27)$$

$$|u|_1 = \sqrt{h \sum_{m=0}^{M-1} (\delta_x u_{m+\frac{1}{2}})^2}, \quad \|u\| = (u, u)^{\frac{1}{2}}, \quad \|u\|_\infty = \max_{1 \leq m \leq M-1} |u_m|. \quad (3.28)$$

Moreover, let

$$\begin{aligned} u \odot v &= \sum_{m=0}^{M-1} h (\delta_x u_{m+\frac{1}{2}}) (\delta_x v_{m+\frac{1}{2}}) - \frac{1}{12} h^3 [(\delta_x^2 u_1)(\delta_x^2 v_1) + (\delta_x^2 u_{M-1})(\delta_x^2 v_{M-1})] \\ &\quad - (q + 3p) h^3 [(\delta_x^2 u_2)(\delta_x^2 v_2) + (\delta_x^2 u_{M-2})(\delta_x^2 v_{M-2})] \\ &\quad - (q + 4p) \sum_{m=3}^{M-3} h^3 (\delta_x^2 u_m)(\delta_x^2 v_m) + p h^5 \sum_{m=2}^{M-3} (\delta_x^3 u_{m+\frac{1}{2}})(\delta_x^3 v_{m+\frac{1}{2}}) \end{aligned}$$

and

$$u * v = u \odot v + p h^3 [(\delta_x^2 u_1)(\delta_x^2 v_1) + (\delta_x^2 u_{M-1})(\delta_x^2 v_{M-1})], \quad (3.29)$$

where p and q are given in (3.25). For any $u, v \in \mathcal{U}_P$, due to the non-negativity, symmetry and linearity of the operator $\odot$, it is found that

$$u \odot v \leq \frac{1}{2} (u \odot u + v \odot v). \quad (3.30)$$

In what follows, we shall present some lemmas which are needed in the convergence analysis. The first result relates the inner products $u * u$, $u \odot u$ with the norm $|u|_1$.

Lemma 3.2. *If $\frac{1}{20} \leq \kappa < \frac{1}{6}$, then*

$$[1 - 4(q + 4p)]|u|_1^2 \leq u \odot u \leq u * u \leq (3 + 16p)|u|_1^2, \quad u \in \mathcal{U}_P \quad (3.31)$$

where p and q are given in (3.25).

Proof. Since $\kappa \geq \frac{1}{20}$, it is clear that $p, q \geq 0$. Hence, $u \odot u \leq u * u$ is immediate. Next, we observe that

$$h^2 \left(\delta_x^3 u_{m+\frac{1}{2}} \right)^2 \leq 2 \left[\left(\delta_x^2 u_{m+1} \right)^2 + \left(\delta_x^2 u_m \right)^2 \right]$$

and

$$h^2 \left(\delta_x^2 u_m \right)^2 \leq 2 \left[\left(\delta_x u_{m+\frac{1}{2}} \right)^2 + \left(\delta_x u_{m-\frac{1}{2}} \right)^2 \right].$$

Using above two results, from (3.29) we find

$$u * u \leq (3 + 16p) \sum_{m=0}^{M-1} h \left(\delta_x u_{m+\frac{1}{2}} \right)^2 = (3 + 16p)|u|_1^2. \quad (3.32)$$

Now, to estimate the negative terms in $u \odot u$, we get, by noting $\frac{1}{12} < q + 4p$ ($= \kappa + \frac{1}{12}$), $q + 3p \leq q + 4p$ and $ph^5 \sum_{m=2}^{M-3} \left(\delta_x^3 u_{m+\frac{1}{2}} \right)^2$ is non-negative and above results,

$$u \odot u \geq h \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2}} \right)^2 - 4(q + 4p)|u|_1^2 = [1 - 4(q + 4p)]|u|_1^2.$$

The proof is complete. $\square$

Remark 3.1. In the inequality (3.31), we know that the constant $[1 - 4(q + 4p)]$ ($= \frac{2}{3} - 4\kappa$) is positive since $\kappa < \frac{1}{6}$.

The next two lemma plays an important role in proving the convergence of the proposed scheme.

Lemma 3.3. [2, 37, 53, 57, 118] *For any $u \in \mathcal{U}_P$, we have*

$$\|u\|_\infty \leq \frac{\sqrt{L}}{2} |u|_1.$$

Lemma 3.4. [27, 37] *For $0 < \gamma < 1$ and a_j defined in (2.19), we have*

$$(a) \quad 1 = a_{k-1} > a_{k-2} > \cdots > a_j > a_{j-1} \cdots > a_1 > a_0 > 0;$$

$$(b) \quad a_j > \frac{1-\gamma}{(k-j)^\gamma}, \quad 0 \leq j \leq k-1.$$

Now, recall that $U_m^k = U(x_m, t_k)$ is the exact solution of (3.1) at $x = x_m$ and $t = t_k$, and u_m^k is an approximate value of U_m^k , and $e_m^k = U_m^k - u_m^k$ is the error, where $0 \leq m \leq M$, $0 \leq k \leq K$. Obviously, $e^k \in \mathcal{U}_P$ since $e_0^k = e_M^k = 0$.

For our analysis, let us first consider $t = t_k$ where $k \geq 2$. Since U_m^k is the exact solution, from (3.16) and (3.20) respectively we have for $m = 1, M-1$

$$\begin{aligned} A_1^* U_{m-1}^k + A_2^* U_m^k + A_1^* U_{m+1}^k &= \frac{\mu}{12d} \sum_{j=0}^{k-1} a_j^\gamma (U_{m-1}^j + 10U_m^j + U_{m+1}^j) \\ &\quad + \frac{f_{m-1}^k + 10f_m^k + f_{m+1}^k}{12d} - T_m^k, \end{aligned}$$

and for $2 \leq m \leq M-2$

$$A_1 (U_{m-2}^k + U_{m+2}^k) + A_2 (U_{m-1}^k + U_{m+1}^k) + A_3 U_m^k = \frac{\mu}{d} \sum_{j=0}^{k-1} a_j^\gamma (\wedge U_m^j) + \frac{1}{d} \wedge f_m^k - T_m^k.$$

Together with (3.16) and (3.20), it is clear that e_m^k is the solution of

$$A_1^* e_{m-1}^k + A_2^* e_m^k + A_1^* e_{m+1}^k = \frac{\mu}{12d} \sum_{j=0}^{k-1} a_j^\gamma (e_{m-1}^j + 10e_m^j + e_{m+1}^j) - T_m^k, \quad m = 1, M-1 \quad (3.33)$$

and for $2 \leq m \leq M-2$

$$A_1 (e_{m-2}^k + e_{m+2}^k) + A_2 (e_{m-1}^k + e_{m+1}^k) + A_3 e_m^k = \frac{\mu}{d} \sum_{j=0}^{k-1} a_j^\gamma (\wedge e_m^j) - T_m^k. \quad (3.34)$$

For notational simplicity, for $0 \leq j \leq k$, define

$$\begin{aligned} A(j) &= \sum_{m=1}^{M-1} (-h\delta_x^2 e_m^k) e_m^j - \frac{h^3}{12} [(\delta_x^2 e_1^k)(\delta_x^2 e_1^j) + (\delta_x^2 e_{M-1}^k)(\delta_x^2 e_{M-1}^j)] \\ &\quad - (q + 4p)h^3 \sum_{m=2}^{M-2} (\delta_x^2 e_m^k)(\delta_x^2 e_m^j) + \sum_{m=2}^{M-2} (-h\delta_x^2 e_m^k)(ph^4 \delta_x^4 e_m^j). \end{aligned} \quad (3.35)$$

Now, we multiply both sides of (3.33) and (3.34) by $\frac{d}{d\mu}(-h\delta_x^2 e_m^k)$ and then sum from 1 to $(M-1)$. After some substantial manipulation, we get

$$A(k) = \sum_{j=0}^{k-1} a_j^\gamma A(j) - \frac{dh}{\mu} \sum_{m=1}^{M-1} (\delta_x^2 e_m^k)^2 - \frac{\kappa dh^3}{\mu} \sum_{m=2}^{M-2} (\delta_x^2 e_m^k)(\delta_x^4 e_m^k) + \frac{dh}{\mu} \sum_{m=1}^{M-1} (\delta_x^2 e_m^k) T_m^k. \quad (3.36)$$

Next, since $e^j \in \mathcal{U}_P$, after some simple calculation we find $A(j)$ in (3.36) can be rewritten as

$$A(j) = e^k \odot e^j - ph^3 [(\delta_x^2 e_{M-2}^k)(\delta_x^2 e_{M-1}^j) + (\delta_x^2 e_2^k)(\delta_x^2 e_1^j)]. \quad (3.37)$$

Moreover, using (3.30), the inequality $-xy \leq \frac{1}{2}(x^2 + y^2)$ and (3.29), it follows from (3.37) that

$$A(j) \leq \frac{e^k * e^k + e^j * e^j}{2} + \frac{1}{2} ph^3 [(\delta_x^2 e_2^k)^2 + (\delta_x^2 e_{M-2}^k)^2 - (\delta_x^2 e_1^k)^2 - (\delta_x^2 e_{M-1}^k)^2]. \quad (3.38)$$

We are now ready to show the convergence of the proposed numerical scheme.

Theorem 3.2. Suppose $U(x, t) \in \mathcal{C}^{8,2}(\Omega)$. Further, let $\frac{1}{20} \leq \kappa < \frac{1}{6}$ and $\frac{\kappa d}{2\mu} \geq ph^2$ hold. Then,

$$\|e^k\|_\infty^2 \leq CE, \quad 1 \leq k \leq K \quad (3.39)$$

where

$$C = \frac{LT^\gamma \Gamma(3-\gamma)d}{16[1-4(q+4p)](3-4\kappa)}, \quad E = 2h(C_1)^2(\tau^{2-\gamma} + h^4)^2 + L(C_2)^2(\tau^{2-\gamma} + h^6)^2,$$

C_i , $i = 1, 2$ are some positive constants, and p and q are given in (3.25).

Proof. From Lemma 3.4, it is obvious that $a_j^\gamma > 0$ for $0 \leq j \leq k-1$ and $\sum_{j=1}^{k-1} a_j^\gamma < 1$. Moreover, $A(0) = 0$ since $e^0 = 0$. Noting these, we apply (3.38) for $1 \leq k \leq n-1$ in the right side of (3.36) and substitute the left side of (3.36) by (3.37), to obtain

$$\frac{1}{2} e^k * e^k \leq \frac{1}{2} \sum_{j=1}^{k-1} a_j^\gamma \langle e^j, e^j \rangle + \Xi_1 + \Xi_2 + \Xi_3 + \Xi_4 \quad (3.40)$$

where

$$\Xi_1 = \frac{\kappa d h^2}{\mu} \sum_{m=2}^{M-2} (-h \delta_x^2 e_m^k) (\delta_x^4 e_m^k), \quad \Xi_2 = -\frac{d}{\mu} h \sum_{m=1}^{M-1} (\delta_x^2 e_m^k)^2, \quad \Xi_3 = \frac{d}{\mu} \sum_{m=1}^{M-1} (h \delta_x^2 e_m^k) T_m^k$$

and

$$\begin{aligned} \Xi_4 = & \frac{1}{2} p h^3 \sum_{j=1}^{k-1} a_j^\gamma [(\delta_x^2 e_2^k)^2 + (\delta_x^2 e_{M-2}^k)^2 - (\delta_x^2 e_1^k)^2 - (\delta_x^2 e_{M-1}^k)^2] \\ & + p h^3 [(\delta_x^2 e_{M-2}^k)(\delta_x^2 e_{M-1}^k) + (\delta_x^2 e_2^k)(\delta_x^2 e_1^k) + (\delta_x^2 e_1^k)^2 + (\delta_x^2 e_{M-1}^k)^2]. \end{aligned}$$

We shall obtain an upper bound for $(\Xi_1 + \Xi_2 + \Xi_3 + \Xi_4)$. First, using $\sum_{j=1}^{k-1} a_j^\gamma < 1$ and the inequality $xy \leq \frac{1}{2}(x^2 + y^2)$, we find

$$\Xi_4 \leq p h^3 [(\delta_x^2 e_2^k)^2 + (\delta_x^2 e_{M-2}^k)^2] + \frac{3}{2} p h^3 [(\delta_x^2 e_1^k)^2 + (\delta_x^2 e_{M-1}^k)^2]. \quad (3.41)$$

Next, mainly using the inequality $-xy \leq \frac{1}{2}(x^2 + y^2)$, we have

$$\Xi_1 \leq \frac{\kappa d h}{\mu} \left\{ 4 \sum_{m=3}^{M-3} (\delta_x^2 e_m^k)^2 + \frac{7 [(\delta_x^2 e_2^k)^2 + (\delta_x^2 e_{M-2}^k)^2]}{2} + \frac{(\delta_x^2 e_1^k)^2 + (\delta_x^2 e_{M-1}^k)^2}{2} \right\}. \quad (3.42)$$

Note that the assumption $\frac{\kappa d}{2\mu} \geq p h^2$ implies $\frac{7\kappa d}{2\mu} + p h^2 \leq \frac{4\kappa d}{\mu}$ and $\frac{\kappa d}{2\mu} + \frac{3}{2} p h^2 \leq \frac{4\kappa d}{\mu}$. Therefore, together with (3.41) and (3.42), we get

$$\Xi_1 + \Xi_2 + \Xi_4 \leq -(1 - 4\kappa) \frac{d}{\mu} h \sum_{m=1}^{M-1} (\delta_x^2 e_m^k)^2. \quad (3.43)$$

Next, using the inequality $xy \leq \frac{x^2 + y^2}{2}$, it is easy to find

$$\Xi_3 \leq (1 - 4\kappa) \frac{d}{\mu} h \sum_{m=1}^{M-1} (\delta_x^2 e_m^k)^2 + \sum_{m=1}^{M-1} \frac{d h}{4(1 - 4\kappa)\mu} (T_m^k)^2. \quad (3.44)$$

Now, we combine (3.43) and (3.44) and substitute $\mu = \frac{1}{\tau^\gamma \Gamma(2-\gamma)}$, to obtain

$$\Xi_1 + \Xi_2 + \Xi_3 + \Xi_4 \leq \sum_{m=1}^{M-1} \frac{d h}{4(1 - 4\kappa)\mu} (T_m^k)^2 = \tau^\gamma \frac{\Gamma(2-\gamma)d}{4(1 - 4\kappa)} \|T^k\|^2 \quad (3.45)$$

Since p and q are as in (3.25) which is the result of $Z_1 = Z_2 = Z_3 = 0$, it follows from (3.22) that

$$|T_m^k| \leq \frac{1}{\sqrt{2}} \begin{cases} C_1(\tau^{2-\gamma} + h^4), & m = 1, M-1 \\ C_2(\tau^{2-\gamma} + h^6), & 2 \leq m \leq M-2 \end{cases}$$

where C_1 and C_2 are some positive constants. Hence, we have

$$2\|T^k\|^2 = h \sum_{m=1}^{M-1} (T_m^k)^2 \leq 2h(C_1)^2(\tau^{2-\gamma} + h^4)^2 + L(C_2)^2(\tau^{2-\gamma} + h^6)^2 = E. \quad (3.46)$$

Now, using (3.45) and (3.46) in (3.40), we obtain for $k \geq 2$,

$$e^k * e^k \leq \sum_{j=1}^{k-1} a_j^\gamma (e^j * e^j) + \tau^\gamma \left(\frac{\Gamma(2-\gamma)d}{4(3-4\kappa)} E \right). \quad (3.47)$$

To complete the analysis, we need to estimate the term $\langle e^k, e^k \rangle$ in the right side of (3.47). To this aim, we shall first estimate $\langle e^1, e^1 \rangle$. Using a similar technique as in the derivation of (3.45) and (3.46), (3.47) is true when $k = 1$. Thus, by induction method, from (3.47), we have

$$e^k * e^k \leq \frac{1}{a_k^\gamma} \tau^\gamma \left(\frac{\Gamma(2-\gamma)d}{4(3-4\kappa)} E \right), \quad k \geq 1. \quad (3.48)$$

Finally, in view of Lemmas 3.2, 3.3, 3.4(b) and (3.48), we could get (3.39). The proof is complete. $\square$

Remark 3.2.

- (a) From the error inequality (3.25) of Theorem 3.2, we can conclude that $\|e^k\|_\infty = O(\tau^{2-\gamma} + h^{4.5})$. Hence, our proposed scheme improves the compact finite difference method in [37] which has a global convergence order of $O(\tau^{2-\gamma} + h^4)$ and has been the best result until our current work.
- (b) The constant C in the error inequality (3.39) can be written as

$$C = \frac{LT^\gamma \Gamma(1-\gamma)d}{16[1-4(q+4p)](1-4\kappa)} = \frac{LT^\gamma \Gamma(1-\gamma)d}{16(2/3-4\alpha)(1-4\kappa)}.$$

Hence, it is clear that the maximum error bound is smallest when α is smallest, i.e., the smallest α that satisfies $\frac{1}{20} \leq \kappa < \frac{1}{6}$ and $\frac{\kappa d}{2\mu} \geq ph^2$. However, this is only the *error bound* and we have no information about the behavior of *actual errors* with respect to κ . In Section 3.4, we shall investigate the effect of κ on actual errors of particular problems.

- (c) Note that the error inequality (3.39) gives an error bound but it is not a tight bound. Thus, it is possible that the actual convergence order is higher than the theoretical one. To explain this further, denote E (in (3.39)) as $\mathbb{E}(h)$. Then, for sufficiently small τ , we have

$$\mathbb{E}(h) \approx 2(C_1)^2 h^9 + L(C_2)^2 h^{12}$$

and

$$\mathbb{E}\left(\frac{h}{2}\right) \approx 2(C_1)^2 \left(\frac{h}{2}\right)^9 + L(C_2)^2 \left(\frac{h}{2}\right)^{12}.$$

Hence,

$$\frac{\mathbb{E}(h)}{\mathbb{E}\left(\frac{h}{2}\right)} \approx 2^{12} C_3$$

where

$$C_3 = \frac{2(C_1)^2 + L(C_2)^2 h^3}{2^3[2(C_1)^2] + L(C_2)^2 h^3} \quad (C_3 \text{ is minimum when } h = 0).$$

If $h \rightarrow 0$, then we have $\mathbb{E}(h) / \mathbb{E}\left(\frac{h}{2}\right) \approx 2^9$ which gives a convergence order of $O(h^{4.5})$ in the spatial dimension. However, if h is not that small, then it is possible to expect higher convergence order than $O(h^{4.5})$. In fact, we are able to observe this in the numerical examples in Section 3.4.

Remark 3.3. Note that the range of κ in Theorem 3.1 (solvability) contains the range of κ in Theorem 3.2 (convergence).

Remark 3.4. Our convergence analysis requires that the solution be $\mathcal{C}^8([0, L])$ in the spatial dimension. However, for some engineering problems, the solutions may not be so smooth. It is reasonable to expect lower convergence order for such problems.

Now, let us present the stability result. Similarly, let $v^k \in \mathcal{U}_P$ satisfy that for $m = 1, M - 1$

$$\begin{aligned} A_1^* v_{m-1}^k + A_2^* v_m^k + A_1^* v_{m+1}^k &= \frac{\mu}{12d} \sum_{j=0}^{k-1} a_j^\gamma (v_{m-1}^j + 10v_m^j + v_{m+1}^j) \\ &+ \frac{1}{12d} (f_{m-1}^k + 10f_m^k + f_{m+1}^k), \end{aligned} \quad (3.49)$$

and for $2 \leq m \leq M - 2$

$$A_1 (v_{m-2}^k + v_{m+2}^k) + A_2 (v_{m-1}^k + v_{m+1}^k) + A_3 v_m^k = \frac{\mu}{d} \sum_{j=0}^{k-1} a_j^\gamma (\wedge v_m^j) + \frac{1}{d} \wedge f_m^k, \quad (3.50)$$

with $v_m^0 = \psi(x_m) - \theta_m$, $v_0^k = \phi_1(t_k)$, $v_M^k = \phi_2(t_k)$. Let $\epsilon_m^k = u_m^k - v_m^k$, $0 \leq m \leq M$, $0 \leq k \leq K$.

Then, in view of (3.49)–(3.50), (3.16) and (3.20), ϵ_m^k satisfies

$$A_1^* \epsilon_{m-1}^k + A_2^* \epsilon_m^k + A_1^* \epsilon_{m+1}^k = \frac{\mu}{12d} \sum_{j=0}^{k-1} a_j^\gamma (\epsilon_{m-1}^j + 10\epsilon_m^j + \epsilon_{m+1}^j), \quad m = 1, M - 1 \quad (3.51)$$

and

$$A_1 (\epsilon_{m-2}^k + \epsilon_{m+2}^k) + A_2 (\epsilon_{m-1}^k + \epsilon_{m+1}^k) + A_3 \epsilon_m^k = \frac{\mu}{d} \sum_{j=0}^{k-1} a_k^\gamma (\wedge \epsilon_m^j), \quad 2 \leq m \leq M - 2 \quad (3.52)$$

with $\epsilon_0^k = \epsilon_M^k = 0$, $\epsilon_m^k = \theta_m$. It is noted that $\epsilon^k \in \mathcal{U}_P$.

The theorem below establishes the stability of the proposed scheme with respect to initial values.

Theorem 3.3. *Let $\frac{1}{20} \leq \kappa < \frac{1}{6}$ and $\frac{\kappa d}{2\mu} \geq ph^2$ hold. Then,*

$$\|\epsilon^k\|_\infty^2 \leq \frac{L(3 + 16p)}{4[1 - 4(q + 4p)]} |\epsilon^0|_1^2, \quad 1 \leq k \leq K \quad (3.53)$$

where p and q are given in (3.25).

Proof. Using a similar technique as in the convergence analysis, with e_m^k (in theorem 3.2) replaced by ϵ_m^k and noting that $A(0) \neq 0$, we can obtain an analog of (3.47) as

$$\epsilon^k * \epsilon^k \leq \sum_{j=0}^{k-1} a_j^\gamma (\epsilon^j * \epsilon^j). \quad (3.54)$$

By induction method, from (3.54), we have

$$\epsilon^k * \epsilon^k \leq \epsilon^0 * \epsilon^0, \quad k \geq 1. \quad (3.55)$$

Finally, applying Lemmas 3.3 and 3.4 as well as (3.55), (3.53) is achieved. The proof is complete. $\square$

3.4 Experiment

In this section, we shall present three examples from [29, 37, 50] to demonstrate the efficiency of the proposed parametric quintic spline (PQS) method. We shall also compare the performance of PQS method, compact finite difference (CFD) method [37] and quintic spline (QS) method. Note that QS method is a special case of PQS method when $\kappa = \frac{1}{6}$ and $\rho = \frac{1}{3}$.

In the examples, we consider the generalized diffusion constant $d = 1$. In view of Theorems 3.1 and 3.2, we require $\frac{1}{20} \leq \kappa < \frac{1}{6}$ and $\frac{\kappa d}{2\mu} \geq ph^2$. Noting $d = 1$, the inequality $\frac{\kappa d}{2\mu} \geq ph^2$ is equivalent to

$$\frac{\tau^\gamma \Gamma(2 - \gamma)}{h^2} \geq \frac{1}{6} - \frac{1}{120\kappa}. \quad (3.56)$$

Hence, to ensure convergence and stability, the grid sizes τ , h and parameter κ used in the examples should satisfy $\frac{1}{20} \leq \kappa < \frac{1}{6}$ and (3.56).

For a fixed (τ, h) , denote the maximum absolute error at $t = t_K$ by

$$\|e^K(\tau, h)\|_\infty = \|e^K\|_\infty. \quad (3.57)$$

The spatial convergence order is

$$\mathcal{O}_{\infty,x} = \log_2 \frac{\|e^K(\tau, h)\|_{\infty}}{\|e^K(\tau, \frac{h}{2})\|_{\infty}}. \quad (3.58)$$

Example 3.1. The first example is from [24, 29, 37, 76]. Consider (3.1) with $L = T = d = 1$, $u(x, 0) = 0$,

$$u(0, t) = t^{1+\gamma}, \quad u(1, t) = et^{1+\gamma}, \quad f(x, t) = e^x[\Gamma(2 + \gamma)t - t^{1+\gamma}]. \quad (3.59)$$

The exact solution is $u(x, t) = e^x t^{1+\gamma}$.

TABLE 3.1: (Example 3.1) Maximum absolute error at $t = 1$

γ	h	PQS	$\mathcal{O}_{\infty,x}$	QS	$\mathcal{O}_{\infty,x}$	CFD	$\mathcal{O}_{\infty,x}$
$\frac{1}{4}$	$\frac{1}{5}$	4.62E-07	-	2.51E-07	-	1.25E-06	-
	$\frac{1}{10}$	8.40E-09	5.7814	2.10E-08	3.5792	7.80E-08	4.0023
	$\frac{1}{20}$	1.95E-10	5.4288	1.84E-09	3.5126	4.65E-09	4.0682
$\frac{1}{2}$	$\frac{1}{4}$	1.67E-06	-	1.02E-06	-	2.99E-06	-
	$\frac{1}{8}$	3.14E-08	5.7303	4.39E-08	4.5398	1.86E-07	4.0058
	$\frac{1}{16}$	8.24E-10	5.2531	4.77E-09	3.2037	1.06E-08	4.1302
$\frac{3}{5}$	$\frac{1}{4}$	1.66E-06	-	1.02E-06	-	2.96E-06	-
	$\frac{1}{8}$	3.13E-08	5.7259	4.35E-08	4.5441	1.84E-07	4.0062
	$\frac{1}{16}$	8.67E-10	5.1725	4.77E-09	3.1911	1.05E-08	4.1365

For $\gamma = 0.25$, we take $\kappa = \frac{1}{12}$ and $\tau = \frac{1}{20000}$; for $\gamma = 0.5$, we take $\kappa = \frac{1}{20}$ and $\tau = \frac{1}{100000}$; for $\gamma = 0.6$, we take $\kappa = \frac{1}{20}$ and $\tau = \frac{1}{300000}$. In Table 3.1, we tabulate $\|e^K(\tau, h)\|_{\infty}$ obtained by three methods (PQS, QS, CFD) for various h as well as the corresponding convergence order.

From Table 3.1, we observe that PQS method outperforms CFD method for all cases, and except for the largest h , the errors obtained are also smaller than that of QS method.

We further plot the numerical/exact solutions and the absolute error in Figures 3.1 and 3.2. As stated in Theorem 3.2, the bound of maximum absolute error depends on the choice of κ . Hence, it is interesting to illustrate the influence of κ on error. From Figure 3.2, we see that the maximum absolute error $\|e^K(\tau, h)\|_{\infty}$ increases with κ but the effect is not significant. Regardless of the chosen value of κ , PQS

FIGURE 3.1: (Example 3.1) Approximate (left) and exact solutions (right) when $\gamma = 0.25$, $h = \frac{1}{20}$, $\tau = \frac{1}{20000}$.

FIGURE 3.2: (Example 3.1) Absolute error (left) and influence of κ on maximum absolute error (right) when $\gamma = 0.25$, $h = \frac{1}{20}$, $\tau = \frac{1}{20000}$.

method is still better than CFD method, and it is also better than QS method for smaller h . Therefore, κ has little effect on the performance of PQS method.

Example 3.2. *This example is inspired by Example 2 of [29] and Example 1 of [80]. Here, we consider (3.1) with $L = T = d = 1$,*

$$u(0, t) = u(1, t) = u(x, 0) = 0, \quad f(x, t) = \left[\frac{2}{\Gamma(3 - \gamma)} t^{2-\gamma} + 4\pi^2 t^2 \right] \sin 2\pi x.$$

The exact solution is $u(x, t) = t^2 \sin 2\pi x$.

For $\gamma = 0.25, 0.5$, we take $\kappa = \frac{1}{12}$ and $\tau = \frac{1}{20000}$; for $\gamma = 0.75$, we take $\kappa = \frac{1}{20}$ and $\tau = \frac{1}{100000}$. The values of $\|e^K(\tau, h)\|_\infty$ are presented in Table 3.2 and we observe that PQS method gives the smallest errors in all cases.

TABLE 3.2: (Example 3.2) Maximum absolute error at $t = 1$

γ	h	PQS	$\mathcal{O}_{\infty,x}$	QS	$\mathcal{O}_{\infty,x}$	CFD	$\mathcal{O}_{\infty,x}$
$\frac{1}{4}$	$\frac{1}{10}$	1.13E-04	-	1.66E-04	-	6.08E-04	-
	$\frac{1}{20}$	1.05E-06	6.7498	1.29E-05	3.6857	3.95E-05	3.9441
	$\frac{1}{40}$	8.84E-09	6.8921	8.20E-07	3.9756	2.46E-06	4.0051
$\frac{1}{2}$	$\frac{1}{10}$	1.12E-04	-	1.65E-04	-	6.04E-04	-
	$\frac{1}{20}$	1.05E-06	6.7370	1.28E-05	3.6883	3.92E-05	3.9456
	$\frac{1}{40}$	1.09E-08	6.5899	8.11E-07	3.9803	2.45E-06	4.0000
$\frac{3}{4}$	$\frac{1}{10}$	1.19E-04	-	1.19E-04	-	6.00E-04	-
	$\frac{1}{20}$	1.12E-06	6.7210	1.12E-06	3.6923	3.90E-05	3.9445
	$\frac{1}{40}$	1.32E-08	6.4145	1.32E-08	3.9824	2.43E-06	4.0020

FIGURE 3.3: (Example 3.2) Approximate (left) and exact (right) solutions when $\gamma = 0.25$, $h = \frac{1}{40}$, $\tau = \frac{1}{20000}$.

Figures 3.3 and 3.4 illustrate the numerical/exact solutions and the absolute error. Figure 3.4 shows that as κ increases the maximum absolute error $\|e^K(\tau, h)\|_\infty$ decreases, though the effect is not significant.

Example 3.3. *This example is modified from [50]. Here, we consider (3.1) with $L = T = d = 1$,*

$$u(0, t) = t^{3+\gamma}, \quad u(1, t) = 0, \quad u(x, 0) = x^4(x-1)^4,$$

$$f(x, t) = (x-1)^2 e^{-x} t^3 \left[(x-1)^2 \frac{\Gamma(4+\gamma)}{6} - (21-10x+x^2)t^\gamma \right] - 4x^2(x-1)^2(34x^2-14x+3).$$

The exact solution is $u(x, t) = (x-1)^4 (e^{-x} t^{3+\gamma} + x^4)$.

FIGURE 3.4: (Example 3.2) Absolute error (left) and influence of κ on maximum absolute error (right) when $\gamma = 0.25$, $h = \frac{1}{40}$, $\tau = \frac{1}{20000}$.

TABLE 3.3: (Example 3.3) Maximum absolute error at $t = 1$

γ	h	PQS	$\mathcal{O}_{\infty,x}$	QS	$\mathcal{O}_{\infty,x}$	CFD	$\mathcal{O}_{\infty,x}$
$\frac{1}{4}$	$\frac{1}{10}$	1.19E-05	-	7.46E-06	-	2.85E-05	-
	$\frac{1}{20}$	2.46E-07	5.5962	3.97E-07	4.2320	1.85E-06	3.9454
	$\frac{1}{40}$	4.29E-09	5.8415	3.52E-08	3.4955	1.15E-07	4.0078
	$\frac{1}{80}$						
$\frac{1}{2}$	$\frac{1}{10}$	1.20E-05	-	7.58E-06	-	2.80E-05	-
	$\frac{1}{20}$	2.43E-07	5.6259	3.92E-07	4.2733	1.80E-06	3.9549
	$\frac{1}{40}$	6.65E-09	5.1915	4.41E-08	3.1520	1.04E-07	4.1133
	$\frac{1}{80}$						
$\frac{3}{4}$	$\frac{1}{10}$	1.23E-05	-	7.74E-06	-	2.74E-05	-
	$\frac{1}{20}$	2.51E-07	5.6139	3.75E-07	4.3668	1.75E-06	3.9664
	$\frac{1}{40}$	8.10E-09	4.9552	4.47E-08	3.0681	9.89E-08	4.1462
	$\frac{1}{80}$						

Let $\kappa = \frac{1}{12}$ and $\tau = \frac{1}{20000}$ for $\gamma = 0.25, 0.5$ and $\kappa = \frac{1}{20}$ and $\tau = \frac{1}{200000}$ for $\gamma = 0.75$. The simulation performance is presented in Table 3.3. We observe that PQS method has smaller error than CFD method for all cases. Although QS method has a better performance when $h = \frac{1}{10}$, PQS method tends to be better when h is smaller.

Once again, the numerical/exact solutions and the absolute error are plotted in Figures 3.5 and 3.6, while Figure 3.6 shows that as κ increases the maximum absolute error $\|e^K(\tau, h)\|_{\infty}$ decreases, though the effect is not significant.

FIGURE 3.5: (Example 3.3) Approximate (left) and exact (right) solutions when $\gamma = 0.25$, $h = \frac{1}{40}$, $\tau = \frac{1}{20000}$.

FIGURE 3.6: (Example 3.3) Absolute error (left) and influence of κ on maximum absolute error (right) when $\gamma = 0.25$, $h = \frac{1}{40}$, $\tau = \frac{1}{20000}$.

3.5 Summary

In this chapter, we have developed a numerical scheme for a fractional sub-diffusion problem. Our scheme is obtained by using parametric quintic spline and $L1$ discretization of the Caputo derivative. We have verified the solvability of the scheme and have further used energy method to establish the convergence and stability in maximum norm. The energy method involves the definition of a suitable inner product that plays a vital role in the analysis. Under some conditions, the scheme is shown to achieve accuracy of 4.5 in the spatial grid size and $(2 - \gamma)$ in the temporal grid size. This accuracy improves the earlier work done to date. To demonstrate the theoretical accuracy obtained and also to compare with other numerical methods, three well known numerical examples are presented.

Chapter 4

Second-order Two-dimensional Fractional Sub-diffusion Problems

This chapter extends results in Chapter 3 to a two-dimensional fractional sub-diffusion problem [142]. The problem is formulated as

$$\begin{cases} {}^C_0 D_t^\gamma u = d(u_{xx} + u_{yy}) + f(x, y, t), & (x, y) \in \Omega, \quad t \in [0, T] \\ u(x, y, 0) = \psi(x, y), & (x, y) \in \bar{\Omega} = \Omega \cup \partial\Omega \\ u(x, y, t) = \phi(x, y, t), & (x, y) \in \partial\Omega, \quad t \in [0, T] \end{cases} \quad (4.1)$$

where $\Omega = (0, L) \times (0, L')$ ($L, L' > 0$) is the spatial domain, $\partial\Omega$ is the boundary of Ω and $f(x, y, t)$, $\phi(x, y, t)$, $\psi(x, y)$ are known continuous functions in corresponding domains.

There is only a handful of pioneering work on two-dimensional [1, 26, 58, 142] and three-dimensional [23] fractional sub-diffusion problems. In fact, Chen et. al [26] has developed an implicit numerical scheme for a two-dimensional anomalous sub-diffusion equation using GL method and finite difference method. The stability and convergence of the numerical scheme is established via Fourier method, and it is shown that the convergence order is $O(\tau + h^2 + \ell^2)$ in l_2 norm. Subsequently, Zhang and Sun [142] have proposed two ADI schemes using $L1$ discretization and finite difference method. They have shown that the schemes are unconditionally stable with convergence order of $O(\tau^{\min\{1+\gamma, 2-\gamma\}} + h^2 + \ell^2)$ in H^1 norm. Thereafter, Abbaszadeh and Mohebbi [1] have proposed a numerical scheme for a two-dimensional

fractional sub-diffusion problem with a non-linear source term using GL discretization and compact finite difference method. The stability and convergence are then established via Fourier analysis and it is shown that the convergence order is $O(\tau + h^4 + \ell^4)$ in l_2 norm. Further, Ji and Sun [58] have considered the problem in [142] with zero initial condition, and employed the WSGL method coupled with compact finite difference to improve the global convergence order to $O(\tau^3 + h^4 + \ell^4)$ in $L_1(L_\infty)$ norm for $\gamma \in (0, 0.9569347]$. A kind of ADI technique is also proposed in [58] but the convergence has not been established. Last but not least, a numerical scheme for a three-dimensional problem has been developed using $L1$ discretization and finite difference method [23] which achieves second accuracy in spatial in terms of H^1 norm via energy methodology. From all the above work, we see that the *best spatial convergence order* achieved to date for higher dimensional fractional sub-diffusion problems is 4, i.e., $O(h^4 + \ell^4)$ in the related norms [1, 58].

In this chapter, we shall employ *parametric quintic spline* approach and $L2 - 1_\sigma$ method in the numerical treatment of (4.1). The new numerical scheme is theoretically proven to achieve spatial convergence order of *at least 4.5*, which *improves* the best result to date for higher dimensional fractional sub-diffusion problems. It should be pointed out that higher dimensional problems are much more challenging due to the complexity of computation and the analysis in the current work is *very different* from the one-dimensional case [78].

This chapter is organized as follows. In Section 4.1, we derive a new numerical scheme using parametric quintic spline and $L2 - 1_\sigma$ method. Then, the stability, the solvability and convergence of the numerical scheme in l_2 norm is established through discrete energy methodology in Section 4.2. In Section 4.3, we present numerical results to demonstrate the efficiency and accuracy of the proposed method and to compare with the earlier work. Section 4.4 concludes this chapter.

4.1 Numerical Scheme

In this section, we develop a high order numerical scheme for the two-dimensional problem (4.1) using parametric quintic spline and $L2 - 1_\sigma$ method.

Consider uniform partitions P, P'' in Chapter 3 and uniform partition P' of $[0, L']$ as follows

$$P' : 0 = y_0 < y_1 < \cdots < y_N = L' \quad (4.2)$$

where $y_n = n\ell$ with step size $\ell = \frac{L'}{N}$. For notational simplicity, we define for $u \in \mathcal{U}_{M,N}$ that

$$\begin{aligned} \delta_x u_{m+\frac{1}{2},n} &= \frac{u_{m+1,n} - u_{m,n}}{h}, & \delta_x^2 u_{m,n} &= \frac{\delta_x u_{m+\frac{1}{2},n} - \delta_x u_{m-\frac{1}{2},n}}{h}, \\ \delta_x^3 u_{m+\frac{1}{2},n} &= \frac{\delta_x^2 u_{m+1,n} - \delta_x^2 u_{m,n}}{h}, & \delta_x^4 u_{m,n} &= \frac{\delta_x^3 u_{m+\frac{1}{2},n} - \delta_x^3 u_{m-\frac{1}{2},n}}{h}, \end{aligned} \quad (4.3)$$

and

$$\begin{aligned} \delta_y u_{m,n+\frac{1}{2}} &= \frac{u_{m,n+1} - u_{m,n}}{\ell}, & \delta_y^2 u_{m,n} &= \frac{\delta_y u_{m,n+\frac{1}{2}} - \delta_y u_{m,n-\frac{1}{2}}}{\ell}, \\ \delta_y^3 u_{m,n+\frac{1}{2}} &= \frac{\delta_y^2 u_{m,n+1} - \delta_y^2 u_{m,n}}{\ell}, & \delta_y^4 u_{m,n} &= \frac{\delta_y^3 u_{m,n+\frac{1}{2}} - \delta_y^3 u_{m,n-\frac{1}{2}}}{\ell}. \end{aligned} \quad (4.4)$$

Moreover, let

$$(u, v) = h\ell \sum_{m=1}^{M-1} \sum_{n=1}^{N-1} u_{m,n} v_{m,n}, \quad (4.5)$$

and

$$\|u\| = (u, u)^{\frac{1}{2}}, \quad \|u\|_{\infty} = \max_{m,n} |u_{m,n}|. \quad (4.6)$$

First, we shall construct a two-dimensional parametric quintic spline operator based on the one-dimensional parametric quintic spline [65, 78]. From Definition 3.1, (3.11) and (3.12) in Chapter 3, after omitting k temporally, it is easily found that [78]

$$pW_{m-2} + qW_{m-1} + sW_m + qW_{m+1} + pW_{m+2} = (\delta_x^2 + \kappa h^2 \delta_x^4) u_m, \quad 2 \leq m \leq M-2$$

where $\kappa = \frac{1}{\nu^2} \left(\frac{\nu}{\sin \nu} - 1 \right)$ and p, q, s are in terms of κ satisfying $2p + 2q + s = 1$.

By selecting ξ ($\nu = \xi h$), we can get various numerical schemes with different accuracy. This can be seen from the expression of the local truncation error later. However, due to the consistency relation [65, 78], we can only consider κ in $(0, \frac{1}{2})$. Fortunately, it is sufficient to obtain various schemes in applications using κ in this

range. To facilitate subsequent analysis, we give an equivalent form of the

$$[1 + (q + 4p)h^2\delta_x^2 + ph^4\delta_x^4] W_m = (\delta_x^2 + \kappa h^2\delta_x^4) u_m, \quad 2 \leq m \leq M - 2. \quad (4.7)$$

Besides (4.7), we need two more equations which can be derived from (3.18). Omitting T_m^k then leads to two equations

$$\left(1 + h^2 \frac{\delta_x^2}{12}\right) W_m = \delta_x^2 s_m, \quad m = 1, M - 1. \quad (4.8)$$

Having obtained the relations (4.7) and (4.8), we now define the *two-dimensional parametric quintic spline operator* which plays a vital role in the derivation of the new numerical scheme.

Definition 4.1. For any $u \in \mathcal{U}_{M,N}$, we define the *two-dimensional parametric quintic spline operator* H as

$$H = H_x H_y = H_y H_x,$$

where H_x and H_y are one-dimensional parametric quintic spline operators in x and y dimensions respectively given by

$$H_x u_{m,n} = \begin{cases} \left(1 + h^2 \frac{\delta_x^2}{12}\right) u_{m,n}, & m = 1, M - 1 \\ [1 + (q + 4p)h^2\delta_x^2 + ph^4\delta_x^4] u_{m,n}, & 2 \leq m \leq M - 2 \end{cases} \quad (4.9)$$

and

$$H_y u_{m,n} = \begin{cases} \left(1 + \ell^2 \frac{\delta_y^2}{12}\right) u_{m,n}, & n = 1, N - 1 \\ [1 + (q + 4p)\ell^2\delta_y^2 + p\ell^4\delta_y^4] u_{m,n}, & 2 \leq n \leq N - 2. \end{cases} \quad (4.10)$$

Next, we shall present an important result of H_x and H_y . To this aim, we introduce the notations $\bar{\delta}_x^2$ and $\bar{\delta}_y^2$ as

$$\bar{\delta}_x^2 u_{m,n} = \begin{cases} \delta_x^2 u_{m,n}, & m = 1, M - 1 \\ (\delta_x^2 + \kappa h^2\delta_x^4) u_{m,n}, & 2 \leq m \leq M - 2 \end{cases} \quad (4.11)$$

and

$$\bar{\delta}_y^2 u_{m,n} = \begin{cases} \delta_y^2 u_{m,n}, & n = 1, N-1 \\ (\delta_y^2 + \kappa \ell^2 \delta_y^4) u_{m,n}, & 2 \leq n \leq N-2 \end{cases} \quad (4.12)$$

where $0 < \kappa < \frac{1}{2}$.

Applying Taylor expansion at (x_m, y_n) , we obtain the following result.

Lemma 4.1. *Let $u(x, y, t_k) \in \mathcal{C}^{8,8}(\Omega)$. If*

$$p = \frac{1}{12}\kappa - \frac{1}{240}, \quad q = \frac{8}{12}\kappa + \frac{24}{240}, \quad s = -\frac{3}{2}\kappa + \frac{97}{120}, \quad (4.13)$$

then we have

$$H_x u_{xx}(x_m, y_n, t_k) - \bar{\delta}_x^2 u_{m,n}^k = \begin{cases} -\frac{1}{240} h^4 D_x^6 u(x_m, y_n, t_k) + O(h^6), & m = 1, M-1 \\ Z_1 h^6 D_x^8 u(x_m, y_n, t_k) + O(h^8), & 2 \leq m \leq M-2 \end{cases} \quad (4.14)$$

and

$$H_y u_{yy}(x_m, y_n, t_k) - \bar{\delta}_y^2 u_{m,n}^k = \begin{cases} -\frac{1}{240} \ell^4 D_y^6 u(x_m, y_n, t_k) + O(\ell^6), & n = 1, N-1 \\ Z_1 \ell^6 D_y^8 u(x_m, y_n, t_k) + O(\ell^8), & 2 \leq n \leq N-2 \end{cases} \quad (4.15)$$

where $Z_1 = \frac{1}{20160} + \frac{126\kappa}{10080} - \frac{8}{45}p - \frac{1}{360}q$ and $0 < \kappa < \frac{1}{2}$.

Remark 4.1. For the rest of the paper, we shall fix p , q and s as in (4.13) in order to get high spatial accuracy.

We are now ready to develop the new numerical scheme for the two-dimensional fractional sub-diffusion problem (4.1) using results (4.14)–(4.15). To begin, we discretize (4.1) at $(x_m, y_n, t_{k-1+\sigma})$ to get

$${}^C_0 D_t^\gamma u(x_m, y_n, t_{k-1+\sigma}) = d \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) u(x_m, y_n, t_{k-1+\sigma}) + f(x_m, y_n, t_{k-1+\sigma}). \quad (4.16)$$

We note the well known result below

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) u(x_m, y_n, t_{k-1+\sigma}) = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) u_{m,n}^{k-1+\sigma} + O(\tau^2), \quad (4.17)$$

To derive the new numerical scheme, we first apply the $L2 - 1_\sigma$ approximation (2.21) and the result (4.17) to (4.16), then the two-dimensional parametric quintic spline operator $H = H_x H_y = H_y H_x$ is applied to both sides of (4.16). In view of (4.14) and (4.15) in Lemma 4.1, we achieve, after omitting the small terms,

where the various constants and notations are given in Lemma 2.4 and (4.9)–(4.13).

4.2 Solvability, Stability and Convergence

Let us start with the stability. For simplicity, besides the inner product $(\cdot, \cdot)$, we also introduce the following notations for $u, v \in \mathcal{U}_{M,N}^*$,

We shall first present two lemmas on the one-dimensional parametric quintic spline operator H_x . We remark that these results can be *similarly* obtained for H_y . The first lemma establishes the relation between $(H_x u, H_x u)_{x,n}$ and $(u, u)_{x,n}$.

Lemma 4.2. Let $u \in \mathcal{U}_{M,N}^*$. If $0 < \kappa < \frac{67}{492}$, then

$$\varepsilon_0^2(u, u)_{x,n} \leq (H_x u, H_x u)_{x,n} \leq \left(\frac{61}{60}\right)^2 (u, u)_{x,n}, \quad (4.19)$$

where $\varepsilon_0 > 0$ is given by

$$\varepsilon_0 = \begin{cases} \frac{283}{480} - \frac{71}{24}\kappa, & 0 < \kappa \leq \frac{1}{20} \\ \frac{2}{3} - \frac{9}{2}\kappa, & \kappa = \frac{1}{20} \\ \frac{67}{96} - \frac{41}{8}\kappa, & \frac{1}{20} < \kappa < \frac{67}{492}. \end{cases}$$

Proof. We start with the proof of the first inequality in (4.19). For any positive number ε , applying Young's inequality gives

$$2\varepsilon(H_x u, u)_{x,n} = 2(H_x u, \varepsilon u)_{x,n} \leq (H_x u, H_x u)_{x,n} + \varepsilon^2(u, u)_{x,n}$$

or equivalently

$$(H_x u, H_x u)_{x,n} \geq 2\varepsilon(H_x u, u)_{x,n} - \varepsilon^2(u, u)_{x,n}. \quad (4.20)$$

Hence, to obtain the first inequality of (4.19), it is sufficient to relate $(H_x u, u)_{x,n}$ to $(u, u)_{x,n}$.

Noting the definition of H_x and the fact that $q + 4p = \frac{1}{12} + \kappa$, it is seen that

$$(H_x u, u)_{x,n} = (u, u)_{x,n} + \frac{h^2}{12}(u, \delta_x^2 u)_{x,n} + \kappa h^3 \sum_{m=2}^{M-2} u_{m,n}(\delta_x^2 u_{m,n}) + p h^5 \sum_{m=2}^{M-2} u_{m,n}(\delta_x^4 u_{m,n}). \quad (4.21)$$

Let $\delta_x^2 u_{0,n} = \delta_x^2 u_{M,n} = 0$, using $u_{0,n} = u_{M,n} = 0$, after simple manipulations, we find

$$(u, \delta_x^2 u)_{x,n} = -h \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2 \quad \text{and} \quad h^4 \sum_{m=1}^{M-1} u_{m,n}(\delta_x^4 u_{m,n}) = \mathbf{u}_n^T X^2 \mathbf{u}_n$$

where $\mathbf{u}_n = (u_{1,n}, u_{2,n}, \dots, u_{M-1,n})^T$ and X is a $(M-1) \times (M-1)$ matrix given by

$$X = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}. \quad (4.22)$$

Substituting the above relations into (4.21) gives

$$(H_x u, u)_{x,n} = (u, u)_{x,n} - \left(\frac{1}{12} + \kappa \right) h^3 \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2 + p h \mathbf{u}_n^T X^2 \mathbf{u}_n + h R_1, \quad (4.23)$$

where

$$R_1 = (2\kappa - 5p) \sum_{m=1, M-1} (u_{m,n})^2 + (-\kappa + 4p) \sum_{m=1, M-2} (u_{m,n} u_{m+1,n}) - p \sum_{m=1, M-3} (u_{m,n} u_{m+2,n}).$$

Using Theorem 12.6.1 of [2], it is found that

$$0 \leq h \mathbf{u}_n^T X^2 \mathbf{u}_n \leq 16(u, u)_{x,n} \quad \text{and} \quad h^3 \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2 \leq 4(u, u)_{x,n}. \quad (4.24)$$

Hence, in the equation (4.23) it remains to estimate R_1 . For this, we consider the following cases.

Case 1 $0 < \kappa < \frac{1}{20}$. This implies $p = \frac{\kappa}{12} - \frac{1}{240} < 0$, so

$$h R_1 \geq \left(\frac{-\kappa + 4p}{2} + \frac{p}{2} \right) (u, u)_{x,n} = \left(-\frac{\kappa}{2} + \frac{5}{2}p \right) (u, u)_{x,n}.$$

Together with (4.24), from (4.23) we find

$$\begin{aligned} (H_x u, u)_{x,n} &\geq \left[1 - 4 \left(\frac{1}{12} + \kappa \right) + 16p - \frac{\kappa}{2} + \frac{5}{2}p \right] (u, u)_{x,n} \\ &= \left(\frac{283}{480} - \frac{71}{24}\kappa \right) (u, u)_{x,n}. \end{aligned} \quad (4.25)$$

Case 2 $\kappa = \frac{1}{20}$. This implies $p = 0$. In this case, since $hR_1 \geq -\frac{\kappa}{2}(u, u)_{x,n}$, we have

$$(H_x u, u)_{x,n} \geq \left[1 - 4\left(\frac{1}{12} + \kappa\right) - \frac{\kappa}{2}\right] (u, u)_{x,n} = \left(\frac{2}{3} - \frac{9}{2}\kappa\right) (u, u)_{x,n}. \quad (4.26)$$

Case 3 $\frac{1}{20} < \kappa < 1$. This implies $p > 0$, so

$$hR_1 \geq \left(-5p + \frac{-\kappa - 4p}{2} - \frac{p}{2}\right) (u, u)_{x,n} = -\left(\frac{\kappa}{2} + \frac{15}{2}p\right) (u, u)_{x,n}.$$

Coupling with (4.24), it follows from (4.23) that

$$(H_x u, u)_{x,n} \geq \left[1 - 4\left(\frac{1}{12} + \kappa\right) - \left(\frac{\kappa}{2} + \frac{15}{2}p\right)\right] (u, u)_{x,n} = \left(\frac{67}{96} - \frac{41}{8}\kappa\right) (u, u)_{x,n}. \quad (4.27)$$

Taking $\varepsilon = \varepsilon_0 > 0$ in (4.20), the first inequality in (4.19) follows directly from (4.25)–(4.27).

Now, let us prove the second inequality in (4.19). The matrix representation of $(H_x u, H_x u)_{x,n}$ can be written as

$$(H_x u, H_x u)_{x,n} = h \mathbf{u}_n^T Y^T Y \mathbf{u}_n,$$

where Y is a $(M-1) \times (M-1)$ matrix given by

$$Y = \begin{bmatrix} \frac{10}{12} & \frac{1}{12} & & & & & \\ q & s & q & p & & & \\ p & q & s & q & p & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & p & q & s & q & p \\ & & & p & q & s & q \\ & & & & & \frac{1}{12} & \frac{10}{12} \end{bmatrix}.$$

Note that $s = 1 - 2p - 2q$ and $q > 0$, it is clear that the spectral radius of the matrix $Y^T Y$ satisfies

$$\mathcal{R}(Y^T Y) \leq \|Y^T Y\|_\infty \leq \|Y^T\|_\infty \|Y\|_\infty = (1 - 2p + 2|p|)^2.$$

Thus, from the expression of p , we have

$$(H_x u, H_x u)_{x,n} \leq (1 - 2p + 2|p|)^2 (u, u)_{x,n} \leq \left(\frac{61}{60}\right)^2 (u, u)_{x,n}$$

which completes the proof. $\square$

The next lemma relates $(H_x u, \bar{\delta}_x^2 u)_{x,n}$ to $(u, u)_{x,n}$.

Lemma 4.3. *Let $u \in \mathcal{U}_{M,N}^*$. If $0 < \kappa < \kappa_0 = \frac{-164 + \sqrt{31461}}{220}$ (≈ 0.06), then*

$$(H_x u, \bar{\delta}_x^2 u)_{x,n} \leq -\frac{4\varepsilon_1}{L} (u, u)_{x,n}, \quad (4.28)$$

where $\varepsilon_1 > 0$ is given by

$$\varepsilon_1 = \begin{cases} \varepsilon_{11}, & 0 < \kappa < \kappa^* \\ \varepsilon_{12}, & \kappa = \kappa^* \\ \varepsilon_{13}, & \kappa^* < \kappa \leq \frac{1}{20} \\ \varepsilon_{14}, & \frac{1}{20} < \kappa < \kappa_0. \end{cases}$$

Here,

$$\begin{aligned} \varepsilon_{11} &= 18\kappa^2 - 7\kappa + \frac{71}{120}, & \varepsilon_{12} &= -\left(10\kappa - \frac{2}{3}\right), \\ \varepsilon_{13} &= -\left(6\kappa^2 + 11\kappa - \frac{83}{120}\right), & \varepsilon_{14} &= -\frac{1}{120}(880\kappa^2 + 1312\kappa - 83), \end{aligned}$$

and

$$\kappa_0 = \frac{-164 + \sqrt{31461}}{220} \approx 0.06, \quad \kappa^* = \frac{-5 + 2\sqrt{10}}{60} \approx 0.022$$

are the positive solutions of $\varepsilon_{14} = 0$ and $p + \frac{\kappa}{12} + \kappa^2 = 0$ respectively.

Proof. Using the definition of H_x and $\bar{\delta}_x^2$ in (4.9) and (4.11), we get

$$\begin{aligned}
(\bar{\delta}_x^2 u, H_x u)_{x,n} &= \left(\left(1 + \frac{h^2}{12} \delta_x^2 \right) u, \delta_x^2 u \right)_{x,n} + h \sum_{m=2}^{M-2} \left[\left(1 + \frac{h^2}{12} \delta_x^2 \right) u_{m,n} \right] (\kappa h^2 \delta_x^4 u_{m,n}) \\
&\quad + h \sum_{m=2}^{M-2} [(\kappa h^2 \delta_x^2 + p h^4 \delta_x^4) u_{m,n}] [(\delta_x^2 + \kappa h^2 \delta_x^4) u_{m,n}] \\
&= -h \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2 + \left(\frac{h^2}{12} + \kappa h^2 \right) (\delta_x^2 u, \delta_x^2 u)_{x,n} \\
&\quad + p \kappa h^7 \sum_{m=2}^{M-2} (\delta_x^4 u_{m,n})^2 + h R_2
\end{aligned} \tag{4.29}$$

where

$$\begin{aligned}
R_2 &= \kappa h^2 \sum_{m=2}^{M-2} u_{m,n} (\delta_x^4 u_{m,n}) + \left(\frac{\kappa}{12} + p + \kappa^2 \right) h^4 \sum_{m=2}^{M-2} (\delta_x^2 u_{m,n}) (\delta_x^4 u_{m,n}) \\
&\quad - \kappa h^2 \sum_{m=1, M-1} (\delta_x^2 u_{m,n})^2.
\end{aligned}$$

In order to derive the inequality (4.28), we need to estimate the term R_2 appropriately. First, by simple calculation, we find

$$h \sum_{m=1}^{M-1} u_{m,n} (\delta_x^4 u_{m,n}) = (\delta_x^2 u, \delta_x^2 u)_{x,n}, \quad \sum_{m=1}^{M-1} (\delta_x^2 u_{m,n}) (\delta_x^4 u_{m,n}) = - \sum_{m=1}^{M-2} \left(\delta_x^3 u_{m+\frac{1}{2},n} \right)^2, \tag{4.30}$$

where we have used $\delta_x^2 u_{0,n} = \delta_x^2 u_{M,n} = 0$. Then, applying (4.30) in R_2 yields

$$\begin{aligned}
R_2 &= R_3 + \kappa h^2 \sum_{m=2}^{M-2} (\delta_x^2 u_{m,n})^2 \\
&\quad - \left(\frac{\kappa}{12} + p + \kappa^2 \right) \left[h^4 \sum_{m=1}^{M-2} \left(\delta_x^3 u_{m+\frac{1}{2},n} \right)^2 - h^2 \sum_{m=1, M-1} (\delta_x^2 u_{m,n})^2 \right],
\end{aligned} \tag{4.31}$$

where

$$\begin{aligned}
 R_3 = & -\kappa \left[u_{1,n}(\delta_x^2 u_{2,n} - 2\delta_x^2 u_{1,n}) + u_{M-1,n}(\delta_x^2 u_{M-2,n} - 2\delta_x^2 u_{M-1,n}) \right] \\
 & - \left(\frac{\kappa}{12} + p + \kappa^2 \right) h^2 \sum_{m=1, M-2} (\delta_x^2 u_{m,n})(\delta_x^2 u_{m+1,n}).
 \end{aligned} \tag{4.32}$$

We need a few inequalities to proceed further. First, since $u_{0,n} = u_{M,n} = 0$, using the inequality $\pm ab \leq \frac{1}{2}(a^2 + b^2)$ we get

$$\begin{aligned}
 -u_{1,n}(\delta_x^2 u_{2,n} - 2\delta_x^2 u_{1,n}) &= -\delta_x u_{\frac{1}{2},n} \left(\delta_x u_{\frac{5}{2},n} - 3\delta_x u_{\frac{3}{2},n} \right) \\
 &\leq 2 \left(\delta_x u_{\frac{1}{2},n} \right)^2 + \frac{1}{2} \left(\delta_x u_{\frac{5}{2},n} \right)^2 + \frac{3}{2} \left(\delta_x u_{\frac{3}{2},n} \right)^2 \\
 &\leq 2 \sum_{m=0}^2 \left(\delta_x u_{m+\frac{1}{2},n} \right)^2.
 \end{aligned} \tag{4.33}$$

Similarly, we have

$$-u_{M-1,n}(\delta_x^2 u_{M-2,n} - 2\delta_x^2 u_{M-1,n}) \leq 2 \sum_{m=M-3}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2. \tag{4.34}$$

Next, we note the following inequalities

$$\begin{aligned}
 h^2(\delta_x^2 u_{m,n})^2 &\leq 2 \left(\delta_x u_{m+\frac{1}{2},n} \right)^2 + 2 \left(\delta_x u_{m-\frac{1}{2},n} \right)^2, \\
 \pm(\delta_x^2 u_{m,n})(\delta_x^2 u_{m+1,n}) &\leq \frac{1}{2} \left[(\delta_x^2 u_{m,n})^2 + (\delta_x^2 u_{m+1,n})^2 \right].
 \end{aligned} \tag{4.35}$$

Using the inequalities (4.33)–(4.35), we proceed in the following cases.

Case 1 $\frac{\kappa}{12} + p + \kappa^2 = \kappa^2 + \frac{\kappa}{6} - \frac{1}{240} > 0$. So R_3 satisfies

$$R_3 \leq 2\kappa \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2 + \frac{1}{2} \left(\frac{\kappa}{12} + p + \kappa^2 \right) h^2 \sum_{m=1, M-2} \left[(\delta_x^2 u_{m,n})^2 + (\delta_x^2 u_{m+1,n})^2 \right].$$

Hence, from (4.31) we get

$$\begin{aligned}
R_2 &\leq \left[\kappa + \frac{3}{2} \left(\frac{\kappa}{12} + p + \kappa^2 \right) \right] h^2 \sum_{m=1}^{M-1} (\delta_x^2 u_{m,n})^2 + 2\kappa \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2 \\
&\leq \left\{ 2\kappa + 4 \left[\kappa + \frac{3}{2} \left(\frac{\kappa}{12} + p + \kappa^2 \right) \right] \right\} \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2 \\
&= \left(6\kappa^2 + 7\kappa - \frac{1}{40} \right) \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2.
\end{aligned} \tag{4.36}$$

Case 2 $\frac{\kappa}{12} + p + \kappa^2 = \kappa^2 + \frac{\kappa}{6} - \frac{1}{240} = 0$. Here, it is obvious that

$$R_2 \leq \kappa h^2 \sum_{m=2}^{M-2} (\delta_x^2 u_{m,n})^2 + 2\kappa \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2 \leq 6\kappa \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2. \tag{4.37}$$

Case 3 $\frac{\kappa}{12} + p + \kappa^2 = \kappa^2 + \frac{\kappa}{6} - \frac{1}{240} < 0$. We find

$$R_3 \leq 2\kappa \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2 - \frac{h^2}{2} \left(\frac{\kappa}{12} + p + \kappa^2 \right) \sum_{m=1, M-2} \left[(\delta_x^2 u_{m,n})^2 + (\delta_x^2 u_{m+1,n})^2 \right].$$

Note that $h^2 \left(\delta_x^3 u_{m+\frac{1}{2},n} \right)^2 = (\delta_x^2 u_{m+1,n} - \delta_x^2 u_{m,n})^2 \leq 2(\delta_x^2 u_{m+1,n})^2 + 2(\delta_x^2 u_{m,n})^2$, so it follows from (4.31) that

$$\begin{aligned}
R_2 &\leq \left[\kappa - \frac{9}{2} \left(\frac{\kappa}{12} + p + \kappa^2 \right) \right] h^2 \sum_{m=1}^{M-1} (\delta_x^2 u_{m,n})^2 + 2\kappa \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2 \\
&\leq \left\{ 2\kappa + 4 \left[\kappa - \frac{9}{2} \left(\frac{\kappa}{12} + p + \kappa^2 \right) \right] \right\} \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2 \\
&= \left(-18\kappa^2 + 3\kappa + \frac{3}{40} \right) \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2.
\end{aligned} \tag{4.38}$$

Now, using (4.36)–(4.38) in (4.29), we are able to establish the relation between $(H_x u, \bar{\delta}_x^2 u)_{x,n}$ and $h \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2$. In fact, we have the following cases.

Case (i) $p \geq 0$. Here, we apply the inequality (4.36) in (4.29) to get

$$\begin{aligned} (\bar{\delta}_x^2 u, H_x u)_{x,n} &\leq \left(-1 + \frac{4}{12} + 4\kappa + 16p\kappa + 6\kappa^2 + 7\kappa - \frac{1}{40}\right) h \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n}\right)^2 \\ &= -\varepsilon_{14} h \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n}\right)^2. \end{aligned} \quad (4.39)$$

Case (ii) $p < 0$ and $p + \frac{1}{12}\kappa + \kappa^2 > 0$. In this case, using (4.36) and removing negative terms in (4.29) yields

$$\begin{aligned} (\bar{\delta}_x^2 u, H_x u)_{x,n} &\leq \left(-1 + \frac{4}{12} + 4\kappa + 6\kappa^2 + 7\kappa - \frac{1}{40}\right) h \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n}\right)^2 \\ &= -\varepsilon_{13} h \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n}\right)^2. \end{aligned} \quad (4.40)$$

Case (iii) $p < 0$ and $p + \frac{1}{12}\kappa + \kappa^2 = 0$. From (4.37) and (4.29), we obtain

$$\begin{aligned} (\bar{\delta}_x^2 w, H_x u)_{x,n} &\leq \left(-1 + \frac{4}{12} + 4\kappa + 6\kappa\right) h \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n}\right)^2 \\ &= -\varepsilon_{12} h \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n}\right)^2. \end{aligned} \quad (4.41)$$

Case (iv) $p < 0$ and $p + \frac{1}{12}\kappa + \kappa^2 < 0$. Applying (4.38) in (4.29) gives

$$\begin{aligned} (\bar{\delta}_x^2 u, H_x u)_{x,n} &\leq \left(-1 + \frac{4}{12} + 4\kappa - 18\kappa^2 + 3\kappa + \frac{3}{40}\right) h \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n}\right)^2 \\ &= -\varepsilon_{11} h \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n}\right)^2. \end{aligned} \quad (4.42)$$

Finally, from the discrete Poincaré inequality [103], we have

$$\frac{4}{L} \sum_{m=1}^{M-1} (u_{m,n})^2 \leq \left(\frac{2 \sin \frac{\pi h}{2L}}{h}\right)^2 \sum_{m=1}^{M-1} (u_{m,n})^2 \leq \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n}\right)^2$$

which, in view of the inequalities (4.39)–(4.42), leads to

$$(\bar{\delta}_x^2 u, H_x u)_{x,n} \leq -\varepsilon_1 h \sum_{m=0}^{M-1} \left(\delta_x u_{m+\frac{1}{2},n} \right)^2 \leq -\frac{4\varepsilon_1}{L} (u, u)_{x,n}.$$

This completes the proof. $\square$

Remark 4.2. By a similar technique, the analogues of (4.19) and (4.28) for H_y are respectively obtained as

$$\varepsilon_0^2 (u, u)_{y,m} \leq (H_y u, H_y u)_{y,m} \leq \left(\frac{61}{60} \right)^2 (u, u)_{y,m} \quad (4.43)$$

and

$$(H_y u, \bar{\delta}_y^2 u)_{y,m} \leq -\frac{4\varepsilon_1}{L'} (u, u)_{y,m}. \quad (4.44)$$

Using Lemmas 4.2 and 4.3 as well as (4.43) and (4.44), we shall give another two lemmas that are directly used to prove the main theorem. The first result investigates the relation between $\|Hu\|^2$ and $\|u\|^2$.

Lemma 4.4. *Let $u \in \mathcal{U}_{M,N}^*$. If $0 < \kappa < \frac{67}{492}$, then*

$$\varepsilon_0^4 \|u\|^2 \leq \|Hu\|^2 \leq \left(\frac{61}{60} \right)^4 \|u\|^2, \quad (4.45)$$

where $\varepsilon_0 > 0$ is given in Lemma 4.2.

Proof. Let $v = H_y u$. Obviously, $v \in \mathcal{U}_{M,N}^*$. From the definition of $\|Hu\|$, we have

$$\|Hu\|^2 = h\ell \sum_{m=1}^{M-1} \sum_{n=1}^{N-1} (H_x H_y u_{m,n})(H_x H_y u_{m,n}) = \ell \sum_{n=1}^{N-1} (H_x v, H_x v)_{x,n}. \quad (4.46)$$

Applying Lemma 4.2 and (4.43) successively to (4.46), we obtain

$$\begin{aligned} \|Hu\|^2 &\leq \left(\frac{61}{60} \right)^2 \ell \sum_{n=1}^{N-1} (v, v)_{x,n} = \left(\frac{61}{60} \right)^2 h \sum_{m=1}^{M-1} (H_y u, H_y u)_{y,m} \\ &\leq \left(\frac{61}{60} \right)^4 h \sum_{m=1}^{M-1} (u, u)_{y,m} = \left(\frac{61}{60} \right)^4 \|u\|^2, \end{aligned}$$

which gives the second inequality in (4.45).

The first inequality in (4.45) can be similarly derived. The proof is complete. $\square$

The next lemma gives an estimation of $((H_y \bar{\delta}_x^2 + H_x \bar{\delta}_y^2) u, Hu)$ that is vital in the proof of the main theorem.

Lemma 4.5. *Let $u \in \mathcal{U}_{M,N}^*$. If $0 < \kappa < \kappa_0$, then*

$$((H_y \bar{\delta}_x^2 + H_x \bar{\delta}_y^2) u, Hu) \leq -4\varepsilon_1 \varepsilon_0^2 \left(\frac{1}{L} + \frac{1}{L'} \right) \|u\|^2, \quad (4.47)$$

where $\varepsilon_0, \varepsilon_1 > 0$ are given in Lemmas 4.2 and 4.3 respectively.

Proof. Let us deal with $(H_y \bar{\delta}_x^2 u, Hu)$ first. Applying Lemma 4.3 and then (4.43), we are able to get

$$(H_y \bar{\delta}_x^2 u, Hu) \leq -\frac{4\varepsilon_1}{L} h \sum_{m=1}^{M-1} (H_y u, H_y u)_{y,m} \leq -\frac{4\varepsilon_1 \varepsilon_0^2}{L} \|u\|^2.$$

By a similar argument, we obtain

$$(H_x \bar{\delta}_y^2 u, Hu) \leq -\frac{4\varepsilon_1 \varepsilon_0^2}{L'} \|u\|^2.$$

Hence, (4.47) follows directly from the above two inequalities. $\square$

Finally, we need two lemmas from [7] to complete the analysis later. The first lemma presents the properties of r_j 's in (2.22).

Lemma 4.6. [7] *For any fixed $k \geq 1$, r_j ($0 \leq j \leq k$) satisfies*

$$r_k > \frac{1 - \gamma}{2(k + \sigma)\gamma}, \quad (4.48)$$

$$r_0 > r_1 > \cdots > r_{k-1} > r_k, \quad (4.49)$$

$$(2\sigma - 1)r_0 - \sigma r_1 > 0, \quad (4.50)$$

where $0 < \gamma < 1$ and $\sigma = 1 - \frac{\gamma}{2}$.

The second lemma provides an inequality which is essential in analyzing stability.

where $c = \varepsilon_0^{-4}$ and

$$E = \|H\epsilon^0\|^2 + \frac{\Gamma(1-\gamma)T^\gamma}{4\varepsilon_1\varepsilon_0^2\left(\frac{60}{61}\right)^4\left(\frac{1}{L} + \frac{1}{L'}\right)} \max_{1 \leq k \leq K} \|H\hat{f}^{k-1+\sigma}\|^2 \quad (4.55)$$

only depends on initial values and the non-homogeneous term.

Proof. Multiplying both sides of (4.53) by $h\ell H\epsilon_{m,n}^{k-1+\sigma}$, then summing over m and n , we obtain

$$\begin{aligned} & \mu \left[r_0(H\epsilon^{k-1+\sigma}, H\epsilon^k) - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j})(H\epsilon^{k-1+\sigma}, H\epsilon^j) - r_{k-1}(H\epsilon^{k-1+\sigma}, H\epsilon^0) \right] \\ &= d(H\epsilon^{k-1+\sigma}, (H_x\bar{\delta}_y^2 + H_y\bar{\delta}_x^2)\epsilon^{k-1+\sigma}) + (H\epsilon^{k-1+\sigma}, H\hat{f}^{k-1+\sigma}). \end{aligned} \quad (4.56)$$

It is clear that $\epsilon^k \in \mathcal{U}_{M,N}^*$. Therefore, applying Lemma 4.5 we get

$$(H\epsilon^{k-1+\sigma}, (H_x\bar{\delta}_y^2 + H_y\bar{\delta}_x^2)\epsilon^{k-1+\sigma}) \leq -4\varepsilon_1\varepsilon_0^2 \left(\frac{1}{L} + \frac{1}{L'} \right) \|\epsilon^{k-1+\sigma}\|^2. \quad (4.57)$$

Next, for any $\varepsilon > 0$, using Young's inequality and Lemma 4.4, we find

$$\begin{aligned} (H\epsilon^{k-1+\sigma}, H\hat{f}^{k-1+\sigma}) &\leq \varepsilon \|H\epsilon^{k-1+\sigma}\|^2 + \frac{1}{4\varepsilon} \|H\hat{f}^{k-1+\sigma}\|^2 \\ &\leq \varepsilon \left(\frac{61}{60} \right)^4 \|\epsilon^{k-1+\sigma}\|^2 + \frac{1}{4\varepsilon} \|H\hat{f}^{k-1+\sigma}\|^2. \end{aligned} \quad (4.58)$$

Moreover, applying the inequality (4.51) yields

$$\begin{aligned} & r_0(H\epsilon^{k-1+\sigma}, H\epsilon^k) - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j})(H\epsilon^{k-1+\sigma}, H\epsilon^j) - r_{k-1}(H\epsilon^{k-1+\sigma}, H\epsilon^0) \\ &\geq \frac{1}{2} \left[r_0 \|H\epsilon^k\|^2 - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \|H\epsilon^j\|^2 - r_{k-1} \|H\epsilon^0\|^2 \right]. \end{aligned} \quad (4.59)$$

Now, setting $\varepsilon = 4\varepsilon_1\varepsilon_0^2\left(\frac{60}{61}\right)^4\left(\frac{1}{L} + \frac{1}{L'}\right)$ (> 0) and using (4.57)–(4.59) in equation (4.56) leads to

$$r_0\|H\epsilon^k\|^2 - \sum_{j=1}^{k-1}(r_{k-j-1} - r_{k-j})\|H\epsilon^j\|^2 - r_{k-1}\|H\epsilon^0\|^2 \leq \frac{1}{2\mu\varepsilon}\|H\hat{f}^{k-1+\sigma}\|^2. \quad (4.60)$$

In view of (4.48), we see that $\frac{1}{\mu r_{k-1}} < \Gamma(2-\gamma)\tau^{\gamma\frac{2(k-1+\sigma)\gamma}{1-\gamma}} \leq 2\Gamma(1-\gamma)T^\gamma$. It follows from (4.60) that

$$\begin{aligned} r_0\|H\epsilon^k\|^2 - \sum_{j=1}^{k-1}(r_{k-j-1} - r_{k-j})\|H\epsilon^j\|^2 &\leq r_{k-1} \left[\|H\epsilon^0\|^2 + \frac{1}{2\mu r_{k-1}\varepsilon}\|H\hat{f}^{k-1+\sigma}\|^2 \right] \\ &\leq r_{k-1}E, \end{aligned} \quad (4.61)$$

where E is defined in (4.55).

We shall show by mathematical induction that

$$\|H\epsilon^k\|^2 \leq E, \quad 1 \leq k \leq K. \quad (4.62)$$

In fact, when $k = 1$, the inequality (4.61) gives (4.62) $|_{k=1}$. Suppose (4.62) is true up to k . Then, noting the property of r_k 's in (4.49), from (4.61) we find

$$r_0\|H\epsilon^{k+1}\|^2 \leq \sum_{j=1}^k(r_{k-j} - r_{k-j+1})\|H\epsilon^j\|^2 + r_k E \leq \sum_{j=1}^k(r_{k-j} - r_{k-j+1})E + r_k E = r_0 E.$$

Hence, (4.62) is proved. Now, (4.54) follows from (4.62) and the first inequality in (4.45). $\square$

Theorem 4.1 shows that the scheme (4.18) is unconditionally stable with respect to the initial values and the non-homogeneous term. Now, let us analyze the solvability and convergence of the numerical scheme (4.18). The first result is on the solvability.

Theorem 4.2. *If $0 < \kappa < \kappa_0$, the numerical scheme (4.18) is uniquely solvable at each time level $t = t_k$, $1 \leq k \leq K$.*

Proof. It is sufficient to show that the homogeneous scheme of (4.18) with $f = \psi = \phi = 0$ has only the trivial solution.

In fact, applying Theorem 4.1 to the homogeneous scheme gives

$$\|u^k\|^2 \leq 0, \quad 1 \leq k \leq K$$

which results in $u_{m,n}^k = 0$ for all m, n and k . This implies that the homogeneous system has only the trivial solution. $\square$

Next, let $\{U_{m,n}^k = U(x_m, y_n, t_k)\}$ be the exact solution of the problem (4.1). Then, $\{U_{m,n}^k\}$ is the solution of the following system

$$\begin{cases} \mu H \left[r_0 U_{m,n}^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) U_{m,n}^j - r_{k-1} U_{m,n}^0 \right] \\ \qquad \qquad \qquad = d(H_x \bar{\delta}_y^2 + H_y \bar{\delta}_x^2) U_{m,n}^{k-1+\sigma} + H f_{m,n}^{k-1+\sigma} + T_{m,n}^k \\ U_{m,n}^0 = \psi(x_m, y_n), \quad (x_m, y_n) \in \bar{\Omega} \\ U_{m,n}^k = \phi(x_m, y_n, t_k), \quad (x_m, y_n) \in \partial\Omega \end{cases} \quad (4.63)$$

where $T_{m,n}^k$ denotes the local truncation error.

To establish the convergence of the scheme (4.18), we need to estimate the local truncation error $T_{m,n}^k$. In fact, in view of Lemma 2.4, Lemma 4.1 and the result (4.17), we obtain the following result.

Lemma 4.8. *Assume that $U(x, y, t) \in \mathcal{C}^{8,8,3}(\bar{\Omega} \times [0, T])$. The local truncation error $T_{m,n}^k$ satisfies*

$$T_{m,n}^k = \begin{cases} O(\tau^2 + h^4 + \ell^4), & m = 1, M-1, \quad n = 1, N-1 \\ O(\tau^2 + h^6 + \ell^4), & 2 \leq m \leq M-2, \quad n = 1, N-1 \\ O(\tau^2 + h^6 + \ell^6), & 2 \leq m \leq M-2, \quad 2 \leq n \leq N-2 \\ O(\tau^2 + h^4 + \ell^6), & m = 1, M-1, \quad 2 \leq n \leq N-2. \end{cases} \quad (4.64)$$

Let $e_{m,n}^k = U_{m,n}^k - u_{m,n}^k$ be the difference between the exact solution $U_{m,n}^k$ and the numerical solution $u_{m,n}^k$ obtained from the scheme (4.18). Using the discrete energy method, we obtain the convergence theorem as follows.

Theorem 4.3. Assume that the exact solution $U(x, y, t) \in \mathcal{C}^{8,8,3}(\bar{\Omega} \times [0, T])$ and $\kappa \in (0, \kappa_0)$. Then,

$$\|e^k\| \leq O(\tau^2 + h^{4.5} + \ell^{4.5}), \quad 1 \leq k \leq K. \quad (4.65)$$

Proof. Clearly, $\{e_{m,n}^k\}$ is the solution of the following system

$$\mu H \left[r_0 e_{m,n}^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) e_{m,n}^j - r_{k-1} e_{m,n}^0 \right] = d(H_x \bar{\delta}_y^2 + H_y \bar{\delta}_x^2) e_{m,n}^{k-1+\sigma} + T_{m,n}^k, \quad (4.66)$$

with conditions $e_{m,n}^0 = 0$, $(x_m, y_n) \in \bar{\Omega}$ and $e_{m,n}^k = 0$, $(x_m, y_n) \in \partial\Omega$.

Note that $e^k \in \mathcal{U}_{M,N}^*$. Thus, applying Theorem 4.1 to (4.66) yields

$$\|e^k\|^2 \leq c \frac{\Gamma(1-\gamma)T^\gamma}{4\varepsilon_1\varepsilon_0^2 \left(\frac{60}{61}\right)^4 \left(\frac{1}{L} + \frac{1}{L'}\right)} \max_{1 \leq k \leq K} \|T^k\|^2, \quad 1 \leq k \leq K. \quad (4.67)$$

We need to bound the term $\|T^k\|^2$. Implementing (4.64), and noting $(M-3)h \leq L$ and $(N-3)\ell \leq L'$, we find

$$\begin{aligned} \|T^k\|^2 &= h\ell \sum_{m=1}^{M-1} \sum_{n=1}^{N-1} (T_{m,n}^k)^2 \\ &= (4h\ell) O(\tau^2 + h^4 + \ell^4)^2 + [2(M-3)h\ell] O(\tau^2 + h^6 + \ell^4)^2 \\ &\quad + [2(N-3)h\ell] O(\tau^2 + h^4 + \ell^6)^2 \\ &\quad + [(M-3)(N-3)h\ell] O(\tau^2 + h^6 + \ell^6)^2 \\ &\leq O(\tau^2 + h^{4.5}\ell^{0.5} + h^{0.5}\ell^{4.5})^2 + O(\tau^2 + h^6\ell^{0.5} + \ell^{4.5})^2 \\ &\quad + O(\tau^2 + h^{4.5} + \ell^6 h^{0.5})^2 + O(\tau^2 + h^6 + \ell^6)^2 \\ &\leq O(\tau^2 + h^{4.5} + \ell^{4.5})^2. \end{aligned}$$

Substituting the above result into (4.67) leads to (4.65) immediately. The proof is complete. $\square$

Remark 4.3. From the error inequality (4.65), it is obvious that our numerical scheme (4.18) improves the compact finite difference method [1, 58] which achieves

the spatial convergence order of $O(h^4 + \ell^4)$ (the best to date), and the finite difference method [26, 142] which gives the spatial convergence order of $O(h^2 + \ell^2)$. Note that in [1, 26] the convergence is established in l_2 norm, while $L_1(L_\infty)$ norm and H^1 norm are respectively used in [58] and [142].

Remark 4.4. The spatial convergence order of $O(h^{4.5} + \ell^{4.5})$ obtained in Theorem 4.3 is a *theoretical result*. In practice, we may get higher spatial convergence order for some particular problems (see Remark 3.2 (c) in Chapter 3). This is illustrated in the numerical experiments in Section 4.3.

Remark 4.5.

- (a) In Theorem 4.3, we require the exact solution $U(x, y, t)$ to be in $\mathcal{C}^{8,8,3}(\bar{\Omega} \times [0, T])$ to guarantee the accuracy. For some engineering problems, the solution is not smooth so order reduction is expected when we implement the proposed scheme (4.18) to obtain numerical solutions.
- (b) To weaken the continuity requirement, instead of the $L2 - 1_\sigma$ method (which requires $\mathcal{C}^3[0, T]$ and is of $O(\tau^{3-\gamma})$) used in the proposed scheme, we can use $L1$ scheme [60] which is less accurate ($O(\tau)$) but requires no continuity condition. It has been shown in [60] that $L1$ scheme can work well for non-smooth data. By a similar technique as in the present work, it is possible to show that a numerical scheme using parametric quintic spline approach and $L1$ method can achieve $O(\tau + h^{4.5} + \ell^{4.5})$ on the *weaker* condition that the exact solution $U(x, y, t) \in \mathcal{C}^{8,8}(\bar{\Omega})$.

4.3 Experiment

In this section, we shall demonstrate the accuracy and efficiency of the PQS scheme (4.18) through three examples, as well as compare with the CFD method [58] and the FD method [26, 142].

Implementing the numerical scheme (4.18) directly can be very expensive in practice. Therefore, similar to the matrix decomposition method described in [15, 113], we shall in practice convert the original scheme (4.18) to $(M - 1)$ one-dimensional equations if we solve y dimension first, or $(N - 1)$ one-dimensional equations if we solve x dimension first. This technique will greatly reduce the computation cost.

In the examples, for a fixed (τ, h, ℓ) , we shall compute the l_2 norm error and the maximum norm error at $t = T$, namely,

$$\|e^K(\tau, h, \ell)\| = \|e^K\|, \quad \|e^K(\tau, h, \ell)\|_\infty = \|e^K\|_\infty, \quad (4.68)$$

and the spatial convergence order when $h = \ell$ as

$$\mathcal{O}_{2,x} = \log_2 \frac{\|e^K(\tau, h, h)\|}{\|e^K(\tau, \frac{h}{2}, \frac{h}{2})\|}, \quad \mathcal{O}_{\infty,x} = \log_2 \frac{\|e^K(\tau, h, h)\|_\infty}{\|e^K(\tau, \frac{h}{2}, \frac{h}{2})\|_\infty}. \quad (4.69)$$

We also calculate $\mathcal{E}_\infty(\tau, h, \ell)$, the maximum absolute error over all time levels, as

$$\mathcal{E}_\infty(\tau, h, \ell) = \max_{1 \leq k \leq K} \|e^k(\tau, h, \ell)\|_\infty. \quad (4.70)$$

The spatial convergence order in terms of $\mathcal{E}_\infty(\tau, h, \ell)$ is similarly calculated as $\mathcal{O}_{\infty,x}$.

Example 4.1. [58] Consider problem (4.1) with $\Omega = (0, \pi) \times (0, \pi)$, $d = T = 1$, $\phi(x, y, t) = 0$, $\psi(x, y) = 0$ and

$$f(x, y, t) = t^3 \left[\frac{\Gamma(4 + \gamma)}{6} + 2t^\gamma \right] (\sin x)(\sin y).$$

The exact solution is $u(x, y, t) = t^{3+\gamma}(\sin x)(\sin y)$.

In this example, we fix $\kappa = \frac{1}{20}$ and $\tau = \frac{1}{10000}$. In Table 4.1, for various h ($= \ell$) we present the $\mathcal{E}_\infty(\tau, h, \ell)$ (see (4.67)) and the spatial convergence order and compare our results with the CFD methods in [58]. It is easily seen that our PQS method gives the best result for all cases.

TABLE 4.1: (Example 4.1) $\mathcal{E}_\infty(\tau, h, \ell)$ and spatial convergence order

γ	h	Scheme 1 [58]	order	Scheme 2 [58]	order	PQS	order
0.3	$\frac{\pi}{6}$	1.813E-04	-	1.813E-04	-	2.426E-05	-
	$\frac{\pi}{12}$	1.124E-05	4.012	1.124E-05	4.012	2.519E-07	6.589
	$\frac{\pi}{24}$	6.775E-07	4.052	7.000E-07	4.005	1.911E-09	7.042
0.5	$\frac{\pi}{6}$	1.581E-04	-	1.581E-04	-	2.200E-05	-
	$\frac{\pi}{12}$	9.803E-06	4.012	9.803E-06	4.012	2.385E-07	6.528
	$\frac{\pi}{24}$	5.971E-07	4.037	6.113E-07	4.003	3.427E-09	6.121
0.7	$\frac{\pi}{6}$	1.328E-04	-	1.328E-04	-	1.949E-05	-
	$\frac{\pi}{12}$	8.235E-06	4.012	8.237E-06	4.012	2.232E-07	6.448
	$\frac{\pi}{24}$	5.127E-07	4.006	5.137E-07	4.003	5.118E-09	5.447

Note that [58] applies CFD and the WSGL method (not $L2 - 1_\sigma$ method as in our PQS scheme). Hence, to have a *more precise comparison*, we shall apply the $L2 - 1_\sigma$ technique in the temporal dimension while employing CFD in the spatial dimension – we call this the CFD_σ method. In Tables 4.2 and 4.3 respectively, we calculate the errors $\|e^K(\tau, h, h)\|$ and $\|e^K(\tau, h, h)\|_\infty$ for both CFD_σ and PQS methods. Obviously, comparing to the CFD_σ method, the PQS method gives smaller error and higher spatial convergence order both in l_2 norm and maximum norm. In fact, the spatial convergence order is far better than the theoretical one. As stated in Remark 4.4, this is possible for some particular problems.

TABLE 4.2: (Example 4.1) $\|e^K(\tau, h, h)\|$ and spatial convergence order ($\mathcal{O}_{2,x}$)

	h	$\gamma = 0.3$	$\mathcal{O}_{2,x}$	$\gamma = 0.5$	$\mathcal{O}_{2,x}$	$\gamma = 0.7$	$\mathcal{O}_{2,x}$
PQS	$\frac{\pi}{5}$	1.7749E-04	-	1.5719E-04	-	1.3508E-04	-
	$\frac{\pi}{10}$	1.7751E-06	6.6437	1.5903E-06	6.6271	1.3901E-06	6.6024
	$\frac{\pi}{20}$	1.2657E-08	7.1318	9.0869E-09	7.4513	6.3756E-09	7.7684
CFD_σ	$\frac{\pi}{5}$	5.9342E-04	-	5.1744E-04	-	4.3471E-04	-
	$\frac{\pi}{10}$	3.6658E-05	4.0169	3.1962E-05	4.0169	2.6850E-05	4.0170
	$\frac{\pi}{20}$	2.2799E-06	4.0070	1.9847E-06	4.0094	1.6641E-06	4.0121

TABLE 4.3: (Example 4.1) $\|e^K(\tau, h, h)\|_\infty$ and spatial convergence order ($\mathcal{O}_{\infty,x}$)

	h	$\gamma = 0.3$	$\mathcal{O}_{\infty,x}$	$\gamma = 0.5$	$\mathcal{O}_{\infty,x}$	$\gamma = 0.7$	$\mathcal{O}_{\infty,x}$
PQS	$\frac{\pi}{5}$	7.6332E-05	-	6.8124E-05	-	5.9878E-05	-
	$\frac{\pi}{10}$	8.5147E-07	6.4862	7.9974E-07	6.4125	7.4070E-07	6.3370
	$\frac{\pi}{20}$	7.5342E-09	6.8204	6.9875E-09	6.8386	6.4610E-09	6.8410
CFD_σ	$\frac{\pi}{5}$	3.4171E-04	-	2.9796E-04	-	2.5032E-04	-
	$\frac{\pi}{10}$	2.3337E-05	3.8721	2.0348E-05	3.8722	1.7093E-05	3.8722
	$\frac{\pi}{20}$	1.4515E-06	4.0070	1.2635E-06	4.0090	1.0594E-06	4.0121

Next, for visualization, in Figures 4.1 and 4.2 we plot the exact solution, the numerical solution and the absolute error obtained from the PQS scheme at $t = 1$ when $\gamma = 0.5$. It is observed that the PQS method gives a good approximation to the exact values at mesh points.

Finally, we investigate the influence of κ on the actual errors obtained from the PQS scheme. For $\gamma = 0.5$ and $h = \frac{\pi}{5}$, the errors $\|e^K(\tau, h, h)\|$ and $\|e^K(\tau, h, h)\|_\infty$ for different $\kappa \in (0, \kappa_0)$ (in steps of 0.005) are plotted in Figure 4.3. It is observed that the choice of κ does affect the errors but the influence is very little. Therefore, we can choose any $\kappa \in (0, \kappa_0)$ in practice.

FIGURE 4.1: (Example 4.1) Approximate solution by PQS method and exact solution at $t = 1$ when $\kappa = \frac{1}{20}$, $\gamma = 0.5$, $h = \ell = \frac{\pi}{20}$, $\tau = \frac{1}{10000}$.

FIGURE 4.2: (Example 4.1) Absolute error of PQS method at $t = 1$ when $\kappa = \frac{1}{20}$, $\gamma = 0.5$, $h = \ell = \frac{\pi}{20}$, $\tau = \frac{1}{10000}$.

FIGURE 4.3: (Example 4.1) $\|e^K(\frac{1}{1000}, \frac{\pi}{5}, \frac{\pi}{5})\|$ and $\|e^K(\frac{1}{1000}, \frac{\pi}{5}, \frac{\pi}{5})\|_\infty$ for various κ when $\gamma = 0.5$.

Example 4.2. [142] Consider problem (4.1) with $\Omega = (0, \pi) \times (0, \pi)$, $d = 1$, $T = \frac{1}{2}$, $\phi(x, y, t) = 0$, $\psi(x, y) = 0$ and

$$f(x, y, t) = \left[\frac{2}{\Gamma(3 - \gamma)} t^{2-\gamma} + 2t^2 \right] (\sin x)(\sin y).$$

The exact solution is $u(x, y, t) = t^2(\sin x)(\sin y)$.

Here, we fix $\kappa = \frac{1}{20}$. To compare our PQS method with the FD methods (L_1 -ADI and BD-ADI schemes) proposed in [142], we first use the same $K = 2000$ as in [142], i.e., $\tau = \frac{1}{4000}$. The errors $\|e^K(\tau, h, h)\|_\infty$ are displayed in Table 4.4.

It is obvious that our PQS scheme gives far smaller errors but the convergence order is not what we expect – this is due to the temporal step size not sufficiently small enough. When we switch to $K = 10000$, one can see that the spatial convergence order becomes at least 4.5 which is consistent with our theoretical result.

TABLE 4.4: (Example 4.2) $\|e^K(\tau, h, h)\|_\infty$ and spatial convergence order ($\mathcal{O}_{\infty, x}$)

	h	$\gamma = \frac{1}{2}$	$\mathcal{O}_{\infty, x}$	$\gamma = \frac{2}{3}$	$\mathcal{O}_{\infty, x}$
BD-ADI [142] ($\gamma = \frac{1}{2}$)	$\frac{\pi}{8}$	1.5096E-03	-	1.2844E-03	-
	$\frac{\pi}{16}$	3.7696E-04	2.0017	3.2219E-04	1.9951
L_1 -ADI [142] ($\gamma = \frac{2}{3}$)	$\frac{\pi}{32}$	9.3984E-05	2.0039	8.1568E-05	1.9818
	$\frac{\pi}{8}$	8.3254E-07	-	7.6442E-07	-
PQS ($K = 2000$)	$\frac{\pi}{16}$	7.0783E-09	6.8780	6.9518E-09	6.7808
	$\frac{\pi}{32}$	7.7277E-09	-0.1266	9.1601E-09	-0.3980
	$\frac{\pi}{8}$	8.3540E-07	-	7.6780E-07	-
PQS ($K = 10000$)	$\frac{\pi}{16}$	8.5352E-09	6.6129	8.1528E-09	6.5573
	$\frac{\pi}{32}$	2.6806E-10	4.9928	3.2718E-10	4.6391
	$\frac{\pi}{8}$				

Next, with $\tau = \frac{1}{10000}$ we present the errors and spatial convergence orders in l_2 norm and maximum norm in Tables 4.5 and 4.6 respectively. It is observed that the PQS method achieves a better accuracy than the CFD_σ method, and attains at least 4.5 order of spatial convergence which verifies our theoretical result.

Also, the exact and numerical solutions as well as the absolute error from the PQS scheme at $t = \frac{1}{2}$ are plotted in Figure 4.4. Obviously, we get a good approximation that can be visually seen from Figure 4.5.

TABLE 4.5: (Example 4.2) $\|e^K(\tau, h, h)\|$ and spatial convergence order ($\mathcal{O}_{2,x}$)

	h	$\gamma = 0.3$	$\mathcal{O}_{2,x}$	$\gamma = 0.5$	$\mathcal{O}_{2,x}$	$\gamma = 0.7$	$\mathcal{O}_{2,x}$
PQS	$\frac{\pi}{5}$	4.2952E-05	-	3.7277E-05	-	3.1462E-05	-
	$\frac{\pi}{10}$	4.3088E-07	6.6393	3.7943E-07	6.6183	3.2711E-07	6.5877
	$\frac{\pi}{20}$	2.9491E-09	7.1909	2.0974E-09	7.4990	1.5056E-09	7.7633
CFD $_{\sigma}$	$\frac{\pi}{5}$	1.4303E-04	-	1.2176E-04	-	9.9926E-05	-
	$\frac{\pi}{10}$	8.8357E-06	4.0169	7.5211E-06	4.0169	6.1721E-06	4.0170
	$\frac{\pi}{20}$	5.4937E-07	4.0075	4.6686E-07	4.0099	3.8241E-07	4.0125

TABLE 4.6: (Example 4.2) $\|e^K(\tau, h, h)\|_{\infty}$ and spatial convergence order ($\mathcal{O}_{\infty,x}$)

	h	$\gamma = 0.3$	$\mathcal{O}_{\infty,x}$	$\gamma = 0.5$	$\mathcal{O}_{\infty,x}$	$\gamma = 0.7$	$\mathcal{O}_{\infty,x}$
PQS	$\frac{\pi}{5}$	1.8511E-05	-	1.6207E-05	-	1.4240E-05	-
	$\frac{\pi}{10}$	2.0932E-07	6.4666	1.9476E-07	6.3788	1.7915E-07	6.3126
	$\frac{\pi}{20}$	1.8518E-09	6.8207	1.7142E-09	6.8280	1.5915E-09	6.8147
CFD $_{\sigma}$	$\frac{\pi}{5}$	8.2363E-05	-	7.0113E-05	-	5.7540E-05	-
	$\frac{\pi}{10}$	5.6250E-06	3.8721	4.7881E-06	3.8722	3.9293E-06	3.8722
	$\frac{\pi}{20}$	3.4974E-07	4.0075	2.9721E-07	4.0099	2.4345E-07	4.0125

Finally, to investigate the effect of κ in the PQS method, we plot the l_2 norm and maximum norm errors for various $\kappa \in (0, \kappa_0)$ in Figure 4.6. We find that the choice of κ does not make a big difference in the actual errors.

FIGURE 4.4: (Example 4.2) Approximate solution by PQS method and exact solution at $t = \frac{1}{2}$ when $\kappa = \frac{1}{20}$, $\gamma = 0.5$, $h = \ell = \frac{\pi}{20}$, $\tau = \frac{1}{10000}$.

Example 4.3. [26, 142] Consider problem (4.1) with $\Omega = (0, 1) \times (0, 1)$, $d = T = 1$, $\phi(x, y, t) = e^{x+y}t^{1+\gamma}$, $\psi(x, y) = 0$ and

$$f(x, y, t) = e^{x+y} [\Gamma(2 + \gamma)t - 2t^{1+\gamma}].$$

The exact solution is $u(x, y, t) = e^{x+y}t^{1+\gamma}$.

FIGURE 4.5: (Example 4.2) Absolute error of PQS method at $t = \frac{1}{2}$ when $\kappa = \frac{1}{20}$, $\gamma = 0.5$, $h = \ell = \frac{\pi}{20}$, $\tau = \frac{1}{10000}$.

FIGURE 4.6: (Example 4.2) $\|e^K(\frac{1}{1000}, \frac{\pi}{5}, \frac{\pi}{5})\|$ and $\|e^K(\frac{1}{1000}, \frac{\pi}{5}, \frac{\pi}{5})\|_\infty$ for various κ when $\gamma = 0.5$.

Here, we fix $\kappa = \frac{1}{20}$ and $h = \ell$. For $\tau = \frac{1}{400}$, the $\mathcal{E}_\infty(\tau, h, \ell)$ (see (4.67)) and CPU time of various methods are presented in Table 4.7. It is clearly seen that the PQS scheme can be implemented efficiently using the matrix decomposition method [15, 113]. Also, the $\mathcal{E}_\infty(\tau, h, \ell)$ of the PQS scheme is far smaller than that of L_1 -ADI, BD-ADI [142] and implicit method [26], which are FD methods. However, it is observed that the $\mathcal{E}_\infty(\tau, h, \ell)$ of the PQS scheme becomes only a little bit smaller or even larger as h decreases. This is due to the temporal step size τ not sufficiently small so that minor change in h cannot affect the $\mathcal{E}_\infty(\tau, h, \ell)$ much.

Next, to compare PQS and CFD_σ methods, we fix $\tau = \frac{1}{10000}$ and present l_2 norm error and maximum norm error at $t = 1$ respectively in Tables 4.8 and 4.9. From these two tables, we observe that smaller errors and higher spatial convergence order are achieved by the PQS scheme in both l_2 norm and maximum norm. Obviously, the numerical spatial convergence order is far better than the theoretical

TABLE 4.7: (Example 4.3) $\mathcal{E}_\infty(\tau, h, \ell)$ and CPU time when $\gamma = 0.75$ ($\tau = 1/400$)

	h	$\mathcal{E}_\infty(\tau, h, \ell)$	CPU time (second)
L_1 -ADI [142]	$\frac{1}{8}$	5.2328E-04	4.0790
	$\frac{1}{16}$	1.5076E-04	18.1710
	$\frac{1}{32}$	5.4544E-05	75.3440
BD-ADI [142]	$\frac{1}{8}$	5.4741E-04	1.2180
	$\frac{1}{16}$	1.7523E-04	4.9220
	$\frac{1}{32}$	7.9027E-05	19.8750
Implicit scheme [26]	$\frac{1}{8}$	6.9466E-04	11.3120
	$\frac{1}{16}$	2.8969E-04	143.4690
	$\frac{1}{32}$	7.8882E-05	1895.0630
PQS method	$\frac{1}{8}$	3.2445E-06	0.4176
	$\frac{1}{16}$	3.2410E-06	0.5058
	$\frac{1}{32}$	3.2756E-06	1.0897

one obtained in (4.65). This is possible in practice as the bound in (4.65) is not a tight bound.

TABLE 4.8: (Example 4.3) $\|e^K(\tau, h, h)\|$ and spatial convergence order ($\mathcal{O}_{2,x}$)

	h	$\gamma = 0.3$	$\mathcal{O}_{2,x}$	$\gamma = 0.5$	$\mathcal{O}_{2,x}$	$\gamma = 0.7$	$\mathcal{O}_{2,x}$
PQS	$\frac{1}{5}$	5.7945E-07	-	5.7529E-07	-	5.6971E-07	-
	$\frac{1}{10}$	1.0367E-08	5.8046	1.0209E-08	5.8164	9.9892E-09	5.8337
	$\frac{1}{20}$	1.2775E-10	6.3426	6.9171E-11	7.2055	1.9507E-10	5.6783
CFD_σ	$\frac{1}{5}$	1.4901E-06	-	1.4781E-06	-	1.4620E-06	-
	$\frac{1}{10}$	9.3523E-08	3.9939	9.2670E-08	3.9955	9.1516E-08	3.9977
	$\frac{1}{20}$	5.7919E-09	4.0132	5.6371E-09	4.0391	5.4191E-09	4.0779

TABLE 4.9: (Example 4.3) $\|e^K(\tau, h, h)\|_\infty$ and spatial convergence order ($\mathcal{O}_{\infty,x}$)

	h	$\gamma = 0.3$	$\mathcal{O}_{\infty,x}$	$\gamma = 0.5$	$\mathcal{O}_{\infty,x}$	$\gamma = 0.7$	$\mathcal{O}_{\infty,x}$
PQS	$\frac{1}{5}$	1.1803E-06	-	1.1757E-06	-	1.1694E-06	-
	$\frac{1}{10}$	2.3872E-08	5.6277	2.3784E-08	5.6274	2.3660E-08	5.6272
	$\frac{1}{20}$	4.1679E-10	5.8398	3.9626E-10	5.9074	4.1279E-10	5.8409
CFD_σ	$\frac{1}{5}$	2.7018E-06	-	2.6794E-06	-	2.6492E-06	-
	$\frac{1}{10}$	1.6884E-07	4.0002	1.6725E-07	4.0018	1.6510E-07	4.0042
	$\frac{1}{20}$	1.0453E-08	4.0136	1.0170E-08	4.0396	9.7718E-09	4.0786

The exact solution, the numerical solution and the absolute error obtained from the PQS scheme at $t = 1$ are plotted in Figures 4.7 and 4.8. It is seen that the

error is sufficiently small at mesh points which shows the high accuracy of the PQS scheme.

FIGURE 4.7: (Example 4.3) Approximate solution by PQS method and exact solution at $t = 1$ when $\kappa = \frac{1}{20}$, $\gamma = 0.5$, $h = \ell = \frac{1}{20}$, $\tau = \frac{1}{10000}$.

FIGURE 4.8: (Example 4.3) Absolute error of PQS method at $t = 1$ when $\kappa = \frac{1}{20}$, $\gamma = 0.5$, $h = \ell = \frac{1}{20}$, $\tau = \frac{1}{10000}$.

Finally, the influence of $\kappa \in (0, \kappa_0)$ on the actual errors obtained from the PQS scheme is presented visually in Figure 4.9. Once again we see that the choice of κ has little influence.

4.4 Summary

We develop an efficient numerical scheme for two-dimensional fractional sub-diffusion problems using parametric quintic spline in the spatial dimensions and $L2 - 1_\sigma$ approximation in the temporal dimension in this chapter. Under appropriate assumptions, it is proved that the numerical scheme is uniquely solvable, stable in

FIGURE 4.9: (Example 4.3) $\|e^K(\frac{1}{1000}, \frac{1}{5}, \frac{1}{5})\|$ and $\|e^K(\frac{1}{1000}, \frac{1}{5}, \frac{1}{5})\|_\infty$ for various κ when $\gamma = 0.5$.

l_2 norm sense and convergent with accuracy of $O(\tau^2 + h^{4.5} + \ell^{4.5})$. The spatial convergence order of $O(h^{4.5} + \ell^{4.5})$ improves that of the compact finite difference method, which is $O(h^4 + \ell^4)$ and is the best result until the current work. Finally, simulation is carried out to further demonstrate the efficiency and accuracy of the proposed method. The numerical results show that the spatial convergence order is at least 4.5 which verifies the theoretical result.

Chapter 5

Fourth-order Fractional Sub-diffusion problems

In Chapters 3 and 4, we have considered the classical fractional sub-diffusion equation which contains a second-order space derivative. But in some models such as transverse vibration of beams [114], and groove formation on the surface of metal by a grain boundary [102], a fourth-order space derivative may be necessary. In present chapter, we study the fourth-order fractional sub-diffusion problem [53]:

$$\left\{ \begin{array}{l} {}^C_0 D_t^\gamma u(x, t) + du_{xxxx} = f(x, t), \quad x \in [0, L], \quad t \in [0, T] \\ u(x, 0) = \psi(x), \quad x \in [0, L] \\ u(0, t) = \phi_1(t), \quad u(L, t) = \phi_2(t), \quad u_{xx}(0, t) = \phi_3(t), \quad u_{xx}(L, t) = \phi_4(t), \end{array} \right. \quad (5.1)$$

where $0 < \gamma < 1$, d is a positive constant, $\phi_3(t)$ and $\phi_4(t)$ are known continuous functions. In the physical context, u is the transverse displacement of the beam, t and x are the time and distance variables respectively, d is the ratio of flexural rigidity of the beam to its mass per unit length, and f is the dynamic driving force per unit mass.

The existence and uniqueness of solution of problem (5.1) has been discussed as a special case in the paper by Berdyshev et al. [13]. Here, the authors apply the method of separation of variables to prove the unique solvability of direct and inverse problems for a fourth-order mixed type equation, which coincides with (5.1) for $t > 0$, and for $t < 0$ it is (5.1) with $\gamma = 2$. Moreover, Agrawal [3, 4] has

presented a general solution for a special case of (5.1) when $f = 0$ and $\phi_1(t) = \phi_2(t) = \phi_3(t) = \phi_4(t) = 0$. Here, the finite sine and Laplace transforms are used to reduce the fractional differential equation to an ordinary differential equation, then the solution is obtained by inverse Laplace and inverse finite sine transforms. We note that the method in [3, 4] can be similarly used to derive an analytical solution for problem (5.1).

The attention on the numerical treatment of fractional diffusion equations containing *fourth-order* space derivatives is also aplenty. In fact, numerical methods such as decomposition method [56], homotopy perturbation method [44], local discontinuous Galerkin method [125], and finite element [81, 82] are applied successfully. Further, a collocation method with quintic B-spline basis functions [115] has been used to deal with various boundary conditions, however only error analysis for the semi-discrete scheme is given and no explicit spatial convergence order is established. Very recently, a fully discrete numerical scheme using quintic spline has been developed by Tariq and Akram [120] – it is shown that $O(h^4)$ is obtained in spatial convergence and this improves the result in [115]. On finite difference methods, Hu and Zhang have discussed finite difference method [53] for sub-diffusion problem, compact finite difference method [52, 54] for diffusion-wave problem, and provided convergence and stability analysis. Also, Vong and Wang [122] have constructed a different compact method for a sub-diffusion problem involving *different* boundary conditions from [53], and the spatial convergence order of this compact finite difference method is $O(h^4)$. In summary, $O(h^4)$ is the *best spatial convergence* achieved to date in the literature of fractional diffusion problems.

Motivated by the above mentioned research, in this chapter we shall discuss the numerical treatment of a *fourth-order* fractional sub-diffusion problem which has also been considered in [53]. Our aims are to improve the spatial convergence order to *above* 4, to provide rigorous proof of solvability, convergence and stability in maximum norm, and to demonstrate the efficacy by numerical experiments. To achieve our objectives, we shall apply a *parametric quintic spline method* in the spatial dimension, and use a higher order approximation for fractional derivatives, namely $L2 - 1_\sigma$ scheme [7], to increase the efficiency further. It is noted that parametric quintic spline method has been effective in solving boundary value problems of *integer-order* differential equations [65, 68], and subsequently parametric *cubic* spline has been applied to fractional differential equations [35, 50], while the first

application of parametric *quintic* spline to a *second-order* fractional sub-diffusion problem appears in [78].

The plan of the chapter is as follows. The numerical scheme involving parametric quintic spline and $L2 - 1_\sigma$ approximation is derived in Section 5.1. Then, we prove the stability, solvability and convergence in Section 5.2. In Section 5.3, numerical experiments are carried out to illustrate the efficiency of the proposed scheme as well as to compare with other methods. Finally, we end with a summary in Section 5.4.

5.1 Numerical Scheme

In this section, we shall develop a numerical scheme for problem (5.1) using parametric quintic spline in the spatial dimension and $L2 - 1_\sigma$ approximation (2.21) for the Caputo fractional derivative.

We consider uniform meshes P and P'' . Applying (3.8)(a) and (3.8)(b) obtained in Chapter 3, it is easy to get an explicit expression of W_m^k , in terms of F_j^k and u_j^k , $j = m - 1, m, m + 1$, as follows

$$W_m^k = \delta_x^2 u_m^k - \left[\left(\kappa_1 + \frac{\kappa}{6} \right) F_{m+1}^k + 2 \left(\rho_1 + \frac{\rho}{6} \right) F_{m+1}^k + \left(\kappa_1 + \frac{\kappa}{6} \right) F_{m-1}^k \right].$$

By replacing m by $(m + 1)$ and $(m - 1)$ respectively, W_{m+1}^k and W_{m-1}^k can be obtained. Upon substituting W_{m-1}^k , W_m^k and W_{m+1}^k into (3.8)(a), we derive the following equation which connects the fourth derivatives and the function values

$$p(F_{m-2}^k + F_{m+2}^k) + q(F_{m-1}^k + F_{m+1}^k) + sF_m^k = \delta_x^4 u_m^k, \quad 2 \leq m \leq M - 2 \quad (5.2)$$

where p , q and s are the same as in (3.12).

Similar to previous chapters, we need two more relations besides (5.2). Since we would like these two relations to involve u_m^k 's and F_m^k 's, to incorporate the boundary conditions in (5.1), and to have local truncation error of $O(h^4)$ in the spatial dimension, we consider the following equations:

$$-T_1^k = \frac{c_0 u_0^k + c_1 u_1^k + c_2 u_2^k + c_3 u_3^k}{h^4} + \frac{c_4 h^2 W_0^k + (b_0 F_0^k + b_1 F_1^k + b_2 F_2^k + b_3 F_3^k)}{h^4},$$

and

$$-T_{M-1}^k = \frac{c_M u_M^k + c_{M-1} u_{M-1}^k + c_{M-2} u_{M-2}^k + c_{M-3} u_{M-3}^k}{h^4} + \frac{\bar{c}_4 h^2 W_M^k + h^4 (b_M F_M^k + b_{M-1} F_{M-1}^k + b_{M-2} F_{M-2}^k + b_{M-3} F_{M-3}^k)}{h^4}$$

where the constants are to be determined. By Taylor expansion of above two formulas at $x = x_1$ and $x = x_{M-1}$ respectively, we are able to select the constants such that $T_m^k = O(h^4)$, $m = 1, M-1$. Upon substituting the constants and omitting the local truncation errors, we get

$$\frac{1}{360} (28F_0^k + 245F_1^k + 56F_2^k + F_3^k) = \frac{W_0^k - 2\delta_x^2 u_1 + \delta_x^2 u_2}{h^2}, \quad (5.3)$$

and

$$\frac{1}{360} (28F_M^k + 245F_{M-1}^k + 56F_{M-2}^k + F_{M-3}^k) = \frac{W_M^k - \delta_x^2 u_{M-1}^k + \delta_x^2 u_{M-2}^k}{h^2}. \quad (5.4)$$

We are now ready to combine (5.2)-(5.4) and the $L2 - 1_\sigma$ approximation to obtain a numerical scheme for problem (5.1). To begin, for $u \in \mathcal{U}_P^*$ we define a new parametric quintic spline operator $\mathcal{H}$ as

$$\mathcal{H}u_m = \begin{cases} \frac{1}{360}(28u_0 + 245u_1 + 56u_2 + u_3), & m = 1 \\ p(u_{m-2} + u_{m+2}) + q(u_{m-1} + u_{m+1}) + su_m, & 2 \leq m \leq M-2 \\ \frac{1}{360}(u_{M-3} + 56u_{M-2} + 245u_{M-1} + 28u_M), & m = M-1. \end{cases} \quad (5.5)$$

Let $\sigma = 1 - \frac{\gamma}{2}$ and $t_{k-1+\sigma} = (k-1+\sigma)\tau$. At the node $(x_m, t_{k-1+\sigma})$, it follows from (5.1) that

$${}_0^C D_t^\gamma u(x_m, t_{k-1+\sigma}) + du_{xxxx}(x_m, t_{k-1+\sigma}) = f(x_m, t_{k-1+\sigma}),$$

or

$$u_{xxxx}(x_m, t_{k-1+\sigma}) = \frac{1}{d} [f_m^{k-1+\sigma} - {}_0^C D_t^\gamma u(x_m, t_{k-1+\sigma})] = F_m^{k-1+\sigma} \quad (5.6)$$

where we have also used the fourth derivative of the parametric quintic spline to approximate u_{xxxx} .

To handle the time node at $t_{k-1+\sigma}$, we employ

$$\begin{aligned} u_{xxxx}(x_m, t_{k-1+\sigma}) &= \sigma u_{xxxx}(x_m, t_k) + (1 - \sigma) u_{xxxx}(x_m, t_{k-1}) + O(\tau^2) \\ &= \sigma F_m^k + (1 - \sigma) F_m^{k-1} + O(\tau^2). \end{aligned}$$

Using (5.6) in the above gives

$$\frac{1}{d} [f_m^{k-1+\sigma} - {}^C_0 D_t^\gamma u(x_m, t_{k-1+\sigma})] = \sigma F_m^k + (1 - \sigma) F_m^{k-1} + O(\tau^2). \quad (5.7)$$

Then, we apply the operator $\mathcal{H}$ to (5.7). In view of (5.2)-(5.4) and $2p + 2q + s = 1$, we get

$$\frac{1}{d} \mathcal{H} [f_m^{k-1+\sigma} - {}^C_0 D_t^\gamma u(x_m, t_{k-1+\sigma})] = \delta_x^4 u_m^{k-1+\sigma} + O(\tau^2), \quad 1 \leq m \leq M - 1. \quad (5.8)$$

where $\delta_x^4 u_m^{k-1+\sigma} = \sigma \delta_x^4 u_m^k + (1 - \sigma) \delta_x^4 u_m^{k-1}$.

Now, employing $L2 - 1_\sigma$ approximation (Lemma 2.4) for the Caputo fractional derivative in (5.8) yields, after omitting the small terms, the following *parametric quintic spline scheme*:

$$\begin{cases} \bar{\mu} \mathcal{H} \left[r_0 u_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) u_m^j - r_{k-1} u_m^0 \right] + \delta_x^4 u_m^{k-1+\sigma} = \frac{1}{d} \mathcal{H} f_m^{k-1+\sigma}, \\ u_m^0 = \psi(x_m), \\ u_0^k = \phi_1(t_k), \quad u_M^k = \phi_2(t_k), \quad \delta_x^2 u_0^k = \phi_3(t_k), \quad \delta_x^2 u_M^k = \phi_4(t_k), \end{cases} \quad (5.9)$$

where $\bar{\mu} = \frac{\mu}{d} = \frac{1}{d\Gamma(2-\gamma)\tau^\gamma}$.

We have now derived the parametric quintic spline scheme (5.9). In practice, in view of the initial condition there, if the scheme (5.9) admits a unique solution at each time $t = t_k$, the approximate solution u_m^k , $1 \leq m \leq M - 1$ can be obtained for $1 \leq k \leq K$ as in Chapter 3. In fact, the system (5.9) is indeed *uniquely solvable* and this will be shown in Section 5.2.

5.2 Solvability, Stability and Convergence

In this section, we shall analyze the solvability, stability and convergence of the scheme (5.9). To this aim, we shall first deal with the local truncation error of the parametric quintic spline scheme and then establish the stability since the proof of solvability and convergence employs a similar technique as in the proof of stability.

The first result deals with the local truncation error of the parametric quintic spline scheme.

Lemma 5.1. *Let $u(x, t) \in \mathcal{C}^{8,3}([0, L] \times [0, T])$ and T_m^k be the local truncation error of the k -th equation in the numerical scheme (5.9). We have*

$$T_m^k = \begin{cases} \frac{h^4}{1334} D_x^8 u_m^{k-1+\sigma} + O(h^5 + \tau^2), & m = 1, M-1 \\ -(2p+2q+s-1) D_x^4 u_m^{k-1+\sigma} - \left(4p+q-\frac{1}{6}\right) h^2 D_x^6 u_m^{k-1+\sigma} \\ - \left(\frac{4}{3}p + \frac{1}{12}q - \frac{1}{80}\right) h^4 D_x^8 u_m^{k-1+\sigma} + O(h^6 + \tau^2), & 2 \leq m \leq M-2 \end{cases} \quad (5.10)$$

Proof. For $1 \leq m \leq M-1$, we find, in view of (5.7) and (2.21),

$$\begin{aligned} T_m^k &= \bar{\mu} \mathcal{H} \left[r_0 u_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) u_m^k - r_{k-1} u_m^0 \right] + \delta_x^4 u_m^{k-1+\sigma} - \frac{1}{d} \mathcal{H} f_m^{k-1+\sigma} \\ &= \bar{\mu} \mathcal{H} \left[r_0 u_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) u_m^k - r_{k-1} u_m^0 \right] - \frac{1}{d} \mathcal{H} {}^C_0 D_t^\gamma u(x_m, t_{k-1+\sigma}) \\ &\quad - \mathcal{H} u_{xxxx}(x_m, t_{k-1+\sigma}) + \delta_x^4 u_m^{k-1+\sigma} \\ &= O(\tau^{3-\gamma}) - \mathcal{H} u_{xxxx}(x_m, t_{k-1+\sigma}) + \delta_x^4 u(x_m, t_{k-1+\sigma}) + O(\tau^2) \end{aligned}$$

Then, taking Taylor expansion at $x = x_m$ gives (5.10). $\square$

Remark 5.1. From Lemma 5.1, we see that T_m^k , $2 \leq m \leq M-2$ will be of $O(h^6)$ if

$$2p+2q+s-1=0, \quad 4p+q-\frac{1}{6}=0, \quad \frac{4}{3}p+\frac{1}{12}q-\frac{1}{80}=0,$$

which upon solving yields

$$p = -\frac{1}{720}, \quad q = \frac{31}{180}, \quad s = \frac{79}{120}. \quad (5.11)$$

As a result, there exist constants C_1 and C_2 such that

$$|T_m^k| \leq \begin{cases} C_1(h^4 + \tau^2), & m = 1, M-1 \\ C_2(h^6 + \tau^2), & 2 \leq m \leq M-2 \end{cases} \quad (5.12)$$

In the current work, we shall fix p , q and s as in (5.11). Note that this is the only way to get higher convergence order.

We shall now define an inner product that is vital in subsequent analysis. For any $u, v \in \mathcal{U}_P^*$,

$$\langle u, v \rangle = (\delta_x^2 u, \delta_x^2 v) - \frac{h^3}{6} \sum_{m=0}^{M-1} \left(\delta_x^3 u_{m+\frac{1}{2}} \right) \left(\delta_x^3 v_{m+\frac{1}{2}} \right) - h^4 \eta (\delta_x^4 u, \delta_x^4 v), \quad (5.13)$$

where $\eta = \frac{1}{720}$ for $2 \leq m \leq M-2$ and $\eta = -\frac{1}{360}$ for $m = 1, M-1$.

The next few lemmas will be used to establish the stability of the parametric quintic spline scheme. The first result relates $\langle \cdot, \cdot \rangle$ with $\|\delta_x^2 \cdot\|^2$.

Lemma 5.2. *For any $u \in \mathcal{U}_P^*$, the following inequality holds*

$$\frac{14}{45} \|\delta_x^2 u\|^2 \leq \langle u, u \rangle \leq \frac{47}{45} \|\delta_x^2 u\|^2. \quad (5.14)$$

Proof. The definition (5.13) gives

$$\langle u, u \rangle = \|\delta_x^2 u\|^2 - \frac{h^2}{6} |\delta_x^3 u|_1^2 - \frac{h^5}{720} \sum_{m=2}^{M-2} (\delta_x^4 u_m)^2 + \frac{h^5}{360} (\delta_x^4 u_1)^2 + \frac{h^5}{360} (\delta_x^4 u_{M-1})^2$$

which leads to

$$\begin{cases} \langle u, u \rangle \leq \|\delta_x^2 u\|^2 + \frac{h^5}{360} (\delta_x^4 u_1)^2 + \frac{h^5}{360} (\delta_x^4 u_{M-1})^2, \\ \langle u, u \rangle \geq \|\delta_x^2 u\|^2 - \frac{h^2}{6} |\delta_x^3 u|_1^2 - \frac{h^5}{720} \sum_{m=2}^{M-2} (\delta_x^4 u_m)^2. \end{cases} \quad (5.15)$$

To establish (5.14), we shall first estimate $h^4 \|\delta_x^4 u\|^2$ and $h^2 |\delta_x^3 u|_1^2$. In fact, using the inequality $(a \pm b)^2 \leq 2(a^2 + b^2)$ ($\forall a, b \in \mathcal{R}$), we find

$$\begin{aligned} h^4 \|\delta_x^4 u\|^2 &= h^3 \sum_{m=1}^{M-1} \left(\delta_x^3 u_{m+\frac{1}{2}} - \delta_x^3 u_{m-\frac{1}{2}} \right)^2 \\ &\leq 2h^3 \sum_{m=1}^{M-1} \left[\left(\delta_x^3 u_{m+\frac{1}{2}} \right)^2 + \left(\delta_x^3 u_{m-\frac{1}{2}} \right)^2 \right] \leq 4h^2 |\delta_x^3 u|_1^2 \end{aligned}$$

and

$$\begin{aligned} h^2 |\delta_x^3 u|_1^2 &= h \sum_{m=0}^{M-1} \left(\delta_x^2 u_{m+1} - \delta_x^2 u_m \right)^2 \\ &\leq 2h \sum_{m=0}^{M-1} \left[\left(\delta_x^2 u_{m+1} \right)^2 + \left(\delta_x^2 u_m \right)^2 \right] = 4 \|\delta_x^2 u\|^2. \end{aligned} \tag{5.16}$$

Combining the above two inequalities, we get

$$h^4 \|\delta_x^4 u\|^2 \leq 4h^2 |\delta_x^3 u|_1^2 \leq 16 \|\delta_x^2 u\|^2. \tag{5.17}$$

Applying (5.17) and (5.15), it follows from (5.14) that

$$\langle u, u \rangle \leq \|\delta_x^2 u\|^2 + \frac{h^5}{360} (\delta_x^4 u_1)^2 + \frac{h^5}{360} (\delta_x^4 u_{M-1})^2 \leq \left(1 + \frac{16}{360} \right) \|\delta_x^2 u\|^2 = \frac{47}{45} \|\delta_x^2 u\|^2$$

and

$$\langle u, u \rangle \geq \|\delta_x^2 u\|^2 - \frac{h^2}{6} |\delta_x^3 u|_1^2 - \frac{h^5}{720} \sum_{m=2}^{K-2} (\delta_x^4 u_m)^2 \geq \left(1 - \frac{4}{6} - \frac{16}{720} \right) \|\delta_x^2 u\|^2 = \frac{14}{45} \|\delta_x^2 u\|^2.$$

The proof is complete. $\square$

The next lemma relates $\|\delta_x^2 \cdot\|$ with the maximum norm $\|\cdot\|_\infty$.

Lemma 5.3. [2, 52–54, 103] For any $u \in \mathcal{U}_P$ and $0 < h < L$, we have

$$\left(\frac{2 \sin \frac{\pi h}{2L}}{h} \right)^2 |\delta_x u|_1^2 \leq \|\delta_x^2 u\|^2, \tag{5.18}$$

and

$$\|u\|_\infty \leq \frac{\sqrt{L}}{2} |\delta_x u|_1. \quad (5.19)$$

Remark 5.2. The inequality (5.18) when $L = 1$ is given in [103]. For any positive constant L , the inequality (5.18) can be derived from [2] (Theorem 12.6.1). Note that in [52–54], they also refer to [103] and use (5.18) without the term L , but this is not exactly what [103] provided since only $L = 1$ is considered in [103].

Now, we present an inequality which is a general case of Lemma 4.7 that is first constructed in [7].

Lemma 5.4. *Let $0 < \gamma < 1$ and $\sigma = 1 - \frac{\gamma}{2}$. For any sequence $\{\mathbb{G}^j\}_{j=0}^k$ ($k \geq 0$) where $\mathbb{G}^j \in \mathcal{U}_P^*$, we have the inequality*

$$\sigma \mathcal{Q}_1 + (1 - \sigma) \mathcal{Q}_2 \geq \mathcal{Q}_0, \quad (5.20)$$

where

$$\mathcal{Q}_0 = \frac{1}{2} \left[r_0 \langle \mathbb{G}^k, \mathbb{G}^k \rangle - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle \mathbb{G}^j, \mathbb{G}^j \rangle - r_{k-1} \langle \mathbb{G}^0, \mathbb{G}^0 \rangle \right],$$

$$\mathcal{Q}_1 = r_0 \langle \mathbb{G}^k, \mathbb{G}^k \rangle - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle \mathbb{G}^k, \mathbb{G}^j \rangle - r_{k-1} \langle \mathbb{G}^k, \mathbb{G}^0 \rangle,$$

$$\mathcal{Q}_2 = r_0 \langle \mathbb{G}^{k-1}, \mathbb{G}^k \rangle - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle \mathbb{G}^{k-1}, \mathbb{G}^j \rangle - r_{k-1} \langle \mathbb{G}^{k-1}, \mathbb{G}^0 \rangle$$

and r_j 's are given in (2.22).

Proof. Note that the operator $\langle \cdot, \cdot \rangle$ is symmetrical. By writing $r_0 = \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) + r_{k-1}$, we get by direct computation,

$$\mathcal{Q}_1 - \mathcal{Q}_0 = \frac{1}{2} \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle \mathbb{G}^k - \mathbb{G}^j, \mathbb{G}^k - \mathbb{G}^j \rangle + \frac{r_{k-1}}{2} \langle \mathbb{G}^k - \mathbb{G}^0, \mathbb{G}^k - \mathbb{G}^0 \rangle.$$

Next, we find

$$\begin{aligned}
\mathcal{Q}_2 - \mathcal{Q}_0 &= r_0 \langle \mathbb{G}^j, \mathbb{G}^k \rangle - \frac{r_0}{2} \langle \mathbb{G}^k, \mathbb{G}^k \rangle - \frac{r_0}{2} \langle \mathbb{G}^j, \mathbb{G}^j \rangle + \frac{r_{k-1}}{2} \langle \mathbb{G}^{k-1} - \mathbb{G}^0, \mathbb{G}^{k-1} - \mathbb{G}^0 \rangle \\
&\quad + \frac{1}{2} \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle \mathbb{G}^{k-1} - \mathbb{G}^j, \mathbb{G}^{k-1} - \mathbb{G}^j \rangle \\
&= -\frac{r_0}{2} \langle \mathbb{G}^k - \mathbb{G}^j, \mathbb{G}^k - \mathbb{G}^j \rangle + \frac{r_{k-1}}{2} \langle \mathbb{G}^{k-1} - \mathbb{G}^0, \mathbb{G}^{k-1} - \mathbb{G}^0 \rangle \\
&\quad + \frac{1}{2} \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle \mathbb{G}^{k-1} - \mathbb{G}^j, \mathbb{G}^{k-1} - \mathbb{G}^j \rangle.
\end{aligned}$$

Therefore, for $k = 1$, it is obvious that

$$\sigma \mathcal{Q}_1 + (1-\sigma) \mathcal{Q}_2 - \mathcal{Q}_0 = \sigma(\mathcal{Q}_1 - \mathcal{Q}_0) + (1-\sigma)(\mathcal{Q}_2 - \mathcal{Q}_0) = \frac{r_0}{2} (2\sigma - 1) \langle \mathbb{G}^1 - \mathbb{G}^0, \mathbb{G}^1 - \mathbb{G}^0 \rangle \geq 0$$

since $r_0 = a_0 = \sigma^{1-\gamma} > 0$.

For $k \geq 2$, noting the properties of r_j 's (4.50), we find

$$\begin{aligned}
\sigma \mathcal{Q}_1 + (1-\sigma) \mathcal{Q}_2 - \mathcal{Q}_0 &= \sigma(\mathcal{Q}_1 - \mathcal{Q}_0) + (1-\sigma)(\mathcal{Q}_2 - \mathcal{Q}_0) \\
&\geq \left[\sigma \frac{(r_0 - r_1)}{2} - (1-\sigma) \frac{r_0}{2} \right] \langle \mathbb{G}^k - \mathbb{G}^j, \mathbb{G}^k - \mathbb{G}^j \rangle \\
&= \frac{(2\sigma - 1)r_0 - \sigma r_1}{2} \langle \mathbb{G}^k - \mathbb{G}^j, \mathbb{G}^k - \mathbb{G}^j \rangle \geq 0
\end{aligned}$$

where the last inequality follows from (5.14). Hence, (5.20) holds for any integer $k \geq 1$. $\square$

With the above lemmas, we are now ready to show that the parametric quintic spline scheme (5.9) depends continuously on the initial condition and the non-linear term. Let v_m^k be the solution of the following problem:

$$\begin{cases} \bar{\mu} \mathcal{H} \left[r_0 v_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) v_m^j - r_{k-1} v_m^0 \right] + \delta_x^4 v_m^{k-1+\sigma} = \frac{\mathcal{H} \bar{f}_m^{k-1+\sigma}}{d}, \\ v_m^0 = \psi(x_m) - \theta_m, \\ v_0^k = \phi_1(t_k), \quad v_M^k = \phi_2(t_k), \quad \delta_x^2 v_0^k = \phi_3(t_k), \quad \delta_x^2 v_M^k = \phi_4(t_k), \end{cases} \quad (5.21)$$

where $\theta_0 = \theta_M = 0$.

Let $\epsilon_m^k = u_m^k - v_m^k$, $0 \leq m \leq M$, $0 \leq k \leq K$. Obviously, ϵ_m^k satisfies

$$\begin{cases} \bar{\mu} \mathcal{H} \left[r_0 \epsilon_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \epsilon_m^j - r_{k-1} \epsilon_m^0 \right] + \delta_x^4 \epsilon_m^{k-1+\sigma} = \frac{\mathcal{H} \hat{f}_m^{k-1+\sigma}}{d}, \\ \epsilon_m^0 = \theta_m, \quad \epsilon_0^k = \epsilon_M^k = \delta_x^2 \epsilon_0^k = \delta_x^2 \epsilon_M^k = 0, \end{cases} \quad (5.22)$$

where $\hat{f}_m^{k-1+\sigma} = f_m^{k-1+\sigma} - \bar{f}_m^{k-1+\sigma}$. It is clear that $\epsilon^k \in \mathcal{U}_P^*$, $0 \leq k \leq K$.

The next theorem establishes the stability of the parametric quintic spline scheme with respect to the initial condition and the non-linear term. To simplify the proof, for $u, v \in \mathcal{U}_P^*$, we note that by direct calculation we have

$$(a) \quad \mathcal{H}u_m = \begin{cases} u_m + \frac{h^2}{6} \delta_x^2 u_m + \frac{h^4}{360} \delta_x^4 u_m, & m = 1, M-1 \\ u_m + \frac{h^2}{6} \delta_x^2 u_m - \frac{h^4}{720} \delta_x^4 u_m, & 2 \leq m \leq M-2 \end{cases} \quad (5.23)$$

(b)

$$(u, \delta_x^4 v) = (\delta_x^2 u, \delta_x^2 v) \quad (\delta_x^2 u, \delta_x^4 v) = - \sum_{m=0}^{M-1} \left(\delta_x^3 u_{m+\frac{1}{2}} \right) \left(\delta_x^3 v_{m+\frac{1}{2}} \right). \quad (5.24)$$

(c) Using (5.23) and (5.24), we find

$$\begin{aligned} (\delta_x^4 v, \mathcal{H}u) &= (\delta_x^4 v, u) + \frac{h^2}{6} (\delta_x^4 v, \delta_x^2 u) - h^4 \eta (\delta_x^4 v, \delta_x^4 u) \\ &= (\delta_x^2 v, \delta_x^2 u) - \frac{h^2}{6} (\delta_x^3 v, \delta_x^3 u)_1 - h^4 \eta (\delta_x^4 v, \delta_x^4 u) \\ &= \langle u, v \rangle. \end{aligned} \quad (5.25)$$

Theorem 5.1. (Stability) Let $\epsilon^k \in \mathcal{U}_P^*$, $0 \leq k \leq K$ satisfy (5.22). Then,

$$\|\epsilon^k\|_\infty^2 \leq c \left[\langle \epsilon^0, \epsilon^0 \rangle + \frac{\Gamma(1-\gamma)T^\gamma}{d} \max_{1 \leq k \leq K} \|\mathcal{H} \hat{f}^{k-1+\sigma}\|^2 \right], \quad 1 \leq k \leq K \quad (5.26)$$

where $c = \frac{45}{224} L^3$.

Proof. First, we multiply both sides of (5.22) by $h\delta_x^4\epsilon_m^{k-1+\sigma}$ and sum m from 1 to $(M-1)$, giving

$$\begin{aligned} & \bar{\mu} \left(\delta_x^4 \epsilon^{k-1+\sigma}, r_0 \mathcal{H} \epsilon^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \mathcal{H} \epsilon^j - r_{k-1} \mathcal{H} \epsilon^0 \right) + \|\delta_x^4 \epsilon^{k-1+\sigma}\|^2 \\ &= \frac{1}{d} \left(\delta_x^4 \epsilon^{k-1+\sigma}, \mathcal{H} \hat{f}^{k-1+\sigma} \right). \end{aligned} \quad (5.27)$$

Noting $\epsilon^k, \epsilon^{k-1+\sigma} \in \mathcal{U}_P^*$ and (5.25), (5.27) can be rewritten as

$$\begin{aligned} & \bar{\mu} \left[r_0 \langle \epsilon^{k-1+\sigma}, \epsilon^k \rangle - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle \epsilon^{k-1+\sigma}, \epsilon^j \rangle - r_{k-1} \langle \epsilon^{k-1+\sigma}, \epsilon^0 \rangle \right] \\ &= \frac{1}{d} (\delta_x^4 \epsilon^{k-1+\sigma}, \mathcal{H} \hat{f}^{k-1+\sigma}) - \|\delta_x^4 \epsilon^{k-1+\sigma}\|^2. \end{aligned} \quad (5.28)$$

Considering the the left side of (5.28), it is easily seen by Lemma 5.4 that

$$\begin{aligned} & \bar{\mu} \left[r_0 \langle \epsilon^{k-1+\sigma}, \epsilon^k \rangle - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle \epsilon^{k-1+\sigma}, \epsilon^j \rangle - r_{k-1} \langle \epsilon^{k-1+\sigma}, \epsilon^0 \rangle \right] \\ & \geq \frac{\mu}{2} \left[r_0 \langle \epsilon^k, \epsilon^k \rangle - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle \epsilon^j, \epsilon^j \rangle - r_{k-1} \langle \epsilon^0, \epsilon^0 \rangle \right]. \end{aligned} \quad (5.29)$$

On the other hand, by Young's inequality, we get

$$\frac{1}{d} (\delta_x^4 \epsilon^{k-1+\sigma}, \mathcal{H} \hat{f}^{k-1+\sigma}) \leq \frac{1}{d} \left[\varepsilon \|\delta_x^4 \epsilon^{k-1+\sigma}\|^2 + \frac{1}{4\varepsilon} \|\mathcal{H} \hat{f}^{k-1+\sigma}\|^2 \right] \quad (5.30)$$

where ε is any positive number. Now, employing (5.29) and (5.30)| $_{\varepsilon=d}$ in (5.28), we obtain

$$\begin{aligned} & \frac{\mu}{2} \left[r_0 \langle \epsilon^k, \epsilon^k \rangle - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle \epsilon^j, \epsilon^j \rangle - r_{k-1} \langle \epsilon^0, \epsilon^0 \rangle \right] + \|\delta_x^4 \epsilon^{k-1+\sigma}\|^2 \\ & \leq \frac{1}{d} \left[d \|\delta_x^4 \epsilon^{k-1+\sigma}\|^2 + \frac{1}{4d} \|\mathcal{H} \hat{f}^{k-1+\sigma}\|^2 \right], \end{aligned}$$

or equivalently

$$r_0 \langle \epsilon^k, \epsilon^k \rangle - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle \epsilon^j, \epsilon^j \rangle - r_{k-1} \langle \epsilon^0, \epsilon^0 \rangle \leq \frac{\Gamma(2-\gamma)\tau^\gamma}{2d} \|\mathcal{H}\hat{f}^{k-1+\sigma}\|^2. \quad (5.31)$$

From Lemma 4.6, we know that $r_{k-1} > \frac{1-\gamma}{2(k-1+\sigma)^\gamma}$ is true for any fixed $k \geq 2$. Note that this is also correct for $k = 1$, since $r_0 = \sigma^{1-\gamma} = \frac{\sigma}{\sigma^\gamma} > \frac{1-\gamma}{2\sigma^\gamma}$. Hence,

$$r_{k-1} > \frac{1-\gamma}{2(k-1+\sigma)^\gamma}, \quad k \geq 1.$$

Using the above inequality and $(k-1+\sigma)\tau \leq T$, we get $\frac{\Gamma(2-\gamma)\tau^\gamma}{2r_{k-1}} \leq \Gamma(1-\gamma)T^\gamma$. Then from (5.31) we find

$$\begin{aligned} r_0 \langle \epsilon^k, \epsilon^k \rangle &\leq \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle \epsilon^j, \epsilon^j \rangle + r_{k-1} \left[\langle \epsilon^0, \epsilon^0 \rangle + \frac{\Gamma(2-\gamma)\tau^\gamma}{2dr_{k-1}} \|\mathcal{H}\hat{f}^{k-1+\sigma}\|^2 \right] \\ &\leq \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle \epsilon^j, \epsilon^j \rangle + r_{k-1} E \end{aligned} \quad (5.32)$$

where

$$E = \langle \epsilon^0, \epsilon^0 \rangle + \frac{\Gamma(1-\gamma)T^\gamma}{d} \max_{1 \leq k \leq K} \|\mathcal{H}\hat{f}^{k-1+\sigma}\|^2.$$

Next, by mathematical induction, we can prove as in Theorem 4.1 of Chapter 4 that

$$\langle \epsilon^k, \epsilon^k \rangle \leq E, \quad 1 \leq k \leq K. \quad (5.33)$$

Now, since $\epsilon^k \in \mathcal{U}_P^*$, from Lemmas 5.2 and 5.3, we obtain

$$\langle \epsilon^k, \epsilon^k \rangle \geq \frac{14}{45} \|\delta_x^2 \epsilon^k\|^2 \quad (5.34)$$

and

$$\|\delta_x^2 \epsilon^k\|^2 \geq \left(\frac{2 \sin \frac{\pi h}{2L}}{h} \right)^2 |\delta_x \epsilon^k|_1^2 \geq \left(\frac{2 \sin \frac{\pi h}{2L}}{h} \right)^2 \frac{4}{L} \|\epsilon^k\|_\infty^2. \quad (5.35)$$

Note that the function $\frac{\sin x}{x}$ is decreasing on $[0, \frac{\pi}{2}]$. For $0 < h < L$, we have $0 < \frac{\pi h}{2L} < \frac{\pi}{2}$ and so

$$\frac{2 \sin \frac{\pi h}{2L}}{h} = \frac{\pi}{L} \cdot \frac{\sin \frac{\pi h}{2L}}{\frac{\pi h}{2L}} \geq \frac{\pi}{L} \cdot \frac{\sin \frac{\pi}{2}}{\frac{\pi}{2}} = \frac{2}{L}.$$

Using the above inequality in (5.35) yields

$$\|\delta_x^2 \epsilon^k\|^2 \geq \left(\frac{2 \sin \frac{\pi h}{2L}}{h} \right)^2 \frac{4}{L} \|\epsilon^k\|_\infty^2 \geq \left(\frac{4}{L^2} \right) \frac{4}{L} \|\epsilon^k\|_\infty^2 = \frac{16}{L^3} \|\epsilon^k\|_\infty^2. \quad (5.36)$$

Finally, combining (5.34) and (5.36), it follows from (5.33) that

$$E \geq \langle \epsilon^k, \epsilon^k \rangle \geq \frac{14}{45} \|\delta_x^2 \epsilon^k\|^2 \geq \frac{224}{45L^3} \|\epsilon^k\|_\infty^2 \quad (5.37)$$

which is exactly (5.26). $\square$

From the bound established in Theorem 5.1, we see that the parametric quintic spline scheme is stable with respect to the initial condition and the non-linear term. Next, we shall prove that the parametric quintic spline scheme has a unique solution and thereafter establish the convergence of the scheme in maximum norm.

Theorem 5.2. (Solvability) *The parametric quintic spline scheme (5.9) is uniquely solvable.*

Proof. The scheme (5.9) is a system of linear equations and so to prove that the system is uniquely solvable, it is sufficient to show that the corresponding homogeneous system has only the trivial solution. Consider the homogeneous system

$$\begin{cases} \bar{\mu} \mathcal{H} \left[r_0 u_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) u_m^j - r_{k-1} u_m^0 \right] + \delta_x^4 u_m^{k-1+\sigma} = 0 \\ u_m^0 = 0, \quad u_0^k = u_M^k = \delta_x^2 u_0^k = \delta_x^2 u_M^k = 0. \end{cases} \quad (5.38)$$

Clearly, any solution u^k of (5.38) satisfies $u^k \in \mathcal{U}_P^*$, $0 \leq k \leq K$. Similar to the proof of Theorem 5.1, we are able to get the analog of (5.26) (with ϵ^k replaced by u^k and $\hat{f}^{k-1+\sigma} \equiv 0$) as

$$\|u^k\|_\infty^2 = 0, \quad 1 \leq k \leq K \quad (5.39)$$

since $\mathcal{H}(0) = 0$ and $u_m^0 = 0$, $0 \leq m \leq M$. Hence, it follows from (5.39) that $u_m^k = 0$ for $1 \leq m \leq M$, $1 \leq k \leq K$, i.e., (5.38) has only the trivial solution for each time level. This shows that (5.9) is uniquely solvable. $\square$

We shall now investigate the convergence of the parametric quintic spline scheme. Let u_m^k denote the numerical solution of (5.1) at (x_m, t_n) obtained from the parametric quintic spline scheme (5.9), and let U_m^k be the corresponding exact solution. Let $e_m^k = U_m^k - u_m^k$ be the error at (x_m, t_n) .

Theorem 5.3. (Convergence) Let $u(x, t) \in \mathcal{C}^{8,3}([0, L] \times [0, T])$. Then, we have

$$\|e^k\|_\infty \leq O(h^{4.5} + \tau^2), \quad 1 \leq k \leq K. \quad (5.40)$$

Proof. The exact solution U_m^k satisfies

$$\begin{cases} \bar{\mu}\mathcal{H} \left[r_0 U_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) U_m^j - r_{k-1} U_m^0 \right] + \delta_x^4 U_m^{k-1+\sigma} = \frac{\mathcal{H} f_m^{k-1+\sigma}}{d} + T_m^k \\ U_m^0 = \psi(x_m), \\ U_m^k = \phi_1(t_n), \quad U_M^k = \phi_2(t_n), \quad \delta_x^2 U_m^k = \phi_3(t_n), \quad \delta_x^2 U_M^k = \phi_4(t_n). \end{cases} \quad (5.41)$$

Since $e_m^k = U_m^k - u_m^k$, it follows from (5.9) and (5.41) that

$$\begin{cases} \bar{\mu}\mathcal{H} \left[r_0 e_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) e_m^j - r_{k-1} e_m^0 \right] + \delta_x^4 e_m^{k-1+\sigma} = T_m^k, \\ e_m^0 = 0, \quad e_0^k = e_M^k = \delta_x^2 e_0^k = \delta_x^2 e_M^k = 0. \end{cases} \quad (5.42)$$

Clearly, $e^k \in \mathcal{U}_P^*$, $0 \leq k \leq K$. Moreover, we observe that (5.42) is the same as (5.22) if ϵ_m^k , θ_m and $\frac{1}{d} H \hat{f}_m^{k-1+\sigma}$ are replaced by e_m^k , 0 and T_m^k respectively. Therefore, following the steps as in (5.27)–(5.31), we are able to get the analog of

(5.32) as follows

$$\begin{aligned} r_0 \langle e^k, e^k \rangle &\leq \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle e^j, e^j \rangle + r_{k-1} \left[\langle e^0, e^0 \rangle + \frac{\Gamma(2-\gamma)\tau^\gamma}{2dr_{k-1}} \|dT^k\|^2 \right] \\ &= \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \langle e^j, e^j \rangle + r_{k-1} d\Gamma(1-\gamma)T^\gamma \max_{1 \leq k \leq K} \|T^k\|^2 \end{aligned}$$

since $e_m^0 = 0$, $0 \leq m \leq M$.

Proceeding as in the proof of Theorem 5.1, we can obtain the analogue of (5.33) as

$$\langle e^k, e^k \rangle \leq d\Gamma(1-\gamma)T^\gamma \max_{1 \leq k \leq K} \|T^k\|^2, \quad 1 \leq k \leq K. \quad (5.43)$$

Then, from Lemmas 5.2 and 5.3, the analog of (5.37) is found to be

$$\langle e^k, e^k \rangle \geq \frac{14}{45} \|\delta_x^2 e^k\|^2 \geq \frac{224}{45L^3} \|e^k\|_\infty^2. \quad (5.44)$$

Next, noting (5.10) and the fact $(M-3)h \leq Mh = L$, we get

$$\begin{aligned} \|T^k\|^2 &= h \sum_{m=1}^{M-1} (T_m^k)^2 \leq 2hC_1^2(h^4 + \tau^2)^2 + (M-3)hC_2^2(h^6 + \tau^2)^2 \\ &\leq 2hC_1^2(h^4 + \tau^2)^2 + LC_2^2(h^6 + \tau^2)^2 \leq C(h^{4.5} + \tau^2)^2 \end{aligned} \quad (5.45)$$

where C_1 , C_2 and C are some positive constants, and C does not depend on h or k . Hence, using (5.45) in (5.44) gives for $1 \leq k \leq K$ that

$$\|e^k\|_\infty^2 \leq \frac{45L^3}{224} d\Gamma(1-\gamma)T^\gamma \max_{1 \leq k \leq K} \|T^k\|^2 \leq \frac{45L^3}{224} d\Gamma(1-\gamma)T^\gamma C(h^{4.5} + \tau^2)^2$$

which yields (5.40). □

Remark 5.3.

- (a) From the error inequality (5.40) in Theorem 5.3, we can conclude that the *PQS scheme* (5.9) achieves convergence of $O(h^{4.5} + \tau^2)$. In comparison, the *FD method* applied to the same problem (5.1) in [53] achieves $O(h^2 + \tau^{2-\gamma})$, while the *quintic spline method* in [120] gives $O(h^4 + \tau^{2-\gamma})$; moreover the *CFD*

scheme administered to a different sub-diffusion problem in [122] achieves $O(h^4 + \tau^{2-\gamma})$. Note that $O(h^4)$ has been the *best* spatial convergence until the present work. The numerical experiments in the next section will further demonstrate the outperformance of the parametric quintic spline scheme.

- (b) In our earlier paper [78] we have considered a *different* fractional sub-diffusion problem – it involves a *second-order* space derivative u_{xx} instead of the fourth-order space derivative in the current work. By using a *different* parametric quintic spline operator with *different* properties from $\mathcal{H}$, we have derived a scheme in [78] that is better than other finite difference type methods for the second-order fractional sub-diffusion problem. The stability of that scheme is, however, not unconditional as in the current work.

Remark 5.4. The spatial convergence order of $O(h^{4.5})$ is *theoretically* derived in Theorem 5.3. In practice, a higher spatial convergence order is possible – in fact this is illustrated by the numerical experiments in Section 5.3. To have a better understanding, one can refer to Remark 3.2(c) in Chapter 3.

Remark 5.5. In some engineering problems, the solution may not be smooth in the temporal dimension and it may have a weak singularity at the initial time $t = 0$. There are some excellent papers on this non-smooth solution issue, see [60, 61, 132]. In fact, if we do not use $L2 - 1_\sigma$ formula (Lemma 2.4) for the Caputo fractional derivative, we can employ one of the techniques in [60, 61, 132] and still use the parametric quintic spline method which is our main contribution. This will then relax the continuity condition in the temporal dimension. However, in this scheme we employ the $L2 - 1_\sigma$ method in the temporal dimension for several reasons:

- It is a high order method ($O(\tau^2)$) when the solution is smooth on the closed domain;
- The numerical scheme (5.9) can still be performed even if the solution has a weak singularity at $t = 0$, just that we will observe order reduction (illustrated in Example 5.4). Most importantly, we can still observe the improvement in the spatial convergence order, which is our main contribution.

5.3 Experiment

In this section, we shall present four numerical examples to verify the efficiency of the PQS scheme (5.9), and also to compare the performance with CFD method, quintic B-spline collocation (BC) method [115] and quintic spline (QS) method [120]. The numerical calculation is performed using a computer with Intel(R) Core(TM) i7-4770 CPU @ 3.40GHz processor and 8GB RAM, and 64-bit Windows 7 Enterprise operating system.

Example 5.1. [53, 145] Consider the following fourth-order fractional sub-diffusion problem ($x \in (0, 1)$, $t \in (0, 1]$)

$$\begin{cases} {}^C_0 D_t^\gamma u(x, t) + u_{xxxx} = e^x \left[\frac{\Gamma(\gamma + 4)}{6} t^3 + t^{3+\gamma} \right], \\ u(x, 0) = 0, \\ u(0, t) = t^{3+\gamma}, \quad u(1, t) = e t^{3+\gamma}, \quad \frac{\partial^2 u(0, t)}{\partial x^2} = t^{3+\gamma}, \quad \frac{\partial^2 u(1, t)}{\partial x^2} = e t^{3+\gamma}. \end{cases} \quad (5.46)$$

The exact solution of (5.46) is given as $u(x, t) = e^x t^{3+\gamma}$.

First, to observe the spatial convergence of PQS method, we fix the temporal step size $\tau = \frac{1}{200000}$ and let the spatial step size h vary. The maximum absolute errors at $t = t_K = 1$, $\|e^K(\tau, h)\|_\infty$ (see (3.57) in Chapter 3), and the convergence orders are displayed in Table 5.1. From Table 5.1, it is observed that the spatial convergence order of the PQS scheme is above 4.5 – the *theoretical* order obtained in Theorem 5.3. As elaborated in Remark 5.4, a higher spatial convergence order is possible in practice for h that is not that small, and this is illustrated in this example.

TABLE 5.1: (Example 5.1) $\|e^K(\tau, h)\|_\infty$ and spatial convergence order of PQS method

τ	h	$\gamma = 0.1$	$\mathcal{O}_{\infty, x}$	$\gamma = 0.5$	$\mathcal{O}_{\infty, x}$	$\gamma = 0.9$	$\mathcal{O}_{\infty, x}$
$\frac{1}{200000}$	$\frac{1}{5}$	5.2837E-08	-	5.2410E-08	-	5.1615E-08	-
	$\frac{1}{10}$	8.7072E-10	5.9232	8.6680E-10	5.9180	8.5622E-10	5.9137
	$\frac{1}{20}$	1.4721E-11	5.8870	1.8847E-11	5.5233	2.0668E-11	5.3725

Next, to observe the temporal convergence of PQS method, we fix $h = \frac{1}{100}$ and let τ vary. The maximum absolute errors $\|e^K(\tau, h)\|_\infty$ and the temporal convergence

orders, namely,

$$\mathcal{O}_{\infty,t} = \log_2 \frac{\|e^K(\tau, h)\|_{\infty}}{\|e^K(\frac{\tau}{2}, h)\|_{\infty}}, \quad (5.47)$$

are presented in Table 5.2. Clearly, the simulation results verify that the temporal convergence order of the PQS scheme is 2 – same as the theoretical result given in Theorem 5.3.

TABLE 5.2: (Example 5.1) $\|e^K(\tau, h)\|_{\infty}$ and temporal convergence order of PQS method

h	τ	$\gamma = 0.1$	$\mathcal{O}_{\infty,t}$	$\gamma = 0.5$	$\mathcal{O}_{\infty,t}$	$\gamma = 0.9$	$\mathcal{O}_{\infty,t}$
$\frac{1}{100}$	$\frac{1}{10}$	3.1131E-04	-	1.6414E-03	-	2.7341E-03	-
	$\frac{1}{20}$	7.9341E-05	1.9722	4.1754E-04	1.9749	6.8917E-04	1.9882
	$\frac{1}{40}$	2.0034E-05	1.9856	1.0541E-04	1.9858	1.7316E-04	1.9928

Then for visualization, the graphs of the numerical solution, exact solution and absolute error for the case $\gamma = 0.1$, $h = \frac{1}{20}$, $\tau = \frac{1}{200000}$ are provided in Figures 5.1 and 5.2.

FIGURE 5.1: (Example 5.1) Approximate and exact solutions when $\gamma = 0.1$, $h = \frac{1}{20}$, $\tau = \frac{1}{200000}$

Finally, we shall compare the performance of PQS and CFD methods, which have *theoretical* spatial convergence orders of $O(h^{4.5})$ and $O(h^4)$ respectively. To have proper comparison, we shall solve (5.46) using $L2 - 1_{\sigma}$ formula (Lemma 2.4) to approximate the Caputo fractional derivative, while employing one of the two methods (PQS, CFD) in the spatial dimension. Here, we fix $\tau = \frac{1}{200000}$ and let h vary. Table 5.3 gives the maximum absolute errors $\|e^K(\tau, h)\|_{\infty}$, the convergence orders and the computation times (in minutes). Clearly, the simulation results indicate that PQS method not only *outperforms* in terms of convergence, but also achieves

FIGURE 5.2: (Example 5.1) Absolute error when $\gamma = 0.1$, $h = \frac{1}{20}$, $\tau = \frac{1}{200000}$

the *smallest* absolute error in all cases with no significant increase of the computation time compared to CFD methods.

TABLE 5.3: (Example 5.1) Comparison of PQS and CFD methods (time is in minutes)

γ	h	PQS	$\mathcal{O}_{\infty,x}$	time	CFD	$\mathcal{O}_{\infty,x}$	time
0.3	$\frac{1}{5}$	5.266E-08	-	88.4	8.200E-08	-	90.2
	$\frac{1}{10}$	8.693E-10	5.9206	94.6	3.597E-09	4.5107	95.0
	$\frac{1}{20}$	1.787E-11	5.6047	107.6	2.004E-10	4.1660	107.8
0.6	$\frac{1}{5}$	5.226E-08	-	89.8	8.137E-08	-	88.5
	$\frac{1}{10}$	8.650E-10	5.9167	96.3	3.572E-09	4.5098	95.4
	$\frac{1}{20}$	2.152E-11	5.3292	109.0	2.014E-10	4.1484	109.9
0.9	$\frac{1}{5}$	5.162E-08	-	89.0	8.038E-08	-	88.2
	$\frac{1}{10}$	8.562E-10	5.9137	95.0	3.530E-09	4.5093	94.4
	$\frac{1}{20}$	2.067E-11	5.3725	108.0	2.005E-10	4.1376	107.1

The next two examples have been considered in [115, 120], where quintic B-spline collocation (BC) and quintic spline (QS) methods are respectively applied in the spatial dimension, while $L1$ discretization is used to approximate the fractional derivative. Hence, for proper comparison with BC and QS methods, we shall employ *PQS method with $L1$ discretization* (PQS- $L1$), in addition to the original PQS method with $L2 - 1_\sigma$ approximation.

Example 5.2. [115, 120] Consider the following fourth-order fractional sub-diffusion problem ($x \in (0, 1)$, $t \in (0, 1]$)

$$\begin{cases} {}^C_0 D_t^\gamma u(x, t) + 0.05 u_{xxxx} = \left[\frac{t^{1-\gamma}}{\Gamma(2-\gamma)} + 0.05\pi^4(t+1) \right] \sin(\pi x), \\ u(x, 0) = 0, \quad u(0, t) = u(1, t) = 0, \quad \frac{\partial^2 u(0, t)}{\partial x^2} = \frac{\partial^2 u(1, t)}{\partial x^2} = 0. \end{cases} \quad (5.48)$$

The exact solution of (5.48) is given as $u(x, t) = (t+1) \sin(\pi x)$.

In this example, we fix $\tau = \frac{1}{100000}$ and $h = \frac{1}{40}$. The maximum absolute errors $\|e^k(\tau, h)\|_\infty$ at various $t = t_k$ are obtained by different methods (PQS, PQS–L1, QS, BC) and presented in Table 5.4. As one can observe, our methods – PQS (with $L2 - 1_\sigma$ approximation) as well as PQS–L1 (with $L1$ discretization) give the *best* results compared to QS and BC methods [115, 120] in all cases.

TABLE 5.4: (Example 5.2) $\|e^K(\tau, h)\|_\infty$ of PQS, PQS–L1, QS and BC methods

γ	k	PQS	PQS–L1	QS [120]	BC [115]
0.5	500	4.5633E-11	4.9374E-11	1.4312E-04	2.3241E-04
	1000	5.9448E-11	6.4284E-11	1.8609E-04	2.8285E-04
	1500	6.8472E-11	7.4006E-11	2.1423E-04	3.1247E-04
1	500	5.3671E-12	5.1544E-12	2.4260E-06	1.2161E-05
	1000	8.0694E-12	7.5583E-12	1.4590E-05	2.4091E-05
	1500	1.0783E-11	9.9174E-12	2.6524E-05	3.5796E-05

Example 5.3. [120] Consider the following fourth-order fractional sub-diffusion problem ($x \in (0, 1)$, $t \in (0, 1]$)

$$\begin{cases} {}^C_0 D_t^\gamma u(x, t) + 0.05 u_{xxxx} = \left[\frac{t^{1-\gamma}}{\Gamma(2-\gamma)} + 0.05\pi^4 t \right] \sin(\pi x), \\ u(x, 0) = 0, \quad u(0, t) = u(1, t) = \frac{\partial^2 u(0, t)}{\partial x^2} = \frac{\partial^2 u(1, t)}{\partial x^2} = 0. \end{cases} \quad (5.49)$$

The exact solution of (5.49) is given as $u(x, t) = t \sin(\pi x)$.

Here, we consider $\gamma = 0.5$ and let h vary. To have proper comparison, we shall take $\tau = h^4$ as in [120], and apply both PQS and PQS–L1 methods (note that $L1$ discretization is used in [120]). Table 5.5 presents the maximum absolute errors

at $t = t_K = 1$, $\|e^K(\tau, h)\|_\infty$, and the convergence orders. As seen from the table, PQS and PQS–L1 methods give the *best* results compared to QS method [120] in all cases. Further, the numerical convergence order is much better than the theoretical $O(h^{4.5})$. As stated in Remark 5.4, this phenomenon can happen for particular problems in practice.

TABLE 5.5: (Example 5.3) Comparison of PQS, PQS–L1 and QS methods

γ	h	PQS	$\mathcal{O}_{\infty,x}$	PQS–L1	$\mathcal{O}_{\infty,x}$	QS [120]	$\mathcal{O}_{\infty,x}$
0.5	$\frac{1}{6}$	4.6075E-05	-	4.6075E-05	-	2.0201E-03	-
	$\frac{1}{12}$	4.2491E-07	6.7607	4.2491E-07	6.7607	1.3888E-04	3.8625
	$\frac{1}{24}$	4.0338E-09	6.7189	4.0334E-09	6.7190	9.0745E-06	3.9359

In the next example, we shall illustrate the efficiency of PQS scheme (5.9) when the solution has a *weak singularity* at $t = 0$.

Example 5.4. Consider the following fourth-order fractional sub-diffusion problem ($x \in (0, \pi)$, $t \in (0, 1)$)

$$\begin{cases} {}^C_0 D_t^\gamma u(x, t) + u_{xxxx} = 0, \\ u(x, 0) = \sin(x), \\ u(0, t) = u(\pi, t) = \frac{\partial^2 u(0, t)}{\partial x^2} = \frac{\partial^2 u(\pi, t)}{\partial x^2} = 0. \end{cases} \quad (5.50)$$

Using the method in [4], the exact solution of (5.50) is given as

$$u(x, t) = \sin(x) E_\gamma(-t^\gamma),$$

where $E_\gamma(\cdot)$ is the Mittag-Leffler function.

In this example, the solution $u(x, t)$ has a *weak singularity* at $t = 0$ which is possible in engineering problems, as observed in [60, 61, 132] and the references cited therein. Here, even though the condition in Lemma 2.4 is not satisfied anymore, we can still perform the PQS scheme (5.9) since the scheme only involves function values and it does not require any regularity of the exact solution itself. Further, to compute the exact solution at grid points, we refer to [112] to evaluate the Mittag-Leffler function.

In Table 5.6, we fix $h = \frac{\pi}{1000}$ and present the maximum absolute errors at $t = 0.1$ as well as the temporal convergence orders. We observe severe temporal order reduction due to the weak singularity of the solution at $t = 0$.

TABLE 5.6: (Example 5.4) Temporal convergence order of PQS method when singularity exists

τ	$\gamma = 0.3$	$\mathcal{O}_{\infty,t}$	$\gamma = 0.6$	$\mathcal{O}_{\infty,t}$	$\gamma = 0.9$	$\mathcal{O}_{\infty,t}$
$\frac{0.1}{10}$	2.0169E-03	-	1.7419E-03	-	3.6065E-04	-
$\frac{0.1}{20}$	1.0054E-03	1.0043	8.7244E-04	0.9975	1.8106E-04	0.9941
$\frac{0.1}{40}$	5.0150E-04	1.0035	4.3733E-04	0.9963	9.1242E-05	0.9887

To observe the spatial convergence, we let h vary while setting $\tau = \frac{0.1}{400000}$ for $\gamma = 0.3, 0.6$ and $\tau = \frac{0.1}{200000}$ for $\gamma = 0.9$. The maximum absolute errors at $t = 0.1$ and the spatial convergence orders are presented in Table 5.7. It is observed that the PQS scheme achieves at least $O(h^{4.5})$ which is consistent with our theoretical result even though the solution has a weak singularity at $t = 0$.

TABLE 5.7: (Example 5.4) Spatial convergence order of PQS method when singularity exists

h	$\gamma = 0.3$	$\mathcal{O}_{\infty,x}$	$\gamma = 0.6$	$\mathcal{O}_{\infty,x}$	$\gamma = 0.9$	$\mathcal{O}_{\infty,x}$
$\frac{\pi}{4}$	1.9496E-04	-	1.4851E-04	-	8.4157E-05	-
$\frac{\pi}{8}$	1.9444E-06	6.6477	1.4895E-06	6.6396	8.1766E-07	6.6854
$\frac{\pi}{16}$	6.6928E-08	4.8605	5.7302E-08	4.7001	2.5479E-08	5.0041

5.4 Summary

In this chapter, we have developed a numerical method for a fourth-order fractional sub-diffusion problem. Our method is built on deploying a parametric quintic spline scheme in the spatial dimension and a higher order non-uniform approximation for Caputo fractional derivatives. The solvability, convergence and stability in maximum norm are proved using energy method, where the definition of an appropriate inner product is vital in the analysis. It is shown that the proposed method achieves the convergence order of $O(h^{4.5} + \tau^2)$, which improves the earlier work done to date. Finally, through some numerical simulation, we confirm the theoretical accuracy

and also demonstrate the outperformance of the proposed method over finite difference, compact finite difference, quintic B-spline collocation and quintic spline methods.

Chapter 6

Fourth-order Fractional Diffusion-wave Model I

In previous chapters, we aim to construct high order accuracy methods for fractional sub-diffusion ($0 < \gamma < 1$) problems which describe a slow diffusion comparing to standard Brownian motion, see [95]. In fact, there is another kind of diffusion process called super-diffusion or diffusion-wave ($1 < \gamma < 2$) as one can observe diffusion and wave simultaneously [3, 4], which intuitively is true and interesting. In this chapter, we shall discuss the numerical treatment of a fourth-order fractional diffusion-wave problem which has also been considered in [52–54]. The problem is

$$\left\{ \begin{array}{l} {}^C_0 D_t^\gamma u(x, t) + du_{xxxx} = f(x, t), \quad x \in (0, L), \quad t \in [0, T] \\ u(x, 0) = \psi(x), \quad u_t(x, 0) = \psi_1(x), \\ u(0, t) = \phi_1(t), \quad u(L, t) = \phi_2(t), \quad u_{xx}(0, t) = \phi_3(t), \quad u_{xx}(L, t) = \phi_4(t). \end{array} \right. \quad (6.1)$$

where $1 < \gamma < 2$, $\psi_1(x)$ is a known continuous function and the rest has the same constraints as in Chapter 5.

The well-posedness of the problem (6.1) has been deeply studied in a series of works done in [8–11]. These excellent works lay a good foundation for numerical investigations. However, the numerical treatment on fourth-order fractional diffusion-wave problems is scarce and $O(h^4)$ is the *best spatial convergence* achieved in the literature, see [52–54]. Our aims are to improve the spatial convergence order to *above*

4, and to provide rigorous proof of solvability, convergence and stability of the proposed method.

In what follows, Section 6.1 presents numerical scheme using PQS operator and a well known approximation of the Caputo fractional derivative at half-points. Then, in Section 6.2, we establish the solvability, stability and convergence of the proposed scheme rigorously by energy method. To confirm the theoretical results and to demonstrate the efficiency of the proposed scheme, numerical simulations are presented in Section 6.3. Section 6.4 ends with a brief summary.

6.1 Non-polynomial Numerical Scheme

In this section, we shall derive a higher order numerical scheme for the diffusion-wave model (6.1) by employing parametric quintic spline in the spatial dimension and using $L1$ discretization with Crank-Nicolson technique [118] in the temporal dimension, i.e. Lemma 2.8.

We begin with lemmas that will be used throughout the work. The first lemma is important, especially in the convergence analysis later.

Lemma 6.1. *For fixed t , let $u(x, t) \in \mathcal{C}^8[0, L]$ and $\mathcal{H}$ be the PQS operator in (5.5). If*

$$p = -\frac{1}{720}, \quad q = \frac{31}{180}, \quad s = \frac{79}{120}, \quad (6.2)$$

then the following holds

$$\mathcal{H}u_{xxxx}(x_m, t) = \delta_x^4 u_m + O(h^r) \quad (6.3)$$

where $r = 4$ for $m = 1, M - 1$; and $r = 6$ for $2 \leq m \leq M - 2$.

Proof. Taking Taylor expansion of $Hu_{xxxx}(x_m, t)$ at $x = x_m$ readily gives (6.3). $\square$

Remark 6.1. (a) Having established Lemma 6.1, for the rest of the paper we shall take the values of p , q and s as in (6.2); (b) When $m = 1, M - 1$, we have $\delta_x^4 u_1 = [\delta_x^2 u_0 - 2\delta_x^2 u_1 + \delta_x^2 u_2]/h^2$ and $\delta_x^4 u_{M-1} = [\delta_x^2 u_M - 2\delta_x^2 u_{M-1} + \delta_x^2 u_{M-2}]/h^2$. Here, we let $\delta_x^2 u_0 = u_{xx}(x_0, t)$ and $\delta_x^2 u_M = u_{xx}(x_M, t)$, so that $\delta_x^4 u_1$ and $\delta_x^4 u_{M-1}$ are well defined.

We are now ready to develop the numerical scheme for (6.1). Suppose that the exact solution is sufficiently smooth. Discretizing (6.1) at $(x_m, t_{k-\frac{1}{2}})$ yields

$${}_0^C D_t^\gamma u(x_m, t_{k-\frac{1}{2}}) + du_{xxxx}(x_m, t_{k-\frac{1}{2}}) = f(x_m, t_{k-\frac{1}{2}}). \quad (6.4)$$

Note that

$$u_{xxxx}(x_m, t_{k-\frac{1}{2}}) = \frac{1}{2} [u_{xxxx}(x_m, t_k) + u_{xxxx}(x_m, t_{k-1})] + O(\tau^2).$$

Upon substituting the above formula into (6.4) and applying the PQS operator $\mathcal{H}$ on both sides of the equation, we get

$$\mathcal{H} \left[{}_0^C D_t^\gamma u(x_m, t_{k-\frac{1}{2}}) \right] + \frac{d}{2} \mathcal{H} [u_{xxxx}(x_m, t_k) + u_{xxxx}(x_m, t_{k-1})] = \mathcal{H} f_j^{k-\frac{1}{2}} + O(\tau^2). \quad (6.5)$$

Now, using (2.27) and (6.3) in (6.5) and then omitting the small terms, we finally achieve the following *PQS scheme*

$$\begin{cases} \tilde{\mu} \mathcal{H} \left[\tilde{a}_0 \delta_t u_m^{k-\frac{1}{2}} - \sum_{j=1}^{k-1} (\tilde{a}_{k-j-1} - \tilde{a}_{k-j}) \delta_t u_m^{j-\frac{1}{2}} - \tilde{a}_{k-1} \psi_1(x_m) \right] + d \delta_x^4 u_m^{k-\frac{1}{2}} = \mathcal{H} f_m^{k-\frac{1}{2}} \\ u_m^0 = \psi(x_m), \\ u_0^k = \phi_1(t_k), \quad u_M^k = \phi_2(t_k), \quad \delta_x^2 u_0^k = \phi_3(t_k), \quad \delta_x^2 u_M^k = \phi_4(t_k), \end{cases} \quad (6.6)$$

where $\delta_x^4 u_m^{k-\frac{1}{2}} = (\delta_x^4 u_m^k + \delta_x^4 u_m^{k-1}) / 2$, p , q and s in $\mathcal{H}$ are as in (6.2) and (5.5) and

$$\delta_t u_m^{k-\frac{1}{2}} = \frac{u_m^k - u_m^{k-1}}{\tau}. \quad (6.7)$$

We can similarly implement the PQS scheme (6.6) as in Chapter 3 to obtain the numerical solution once we have the solvability of the scheme which will be proved in next section.

6.2 Solvability, Stability and Convergence

The solvability and stability of the PQS scheme in terms of maximum norm will be analyzed in this section. Our methodology is that of energy method. To begin,

we shall present a series of lemmas which are needed in subsequent analysis.

The first lemma, which is stated in [52–54, 118], will be needed in subsequent results.

Lemma 6.2. [52–54, 118] *Let $\{G^1, G^2, \dots, G^k\}$ be a sequence, χ be a number, $\gamma \in (1, 2)$ and $\tilde{a}_j$'s be defined as in Lemma 2.8. Then, the following inequality holds*

$$\sum_{i=1}^k \left[\tilde{a}_0 G^i - \sum_{j=1}^{i-1} (\tilde{a}_{i-j-1} - \tilde{a}_{i-j}) G^j - \tilde{a}_{i-1} \chi \right] G^i \geq \frac{(2-\gamma)t_k^{1-\gamma}}{2\tau^{1-\gamma}} \sum_{i=1}^k (G^i)^2 - \frac{t_k^{2-\gamma}}{2\tau^{2-\gamma}} \chi^2 \quad (6.8)$$

where $t_k = k\tau$.

To proceed further, we shall establish an estimation of the solutions of the PQS scheme (6.6) with zero boundary conditions

$$u_0^k = u_M^k = \delta_x^2 u_0^k = \delta_x^2 u_M^k = 0, \quad 0 \leq k \leq K. \quad (6.9)$$

Lemma 6.3. *Let u^k satisfy (6.6) with (6.9). Then, for $1 \leq k \leq K$,*

$$\langle u^k, u^k \rangle \leq \langle u^0, u^0 \rangle + \frac{t_k^{2-\gamma}}{d\Gamma(3-\gamma)} \|\mathcal{H}\psi_1\|^2 + \frac{\Gamma(2-\gamma)t_k^{\gamma-1}\tau}{d} \sum_{i=1}^k \|\mathcal{H}f^{i-\frac{1}{2}}\|^2, \quad (6.10)$$

where $t_k = k\tau$.

Proof. In view of (6.9), it is clear that the numerical solution $u^i \in \mathcal{U}_P^*$, $0 \leq i \leq N$. To begin, we multiply both sides of (6.6) $|_{k=i}$ by $h\tau\mathcal{H}\delta_t u_m^{i-\frac{1}{2}}$ and then sum, giving

$$\begin{aligned} & \tilde{\mu}\tau \sum_{i=1}^k \left(\mathcal{H}\delta_t u^{i-\frac{1}{2}}, a_0 \mathcal{H}\delta_t u^{i-\frac{1}{2}} - \sum_{j=1}^{i-1} (\tilde{a}_{i-j-1} - \tilde{a}_{i-j}) \mathcal{H}\delta_t u^{j-\frac{1}{2}} - a_{i-1} \mathcal{H}\psi_1 \right) \\ &= -d\tau \sum_{i=1}^k \left(\mathcal{H}\delta_t u^{i-\frac{1}{2}}, \delta_x^4 u^{i-\frac{1}{2}} \right) + \tau \sum_{i=1}^k \left(\mathcal{H}\delta_t u^{i-\frac{1}{2}}, \mathcal{H}f^{i-\frac{1}{2}} \right). \end{aligned} \quad (6.11)$$

We shall estimate the various terms in (6.11). To proceed, Lemma 6.2 is first applied to each element to get

$$\begin{aligned}
& \sum_{i=1}^k \left(\mathcal{H}\delta_t u^{i-\frac{1}{2}}, a_0 \mathcal{H}\delta_t u^{i-\frac{1}{2}} - \sum_{j=1}^{i-1} (\tilde{a}_{i-j-1} - \tilde{a}_{i-j}) \mathcal{H}\delta_t u^{j-\frac{1}{2}} - a_{i-1} \mathcal{H}\psi_1 \right) \\
& \geq \sum_{j=1}^{M-1} \left[\frac{(2-\gamma)t_k^{1-\gamma}}{2\tau^{1-\gamma}} h \sum_{i=1}^k \left(\mathcal{H}\delta_t u_m^{i-\frac{1}{2}} \right)^2 - \frac{t_k^{2-\gamma}}{2\tau^{2-\gamma}} (\mathcal{H}\psi(x_m))^2 \right] \\
& = \frac{(2-\gamma)t_k^{1-\gamma}}{2\tau^{1-\gamma}} \sum_{i=1}^k \|\mathcal{H}\delta_t u^{i-\frac{1}{2}}\|^2 - \frac{t_k^{2-\gamma}}{2\tau^{2-\gamma}} \|\mathcal{H}\psi_1\|^2.
\end{aligned} \tag{6.12}$$

Next, noting the result (5.25), it is easily found that

$$\tau \sum_{i=1}^k \left(\mathcal{H}\delta_t u^{i-\frac{1}{2}}, \delta_x^4 u^{i-\frac{1}{2}} \right) = \sum_{i=1}^k [\langle u^i, u^i \rangle - \langle u^{i-1}, u^{i-1} \rangle] = \frac{1}{2} [\langle u^k, u^k \rangle - \langle u^0, u^0 \rangle]. \tag{6.13}$$

Moreover, employing the inequality $ab \leq \frac{1}{2}(a^2 + b^2)$, we have

$$\left(\mathcal{H}\delta_t u_m^{i-\frac{1}{2}} \right) \left(\mathcal{H}f_m^{i-\frac{1}{2}} \right) = \left(\sqrt{2}c \mathcal{H}\delta_t u_m^{i-\frac{1}{2}} \right) \left(\frac{\mathcal{H}f_m^{i-\frac{1}{2}}}{\sqrt{2}c} \right) \leq c^2 \left(\mathcal{H}\delta_t u_m^{i-\frac{1}{2}} \right)^2 + \frac{\left(\mathcal{H}f_m^{i-\frac{1}{2}} \right)^2}{4c^2} \tag{6.14}$$

where

$$c^2 = \tilde{\mu} \frac{(2-\gamma)t_k^{1-\gamma}}{2\tau^{1-\gamma}} = \frac{t_k^{1-\gamma}}{2\Gamma(2-\gamma)}.$$

Therefore, by (6.14), the following inequality is achieved

$$\sum_{i=1}^k \left(\mathcal{H}\delta_t u^{i-\frac{1}{2}}, \mathcal{H}f_j^{i-\frac{1}{2}} \right) \leq c^2 \sum_{i=1}^k \|\mathcal{H}\delta_t u^{i-\frac{1}{2}}\|^2 + \frac{1}{4c^2} \sum_{i=1}^k \|\mathcal{H}f^{i-\frac{1}{2}}\|^2. \tag{6.15}$$

Now, using the inequalities (6.12), (6.14) and (6.15) in (6.11), after some rearrangements we find

$$\begin{aligned}
& \tau c^2 \sum_{i=1}^k \|\mathcal{H}\delta_t u^{i-\frac{1}{2}}\|^2 + \frac{d}{2} [\langle u^k, u^k \rangle - \langle u^0, u^0 \rangle] - \frac{t_k^{2-\gamma}}{2\Gamma(3-\gamma)} \|\mathcal{H}\psi_1\|^2 \\
& \leq \tau \sum_{i=1}^k \left(\mathcal{H}\delta_t u^{i-\frac{1}{2}}, \mathcal{H}f^{i-\frac{1}{2}} \right) \leq \tau c^2 \sum_{i=1}^n \|\mathcal{H}\delta_t u^{i-\frac{1}{2}}\|^2 + \frac{\tau}{4c^2} \sum_{i=1}^n \|\mathcal{H}f^{i-\frac{1}{2}}\|^2.
\end{aligned} \tag{6.16}$$

From inequality (6.16), we finally get

$$\langle u^k, u^k \rangle \leq \langle u^0, u^0 \rangle + \frac{t_k^{2-\gamma}}{d\Gamma(3-\gamma)} \|\mathcal{H}\psi_1\|^2 + \frac{\Gamma(2-\gamma)t_k^{\gamma-1}h\tau}{d} \sum_{i=1}^k \|\mathcal{H}f^{i-\frac{1}{2}}\|^2.$$

The proof is complete. $\square$

We are now ready to establish the *solvability* of the PQS scheme.

Theorem 6.1. (Solvability) *The PQS scheme (6.6) has a unique solution at each time level $t = t_k$, $1 \leq k \leq K$.*

Proof. It suffices to show that the following homogeneous system

$$\begin{cases} \tilde{\mu}\mathcal{H} \left[\tilde{a}_0\delta_t u_m^{k-\frac{1}{2}} - \sum_{j=1}^{k-1} (\tilde{a}_{k-j-1} - \tilde{a}_{k-j})\delta_t u_m^{j-\frac{1}{2}} - \tilde{a}_{k-1} \cdot 0 \right] + d\delta_x^4 u_m^{k-\frac{1}{2}} = 0 \\ u_m^0 = 0, \quad 0 \leq m \leq M \\ u_0^k = u_M^k = 0, \quad \delta_x^2 u_0^k = \delta_x^2 u_M^k = 0, \quad 0 \leq k \leq K \end{cases} \quad (6.17)$$

has only the zero solution at each time level $t = t_k$, i.e., $u_m^k = 0$, $0 \leq m \leq M$.

Clearly, a solution u^k of (6.17) is in $\mathcal{U}^*$. Moreover, by Lemma 6.3, u^k satisfies the following inequality

$$\langle u^k, u^k \rangle \leq \langle u^0, u^0 \rangle + \frac{t_k^{2-\gamma}}{d\Gamma(3-\gamma)} \|(\mathcal{H}0)\|^2 + \frac{\Gamma(2-\gamma)t_k^{\gamma-1}\tau}{d} \sum_{i=1}^k \|(\mathcal{H}0)\|^2 = 0 \quad (6.18)$$

since $u_m^0 = 0$, $0 \leq j \leq M$. Hence, (6.18) implies

$$\langle u^k, u^k \rangle = 0, \quad 0 \leq k \leq K. \quad (6.19)$$

In view of (5.14) of Lemma 5.2, the equation (6.19) leads to

$$\|\delta_x^2 u^k\| = 0, \quad 0 \leq k \leq K$$

or equivalently, by definition of $\|\cdot\|$,

$$\delta_x^2 u_m^k = \frac{1}{h^2} (u_{m+1}^k - 2u_m^k + u_{m-1}^k) = 0, \quad 1 \leq m \leq M-1.$$

Using $u_0^k = u_M^k = 0$, the above relation yields $u_m^k = 0$, $0 \leq m \leq M$. Hence, the homogeneous scheme (6.17) has only the zero solution at each time level $t = t_k$. $\square$

Next, we shall investigate the *stability* of the parametric quintic spline scheme with respect to the initial condition and the non-linear term. Let u^k be the solution of (6.6), while v^k be the solution of the following system

$$\begin{cases} \tilde{\mu}\mathcal{H} \left[\tilde{a}_0 \delta_t v_m^{k-\frac{1}{2}} - \sum_{j=1}^{k-1} (\tilde{a}_{k-j-1} - \tilde{a}_{k-j}) \delta_t v_m^{k-\frac{1}{2}} - \tilde{a}_{k-1} \bar{\psi}_1(x_m) \right] + d\delta_x^4 v_m^{k-\frac{1}{2}} = H\bar{f}_m^{k-\frac{1}{2}} \\ v_m^0 = \psi(x_m) - \theta_m, \\ v_0^k = \phi_1(t_k), \quad v_M^k = \phi_2(t_k), \quad \delta_x^2 v_0^k = \phi_3(t_k), \quad \delta_x^2 v_M^k = \phi_4(t_k), \end{cases} \quad (6.20)$$

where $\theta_0 = \theta_M = 0$. Denote $\epsilon_m^k = u_m^k - v_m^k$, $\hat{f}_m^{k-\frac{1}{2}} = f_m^{k-\frac{1}{2}} - \bar{f}_m^{k-\frac{1}{2}}$, and $\hat{\psi}_1(x_m) = \psi_1(x_m) - \bar{\psi}_1(x_m)$. Then, in view of Theorem 6.1, ϵ^k is the unique solution of the following system

$$\begin{cases} \tilde{\mu}\mathcal{H} \left[\tilde{a}_0 \delta_t \epsilon_m^{k-\frac{1}{2}} - \sum_{j=1}^{k-1} (\tilde{a}_{k-j-1} - \tilde{a}_{k-j}) \delta_t \epsilon_m^{k-\frac{1}{2}} - \tilde{a}_{k-1} \hat{\psi}_1(x_m) \right] + d\delta_x^4 \epsilon_m^{k-\frac{1}{2}} = \mathcal{H}\hat{f}_m^{k-\frac{1}{2}} \\ \epsilon_m^0 = \theta_m, \quad \epsilon_0^k = \epsilon_M^k = \delta_x^2 \epsilon_0^k = \delta_x^2 \epsilon_M^k = 0. \end{cases} \quad (6.21)$$

The next theorem presents an estimate of $\|\epsilon^k\|_\infty$ which leads to the *stability* of the PQS scheme.

Theorem 6.2. (Stability) *The solution ϵ^k of (6.21) satisfies*

$$\|\epsilon^k\|_\infty^2 \leq \frac{45L^3}{224} \left[\frac{47}{45} \|\delta_x^2 \epsilon^0\|^2 + \frac{T^{2-\gamma}}{d\Gamma(3-\gamma)} \|\mathcal{H}\hat{\psi}_1\|^2 + \frac{\Gamma(2-\gamma)T^\gamma}{d} \max_{1 \leq k \leq K} \|\mathcal{H}\hat{f}^{k-\frac{1}{2}}\|^2 \right]. \quad (6.22)$$

Proof. Obviously, $\epsilon^k \in \mathcal{U}_P^*$. Applying (5.18), (5.19) and (5.14), we get an analog as in (5.37) that

$$\|\epsilon^k\|_\infty \leq \sqrt{\frac{45L^3}{224} \langle \epsilon^k, \epsilon^k \rangle}. \quad (6.23)$$

Next, using Lemma 6.3 and $t_k \leq t_K = K\tau = T$, we get

$$\begin{aligned} \langle \epsilon^k, \epsilon^k \rangle &\leq \langle \epsilon^0, \epsilon^0 \rangle + \frac{t_k^{2-\gamma}}{d\Gamma(3-\gamma)} \|\mathcal{H}\hat{\psi}_1\|^2 + \frac{\Gamma(2-\gamma)t_k^{\gamma-1}\tau}{d} \sum_{i=1}^k \|\mathcal{H}\hat{f}^{i-\frac{1}{2}}\|^2 \\ &\leq \langle \epsilon^0, \epsilon^0 \rangle + \frac{T^{2-\gamma}}{d\Gamma(3-\gamma)} \|H\hat{\psi}_1\|^2 + \frac{\Gamma(2-\gamma)T^\gamma}{d} \max_{1 \leq k \leq K} \|\mathcal{H}\hat{f}^{k-\frac{1}{2}}\|^2. \end{aligned} \quad (6.24)$$

Further, we have by (5.14),

$$\langle \epsilon^0, \epsilon^0 \rangle \leq \frac{47}{45} \|\delta_x^2 \epsilon^0\|^2. \quad (6.25)$$

Now, using (6.24) and (6.25) in (6.23) yields (6.22) which completes the proof. $\square$

From the bound established in Theorem 6.2, we can conclude that the PQS scheme (6.6) is stable with respect to initial and inhomogeneous data in maximum norm sense.

Next, we come to analyze the convergence. To this aim, we shall first give the local truncation error of (6.6) and then establish the convergence of the proposed scheme in maximum norm. Let U_m^k be the exact solution of problem (6.1) at (x_m, t_k) . Then, U^k satisfies

$$\begin{cases} \tilde{\mu}\mathcal{H} \left[\tilde{a}_0 \delta_t U_m^{k-\frac{1}{2}} - \sum_{j=1}^{k-1} (\tilde{a}_{k-j-1} - \tilde{a}_{k-j}) \delta_t U_m^{j-\frac{1}{2}} - \tilde{a}_{k-1} \psi_1(x_m) \right] + d\delta_x^4 U_m^{k-\frac{1}{2}} \\ \hspace{25em} = \mathcal{H}f_m^{k-\frac{1}{2}} + T_m^k \\ u_m^0 = \psi(x_m), \\ U_0^k = \phi_1(t_k), \quad U_M^k = \phi_2(t_k), \quad \delta_x^2 U_0^k = \phi_3(t_k), \quad \delta_x^2 U_M^k = \phi_4(t_k), \end{cases} \quad (6.26)$$

where T_m^k is the local truncation error. The order of the local truncation error is obtained in the following lemma.

Lemma 6.4. *Let $u(x, t) \in \mathcal{C}^{8,3}([0, L] \times [0, T])$ be the exact solution of problem (6.1). With p , q and s as in (6.2), we have*

$$T_m^k = \begin{cases} O(\tau^{3-\gamma} + h^4), & m = 1, M-1 \\ O(\tau^{3-\gamma} + h^6), & 2 \leq m \leq M-2. \end{cases} \quad (6.27)$$

Proof. From (6.26), it is obvious that

$$\begin{aligned}
 T_m^k &= \tilde{\mu} \mathcal{H} \left[\tilde{a}_0 \delta_t u_m^{k-\frac{1}{2}} - \sum_{j=1}^{k-1} (\tilde{a}_{k-j-1} - \tilde{a}_{k-j}) \delta_t u_m^{j-\frac{1}{2}} - \tilde{a}_{k-1} \psi_1(x_m) \right] + d \delta_x^4 u_m^{k-\frac{1}{2}} \\
 &\quad - \mathcal{H} f_m^{k-\frac{1}{2}} \\
 &= T_{m,t}^k + T_{m,x}^k + \mathcal{H} \left[{}^C_0 D_t^\gamma u(x_m, t_{k-\frac{1}{2}}) + du_{xxxx}(x_m, t_{k-\frac{1}{2}}) - f(x_m, t_{k-\frac{1}{2}}) \right]
 \end{aligned} \tag{6.28}$$

where

$$\begin{aligned}
 T_{m,t}^k &= \tilde{\mu} \mathcal{H} \left[\tilde{a}_0 \delta_t u_m^{k-\frac{1}{2}} - \sum_{j=1}^{k-1} (\tilde{a}_{k-j-1} - \tilde{a}_{k-j}) \delta_t u_m^{j-\frac{1}{2}} - \tilde{a}_{k-1} u_t(x_m, t_0) \right] \\
 &\quad - \mathcal{H} {}^C_0 D_t^\gamma u(x_m, t_{k-\frac{1}{2}})
 \end{aligned} \tag{6.29}$$

and

$$T_{m,x}^k = d \delta_x^4 u_m^{k-\frac{1}{2}} - d \mathcal{H} u_{xxxx}(x_m, t_{k-\frac{1}{2}}) \tag{6.30}$$

Applying Lemma 2.8 in (6.29) and Lemma 6.1 in (6.30), we get

$$T_{m,t}^k = O(\tau^{3-\gamma}), \quad T_{m,x}^k = O(\tau^2) + O(h^r) \tag{6.31}$$

where $r = 4$ for $m = 1, M-1$ and $r = 6$ for $2 \leq m \leq M-2$.

Moreover, since $u(x, t)$ is the exact solution of (6.1), it is clear that

$${}^C_0 D_t^\gamma u(x_m, t_{k-\frac{1}{2}}) + du_{xxxx}(x_m, t_{k-\frac{1}{2}}) - f(x_m, t_{k-\frac{1}{2}}) = 0 \tag{6.32}$$

for $0 \leq m \leq M$, $0 \leq k \leq K$.

Now, using (6.31) and (6.32) in (6.28), we obtain (6.27) immediately. $\square$

We are now ready to analyze the *convergence* of the parametric quintic spline scheme. Suppose that $\{u_m^k \mid 0 \leq m \leq M, 0 \leq k \leq K\}$ is the numerical solution of (6.1) obtained from (6.6) and let $e_m^k = U_m^k - u_m^k$.

Theorem 6.3. (Convergence) *Let $u(x, t) \in \mathcal{C}^{8,3}([0, L] \times [0, T])$ be the exact solution of problem (6.1). With p , q and s as in (6.2), we have*

$$\|e^k\|_\infty \leq O(\tau^{3-\gamma} + h^{4.5}), \quad 1 \leq k \leq K. \tag{6.33}$$

Proof. Noting (6.26) and (6.6), it is easy to see that e^k satisfies

$$\begin{cases} \tilde{\mu}\mathcal{H}\left[\tilde{a}_0\delta_te_m^{k-\frac{1}{2}} - \sum_{j=1}^{k-1}(\tilde{a}_{k-j-1} - \tilde{a}_{k-j})\delta_te_m^{j-\frac{1}{2}} - \tilde{a}_{k-1} \cdot 0\right] + d\delta_x^4e_m^{k-\frac{1}{2}} = T_m^k \\ e_m^0 = 0, \quad e_0^k = e_M^k = \delta_x^2e_0^k = \delta_x^2e_M^k = 0. \end{cases} \quad (6.34)$$

Clearly, $e^k \in \mathcal{U}_P^*$. Therefore, using a similar argument as in the proof of Theorem 6.2, we are able to get an analog of (6.22) as

$$\begin{aligned} \|e^k\|_\infty &\leq \left\{ \frac{45L^3}{224} \left[\frac{47}{45} \|\delta_x^2e^0\|^2 + \frac{T^{2-\gamma}\|\mathcal{H}0\|^2}{d\Gamma(3-\gamma)} + \frac{\Gamma(2-\gamma)T^\gamma}{d} \max_{1 \leq k \leq K} \|T^k\|^2 \right] \right\}^{\frac{1}{2}} \\ &= \left\{ \frac{45L^3}{224} \frac{\Gamma(2-\gamma)T^\gamma}{d} \max_{1 \leq k \leq K} \|T^k\|^2 \right\}^{\frac{1}{2}}. \end{aligned} \quad (6.35)$$

Next, using (6.27) of Lemma 6.4 and $(M-3)h \leq L$, we find

$$\|T^k\|^2 = h \sum_{m=1}^{M-1} (T_m^k)^2 \leq 2hC_1(\tau^{3-\gamma}+h^4)^2 + (M-3)hC_2(\tau^{3-\gamma}+h^6)^2 \leq C_3(\tau^{3-\gamma}+h^{4.5})^2 \quad (6.36)$$

where C_1 , C_2 and C_3 are constants independent of k .

Now, employing (6.36) in (6.35) yields

$$\|e^k\|_\infty \leq \left[\frac{45L^3}{224} \frac{\Gamma(2-\gamma)T^\gamma}{d} C_3 \right]^{\frac{1}{2}} (\tau^{3-\gamma} + h^{4.5}) = O(\tau^{3-\gamma} + h^{4.5}). \quad (6.37)$$

The proof is complete. $\square$

Remark 6.2. From the error inequality (6.33) in Theorem 6.3, we conclude that the PQS scheme (6.6) achieves convergence order of $O(h^{4.5} + \tau^{3-\gamma})$. In comparison, the CFD method applied to problem (6.1) with zero boundary conditions in [52] and the new CFD scheme administered to the problem (6.1) in [54] both achieve $O(h^4 + \tau^{3-\gamma})$ – note that $O(h^4)$ has been the *best spatial convergence* achieved to date by methods of finite difference nature. Obviously, the PQS scheme *improves* the spatial convergence order to $O(h^{4.5})$ and this theoretical outperformance will be further demonstrated by numerical experiments in the next section.

Remark 6.3. It is noted that the spatial convergence order of $O(h^{4.5})$ is a *theoretical result* in Theorem 6.3. In practice, it is possible to obtain a *higher* spatial convergence order, as illustrated by the numerical simulations in Section 6.3. One can refer to Remark 3.2(c) in Chapter 3 for a more rigorous explanation.

6.3 Numerical Simulation

In this section, we shall present some numerical simulations to verify the efficiency of the PQS scheme (6.6) and also to compare the performance with CFD method [52] and the new compact finite difference (NewCFD) method [54]. To have proper comparison, we shall solve diffusion-wave problems from [53, 54] using Lemma 2.8 to approximate the Caputo derivatives while employing one of the three methods (PQS, CFD, NewCFD) in the spatial dimension.

Example 6.1. [54] Consider the diffusion-wave problem (6.1) with

$$L = T = d = 1, \quad \phi_1(t) = \phi_2(t) = \phi_3(t) = \phi_4(t) = 0, \quad \psi(x) = \psi_1(x) = 0,$$

$$f(x, t) = \left[\frac{1}{6} \Gamma(\gamma + 4) + 16\pi^4 t^\gamma \right] t^3 \sin(2\pi x).$$

The exact solution is $u(x, t) = t^{3+\gamma} \sin(2\pi x)$.

From Theorem 6.3, we know that the convergence order of the PQS scheme, $O(\tau^{3-\gamma} + h^{4.5})$, depends on the fractional order γ and the temporal step size τ . Since our intention is to illustrate the *better spatial convergence* of PQS scheme over other methods (Remark 6.2), it is necessary to take appropriate τ 's for different γ 's in order to mostly eliminate the influence of $\tau^{3-\gamma}$ in the calculation of spatial convergence order. Indeed, a smaller τ should be used for a larger γ . In this example, we use $\tau = \frac{1}{50000}$ for $\gamma = 1.2, 1.5$ and $\tau = \frac{1}{100000}$ for $\gamma = 1.8$.

In Table 6.1, we tabulate the maximum absolute errors $\|e^K(\tau, h)\|_\infty$ and the spatial convergence orders. It is observed that the spatial convergence order of the PQS scheme is higher than the *theoretical* order of 4.5 obtained in Theorem 6.3. As elaborated in Remark 6.3, a higher spatial convergence order is possible in practice for h that is not that small, and this is illustrated in this example.

TABLE 6.1: (Example 6.1) $\|e^K(\tau, h)\|_\infty$ and spatial convergence order of PQS method

h	$\gamma = 1.2$	$\mathcal{O}_{\infty, x}$	$\gamma = 1.5$	$\mathcal{O}_{\infty, x}$	$\gamma = 1.8$	$\mathcal{O}_{\infty, x}$
$\frac{1}{5}$	8.95E-03	-	8.93E-03	-	8.90E-03	-
$\frac{1}{10}$	1.09E-04	6.362	1.09E-04	6.362	1.08E-04	6.362
$\frac{1}{20}$	1.07E-06	6.668	1.07E-06	6.667	1.08E-06	6.651
$\frac{1}{40}$	1.04E-08	6.688	1.08E-08	6.633	2.33E-08	5.532

Further, for visualization we plot the numerical solution of PQS method and the exact solution in Figure 6.1, and the corresponding absolute error in Figure 6.2 for the case $\gamma = 1.2$, $h = \frac{1}{20}$, $\tau = \frac{1}{50000}$. From the figures, it is visually seen that the PQS method can provide a good approximation of the exact solution.

FIGURE 6.1: (Example 6.1) Approximate solution of PQS method and exact solution when $\gamma = 1.2$, $h = \frac{1}{20}$, $\tau = \frac{1}{50000}$.

Finally, we shall compare the performance of PQS, CFD and NewCFD methods, which have *theoretical* spatial convergence orders of $O(h^{4.5})$ (PQS) and $O(h^4)$ (CFD, NewCFD). Note that the CFD method [52] can be obtained by setting

$$p = 0, \quad q = \frac{1}{6}, \quad s = \frac{2}{3}.$$

Table 6.2 presents the maximum absolute errors $\|e^K(\tau, h)\|_\infty$ and the spatial convergence orders of the three methods. Clearly, the simulation results indicate that PQS method not only *outperforms* in terms of convergence, but also achieves the *smallest* maximum absolute error in all cases.

FIGURE 6.2: (Example 6.1) Absolute error of PQS method when $\gamma = 1.2$, $h = \frac{1}{20}$, $\tau = \frac{1}{50000}$.

TABLE 6.2: (Example 6.2) Comparison of PQS, CFD and NewCFD methods

	h	PQS	$\mathcal{O}_{\infty,x}$	CFD	$\mathcal{O}_{\infty,x}$	NewCFD	$\mathcal{O}_{\infty,x}$
$\gamma = 1.2$	$\frac{1}{5}$	8.95E-03	-	9.72E-03	-	2.11E-02	-
	$\frac{1}{10}$	1.09E-04	6.362	2.84E-04	5.095	1.25E-03	4.077
	$\frac{1}{20}$	1.07E-06	6.668	1.43E-05	4.314	8.12E-05	3.945
	$\frac{1}{40}$	1.04E-08	6.688	8.51E-07	4.071	5.06E-06	4.005
$\gamma = 1.5$	$\frac{1}{5}$	8.93E-03	-	9.70E-03	-	2.11E-02	-
	$\frac{1}{10}$	1.09E-04	6.362	2.84E-04	5.095	1.25E-03	4.077
	$\frac{1}{20}$	1.07E-06	6.667	1.43E-05	4.313	8.10E-05	3.945
	$\frac{1}{40}$	1.08E-08	6.633	8.50E-07	4.070	5.05E-06	4.004
$\gamma = 1.8$	$\frac{1}{5}$	8.90E-03	-	9.67E-03	-	2.10E-02	-
	$\frac{1}{10}$	1.08E-04	6.362	2.83E-04	5.095	1.24E-03	4.077
	$\frac{1}{20}$	1.08E-06	6.651	1.42E-05	4.312	8.08E-05	3.945
	$\frac{1}{40}$	2.33E-08	5.532	8.59E-07	4.050	5.04E-06	4.001

Example 6.2. [53] Consider the diffusion-wave problem (6.1) with

$$L = T = d = 1, \quad \phi_1(t) = \phi_3(t) = t^{\gamma+3} + t, \quad \phi_2(t) = \phi_4(t) = e(t^{\gamma+3} + t),$$

$$\psi(x) = 0, \quad \psi_1(x) = e^x, \quad f(x, t) = e^x \left[\frac{t^3}{6} \Gamma(\gamma + 4) + t^{\gamma+3} + t \right].$$

The exact solution is $u(x, t) = e^x (t^{3+\gamma} + t)$.

In this example, we shall perform the simulations of *four* methods – PQS, modified CFD (M-CFD), modified NewCFD (M-NewCFD) and NewCFD. Specifically, the CFD method [52], which is originally developed for *zero* boundary conditions, is *modified* to use the equations (5.3) and (5.4) in the calculation – and this gives *modified CFD* method. Likewise, the difference between NewCFD [54] and *modified NewCFD* methods is that the latter uses (5.3) and (5.4) in the calculation.

Let $\gamma = 1.1$. The temporal convergence is almost $O(\tau^2)$ in general and we fix $\tau = \frac{1}{100000}$. In Table 6.3, we tabulate the maximum absolute errors $\|e^K(\tau, h)\|_\infty$ and the spatial convergence orders of the four methods. Further, the numerical solution of PQS method, the exact solution and the absolute error are plotted in Figures 6.3 and 6.4. From the information presented, it is clear that PQS method once again *excels* in terms of convergence and the size of maximum absolute error in all cases.

TABLE 6.3: (Example 6.2) Comparison of four methods ($\gamma = 1.1$)

h	PQS	$\mathcal{O}_{\infty, x}$	M-CFD	order	M-NewCFD	$\mathcal{O}_{\infty, x}$	NewCFD	$\mathcal{O}_{\infty, x}$
$\frac{1}{5}$	1.04E-07	-	1.62E-07	-	4.51E-07	-	1.49E-03	-
$\frac{1}{10}$	1.72E-09	5.918	7.10E-09	4.510	3.40E-08	3.730	3.76E-04	1.985
$\frac{1}{20}$	3.21E-11	5.742	3.97E-10	4.162	2.21E-09	3.947	9.46E-05	1.991

6.4 Summary

In this chapter, a higher order non-polynomial method – parametric quintic spline scheme – is developed for fourth-order fractional diffusion-wave problems. The solvability, stability and convergence of the numerical scheme have been established rigorously using the well known energy method. We have proved that the spatial

FIGURE 6.3: (Example 6.2) Approximate solution of PQS method and exact solution when $\gamma = 1.1$, $h = \frac{1}{20}$, $\tau = \frac{1}{100000}$.

FIGURE 6.4: (Example 6.2) Absolute error of PQS method when $\gamma = 1.1$, $h = \frac{1}{20}$, $\tau = \frac{1}{100000}$.

convergence order of $O(h^{4.5})$ improves that of compact finite difference methods, which give the best spatial convergence until the current work. Also, experiments are presented to demonstrate the efficiency of our method numerically. As one can see, our scheme outperforms CFD methods both theoretically and numerically in spatial approximation and could achieve a high convergence order in practice.

Chapter 7

Fourth-order Fractional Diffusion-wave Model II

In Chapter 6, we propose an efficient numerical scheme for fourth-order fractional diffusion-wave problems. The global convergence order obtained there is $O(\tau^{3-\gamma} + h^{4.5})$. However, when $\gamma \rightarrow 2$, the scheme (6.6) only achieves first order accuracy which may not meet the demand. In this chapter, we shall develop a different PQS scheme for the problem (6.1) that can obtain $O(\tau^2)$ in temporal while keep $(h^{4.5})$ in spatial. Our numerical method involves using a *parametric quintic spline* (non-polynomial spline) in the spatial dimension and employing Crank-Nicolson technique and the *weighted shifted Grünwald-Letnikov* (WSGL) method for fractional integral [123]. The method is termed *PQS-WSGL* as it involves parametric quintic spline and WSGL approximation. We plan to develop the PQS-WSGL scheme for problem (6.1) in Section 7.1. The solvability, stability and convergence of the numerical scheme are presented in Section 7.2. In Section 7.3, we include some numerical examples to demonstrate the efficiency and also to compare with other methods. Finally, a brief conclusion is made in Section 7.4.

7.1 PQS-WSGL Numerical Scheme

In this section, we develop the PQS-WSGL numerical scheme which employs the parametric quintic spline and the WSGL approximation of the fractional integral. The details are presented in the following subsections.

7.1.1 Equivalent problem and WSGL approximation of fractional integral

We shall obtain an equivalent problem of (6.1) so that we can employ the WSGL method for the fractional integral later. To this aim, we apply the *fractional integral operator* ${}_0I_t^\alpha$ ($\alpha = \gamma - 1 \in (0, 1)$) to both sides of (6.1). Note that ${}_0I_t^\alpha [{}_0^C D_t^\gamma u(x, t)] = u_t(x, t)$, we get the *equivalent problem*

$$\begin{cases} u_t(x, t) + d {}_0I_t^\alpha u_{xxxx} = g(x, t), \\ u(x, 0) = \psi(x), \\ u(0, t) = \phi_1(t), \quad u(L, t) = \phi_2(t), \quad u_{xx}(0, t) = \phi_3(t), \quad u_{xx}(L, t) = \phi_4(t), \end{cases} \quad (7.1)$$

where $g(x, t) = {}_0I_t^\alpha f(x, t) + u_t(x, 0) = {}_0I_t^\alpha f(x, t) + \psi_1(x)$.

The WSGL approximation of fractional integral is given in the following result.

Lemma 7.1. [123] *For $u(x_m, t) \in \mathcal{C}^2[0, T]$, we have*

$${}_0I_t^\alpha u(x_m, t_k) = \tau^\alpha \left[\left(1 - \frac{\alpha}{2}\right) \sum_{j=0}^k \omega_j^{-\alpha} u_m^{k-j} + \frac{\alpha}{2} \sum_{j=0}^{k-1} \omega_j^{-\alpha} u_m^{k-j-1} \right] + O(\tau^2), \quad (7.2)$$

or equivalently

$${}_0I_t^\alpha u(x_m, t_k) = \tau^\alpha \sum_{j=0}^k \lambda_j^{-\alpha} u_m^{k-j} + O(\tau^2), \quad (7.3)$$

where $\alpha = \gamma - 1 \in (0, 1)$, the coefficients $\omega_j^{-\alpha} = (-1)^j \binom{-\alpha}{j}$ for $j \geq 0$, and

$$\lambda_0^{-\alpha} = \left(1 - \frac{\alpha}{2}\right) \omega_0^{-\alpha}, \quad \lambda_j^{-\alpha} = \left(1 - \frac{\alpha}{2}\right) \omega_j^{-\alpha} + \frac{\alpha}{2} \omega_{j-1}^{-\alpha}, \quad k \geq 1. \quad (7.4)$$

7.1.2 Derivation of PQS-WSGL numerical scheme

We are now ready to derive the PQS-WSGL numerical scheme for problem (7.1), which is equivalent to the diffusion-wave problem (6.1). To begin, we discretize (7.1) at $x = x_m$ and $t = t_{k-\frac{1}{2}} = (k - \frac{1}{2})\tau$ to get

$$u_t(x_m, t_{k-\frac{1}{2}}) + d {}_0I_t^\alpha u_{xxxx}(x_m, t_{k-\frac{1}{2}}) = g(x_m, t_{k-\frac{1}{2}}). \quad (7.5)$$

For the first term on the left side of (7.5), we apply the well known Crank-Nicolson technique which yields

$$u_t(x_m, t_{k-\frac{1}{2}}) = \frac{1}{\tau} [u(x_m, t_k) - u(x_m, t_{k-1})] + O(\tau^2). \quad (7.6)$$

For the second term on the left side of (7.5), it is noted that

$${}_0I_t^\alpha u_{xxxx}(x_m, t_{k-\frac{1}{2}}) = \frac{1}{2} [{}_0I_t^\alpha u_{xxxx}(x_m, t_k) + {}_0I_t^\alpha u_{xxxx}(x_m, t_{k-1})] + O(\tau^2). \quad (7.7)$$

Then, using the WSGL formula (7.3) in (7.7) gives

$$\begin{aligned} {}_0I_t^\alpha u_{xxxx}(x_m, t_{k-\frac{1}{2}}) &= \frac{\tau^\alpha}{2} \left[\sum_{j=0}^k \lambda_j^{-\alpha} u_{xxxx}(x_m, t_{k-j}) + \sum_{j=0}^{k-1} \lambda_j^{-\alpha} u_{xxxx}(x_m, t_{k-j-1}) \right] \\ &\quad + O(\tau^2) \\ &= \tau^\alpha \sum_{j=0}^k \mu_j u_{xxxx}(x_m, t_{k-j}) + O(\tau^2), \end{aligned} \quad (7.8)$$

where

$$\mu_0 = \frac{1}{2} \lambda_0^{-\alpha}, \quad \mu_j = \frac{1}{2} (\lambda_j^{-\alpha} + \lambda_{j-1}^{-\alpha}), \quad j \geq 1. \quad (7.9)$$

If we implement the parametric quintic spline operator $\mathcal{H}$ on both sides of (7.8), in view of (6.3) it is clear that

$$\begin{aligned} \mathcal{H} {}_0I_t^\alpha u_{xxxx}(x_m, t_{k-\frac{1}{2}}) &= \tau^\alpha \sum_{j=0}^k \mu_j \mathcal{H} u_{xxxx}(x_m, t_{k-j}) + O(\tau^2) \\ &= \tau^\alpha \sum_{j=0}^k \mu_j \delta_x^4 u_m^{k-j} + O(\tau^2 + h^r), \end{aligned} \quad (7.10)$$

where $r = 4$ for $m = 1, M - 1$ and $r = 6$ for $2 \leq m \leq M - 2$.

Now we implement $\mathcal{H}$ on both sides of (7.5) to get

$$\mathcal{H} u_t(x_m, t_{k-\frac{1}{2}}) + d\mathcal{H} {}_0I_t^\alpha u_{xxxx}(x_m, t_{k-\frac{1}{2}}) = \mathcal{H} g(x_m, t_{k-\frac{1}{2}}). \quad (7.11)$$

Using (7.6) and (7.10) in (7.11) and omitting small terms, we obtain the PQS-WSGL numerical scheme as

$$\begin{cases} \frac{1}{\tau} \mathcal{H}(u_m^k - u_m^{k-1}) + d\tau^\alpha \sum_{j=0}^k \mu_j \delta_x^4 u_m^{k-j} = H g_j^{k-\frac{1}{2}}, \\ u_m^0 = \psi(x_m), \\ u_0^k = \phi_1(t_k), \quad u_M^k = \phi_2(t_k), \quad \delta_x^2 u_0^k = \phi_3(t_k), \quad \delta_x^2 u_M^k = \phi_4(t_k) \end{cases} \quad (7.12)$$

where p , q and s in $\mathcal{H}$ are as in (6.2).

7.2 Solvability, Stability and Convergence

In this section, the solvability, stability and convergence of the newly developed PQS-WSGL scheme are analyzed by discrete energy methodology.

We shall present a few lemmas before proving the main theorems. The first lemma investigates the property of $\lambda_j^{-\alpha}$ defined in (7.4).

Lemma 7.2. *For any real vector sequence $\{\mathbb{G}^1, \mathbb{G}^2, \dots, \mathbb{G}^k\}$ where $\mathbb{G}^j \in \mathcal{U}_P^*$, $1 \leq j \leq k$, we have*

$$\sum_{n=0}^{k-1} \sum_{j=0}^n \lambda_j^{-\alpha} \langle \mathbb{G}^{n+1-j}, \mathbb{G}^{n+1} \rangle \geq 0 \quad (7.13)$$

where $\lambda_j^{-\alpha}$ are given as

$$\lambda_0^{-\alpha} = \left(\frac{3}{2} - \frac{\gamma}{2}\right) \omega_0^{-\alpha}, \quad \lambda_j^{-\alpha} = \left(\frac{3}{2} - \frac{\gamma}{2}\right) \omega_j^{-\alpha} + \left(\frac{\gamma}{2} - \frac{1}{2}\right) \omega_{j-1}^{-\alpha}, \quad j \geq 1,$$

and $\omega_j^{-\alpha} = (-1)^j \binom{1-\gamma}{j}$, $j \geq 0$.

Proof. Since $\langle \cdot, \cdot \rangle$ is an inner product defined on the space $\mathcal{U}_P^*$, there exists a symmetrical and positive semi-definite matrix B such that for any $u, v \in \mathcal{U}_P^*$,

$$\langle u, v \rangle = (\delta_x^2 u)^T B (\delta_x^2 v) \quad (7.14)$$

where $(\delta_x^2 u)^T = (\delta_x^2 u_1, \delta_x^2 u_2, \dots, \delta_x^2 u_{M-1})$.

Using (7.14), we rewrite the left side of (7.13) as

$$\sum_{n=0}^{k-1} \sum_{j=0}^n \lambda_j^{-\alpha} \langle \mathbb{G}^{n+1-j}, \mathbb{G}^{n+1} \rangle = \sum_{n=0}^{k-1} \sum_{j=0}^n \lambda_j^{-\alpha} (\delta_x^2 G^{n+1-j})^T B (\delta_x^2 G^{n+1}) = \mathbb{G} (\Lambda \otimes B) \mathbb{G}^T,$$

where $\mathbb{G} = ((\delta_x^2 \mathbb{G}^1)^T, (\delta_x^2 \mathbb{G}^2)^T, \dots, (\delta_x^2 \mathbb{G}^k)^T)$, Λ is given by

$$\Lambda = \begin{pmatrix} \lambda_0^{-\alpha} & \frac{\lambda_1^{-\alpha}}{2} & \frac{\lambda_2^{-\alpha}}{2} & \dots & \frac{\lambda_{k-1}^{-\alpha}}{2} \\ \frac{\lambda_1^{-\alpha}}{2} & \lambda_0^{-\alpha} & \frac{\lambda_1^{-\alpha}}{2} & \dots & \frac{\lambda_{k-2}^{-\alpha}}{2} \\ \frac{\lambda_2^{-\alpha}}{2} & \frac{\lambda_1^{-\alpha}}{2} & \lambda_0^{-\alpha} & \dots & \frac{\lambda_{k-3}^{-\alpha}}{2} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \frac{\lambda_{k-1}^{-\alpha}}{2} & \dots & \frac{\lambda_2^{-\alpha}}{2} & \frac{\lambda_1^{-\alpha}}{2} & \lambda_0^{-\alpha} \end{pmatrix}$$

and

$$\Lambda \otimes B = \begin{pmatrix} \lambda_0^{-\alpha} B & \frac{\lambda_1^{-\alpha}}{2} B & \frac{\lambda_2^{-\alpha}}{2} B & \dots & \frac{\lambda_{k-1}^{-\alpha}}{2} B \\ \frac{\lambda_1^{-\alpha}}{2} B & \lambda_0^{-\alpha} B & \frac{\lambda_1^{-\alpha}}{2} B & \dots & \frac{\lambda_{k-2}^{-\alpha}}{2} B \\ \frac{\lambda_2^{-\alpha}}{2} B & \frac{\lambda_1^{-\alpha}}{2} B & \lambda_0^{-\alpha} B & \dots & \frac{\lambda_{k-3}^{-\alpha}}{2} B \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \frac{\lambda_{k-1}^{-\alpha}}{2} B & \dots & \frac{\lambda_2^{-\alpha}}{2} B & \frac{\lambda_1^{-\alpha}}{2} B & \lambda_0^{-\alpha} B \end{pmatrix}.$$

From Lemma 4.1 of [123], Λ is a positive semi-definite matrix. Since B is also a positive semi-definite matrix, it follows that the tensor product $\Lambda \otimes B$ is positive semi-definite. Therefore,

$$\sum_{n=0}^{k-1} \sum_{j=0}^n \lambda_j^{-\alpha} \langle \mathbb{G}^{n+1-j}, \mathbb{G}^{n+1} \rangle = \mathbb{G} (\Lambda \otimes B) \mathbb{G}^T \geq 0$$

which completes the proof. $\square$

The next lemma is the discrete Grownall's inequality [105, 123] which plays a vital role in subsequent analysis.

Lemma 7.3. [105, 123] For any sequence $\{\pi_k\}$, non-negative sequences $\{\varrho_k\}$ and $v_0 \geq 0$, if

$$\pi_0 \leq v_0, \quad \pi_k \leq v_0 + \sum_{j=0}^{k-1} \varrho_j \pi_j, \quad k \geq 1, \quad (7.15)$$

then we have

$$\pi_k \leq v_0 \exp \left(\sum_{j=0}^{k-1} \varrho_j \right), \quad k \geq 1. \quad (7.16)$$

The next lemma relates $\|u\|$ to $\|\mathcal{H}u\|$, this is vital in proving solvability, stability and convergence in l_2 norm.

Lemma 7.4. For any $u \in \mathcal{U}_P^*$, we have

$$\left(\frac{109}{360} \right)^2 \|u\|^2 \leq \|\mathcal{H}u\|^2 \leq \left(\frac{725}{720} \right)^2 \|u\|^2. \quad (7.17)$$

Proof. We shall first prove the second inequality in (7.17). Noting that $\|\mathcal{H}u\|^2 = h \sum_{m=1}^{M-1} (\mathcal{H}u_m)^2$ and $u_0 = u_M = 0$, we see that $\|\mathcal{H}u\|^2$ can be written in matrix form as

$$\|\mathcal{H}u\|^2 = h \mathbf{u}^T \mathcal{B}^T \mathcal{B} \mathbf{u}, \quad (7.18)$$

where $\mathbf{u} = (u_1, u_2, \dots, u_{M-1})^T$ and

$$\mathcal{B} = \begin{pmatrix} \frac{245}{360} & \frac{56}{360} & \frac{1}{360} & & & \\ & q & s & q & p & \\ & p & q & s & q & p \\ & & & \ddots & & \\ & & & & p & q & s & q & p \\ & & & & & p & q & s & q \\ & & & & & & \frac{1}{360} & \frac{56}{360} & \frac{245}{360} \end{pmatrix}_{(M-1) \times (M-1)}.$$

By direct computation (note that p , q and s are given in (6.2)), we get $\|\mathcal{B}\|_\infty = \frac{724}{720}$ and $\|\mathcal{B}^T\|_\infty = \frac{725}{720}$. Then

$$\mathcal{R}(\mathcal{B}^T \mathcal{B}) \leq \|\mathcal{B}^T \mathcal{B}\|_\infty \leq \|\mathcal{B}^T\|_\infty \|\mathcal{B}\|_\infty = \frac{725}{720} \frac{724}{720}.$$

It follows that

$$\|\mathcal{H}u\|^2 \leq h\mathcal{R}(\mathcal{B}^T\mathcal{B})\mathbf{u}^T\mathbf{u} = \mathcal{R}(\mathcal{B}^T\mathcal{B})\|u\|^2 \leq \left(\frac{725}{720}\right)^2 \|u\|^2$$

which is the second inequality in (7.17).

Next, we shall prove the first inequality in (7.17). For any $\varepsilon > 0$, using the linearity and symmetry of $(\cdot, \cdot)$, we obtain

$$(\mathcal{H}u - \varepsilon u, \mathcal{H}u - \varepsilon u) = (\mathcal{H}u, \mathcal{H}u) - 2\varepsilon(\mathcal{H}u, u) + \varepsilon^2(u, u) \geq 0,$$

which gives

$$\|\mathcal{H}u\|^2 = (\mathcal{H}u, \mathcal{H}u) \geq 2\varepsilon(\mathcal{H}u, u) - \varepsilon^2(u, u) = 2\varepsilon(\mathcal{H}u, u) - \varepsilon^2\|u\|^2. \quad (7.19)$$

Hence, in subsequent analysis we shall estimate $(\mathcal{H}u, u)$ in terms of $\|u\|^2$.

We require the following relations in our analysis: for $u, v \in \mathcal{U}_P^*$, by direct calculation we have

$$(v, \delta_x^4 u) = (\delta_x^2 v, \delta_x^2 u), \quad (v, \delta_x^2 u) = -(v, u)_1. \quad (7.20)$$

Using the expression (5.5) of $\mathcal{H}u_m$ and (7.20), we find

$$\begin{aligned} (\mathcal{H}u, u) &= h \sum_{m=1}^{M-1} u_m (\mathcal{H}u_m) \\ &= \|u\|^2 + \frac{h^2}{6}(u, \delta_x^2 u) - \frac{h^4}{720}(u, \delta_x^4 u) + \frac{h^5}{240}(u_1 \delta_x^4 u_1 + u_{M-1} \delta_x^4 u_{M-1}) \\ &= \|u\|^2 - \frac{h^2}{6}|u|_1^2 - \frac{h^4}{720}\|\delta_x^2 u\|^2 + R, \end{aligned} \quad (7.21)$$

where

$$\begin{aligned}
R &= \frac{h^5}{240} (u_1 \delta_x^4 u_1 + u_{M-1} \delta_x^4 u_{M-1}) \\
&= \frac{h}{240} (-4u_1 u_2 + u_1 u_3 - 4u_{M-1} u_{M-2} + u_{M-1} u_{M-3}) + \frac{5h}{240} [(u_1)^2 + (u_{M-1})^2] \\
&\geq -\frac{h}{240} \left\{ -\frac{5}{2} \sum_{m=1, M-1} (u_m)^2 + \frac{1}{2} \sum_{m=3, M-3} (u_m)^2 + 2 \sum_{m=2, M-2} (u_m)^2 \right\} \\
&\geq -\frac{h}{240} \frac{2\|u\|^2}{h} = -\frac{1}{120} \|u\|^2.
\end{aligned} \tag{7.22}$$

(Note that we have used $\pm ab \geq -\frac{1}{2}(a^2 + b^2)$ in the first inequality of (7.22).)

Further, by direct computation we have the following inequalities

$$h^4 \|\delta_x^2 u\|^2 \leq 4h^2 |u|_1^2, \quad h^2 |u|_1^2 \leq 4\|u\|^2. \tag{7.23}$$

Now, we apply (7.22) and (7.23) in (7.21) to get

$$(\mathcal{H}u, u) \geq \left(1 - \frac{4}{6} - \frac{16}{720}\right) \|u\|^2 - \frac{1}{120} \|u\|^2 = \frac{109}{360} \|u\|^2. \tag{7.24}$$

Substituting (7.24) into (7.19) yields

$$\|\mathcal{H}u\|^2 \geq \varepsilon \left(\frac{109}{180} - \varepsilon \right) \|u\|^2.$$

The maximum of $\varepsilon \left(\frac{109}{180} - \varepsilon \right)$ is achieved when $\varepsilon = \frac{109}{360}$, so the best that we can get from the above inequality is

$$\|\mathcal{H}u\|^2 \geq \left(\frac{109}{360} \right)^2 \|u\|^2$$

which is the first inequality in (7.17). The proof is complete. $\square$

Having Lemmas 7.2–7.4 ready, we shall proceed to get a priori estimate of the solution of the PQS-WSGL scheme with *zero boundary conditions*, i.e.,

$$\begin{cases} \frac{1}{\tau} \mathcal{H}(u_m^k - u_m^{k-1}) + d\tau^\alpha \sum_{j=0}^k \mu_j \delta_x^4 u_m^{k-j} = \mathcal{H}g_m^{k-\frac{1}{2}}, \\ u_m^0 = \psi(x_m), \\ u_0^k = 0, \quad u_M^k = 0, \quad \delta_x^2 u_0^k = 0, \quad \delta_x^2 u_M^k = 0. \end{cases} \quad (7.25)$$

This a priori estimate is key to establishing the stability and convergence of the PQS-WSGL scheme.

Lemma 7.5. (A priori estimate) *Suppose $\{u_m^k\}$ is the solution of (7.25). Then, we have the following a priori estimate for $1 \leq k \leq K$*

$$\|\mathcal{H}u^k\|^2 \leq \exp(2T) \left[4\tau \sum_{k=1}^K \|\mathcal{H}g^{k-\frac{1}{2}}\|^2 + d^2 T \|\delta_x^4 u^0\|^2 + 2\|\mathcal{H}u^0\|^2 \right]. \quad (7.26)$$

Proof. From the boundary conditions, obviously we have $u^k \in \mathcal{U}_P^*$. Multiplying both sides of the first equation of (7.25) $|_{k=n}$ by $\tau h(\mathcal{H}u_m^n + \mathcal{H}u_m^{n-1})$, followed by summing from $m = 1$ to $(M - 1)$, and from $n = 1$ to k , we obtain

$$\begin{aligned} & \sum_{n=1}^k (\mathcal{H}(u^n - u^{n-1}), \mathcal{H}(u^n + u^{n-1})) + d\tau^{\alpha+1} \sum_{n=1}^k \sum_{j=0}^n \mu_j (\delta_x^4 u^{n-j}, \mathcal{H}(u^n + u^{n-1})) \\ &= \tau \sum_{n=1}^k (\mathcal{H}g^{n-\frac{1}{2}}, \mathcal{H}(u^n + u^{n-1})). \end{aligned} \quad (7.27)$$

Using the linear property of inner product $(\cdot, \cdot)$, it is easy to get the first term on the left side of (7.27) as

$$\sum_{n=1}^k (\mathcal{H}(u^n - u^{n-1}), \mathcal{H}(u^n + u^{n-1})) = \sum_{n=1}^k (\|\mathcal{H}u^n\|^2 - \|\mathcal{H}u^{n-1}\|^2) = \|\mathcal{H}u^k\|^2 - \|\mathcal{H}u^0\|^2. \quad (7.28)$$

Next, we shall estimate the second term on the left side of (7.27). To this aim, applying (5.25), the relations between μ_j and $\lambda_j^{-\alpha}$, and Lemma 7.2 successively, we

find

$$\begin{aligned}
& \sum_{n=1}^k \sum_{j=0}^n \mu_j (\delta_x^4 u^{n-j}, \mathcal{H}(u^n + u^{n-1})) = \sum_{n=1}^k \sum_{j=0}^n \mu_j \langle u^{n-j}, u^n + u^{n-1} \rangle \\
&= \frac{1}{2} \sum_{n=1}^k \sum_{j=0}^{n-1} \lambda_j^{-\alpha} \langle u^{n-j} + u^{n-1-j}, u^n + u^{n-1} \rangle + \frac{1}{2} \sum_{n=1}^k \lambda_n^{-\alpha} (\delta_x^4 u^0, \mathcal{H}(u^n + u^{n-1})) \\
&= \frac{1}{2} \sum_{n=0}^{k-1} \sum_{j=0}^n \lambda_j^{-\alpha} \langle u^{n+1-j} + u^{n-j}, u^{n+1} + u^n \rangle + \frac{1}{2} \sum_{n=1}^k \lambda_n^{-\alpha} (\delta_x^4 u^0, \mathcal{H}(u^n + u^{n-1})) \\
&\geq \frac{1}{2} \sum_{n=1}^k \lambda_n^{-\alpha} (\delta_x^4 u^0, \mathcal{H}(u^n + u^{n-1})).
\end{aligned} \tag{7.29}$$

Substituting (7.28) and (7.29) into (7.27), we derive at the following inequality

$$\|\mathcal{H}u^k\|^2 \leq \|\mathcal{H}u^0\|^2 + \tau \sum_{n=1}^k (\mathcal{H}g^{n-\frac{1}{2}}, \mathcal{H}(u^n + u^{n-1})) - \frac{d\tau^{\alpha+1}}{2} \sum_{n=1}^k \lambda_n^{-\alpha} (\delta_x^4 u^0, \mathcal{H}(u^n + u^{n-1})). \tag{7.30}$$

Now, using the inequality $ab \leq \frac{1}{2}(a^2 + b^2)$, we see that the following hold for any $c_1 > 0$:

$$\begin{aligned}
(\mathcal{H}g^{n-\frac{1}{2}}, \mathcal{H}u^n) &\leq c_1 \|\mathcal{H}g^{n-\frac{1}{2}}\|^2 + \frac{1}{4c_1} \|\mathcal{H}u^n\|^2, \\
(\mathcal{H}g^{n-\frac{1}{2}}, \mathcal{H}u^{n-1}) &\leq c_1 \|\mathcal{H}g^{n-\frac{1}{2}}\|^2 + \frac{1}{4c_1} \|\mathcal{H}u^{n-1}\|^2.
\end{aligned}$$

Hence, upon combining we get the second term on the right side of (7.30) as

$$\sum_{n=1}^k (\mathcal{H}g^{n-\frac{1}{2}}, \mathcal{H}(u^n + u^{n-1})) \leq 2c_1 \sum_{n=1}^k \|\mathcal{H}g^{n-\frac{1}{2}}\|^2 + \frac{1}{4c_1} \sum_{n=1}^k (\|\mathcal{H}u^n\|^2 + \|\mathcal{H}u^{n-1}\|^2). \tag{7.31}$$

Similarly, for the last term on the right side of (7.30), we find

$$-\sum_{n=1}^k (\delta_x^4 u^0, \mathcal{H}(u^n + u^{n-1})) \leq 2c_2 \sum_{n=1}^k \|\delta_x^4 u^0\|^2 + \frac{1}{4c_2} \sum_{n=1}^k (\|\mathcal{H}u^n\|^2 + \|\mathcal{H}u^{n-1}\|^2). \tag{7.32}$$

where c_2 is any positive number.

From Lemma 3.2 of [55], we have $\omega_j^{-\alpha} > 0$ and $\omega_j^{-\alpha} < \omega_{j-1}^{-\alpha}$, $j \geq 1$. Hence, using the relation (7.4), it is obvious that $0 < \lambda_j^{-\alpha} \leq 1$. Moreover, it is reasonable to

assume $\tau < 1$ which leads to $\tau^\alpha < 1$. Using all these, we substitute (7.31) and (7.32) into (7.30) to get

$$\begin{aligned}
\|\mathcal{H}u^k\|^2 &\leq \|\mathcal{H}u^0\|^2 + 2c_1 \sum_{n=1}^k \tau \|\mathcal{H}g^{n-\frac{1}{2}}\|^2 + \frac{1}{4c_1} \tau \sum_{n=1}^k (\|\mathcal{H}u^n\|^2 + \|\mathcal{H}u^{n-1}\|^2) \\
&\quad + \frac{d\tau}{2} \left[2c_2 \sum_{n=1}^i \|\delta_x^4 u^0\|^2 + \frac{1}{4c_2} \sum_{n=1}^k (\|\mathcal{H}u^n\|^2 + \|\mathcal{H}u^{n-1}\|^2) \right] \\
&\leq \|\mathcal{H}u^0\|^2 + 2c_1 \sum_{k=1}^K \tau \|\mathcal{H}g^{k-\frac{1}{2}}\|^2 + c_2 d\tau \sum_{k=1}^K \|\delta_x^4 u^0\|^2 + \\
&\quad + \left(\frac{1}{4c_1} + \frac{d}{8c_2} \right) \left(\|\mathcal{H}u^k\|^2 + 2 \sum_{n=1}^{k-1} \|\mathcal{H}u^n\|^2 + \|\mathcal{H}u^0\|^2 \right). \tag{7.33}
\end{aligned}$$

In (7.33), set $c_1 = 1$ and $c_2 = \frac{1}{2}d$. Then, using $\tau < 1$ when necessary and $K\tau = T$, we obtain

$$\|\mathcal{H}u^k\|^2 \leq 4\tau \sum_{k=1}^K \|\mathcal{H}g^{k-\frac{1}{2}}\|^2 + d^2 T \|\delta_x^4 u^0\|^2 + 2\|\mathcal{H}u^0\|^2 + 2\tau \sum_{n=0}^{k-1} \|\mathcal{H}u^n\|^2. \tag{7.34}$$

In Lemma 7.3, let $\pi_k = \|\mathcal{H}u^k\|^2$ ($k \geq 0$), $\varrho_j = 2\tau$ and

$$v_0 = 4\tau \sum_{k=1}^K \|\mathcal{H}g^{k-\frac{1}{2}}\|^2 + d^2 T \|\delta_x^4 u^0\|^2 + 2\|\mathcal{H}u^0\|^2.$$

Then, (7.15) holds in view of (7.34). Therefore, applying Lemma 7.3 and $k\tau \leq T$, we finally get for $1 \leq k \leq K$

$$\begin{aligned}
\|\mathcal{H}u^k\|^2 &\leq \left[4\tau \sum_{k=1}^K \|\mathcal{H}g^{k-\frac{1}{2}}\|^2 + d^2 T \|\delta_x^4 u^0\|^2 + 2\|\mathcal{H}u^0\|^2 \right] \exp \left(2 \sum_{n=0}^{k-1} \tau \right) \\
&\leq \exp(2T) \left[4\tau \sum_{k=1}^K \|\mathcal{H}g^{k-\frac{1}{2}}\|^2 + d^2 T \|\delta_x^4 u^0\|^2 + 2\|\mathcal{H}u^0\|^2 \right]. \tag{7.35}
\end{aligned}$$

The proof is complete. $\square$

Our first theorem below tackles the *solvability* of the PQS-WSGL scheme.

Theorem 7.1. *The PQS-WSGL scheme (7.12) is uniquely solvable.*

Proof. It suffices to show that the corresponding homogeneous system, namely, (7.12) with $g(x, t) = 0$, $u_m^0 = 0$, $0 \leq m \leq M$, $u_0^k = u_M^k = 0$ and $\delta_x^2 u_0^k = \delta_x^2 u_M^k = 0$ has only the trivial solution. From Lemma 7.5, it is obvious that the solution of the homogeneous system satisfies

$$\|\mathcal{H}u^k\|^2 \leq 0, \quad 1 \leq k \leq K. \quad (7.36)$$

Using Lemma 7.4, (7.36) leads to $\|u^k\| = 0$ which in turn gives $u_m^k = 0$ for $1 \leq k \leq K$ and $1 \leq m \leq M - 1$. Hence, u is a trivial solution. $\square$

Next, we establish the *stability* of the PQS-WSGL scheme.

Theorem 7.2. *The solution of the PQS-WSGL scheme (7.12) depends continuously on the initial data $\psi(x)$ and the inhomogeneous data $g(x, t)$. (Note that $\psi_1(x)$ and $f(x, t)$ from the original problem (6.1) are incorporated into $g(x, t)$.)*

Proof. Let $\{u_m^k\}$ be the solution of (7.12), and let $\{v_m^k\}$ be the solution of the following system

$$\begin{cases} \frac{1}{\tau} \mathcal{H}(v_m^k - v_m^{k-1}) + d\tau^\alpha \sum_{j=0}^k \mu_j \delta_x^4 v_m^{k-j} = \mathcal{H}\bar{g}_m^{k-\frac{1}{2}}, \\ v_m^0 = \psi(x_m) - \theta_m, \\ v_0^k = \phi_1(t_k), \quad v_M^k = \phi_2(t_k), \quad \delta_x^2 v_0^k = \phi_3(t_k), \quad \delta_x^2 v_M^k = \phi_4(t_k). \end{cases} \quad (7.37)$$

Let $\epsilon_m^k = u_m^k - v_m^k$. Then, from (7.12) and (7.37) it is easily obtained that

$$\begin{cases} \frac{1}{\tau} \mathcal{H}(\epsilon_m^k - \epsilon_m^{k-1}) + d\tau^\alpha \sum_{j=0}^k \mu_j \delta_x^4 \epsilon_m^{k-j} = \mathcal{H}\hat{g}_m^{k-\frac{1}{2}}, \\ \epsilon_m^0 = \theta_m, \quad \epsilon_0^k = \epsilon_M^k = \delta_x^2 \epsilon_0^k = \delta_x^2 \epsilon_M^k = 0, \end{cases} \quad (7.38)$$

where $\hat{g}_m^{k-\frac{1}{2}} = g_m^{k-\frac{1}{2}} - \bar{g}_m^{k-\frac{1}{2}}$.

Applying Lemma 7.5, it is clear that

$$\|\mathcal{H}\epsilon^k\|^2 \leq \exp(2T) \left[4\tau \sum_{k=1}^K \left\| \mathcal{H}\hat{g}_m^{k-\frac{1}{2}} \right\|^2 + d^2 T \|\delta_x^4 \epsilon^0\|^2 + 2\|\mathcal{H}\epsilon^0\|^2 \right], \quad (7.39)$$

which implies that the solution of the PQS-WSGL scheme (7.12) continuously depends on the initial and inhomogeneous data. $\square$

Next, we shall establish the convergence of the PQS-WSGL scheme (7.12). For this purpose, let us first analyze the local truncation error which is vital in the convergence analysis. Suppose $U(x, t)$ is the exact solution of the problem (7.1) (or equivalently (6.1)). Then, we have

$$\begin{cases} \frac{1}{\tau} \mathcal{H} (U_m^k - U_m^{k-1}) + d\tau^\alpha \sum_{j=0}^k \mu_j \delta_x^4 U_m^{k-j} = \mathcal{H} g_m^{k-\frac{1}{2}} + T_m^{k-\frac{1}{2}}, \\ U_m^0 = \psi(x_m), \\ U_0^k = \phi_1(t_k), \quad U_M^k = \phi_2(t_k), \quad \delta_x^2 U_0^k = \phi_3(t_k), \quad \delta_x^2 U_M^k = \phi_4(t_k) \end{cases} \quad (7.40)$$

where $T_m^{k-\frac{1}{2}}$ is the local truncation error at $(x_m, t_{k-\frac{1}{2}})$. The following lemma gives an estimate of the local truncation error.

Lemma 7.6. *Suppose that the exact solution $U(x, t) \in \mathcal{C}^{8,2}([0, L] \times [0, T])$. The local truncation error $T_m^{k-\frac{1}{2}}$ in (7.40) satisfies*

$$T_m^{k-\frac{1}{2}} = O(\tau^2 + h^r), \quad 1 \leq m \leq M-1, \quad 1 \leq k \leq K \quad (7.41)$$

where $r = 4$ for $m = 1, M-1$ and $r = 6$ for $2 \leq m \leq M-2$.

Proof. Since $U(x, t)$ is the exact solution of (7.1), it follows from (7.40) that

$$\begin{aligned} T_m^{k-\frac{1}{2}} &= \frac{1}{\tau} \mathcal{H} (U_m^k - U_m^{k-1}) + d\tau^\alpha \sum_{j=0}^k \mu_j \delta_x^4 U_m^{k-j} - \mathcal{H} g_m^{k-\frac{1}{2}} \\ &\quad - \mathcal{H} \left[U_t(x_m, t_{k-\frac{1}{2}}) + d {}_0 I_t^\alpha U_{xxxx}(x_m, t_{k-\frac{1}{2}}) - g(x_m, t_{k-\frac{1}{2}}) \right] \\ &= \mathcal{H} \left[\frac{u_m^k - u_m^{k-1}}{\tau} - U_t(x_m, t_{k-\frac{1}{2}}) \right] \\ &\quad - d \left[\mathcal{H} {}_0 I_t^\alpha U_{xxxx}(x_m, t_{k-\frac{1}{2}}) - \tau^\alpha \sum_{j=0}^k \mu_j \delta_x^4 u_m^{k-j} \right] \\ &= O(\tau^2 + h^r) \end{aligned} \quad (7.42)$$

where we have applied (7.6) and (7.10) to get the last equality. $\square$

We are now ready to establish the *convergence* of the PQS-WSGL numerical scheme in l_2 norm.

Theorem 7.3. *Suppose that $U(x, t) \in \mathcal{C}^{8,2}([0, L] \times [0, T])$ is the exact solution of (7.1) while $\{u_m^k\}$ is the numerical solution obtained from the PQS-WSGL scheme (7.12). Let $e_m^k = U_m^k - u_m^k$ denote the error at (x_m, t_k) . Then, we have*

$$\|e^k\| \leq O(\tau^2 + h^{4.5}), \quad 1 \leq k \leq K. \quad (7.43)$$

Proof. In view of (7.12) and (7.40), it is clear that $\{e_m^k\}$ is the solution of the following system

$$\begin{cases} \frac{1}{\tau} \mathcal{H}(e_m^k - e_m^{k-1}) + d\tau^\alpha \sum_{j=0}^k \mu_j \delta_x^4 e_m^{k-j} = T_m^{k-\frac{1}{2}}, \\ e_m^0 = 0, \quad e_0^k = e_M^k = \delta_x^2 e_0^k = \delta_x^2 e_M^k = 0. \end{cases} \quad (7.44)$$

An application of Lemmas 7.4 and 7.5 gives the following inequality for $1 \leq k \leq K$,

$$\left(\frac{109}{360}\right)^2 \|e^k\|^2 \leq \|\mathcal{H}e^k\|^2 \leq \exp(2T) \left[4\tau \sum_{k=1}^K \|T^{k-\frac{1}{2}}\|^2 \right]. \quad (7.45)$$

Note that from Lemma 7.6, there exist constants C_1 , C_2 and C_3 that are independent of k and h such that

$$\begin{aligned} \|T^{k-\frac{1}{2}}\|^2 &= h \sum_{m=1}^{M-1} \left(T_m^{k-\frac{1}{2}}\right)^2 \leq 2hC_1(\tau^2 + h^4)^2 + (M-3)hC_2(\tau^2 + h^6)^2 \\ &\leq 2hC_1(\tau^2 + h^4)^2 + LC_2(\tau^2 + h^6)^2 \\ &\leq C_3(\tau^2 + h^{4.5})^2. \end{aligned} \quad (7.46)$$

Therefore, we obtain

$$\tau \sum_{k=1}^K \|T^{k-\frac{1}{2}}\|^2 \leq K\tau C_3(\tau^2 + h^{4.5})^2 = TC_3(\tau^2 + h^{4.5})^2. \quad (7.47)$$

Substituting (7.47) into (7.45) immediately yields (7.43). The proof is complete. $\square$

Remark 7.1.

- (a) From the error inequality (7.43) of Theorem 7.3, we conclude that the PQS-WSGL scheme achieves $O(\tau^2 + h^{4.5})$ in l_2 norm. The spatial convergence order of 4.5 *improves* that of the CFD method and FD method in l_2 norm sense – it is well known that CFD and FD methods attain $O(h^4)$ and $O(h^2)$ respectively in maximum norm and $O(h^4)$ has been the best spatial convergence achieved in the literature. In practice, the performance of the PQS-WSGL method is better even in the maximum norm sense. This is illustrated in the numerical experiment in next section.
- (b) Note that the theoretical error bound given in (7.43) is not a tight bound. Thus, for particular problems, the actual convergence order can be *higher* than the theoretical one. In fact, this is observed in the numerical experiment in Section 7.3.

7.3 Numerical Simulation

In this section, we shall present two examples to demonstrate the efficiency and accuracy of the PQS-WSGL scheme (7.12) and also to compare with two other methods, namely, the CFD method and the FD method.

In the examples, we shall compute the errors $e_m^k (= U_m^k - u_m^k)$ for all $1 \leq m \leq M-1$ and $1 \leq k \leq K$, and we shall present the maximum error in l_2 norm as well as in maximum norm. To be precise, for a fixed (τ, h) , we shall use the following notations:

$$\mathcal{E}_2(\tau, h) = \max_{1 \leq k \leq K} \|e^k\|, \quad \mathcal{E}_\infty(\tau, h) = \max_{1 \leq k \leq K} \|e^k\|_\infty. \quad (7.48)$$

The temporal and spatial convergence orders in l_2 norm sense are calculated respectively by the following formula:

$$\mathcal{O}_{2,t} = \log_2 \left[\frac{\mathcal{E}_2(\tau, h)}{\mathcal{E}_2(\tau/2, h)} \right], \quad \mathcal{O}_{2,x} = \log_2 \left[\frac{\mathcal{E}_2(\tau, h)}{\mathcal{E}_2(\tau, h/2)} \right]. \quad (7.49)$$

Likewise, the temporal and spatial convergence orders in maximum norm sense are computed respectively as follows:

$$\mathcal{O}_{\infty,t} = \log_2 \left[\frac{\mathcal{E}_{\infty}(\tau, h)}{\mathcal{E}_{\infty}(\tau/2, h)} \right], \quad \mathcal{O}_{\infty,x} = \log_2 \left[\frac{\mathcal{E}_{\infty}(\tau, h)}{\mathcal{E}_{\infty}(\tau, h/2)} \right]. \quad (7.50)$$

Our first example is taken from [53] in which FD method has been developed to solve (6.1).

Example 7.1. Consider problem in Example 6.2. It is converted to the equivalent problem (7.1) with

$$g(x, t) = \exp(x) \left[\frac{\Gamma(4 + \gamma)}{\Gamma(3 + \gamma)} t^{2+\gamma} + \frac{\Gamma(4 + \gamma)}{\Gamma(3 + 2\gamma)} t^{2+2\gamma} + \frac{1}{\Gamma(1 + \gamma)} t^{\gamma} + 1 \right].$$

First, we fix $h = \frac{1}{30}$ and let τ vary. In Table 7.1, we present the errors in l_2 norm ($\mathcal{E}_2(\tau, h)$) and in maximum norm ($\mathcal{E}_{\infty}(\tau, h)$) resulting from the application of PQS-WSGL scheme, as well as the respective temporal convergence orders calculated using (7.49) and (7.50). It is observed that $O(\tau^2)$ is achieved in both norms, confirming the theoretical result (Theorem 7.3).

TABLE 7.1: (Example 7.1) Errors $\mathcal{E}_{\infty}(\tau, h)$, $\mathcal{E}_2(\tau, h)$ and temporal convergence order

	τ	$\gamma = 1.2$	$\mathcal{O}_{\infty,t}$	$\gamma = 1.5$	$\mathcal{O}_{\infty,t}$	$\gamma = 1.8$	$\mathcal{O}_{\infty,t}$
$\mathcal{E}_{\infty}(\tau, h)$	$\frac{1}{5}$	3.0475E-03	-	4.2773E-03	-	6.3689E-03	-
	$\frac{1}{10}$	7.5393E-04	2.0151	1.1248E-03	1.9270	1.5129E-03	2.0738
	$\frac{1}{20}$	1.8975E-04	1.9903	2.8268E-04	1.9924	3.9281E-04	1.9454
	$\frac{1}{40}$	4.7495E-05	1.9983	7.0901E-05	1.9953	9.9343E-05	1.9834
	$\frac{1}{80}$	1.1883E-05	1.9988	1.7755E-05	1.9976	2.4913E-05	1.9955
	τ	$\gamma = 1.2$	$\mathcal{O}_{\infty,t}$	$\gamma = 1.5$	$\mathcal{O}_{\infty,t}$	$\gamma = 1.8$	$\mathcal{O}_{\infty,t}$
$\mathcal{E}_2(\tau, h)$	$\frac{1}{5}$	2.1659E-03	-	3.0435E-03	-	4.5345E-03	-
	$\frac{1}{10}$	5.3467E-04	2.0182	7.9701E-04	1.9331	1.0743E-03	2.0775
	$\frac{1}{20}$	1.3451E-04	1.9909	2.0073E-04	1.9893	2.7905E-04	1.9448
	$\frac{1}{40}$	3.3722E-05	1.9960	5.0361E-05	1.9949	7.0559E-05	1.9836
	$\frac{1}{80}$	8.4412E-06	1.9982	1.2610E-05	1.9977	1.7694E-05	1.9956

Next, we fix $\tau = \frac{1}{50000}$ and let h vary. Since the main contribution of the current work is in the *higher spatial convergence order*, in this example we shall compare the performance of PQS-WSGL scheme with CFD method and FD method. To have proper comparisons, we apply the *same treatment* of Crank-Nicolson and WSGL

methods in the temporal dimension while employing CFD or FD methods in the spatial dimension to obtain CFD-WSGL or FD-WSGL methods. In Tables 7.2 and 7.3 respectively, the errors $\mathcal{E}_2(\tau, h)$ and $\mathcal{E}_\infty(\tau, h)$ together with the respective spatial convergence orders are presented for the three methods – PQS-WSGL, CFD-WSGL and FD-WSGL. It is observed from the tables that the PQS-WSGL scheme achieves the *smallest* error and the *highest* spatial convergence order for all cases both in l_2 norm and in maximum norm sense. Note that the spatial convergence order is far better than the theoretical one which is possible for a particular problem, refer to Remark 7.1 (b) for some possible illustrations. In fact, it happens not only for the proposed PQS-WSGL method but also for the CFD-WSGL method which gives $O(h^4)$ from a theoretical point of view.

TABLE 7.2: (Example 7.1) Error $\mathcal{E}_2(\tau, h)$ and spatial convergence order

	h	$\gamma = 1.2$	$\mathcal{O}_{2,x}$	$\gamma = 1.5$	$\mathcal{O}_{2,x}$	$\gamma = 1.8$	$\mathcal{O}_{2,x}$
PQS-WSGL	$\frac{1}{5}$	7.730E-08	-	7.615E-08	-	7.425E-08	-
	$\frac{1}{10}$	1.226E-09	5.979	1.197E-09	5.992	1.153E-09	6.009
	$\frac{1}{20}$	1.437E-11	6.414	1.099E-11	6.766	2.630E-11	5.454
CFD-WSGL	$\frac{1}{5}$	1.196E-07	-	1.179E-07	-	1.149E-07	-
	$\frac{1}{10}$	5.023E-09	4.574	4.938E-09	4.577	4.802E-09	4.581
	$\frac{1}{20}$	2.515E-10	4.320	2.416E-10	4.353	2.197E-10	4.450
FD-WSGL	$\frac{1}{5}$	8.889E-04	-	8.750E-04	-	8.541E-04	-
	$\frac{1}{10}$	2.238E-04	1.990	2.204E-04	1.989	2.151E-04	1.990
	$\frac{1}{20}$	5.603E-05	1.998	5.520E-05	1.998	5.385E-05	1.999

TABLE 7.3: (Example 7.1) Error $\mathcal{E}_\infty(\tau, h)$ and spatial convergence order

	h	$\gamma = 1.2$	$\mathcal{O}_{\infty,x}$	$\gamma = 1.5$	$\mathcal{O}_{\infty,x}$	$\gamma = 1.8$	$\mathcal{O}_{\infty,x}$
PQS-WSGL	$\frac{1}{5}$	1.035E-07	-	1.020E-07	-	9.941E-08	-
	$\frac{1}{10}$	1.673E-09	5.951	1.632E-09	5.965	1.571E-09	5.984
	$\frac{1}{20}$	2.032E-11	6.363	1.639E-11	6.638	3.912E-11	5.327
CFD-WSGL	$\frac{1}{5}$	1.612E-07	-	1.588E-07	-	1.549E-07	-
	$\frac{1}{10}$	7.037E-09	4.518	6.917E-09	4.521	6.724E-09	4.526
	$\frac{1}{20}$	3.535E-10	4.315	3.397E-10	4.348	3.091E-10	4.443
FD-WSGL	$\frac{1}{5}$	1.203E-03	-	1.184E-03	-	1.156E-03	-
	$\frac{1}{10}$	3.033E-04	1.988	2.985E-04	1.988	2.909E-04	1.991
	$\frac{1}{20}$	7.660E-05	1.985	7.544E-05	1.985	7.354E-05	1.984

For visualization, in Figures 7.1 and 7.2 we plot the numerical solution obtained from PQS-WSGL scheme, the exact solution, and the absolute error when $\gamma =$

1.2, $\tau = \frac{1}{50000}$ and $h = \frac{1}{20}$. From these diagrams, it is seen that the PQS-WSGL scheme gives a good approximation to the exact solution at mesh points.

FIGURE 7.1: (Example 7.1) Approximate solution by PQS-WSGL method and exact solution when $\gamma = 1.2$, $h = \frac{1}{20}$, $\tau = \frac{1}{50000}$.

FIGURE 7.2: (Example 7.1) Absolute error of PQS-WSGL method when $\gamma = 1.2$, $h = \frac{1}{20}$, $\tau = \frac{1}{50000}$.

Example 7.2. Consider problem (6.1) with $L = T = 1$, $d = 3$, $\psi(x) = 0$, $\psi(x) = \sin(2\pi x)$, $\phi_1(t) = \phi_2(t) = \phi_3(t) = \phi_4(t) = 0$ and

$$f(x, t) = \sin(2\pi x) \left[\Gamma(\gamma + 4) \frac{t^3}{6} + 16\pi^4 d (t^{3+\gamma} + t) \right].$$

The exact solution is $u(x, t) = \sin(2\pi x)(t^{3+\gamma} + t)$.

The above problem is converted to the equivalent problem (7.1) with

$$g(x, t) = \sin(2\pi x) \left\{ \frac{\Gamma(4 + \gamma)}{\Gamma(3 + \gamma)} t^{2+\gamma} + 16\pi^4 d \left[\frac{\Gamma(4 + \gamma)}{\Gamma(3 + 2\gamma)} t^{2+2\gamma} + \frac{t^\gamma}{\Gamma(1 + \gamma)} \right] + 1 \right\}.$$

Then, the PQS-WSGL scheme is applied with different values of γ and (τ, h) .

First, we fix $\tau = \frac{1}{10000}$ and vary h as in Table 7.4 where we compute l_2 norm error $\mathcal{E}_2(\tau, h)$ and maximum absolute error $\mathcal{E}_\infty(\tau, h)$ as well as the corresponding spatial convergence orders. Obviously, our method can achieve at least $O(h^{4.5})$ in l_2 norm which verifies our theoretical result (Theorem 7.3). Also, it is observed that this is true even in maximum norm which is a good sign in practice.

Next, we let $h = \frac{1}{200}$ and vary τ as in Table 7.5 to get temporal convergence orders in l_2 and maximum norms. From this table, it is obvious that second order accuracy is obtained in the temporal dimension which is consistent with our theoretical result (Theorem 7.3).

Finally, we plot the exact and numerical solutions as well as absolute errors when $\gamma = 1.8$, $h = \frac{1}{20}$, $\tau = \frac{1}{10000}$ in Figures 7.3 and 7.4. From these two figures, it is seen that the PQS-WSGL scheme indeed provides a good approximation to the exact solution.

TABLE 7.4: (Example 7.2) Errors $\mathcal{E}_\infty(\tau, h)$, $\mathcal{E}_2(\tau, h)$ and spatial convergence order

	h	$\gamma = 1.2$	$\mathcal{O}_{\infty,x}$	$\gamma = 1.5$	$\mathcal{O}_{\infty,x}$	$\gamma = 1.8$	$\mathcal{O}_{\infty,x}$
$\mathcal{E}_\infty(\tau, h)$	$\frac{1}{5}$	1.7941E-02	-	1.7935E-02	-	1.7926E-02	-
	$\frac{1}{10}$	2.1812E-04	6.3620	2.1804E-04	6.3621	2.1791E-04	6.3621
	$\frac{1}{20}$	2.1262E-06	6.6807	2.1165E-06	6.6867	2.1083E-06	6.6915
	h	$\gamma = 1.2$	$\mathcal{O}_{2,x}$	$\gamma = 1.5$	$\mathcal{O}_{2,x}$	$\gamma = 1.8$	$\mathcal{O}_{2,x}$
$\mathcal{E}_2(\tau, h)$	$\frac{1}{5}$	1.2783E-02	-	1.2778E-02	-	1.2771E-02	-
	$\frac{1}{10}$	1.5744E-04	6.3432	1.5738E-04	6.3433	1.5729E-04	6.3433
	$\frac{1}{20}$	1.5401E-06	6.6756	1.5330E-06	6.6818	1.5269E-06	6.6867

7.4 Summary

In this chapter, we propose the PQS-WSGL numerical scheme for the fourth-order fractional diffusion-wave problem (6.1) (or equivalently (7.1)). The scheme is derived from (i) Crank-Nicolson coupled with weighted shifted Grünwald-Letnikov technique for integral to ensure $O(\tau^2)$ accuracy in temporal dimension, and (ii) parametric quintic spline to guarantee at least $O(h^{4.5})$ accuracy in spatial dimension. Using discrete energy methodology, we prove the solvability, stability and

TABLE 7.5: (Example 7.2) Errors $\mathcal{E}_\infty(\tau, h)$, $\mathcal{E}_2(\tau, h)$ and temporal convergence order

	τ	$\gamma = 1.2$	$\mathcal{O}_{\infty,t}$	$\gamma = 1.5$	$\mathcal{O}_{\infty,t}$	$\gamma = 1.8$	$\mathcal{O}_{\infty,t}$
$\mathcal{E}_\infty(\tau, h)$	$\frac{1}{1000}$	4.2216E-05	-	2.2479E-05	-	1.2042E-05	-
	$\frac{1}{2000}$	1.1417E-05	1.8866	5.6611E-06	1.9894	3.0123E-06	1.9991
	$\frac{1}{4000}$	2.8812E-06	1.9865	1.4243E-06	1.9908	7.5326E-07	1.9997
	τ	$\gamma = 1.2$	$\mathcal{O}_{2,t}$	$\gamma = 1.5$	$\mathcal{O}_{2,t}$	$\gamma = 1.8$	$\mathcal{O}_{2,t}$
$\mathcal{E}_2(\tau, h)$	$\frac{1}{1000}$	2.9852E-05	-	1.5895E-05	-	8.5147E-06	-
	$\frac{1}{2000}$	8.0732E-06	1.8866	4.0030E-06	1.9894	2.1301E-06	1.9991
	$\frac{1}{4000}$	2.0373E-06	1.9865	1.0071E-06	1.9908	5.3264E-07	1.9997

FIGURE 7.3: (Example 7.2) Approximate solution by PQS-WSGL method and exact solution when $\gamma = 1.8$, $h = \frac{1}{20}$, $\tau = \frac{1}{10000}$. FIGURE 7.4: (Example 7.2) Absolute error of PQS-WSGL method when $\gamma = 1.8$, $h = \frac{1}{20}$, $\tau = \frac{1}{10000}$.

convergence of the proposed numerical method in l_2 norm. Finally, to demonstrate the effectiveness and efficiency of the PQS-WSGL scheme, simulations are performed. The numerical results show that the proposed method gives second order accuracy in temporal dimension which is vital for practical use, and at least 4.5 order accuracy in spatial dimension which is consistent with the theoretical result.

Chapter 8

Distributed Order Fractional Sub-diffusion Equations

Previous chapters deal with the classical fractional sub-diffusion and diffusion-wave problems. Though they are known to be more accurate models in applications, a more general *distributed order* fractional differential equation which allows the fractional order to vary, is found to be more appropriate in modeling ultraslow diffusion with the mean square displacement growing as a power of the logarithm of time [21, 22]. Other applications of distributed order fractional differential equation appear, to cite a few, in the modeling of dielectric induction and diffusion [20, 36, 39], and the stress behavior of an elastic medium [18, 36, 39]. The fundamental analytical properties of distributed order fractional differential equations, such as existence and uniqueness of solutions, have been investigated in [46, 86, 89, 90]. Some pioneer work on the numerical treatment of distributed order fractional differential equations can be found in [14, 31, 39, 51, 63, 100, 137, 139]. Motivated by all the above research, our objective in this paper is to *improve* the *spatial convergence order* to at least $O(h^{4.5})$ while keeping the computation cost similar to that of the CFD method [39] which has a convergence of $O(h^4)$.

In this chapter, we shall employ *parametric quintic spline* in the numerical scheme and present theoretical proofs of the stability and convergence by the well known energy method. The distributed order fractional sub-diffusion equation considered

is the following [39, 51]:

$$\begin{cases} {}^C_0 D_t^{\mathcal{D}(\gamma)} u(x, t) = du_{xx}(x, t) + f(x, t), & (x, t) \in \Omega \\ u(x, 0) = 0, & x \in [0, L] \\ u(0, t) = \phi_1(t), \quad u(L, t) = \phi_2(t), & t \in [0, T] \end{cases} \quad (8.1)$$

where $d > 0$ is the diffusion constant, $\Omega = [0, L] \times [0, T]$ ($L, T > 0$), $f(x, t)$, $\phi_1(t)$, $\phi_2(t)$ are continuous functions with $\phi_1(0) = \phi_2(0) = 0$, and the *distributed order fractional derivative* ${}^C_0 D_t^{\mathcal{D}(\gamma)} u(x, t)$ is defined as in (2.10). Note that if the initial condition $u(x, 0) \neq 0$, we can use the transformation $v(x, t) = u(x, t) - u(x, 0)$ and obtain a problem similar to (8.1). Therefore, the problem (8.1) considered is quite general.

The chapter is organized as follows. In Section 8.1, we shall develop the numerical scheme using mid-point quadrature rule, WSGL technique and parametric quintic spline method. The solvability, stability and convergence of the proposed scheme are established rigorously using discrete energy methodology in Section 8.2. To demonstrate the accuracy and efficiency of the proposed scheme, two examples are presented in Section 8.3. Finally, we end with a brief conclusion in Section 8.4.

8.1 Derivation of the Numerical Scheme

In this section, we shall develop a high spatial accuracy numerical scheme using mid-point quadrature rule for distributed order term, WSGL method for fractional terms and parametric quintic spline method in the spatial dimension.

First, To approximate the distributed order term in (8.1), we require the mid-point quadrature rule [51] and a special case of the WSGL method [121], both are stated as follows.

Lemma 8.1. [51] *Let $\gamma_j = \frac{2j-1}{2J}$, $1 \leq j \leq J$. The mid-point quadrature approximation of the distributed order fractional derivative is given by*

$${}^C_0 D_t^{\mathcal{D}(\gamma)} u(x, t) = \eta \sum_{j=1}^J \mathcal{D}(\gamma_j) {}^C_0 D_t^{\gamma_j} u(x, t) + O(\eta^2), \quad (8.2)$$

where $\eta = \frac{1}{j}$.

From Lemma 2.1, Remark (2.4) and $u(x, 0) = 0$, it is clear that

$${}_0^C D_t^{\gamma_j} u(x, t) = {}_0^{RL} D_t^{\gamma_j} u(x, t).$$

Using (2.23) and (2.25), and setting $(\hat{l}, l) = (0, -1)$, upon simplification, we get

$${}_0^C D_t^{\gamma_j} u(x_m, t_k) = \frac{1}{\tau^{\gamma_j}} \sum_{i=0}^{\infty} \lambda_i^{\gamma_j} u(x_m, t_{k-i}) + O(\tau^2), \quad (8.3)$$

where

$$\lambda_0^{\gamma_j} = \left(1 + \frac{\gamma_j}{2}\right) \omega_0^{\gamma_j}, \quad \lambda_i^{\gamma_j} = \left(1 + \frac{\gamma_j}{2}\right) \omega_i^{\gamma_j} - \frac{\gamma_j}{2} \omega_{i-1}^{\gamma_j}, \quad i \geq 1. \quad (8.4)$$

We shall use the WSGL approximation (8.3) in subsequent development.

Next, we shall present the *parametric quintic spline operator* which plays a key role in the numerical scheme. In fact, in Chapter 4, we have defined this operator. For the sake of the convenience, we list some results here. For $u \in \mathcal{U}_P$, we have the parametric quintic spline operator $\mathcal{H}$ in (4.9) in Chapter 4

$$\mathcal{H}u_m = \begin{cases} \left(1 + \frac{h^2}{12}\delta_x^2\right) u_m, & m = 1, M-1 \\ p(u_{m-2} + u_{m+2}) + q(u_{m-1} + u_{m+1}) + su_m, & 2 \leq m \leq M-2. \end{cases} \quad (8.5)$$

where p, q, s are the same as in (4.7). Also, through Taylor expansion at (x_m, t_k) , when

$$p = \frac{1}{12}\kappa - \frac{1}{240}, \quad q = \frac{8}{12}\kappa + \frac{24}{240}, \quad s = -\frac{3}{2}\kappa + \frac{97}{120}, \quad (8.6)$$

we shall get as in Lemma 4.1 that

$$\mathcal{H}u_{xx}(x_m, t_k) - \bar{\delta}_x^2 u_m^k = O(h^r), \quad (8.7)$$

where $\bar{\delta}_x^2 u_m^k$ are similarly defined as in (4.11), and $r = 4$ for $m = 1, M-1$ and $r = 6$ for $2 \leq m \leq M-2$. For the rest of the chapter, we shall fix p, q and s as in (8.6) to get high accuracy in spatial dimension.

Now, we are ready to develop the numerical scheme for the distributed order fractional sub-diffusion problem (8.1). Discretizing the first equation of (8.1) at

(x_m, t_k) , we get

$${}_0^C D_t^{\mathcal{D}(\gamma)} u(x_m, t_k) = du_{xx}(x_m, t_k) + f_m^k. \quad (8.8)$$

Using the mid-point quadrature approximation (8.2) on the distributed order fractional derivative in (8.8) yields

$$\eta \sum_{j=1}^J \mathcal{D}(\gamma_j)_0^C D_t^{\gamma_j} u(x_j, t_k) + O(\eta^2) = du_{xx}(x_m, t_k) + f_m^k. \quad (8.9)$$

Then, WSGL approximation (8.3) is applied to each Caputo fractional term in (8.9) to give

$$\sum_{i=0}^k \lambda_i^* u_m^{k-i} + O(\eta^2) + O(\tau^2) = du_{xx}(x_m, t_k) + f_m^k, \quad (8.10)$$

where λ_i^* is computed using

$$\lambda_i^* = \frac{1}{J} \sum_{j=1}^J \frac{1}{\tau^{\gamma_j}} \mathcal{D}(\gamma_j) \lambda_i^{\gamma_j}, \quad 0 \leq i \leq k. \quad (8.11)$$

Finally, we apply the operator $\mathcal{H}$ on both sides of (8.10). Noting the relation (8.7), we obtain the following numerical scheme, after omitting the small terms,

$$\left\{ \begin{array}{l} \sum_{i=0}^k \lambda_i^* \mathcal{H} u_m^{k-i} = d\bar{\delta}_x^2 u_m^k + \mathcal{H} f_m^k, \quad 1 \leq m \leq M-1 \\ u_m^0 = 0, \quad 0 \leq m \leq M \\ u_0^k = \phi_1(t_k), \quad u_M^k = \phi_2(t_k), \quad 0 \leq k \leq K. \end{array} \right. \quad (8.12)$$

8.2 Theoretical Results

In this section, we shall establish the solvability, stability and convergence of the numerical scheme (8.12) using the well known discrete energy methodology. In what follows, we shall present a series of lemmas that are vital in establishing the main theorems. The first one gives an inequality of the coefficient $\lambda_i^{(\gamma_j)}$ defined in (8.4).

Lemma 8.2. [39, 123] For any real numbers G^i , $0 \leq i \leq k$, we have

$$\sum_{n=0}^k \left(\sum_{i=0}^n \lambda_i^{\gamma_j} G^{n-i} \right) G^n \geq 0. \quad (8.13)$$

Remark 8.1. In view of the expression (8.11), it is clear that (8.13) also holds if $\lambda_i^{\gamma_j}$ is replaced by λ_i^* .

The second lemma relates $\sum_{m=1}^{M-1} (u_m)^2$ to $\sum_{m=0}^{M-1} (u_{m+1} - u_m)^2$ by Wirtinger Type Inequality from **Theorem 12.6.1** in [2].

Lemma 8.3. [2] For any $u \in \mathcal{U}_P$, we have

$$\left(4 \sin^2 \frac{\pi}{2M} \right) \sum_{m=1}^{M-1} (u_m)^2 \leq \sum_{m=0}^{M-1} (u_{m+1} - u_m)^2 \leq \left(4 \cos^2 \frac{\pi}{2M} \right) \sum_{m=1}^{M-1} (u_m)^2. \quad (8.14)$$

Remark 8.2. Using Lemma 8.3, the facts that $h = \frac{L}{M}$ and $\frac{\sin x}{x}$ is decreasing over $x \in (0, \frac{\pi}{2}]$, we find

$$\begin{aligned} |u|_1^2 &\geq \frac{4}{h^2} \sin^2 \frac{\pi}{2M} \|u\|^2 = \frac{4}{h^2} \sin^2 \frac{\pi h}{2L} \|u\|^2 = \frac{4}{h^2} \left(\frac{\pi h}{2L} \right)^2 \frac{\sin^2 \frac{\pi h}{2L}}{\left(\frac{\pi h}{2L} \right)^2} \|u\|^2 \\ &\geq \frac{4}{h^2} \left(\frac{\pi h}{2L} \right)^2 \left(\frac{2}{\pi} \right)^2 \|u\|^2 = \frac{4}{L^2} \|u\|^2. \end{aligned} \quad (8.15)$$

The next three results present three inequalities which are very important in subsequent analysis and have been used in previous chapters. From Lemmas 4.2, 4.3, 3.3 and their proofs, for $u \in \mathcal{U}_P$,

- If $0 < \kappa < \frac{67}{492}$, then

$$\|Hu\|^2 \leq \left(\frac{61}{60} \right)^2 \|u\|^2. \quad (8.16)$$

- If $0 < \kappa < \kappa_0 = \frac{-164 + \sqrt{31461}}{220}$ (≈ 0.06), then

$$(Hu, \bar{\delta}_x^2 u) \leq -\varepsilon_1 |u|_1^2, \quad (8.17)$$

where ρ_1 is the same as in Lemma 4.3.

•

$$\|u\|_\infty \leq \frac{\sqrt{L}}{2} |u|_1. \quad (8.18)$$

Now, we are ready to give *a priori estimate* of a solution of the numerical scheme (8.12) with *zero boundary conditions*, i.e.,

$$\begin{cases} \sum_{i=0}^k \lambda_i^* \mathcal{H} u_m^{k-i} = d \bar{\delta}_x^2 u_m^k + \mathcal{H} f_m^k, & 1 \leq m \leq M-1 \\ u_m^0 = 0, & 0 \leq m \leq M \\ u_0^k = u_M^k = 0, & 0 \leq k \leq K. \end{cases} \quad (8.19)$$

Theorem 8.1. (A priori estimate) Suppose that $0 < \kappa < \kappa_0$. Let $\{u_m^k\}$ be a solution of the linear system (8.19). Then, we have

$$\tau \sum_{i=1}^k \|u^i\|_\infty^2 \leq \left(\frac{61}{60}\right)^2 \frac{L^3 T}{16\varepsilon_1^2 d^2} \max_{1 \leq k \leq K} \|\mathcal{H} f^k\|^2 + \frac{L}{2\varepsilon_1 d} \tau \lambda_0^* \|\mathcal{H} u^0\|^2, \quad 1 \leq k \leq K \quad (8.20)$$

where $\tau \lambda_0^* = \tau \frac{1}{J} \sum_{j=1}^J \frac{1}{\tau^{\gamma_j}} \mathcal{D}(\gamma_j) \lambda_0^{\gamma_j} = O\left(\frac{1}{|\ln(\tau)|}\right)$ is given in [39].

Proof. We multiply both sides of the first equation in (8.19) $|_{k=n}$ by $\tau h \mathcal{H} u_m^n$, then sum over j from 1 to $(M-1)$, and sum over n from 1 to k , to get

$$\tau \sum_{n=1}^k \sum_{i=0}^n \lambda_i^* (\mathcal{H} u^{n-i}, \mathcal{H} u^n) = \tau d \sum_{n=1}^k (\mathcal{H} u^n, \bar{\delta}_x^2 u^n) + \tau \sum_{n=1}^k (\mathcal{H} u^n, \mathcal{H} f^n). \quad (8.21)$$

Using Lemma 8.2 and Remark 8.2, we see that the left side of (8.21) satisfies

$$\begin{aligned} \tau \sum_{n=1}^k \sum_{i=0}^n \lambda_i^* (\mathcal{H} u^{n-i}, \mathcal{H} u^n) &= \tau \sum_{n=0}^k \sum_{i=0}^n \lambda_i^* (\mathcal{H} u^{n-i}, H u^n) - \tau \lambda_0 \|\mathcal{H} u^0\|^2 \\ &\geq -\tau \lambda_0 \|\mathcal{H} u^0\|^2. \end{aligned} \quad (8.22)$$

Next, applying the inequality (8.17) to the first term on the right side of (8.21) yields

$$\tau d \sum_{n=1}^k (\mathcal{H} u^n, \bar{\delta}_x^2 u^n) \leq -\varepsilon_1 \tau d \sum_{n=1}^k |u^n|_1^2. \quad (8.23)$$

To estimate the second term on the right side of (8.21), using Young's inequality, (8.16) and (8.18) successively, we get for any constant $c > 0$,

$$\begin{aligned}
\tau \sum_{n=1}^k (\mathcal{H}u^n, \mathcal{H}f^n) &\leq \frac{\tau}{4c} \sum_{n=1}^k \|\mathcal{H}f^n\|^2 + c\tau \sum_{n=1}^k \|\mathcal{H}u^n\|^2 \\
&\leq \frac{\tau}{4c} \sum_{n=1}^k \|\mathcal{H}f^n\|^2 + c\tau \left(\frac{61}{60}\right)^2 \sum_{n=1}^k \|u^n\|^2 \\
&\leq \frac{\tau}{4c} \sum_{n=1}^k \|\mathcal{H}f^n\|^2 + \frac{cL^2}{4} \left(\frac{61}{60}\right)^2 \tau \sum_{n=1}^k |u^n|_1^2.
\end{aligned} \tag{8.24}$$

Now, deploying the inequalities (8.22)–(8.24) in equation (8.21), we find, after some manipulation,

$$\left(\varepsilon_1 d - \frac{cL^2}{4} \left(\frac{61}{60}\right)^2 \right) \tau \sum_{n=1}^k |u^n|_1^2 \leq \frac{\tau}{4c} \sum_{n=1}^k \|\mathcal{H}f^n\|^2 + \tau \lambda_0^* \|\mathcal{H}u^0\|^2. \tag{8.25}$$

In (8.25), let $c = \left(\frac{60}{61}\right)^2 \frac{2}{L^2} \varepsilon_1 d$ and apply (8.18) to $|u^n|_1^2$. It follows that

$$\begin{aligned}
\tau \sum_{n=1}^k \|u^n\|_\infty^2 &\leq \left(\frac{61}{60}\right)^2 \frac{L^3}{16\varepsilon_1^2 d^2} k\tau \max_{1 \leq k \leq K} \|\mathcal{H}f^k\|^2 + \frac{L}{2\varepsilon_1 d} \tau \lambda_0^* \|\mathcal{H}u^0\|^2 \\
&\leq \left(\frac{61}{60}\right)^2 \frac{L^3 T}{16\varepsilon_1^2 d^2} \max_{1 \leq k \leq K} \|\mathcal{H}f^k\|^2 + \frac{L}{2\varepsilon_1 d} \tau \lambda_0^* \|\mathcal{H}u^0\|^2,
\end{aligned} \tag{8.26}$$

where we have used $k\tau \leq T$ in the last inequality. This completes the proof. $\square$

We are now in a position to analyze the solvability, stability and convergence of the proposed numerical scheme (8.12). Let us first show that (8.12) always admits a unique solution at each time level.

Theorem 8.2. (Solvability) *The numerical scheme (8.12) is uniquely solvable at each time level $t = t_k$ for any $\kappa \in (0, \kappa_0)$.*

Proof. Since the numerical scheme (8.12) is actually a linear system, it suffices to show that the corresponding homogeneous system

$$\begin{cases} \sum_{i=0}^k \lambda_i^* \mathcal{H} u_m^{k-i} = d \bar{\delta}_x^2 u_m^k, & 1 \leq m \leq M-1 \\ u_m^0 = 0, & 0 \leq m \leq M \\ u_0^k = u_M^k = 0, & 0 \leq k \leq K \end{cases} \quad (8.27)$$

has only the trivial solution $u_m^k = 0$, $0 \leq m \leq M$, $0 \leq k \leq K$.

Applying Theorem 8.1 to the linear system (8.27), we see that a solution of (8.27) satisfies for $1 \leq k \leq K$

$$\tau \sum_{i=1}^k \|u^i\|_\infty^2 \leq \left(\frac{61}{60}\right)^2 \frac{L^3 T}{16 \varepsilon_1^2 d^2} \max_{1 \leq k \leq K} \|\mathcal{H} f^k\|^2 + \frac{L}{2 \varepsilon_1 d} \tau \lambda_0^* \|\mathcal{H} u^0\|^2. \quad (8.28)$$

Since $f = 0$ and $u_m^0 = 0$, $0 \leq m \leq M$, it follows from (8.28) that $\|u^k\|_\infty^2 = 0$, $1 \leq k \leq K$ which leads to $u_m^k = 0$, $0 \leq m \leq M$, $0 \leq k \leq K$. The proof is complete. $\square$

Theorem 8.3. (Stability) *The numerical scheme (8.12) depends continuously on the initial and non-homogeneous data for any $\kappa \in (0, \kappa_0)$.*

Proof. It is a direct result of Theorem 8.1. $\square$

Let $U(x, t)$ be the exact solution of the distributed order fractional sub-diffusion problem (8.1) and $\{u_j^k\}$ be the numerical solution obtained from the scheme (8.12). Let $e_m^k = U(x_m, t_k) - u_m^k$ be the error at (x_m, t_k) . The next result gives the convergence of the numerical scheme (8.12).

Theorem 8.4. (Convergence) *Suppose that $U(x, t) \in \mathcal{C}^{8,4}([0, L] \times [0, T])$ and $\kappa \in (0, \kappa_0)$. Then, we have*

$$\sqrt{\tau \sum_{i=1}^k \|e^i\|_\infty^2} = O(\tau^2 + h^{4.5} + \eta^2), \quad 1 \leq k \leq K \quad (8.29)$$

where $\tau = \frac{T}{K}$, $h = \frac{L}{M}$ and $\eta = \frac{1}{J}$ are the step sizes in time, space and distributed order respectively.

Proof. Since $U(x, t)$ is the exact solution of the problem (8.1), it follows that

$$\begin{cases} \sum_{i=0}^k \lambda_i^* \mathcal{H} U_m^{k-i} = d \bar{\delta}_x^2 U_m^k + \mathcal{H} f_m^k + T_m^k, & 1 \leq m \leq M-1 \\ U_m^0 = 0, & 0 \leq m \leq M \\ U_0^k = \phi_1(t_k), & U_M^k = \phi_2(t_k), \quad 0 \leq k \leq K \end{cases} \quad (8.30)$$

where T_m^k denotes the local truncation error incurred from the numerical scheme.

From (8.12) and (8.30), it is clear that

$$\begin{cases} \sum_{i=0}^k \lambda_i^* \mathcal{H} e_m^{k-i} = d \bar{\delta}_x^2 e_m^k + T_m^k, & 1 \leq m \leq M-1 \\ e_m^0 = 0, & 0 \leq m \leq M \\ e_0^k = e_M^k = 0, & 0 \leq k \leq K. \end{cases} \quad (8.31)$$

Applying Theorem 8.1 to the above system (8.31), we find, noting that $e^0 = 0$,

$$\begin{aligned} \tau \sum_{i=1}^k \|e^i\|_\infty^2 &\leq \left(\frac{61}{60}\right)^2 \frac{L^3 T}{16 \varepsilon_1^2 d^2} \max_{1 \leq k \leq K} \|T^k\|^2 + \frac{L}{2 \varepsilon_1 d} \tau \lambda_0^* \|\mathcal{H} e^0\|^2 \\ &= \left(\frac{61}{60}\right)^2 \frac{L^3 T}{16 \varepsilon_1^2 d^2} \max_{1 \leq k \leq K} \|T^k\|^2. \end{aligned} \quad (8.32)$$

On the other hand, using (8.2), (8.3), (8.7), it is obvious that

$$T_m^k = \begin{cases} O(\tau^2 + h^4 + \eta^2), & m = 1, M-1 \\ O(\tau^2 + h^6 + \eta^2), & 2 \leq m \leq M-2. \end{cases} \quad (8.33)$$

Therefore, we have

$$\begin{aligned} \max_{1 \leq k \leq K} \|T^k\|^2 &= \max_{1 \leq k \leq K} h \sum_{m=1}^{M-1} (T_m^k)^2 \\ &\leq 2hC_1 (\tau^2 + h^4 + \eta^2)^2 + (M-3)hC_2 (\tau^2 + h^6 + \eta^2)^2 \\ &\leq 2hC_1 (\tau^2 + h^4 + \eta^2)^2 + LC_2 (\tau^2 + h^6 + \eta^2)^2 \\ &\leq C (\tau^2 + h^{4.5} + \eta^2)^2, \end{aligned} \quad (8.34)$$

where C_1 , C_2 and C are some positive constants.

The error estimate (8.29) is immediate upon substituting (8.34) into (8.32). $\square$

Remark 8.3. The error estimate (8.29) implies immediately that the average maximum error

$$\frac{1}{K} \sum_{k=1}^K \|e^k\|_{\infty} = O(\tau^2 + h^{4.5} + \eta^2), \quad (8.35)$$

since

$$\begin{aligned} \frac{1}{K} \sum_{k=1}^K (\|e^k\|_{\infty} \cdot 1) &\leq \frac{1}{K} \sqrt{\left(\sum_{k=1}^K \|e^k\|_{\infty}^2 \right) \left(\sum_{k=1}^K 1^2 \right)} = \sqrt{\frac{1}{K} \sum_{k=1}^K \|e^k\|_{\infty}^2} \\ &= \frac{1}{\sqrt{T}} \sqrt{\tau \sum_{k=1}^K \|e^k\|_{\infty}^2}. \end{aligned}$$

Remark 8.4. The error estimate (8.29) in Theorem 8.4 (or (8.35)) indicates that the numerical scheme (8.12) achieves a spatial convergence order of $O(h^{4.5})$ – this is *higher* than $O(h^4)$ attained by the CFD method [39].

Remark 8.5. The error estimate (8.29) (or (8.35)) is not a tight one. Indeed, it is possible to obtain even higher spatial convergence order in practice. This is illustrated in the numerical experiment in the next section.

8.3 Numerical Experiment

In this section, we shall demonstrate the efficiency of the proposed numerical scheme (8.12). To this aim, in the examples we shall present the E_{∞} and E_2 errors given respectively by

$$E_{\infty}(\tau, h, \eta) = \max_{1 \leq k \leq K} \|e^k\|_{\infty}, \quad E_2(\tau, h, \eta) = \sqrt{\tau \sum_{k=1}^K \|e^k\|_{\infty}^2}, \quad (8.36)$$

and also the corresponding convergence orders in distributed order, time and space, computed as

$$\begin{aligned}\mathbb{O}_{dist,\infty} &= \log_2 \frac{E_\infty(\tau, h, \eta)}{E_\infty(\tau, h, \frac{\eta}{2})}, & \mathbb{O}_{dist,2} &= \log_2 \frac{E_2(\tau, h, \eta)}{E_2(\tau, h, \frac{\eta}{2})}, \\ \mathbb{O}_{t,\infty} &= \log_2 \frac{E_\infty(\tau, h, \eta)}{E_\infty(\frac{\tau}{2}, h, \eta)}, & \mathbb{O}_{t,2} &= \log_2 \frac{E_2(\tau, h, \eta)}{E_2(\frac{\tau}{2}, h, \eta)}, \\ \mathbb{O}_{x,\infty} &= \log_2 \frac{E_\infty(\tau, h, \eta)}{E_\infty(\tau, \frac{h}{2}, \eta)}, & \mathbb{O}_{x,2} &= \log_2 \frac{E_2(\tau, h, \eta)}{E_2(\tau, \frac{h}{2}, \eta)}.\end{aligned}\tag{8.37}$$

Note that Theorem 8.4 shows the convergence in terms of E_2 error, nonetheless it would also be interesting to see the E_∞ error and the corresponding convergence.

Moreover, we shall compare the proposed PQS approach employed in the numerical scheme (8.12) with CFD method which is used in [39]. To have a proper comparison, we shall implement the same technique for the distributed order term while employing either PQS method or CFD method in the spatial dimension.

In the examples, we shall fix $\kappa = \frac{1}{20}$ for all calculations. The first example is modified from Example 5.2 in [39] where a two-dimensional case is considered.

Example 8.1. [39] Consider problem (8.1) with $d = L = 1$, $T = 0.5$, $\mathcal{D}(\gamma) = \Gamma(5 - \gamma)$ and

$$\phi_1(t) = 16t^4, \quad \phi_2(t) = 16e^{-1}t^4, \quad f(x, t) = 32 \left[\frac{12(t^4 - t^3)}{\ln(t)} - t^4 \right] e^{-x} + 16t^4 e^{-x}.$$

The exact solution is $u(x, t) = 16t^4 e^{-x}$.

First, we fix $(\tau, h) = (\frac{0.5}{10000}, \frac{1}{200})$ and vary η . In Table 8.1, the E_∞ and E_2 errors and the corresponding convergence orders in distributed order are presented. We observe that $O(\eta^2)$ is obtained thus confirming the theoretical result (Theorem 8.4). Then, we check the convergence in time. Let $(h, \eta) = (\frac{1}{200}, \frac{1}{2000})$ and τ vary. The numerical results are displayed in Table 8.2. It is seen that $O(\tau^2)$ is achieved thus confirming the theoretical result (Theorem 8.4).

Now we shall compare the accuracy of the PQS method proposed in the scheme (8.12) with CFD method [39]. As noted earlier, we shall implement the same technique for the distributed order term while employing either PQS method or

TABLE 8.1: (Example 8.1) Convergence order in distributed order

η	$E_\infty(\tau, h, \eta)$	$\mathbb{O}_{dist,\infty}$	$E_2(\tau, h, \eta)$	$\mathbb{O}_{dist,2}$
$\frac{1}{2}$	4.08E-03	-	1.34E-03	-
$\frac{1}{4}$	1.03E-03	1.9895	3.38E-04	1.9897
$\frac{1}{8}$	2.58E-04	1.9973	8.47E-05	1.9974

TABLE 8.2: (Example 8.1) Convergence order in temporal dimension

τ	$E_\infty(\tau, h, \eta)$	$\mathbb{O}_{t,\infty}$	$E_2(\tau, h, \eta)$	$\mathbb{O}_{t,2}$
$\frac{0.5}{10}$	8.94E-03	-	3.27E-03	-
$\frac{0.5}{20}$	2.36E-03	1.9208	8.31E-04	1.9765
$\frac{0.5}{40}$	6.06E-04	1.9612	2.09E-04	1.9886

CFD method in the spatial dimension. In Table 8.3, we fix $(\tau, \eta) = (\frac{0.5}{80000}, \frac{1}{20000})$ and let h vary. The numerical results show that

- (a) the numerical solution obtained from the scheme (8.12) achieves smaller errors and higher spatial convergence order than the CFD method;
- (b) the PQS scheme gives at least $O(h^{4.5})$ while the CFD method obtains $O(h^4)$ in regards to both E_∞ and E_2 errors, thus confirming the theoretical result;
- (c) as indicated in Remark 8.5, the spatial convergence of the scheme (8.12) can be higher than the theoretical $O(h^{4.5})$ in practice.

TABLE 8.3: (Example 8.1) Convergence order in spatial dimension

h	E_∞ error				E_2 error			
	PQS	$\mathbb{O}_{x,\infty}$	CFD	$\mathbb{O}_{x,\infty}$	PQS	$\mathbb{O}_{x,2}$	CFD	$\mathbb{O}_{x,2}$
$\frac{1}{4}$	2.14E-07	-	2.54E-07	-	4.86E-08	-	5.73E-08	-
$\frac{1}{8}$	6.66E-09	5.007	1.62E-08	3.973	1.53E-09	4.994	3.61E-09	3.988
$\frac{1}{16}$	1.78E-10	5.230	8.32E-10	4.284	6.21E-11	4.620	1.72E-10	4.396

Next, we investigate the effect of κ in the numerical scheme (8.12). Let $(\tau, h, \eta) = (\frac{0.5}{10000}, \frac{1}{4}, \frac{1}{200})$. For $\kappa \in (0, \kappa_0)$, in steps of 0.0005, we compute the E_∞ and E_2 errors. The results are shown in Figure 8.1. We observe that different choices of κ do result in different errors but the difference is very small. Therefore, κ does not have a profound influence on the theoretical and practical results.

Finally, for visualization, the numerical solution obtained from (8.12), the exact solution as well as the absolute error when $(\tau, h, \eta) = (\frac{0.5}{80000}, \frac{1}{4}, \frac{1}{20000})$ are plotted in Figures 8.2 and 8.3. It is obvious that the scheme (8.12) can provide a good approximation to the exact solution.

FIGURE 8.1: (Example 8.1) E_2 and E_∞ errors for $\kappa \in (0, \kappa_0)$

FIGURE 8.2: (Example 8.1) Approximate solution by (8.12) and exact solution when $\tau = \frac{0.5}{80000}$, $h = \frac{1}{4}$, $\eta = \frac{1}{20000}$

Example 8.2. [14] Consider problem (8.1) with $d = 2$, $L = T = 0.5$, $\mathcal{D}(\gamma) = \Gamma(5 - \gamma)$, $\phi_1(t) = \phi_2(t) = 0$ and

$$f(x, t) = 2400 \frac{t^4 - t^3}{\ln t} \sin(2\pi x) + 800\pi^2 t^4 \sin(2\pi x).$$

The exact solution is $u(x, t) = 100t^4 \sin(2\pi x)$.

In this example, we shall focus on illustrating the improvement in the spatial convergence order achieved by the PQS method in the scheme (8.12). For this purpose, we fix $(\tau, \eta) = (\frac{0.5}{80000}, \frac{1}{20000})$ and vary h . In Table 8.4, we present the

FIGURE 8.3: (Example 8.1) Absolute error when $\tau = \frac{0.5}{80000}$, $h = \frac{1}{4}$, $\eta = \frac{1}{20000}$

E_∞ and E_2 errors as well as the corresponding spatial convergence orders for both PQS and CFD methods. We observe that the PQS method gives at least $O(h^{4.5})$ while the CFD method obtains $O(h^4)$ in regards to both E_∞ and E_2 errors. Also, the PQS method always achieves a higher accuracy than the CFD method which indicates a better performance in practice.

TABLE 8.4: (Example 8.2) Convergence order in spatial dimension

h	E_∞ error				E_2 error			
	PQS	$\mathbb{O}_{x,\infty}$	CFD	$\mathbb{O}_{x,\infty}$	PQS	$\mathbb{O}_{x,2}$	CFD	$\mathbb{O}_{x,2}$
$\frac{0.5}{4}$	3.00E-03	-	7.01E-03	-	6.95E-04	-	1.62E-03	-
$\frac{0.5}{8}$	3.03E-05	6.628	4.30E-04	4.026	7.08E-06	6.617	9.93E-05	4.026
$\frac{0.5}{16}$	2.65E-07	6.839	2.68E-05	4.007	6.21E-08	6.833	6.18E-06	4.007

Further, the influence of κ (in (8.12)) on the errors is shown in Figure 8.4. Here, we fix $(\tau, h, \eta) = (\frac{0.5}{10000}, \frac{0.5}{4}, \frac{1}{200})$ and calculate the errors for $\kappa \in (0, \kappa_0)$ in steps of 0.0005. It is observed that κ does influence the errors, however it does not make a dominant difference.

Finally, in Figures 8.5 and 8.6 we plot the numerical solution obtained by (8.12), the exact solution as well as the absolute error. The numerical solution is seen to approximate the exact solution very accurately.

FIGURE 8.4: (Example 8.2) E_2 and E_∞ errors for $\kappa \in (0, \kappa_0)$ FIGURE 8.5: (Example 8.2) Approximate solution by (8.12) and exact solution when $\tau = \frac{0.5}{80000}$, $h = \frac{0.5}{8}$, $\eta = \frac{1}{20000}$ FIGURE 8.6: (Example 8.2) Absolute error when $\tau = \frac{0.5}{80000}$, $h = \frac{0.5}{8}$, $\eta = \frac{1}{20000}$

8.4 Summary

For a distributed order fractional sub-diffusion problem, we have proposed an efficient numerical scheme using mid-point quadrature, WSGL approximation and parametric quintic spline operator. The solvability, stability and convergence are analyzed rigorously using the well known energy methodology. To demonstrate both efficiency and accuracy of the constructed scheme, simulation is carried out. It is shown that the numerical results are consistent with the theoretical ones, and the spatial accuracy clearly *improves* that achieved by CFD method.

Part II

Non-uniform Mesh Method

Chapter 9

New Generalized Fractional Sub-diffusion Problems I

In this chapter, we shall develop an efficient numerical scheme for the new generalized fractional sub-diffusion equation that is first studied in [130]

$$\begin{cases} {}_0^C D_{t;[\mathcal{Z},\mathcal{W}]}^\gamma u(x,t) = du_{xx}(x,t) + f(x,t), & (x,t) \in (0,L) \times (0,T) \\ u(x,0) = \psi(x), & x \in (0,L) \\ u(0,t) = \phi_1(t), \quad u(L,t) = \phi_2(t), & t \in (0,T) \end{cases} \quad (9.1)$$

where $0 < \gamma < 1$ is the fractional order, $d(> 0)$ is the diffusion constant and $\phi_1(t)$, $\phi_2(t)$ and $f(x,t)$ are continuous functions in corresponding domain. The generalized Caputo fractional derivative ${}_0^C D_{t;[\mathcal{Z},\mathcal{W}]}^\gamma u(x,t)$ is defined in (2.12) as

$${}_0^C D_{t;[\mathcal{Z},\mathcal{W}]}^\gamma u(x,t) = \frac{[\mathcal{W}(t)]^{-1}}{\Gamma(1-\gamma)} \int_0^t \frac{1}{[\mathcal{Z}(t) - \mathcal{Z}(s)]^\gamma} \frac{\partial (\mathcal{W}(s)u(x,s))}{\partial s} ds. \quad (9.2)$$

Though this new generalization of the Caputo or RL fractional integral or derivative brings convenience in expression as stated in [6], it is very challenging to get analytical solutions of related equations unless for some particular problems, e.g. [17, 70, 130]. Therefore, numerical considerations on this kind of problem is extremely important.

There has been some pioneer works on numerical treatment for various generalized fractional problems covering fractional Burgers equation [128], fractional subdiffusion equation [130], fractional advection-diffusion equation [131], generalized van der Pol equation [127] as well as oscillator equation [129]. To my best knowledge, these topics are all new and first discussed therein since the new generalized fractional operator is proposed in [6]. To get these equations, one can simply replace the original fractional operator by this new generalized fractional operator, like in [128, 130, 131] or an even more general operator involving a kernel function, e.g. [5, 127, 129]. The main difficulty in deriving numerical scheme lies in the approximation of the generalized fractional operator. In tackling this problem, a useful approximation that generalizes the classical $L1$ discretization [53] in the sense that it coincides with $L1$ when $\mathcal{W}(t) \equiv 1$ and $\mathcal{Z}(t) = t$, is constructed in [130]. After that, this approximation has been applied successfully to problem in [128, 131]. As for generalized van der Pol equation [127] and oscillator problem [129], they follow a similar procedure to approximate the generalized fractional derivative, that is, using linear approximation to the first derivative of the function in each subinterval and then computing the integral. However, this is not easy in practice if the kernel function is complex.

This chapter will develop a new numerical scheme for the equivalent generalized fractional problem (9.1) using a generalized weighted shifted Grünwald-Letnikov (gWSGL) method in Section 9.1. Then, we shall establish a priori estimate of solution of (9.1) with zero boundary conditions through energy methodology in Section 9.2 and thereafter analyze the stability and convergence using this estimate in Section 9.3. Next, in Section 9.4, the numerical results are presented to demonstrate the efficiency and accuracy of the proposed numerical scheme. Finally, we end with a brief conclusion in Section 9.5.

9.1 Numerical Scheme

From the definition (9.2), we can multiply both sides of (9.1) by $\mathcal{W}(t)$ and solve $\mathcal{W}(t)u(x, t)$ first. Also, we can just consider $\psi(x) \equiv 0$ for simplicity as it is always possible to use

$$v(x, t) = \mathcal{W}(t)u(x, t) - \mathcal{W}(0)\psi(x)$$

to transform (9.1) into an equivalent problem with zero initial condition. Therefore, in this chapter, it is sufficient to derive a new numerical algorithm for problem (9.1) when $\mathcal{W}(t) \equiv 1$ and $\psi(x) \equiv 0$.

To begin, denote $\mathcal{Z} : t \rightarrow \mathcal{Z}(t)$ as a mapping function from $[0, T]$ to $[\mathcal{Z}(0), \mathcal{Z}(T)]$ such that

$$\mathcal{Z}(t) = \mathcal{Z}(t)$$

where $\mathcal{Z}(t)$ is a strictly increasing function and let P be the uniform mesh of $[0, L]$ and

$$\mathcal{P}'' : 0 = t_0 < t_1 < \cdots < t_{K-1} < t_K = T,$$

be a mesh of $[0, T]$ such that $\mathcal{Z}(t_k) - \mathcal{Z}(t_{k-1})$, $1 \leq k \leq K$ is a constant denoted by τ_z .

Next, we shall develop a gWSGL approximation for the generalized Caputo fractional derivative (9.2) when $\mathcal{W}(t) \equiv 1$. For this purpose, we need the result that relates a subspace of C^{2+m} to $\mathcal{C}^{\gamma+m}$ below.

Lemma 9.1. [39, 121, 147] *If $\gamma \in (0, 1)$, $\phi(t) \in C^{2+m}(\mathcal{R})$ and $\phi^{(i)}(t) \in L_1(\mathcal{R})$ for $0 \leq i \leq m + 2$, then we have $\phi(t) \in \mathcal{C}^{\gamma+m}(\mathcal{R})$.*

Now, we can derive gWSGL approximation.

Lemma 9.2. (gWSGL) *If $u(\cdot, \mathcal{Z}^{-1}(z)) = \bar{u}(\cdot, z) \in C^4[\mathcal{Z}(0), \mathcal{Z}(T)]$, $u(x, 0) = 0$ and $\frac{\partial^i \bar{u}(x, \mathcal{Z}(0))}{\partial z^i} = 0, i = 0, 1, 2, 3, 4$, the approximation of generalized Caputo fractional derivative (9.2) at (x_m, t_k) is given by*

$${}_0^C D_{t;[\mathcal{Z}, 1]}^\gamma u(x_m, t_k) = \frac{\gamma - 2l}{2(\hat{l} - l)} \mathcal{G}_l^\gamma u_m^k + \frac{2\hat{l} - \gamma}{2(\hat{l} - l)} \mathcal{G}_l^\gamma u_m^k + O(\tau_z^2), \quad (9.3)$$

where $\hat{l}$, l are integers and $\hat{l} \neq l$, $\tau_z = \frac{z(T) - z(0)}{K}$ is the step size and

$$\mathcal{G}_l^\gamma u_m^k = \tau_z^{-\gamma} \sum_{j=0}^{k+l} \omega_j^\gamma u_m^{k+l-j}, \quad (9.4)$$

and $\omega_0^\gamma = 1$, $\omega_j^\gamma = \left(1 - \frac{\gamma+1}{j}\right) \omega_{j-1}^\gamma$, $j \geq 1$.

Proof. To prove it, we first extend $u(x, \mathcal{Z}^{-1}(z)) = \bar{u}(x, z)$ as follows:

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

where $\Psi(z)$ can be carefully chosen such that $\bar{u}_e(x, z) \in \mathcal{C}^4(\mathcal{R})$ for any given x . Actually, we can apply Hermite interpolation to get a $\Psi(z)$ to ensure the continuity at $z = \mathcal{Z}(T)$ and $z = 2\mathcal{Z}(T)$. Obviously, $\bar{u}_e(x, z) \in L_1(\mathcal{R})$. Also, using Lemma 9.1, we get $\bar{u}_e(x, z) \in \mathcal{C}^{\gamma+2}(\mathcal{R})$. Therefore, $\bar{u}_e(x, z) \in L_1(\mathcal{R}) \cap \mathcal{C}^{\gamma+2}(\mathcal{R})$.

Noticing that $P_z'' : \mathcal{Z}(0) = z_0 < z_1 < \dots < z_{K-1} < z_K = \mathcal{Z}(T)$ is the uniform mesh of $[\mathcal{Z}(0), \mathcal{Z}(T)]$ with step size $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{K}$ and then applying Lemma 2.6 in Chapter 2, we obtain

$${}^{RL}_{-\infty} D_z^\gamma \bar{u}_e(x_m, z_k) = \frac{\gamma - 2l}{2(\hat{l} - l)} \mathcal{A}_{\tau_z, \hat{l}}^\gamma \bar{u}_e(x_m, z_k) + \frac{2\hat{l} - \gamma}{2(\hat{l} - l)} \mathcal{A}_{\tau_z, l}^\gamma \bar{u}_e(x_m, z_k) + O(\tau_z^2). \quad (9.5)$$

Since $\bar{u}_e(x, z) = 0$ for $z < \mathcal{Z}(0)$ and $u(x, \mathcal{Z}^{-1}(z)) = \bar{u}(x, z)$, from the definition (9.2), we have

$${}^{RL}_{-\infty} D_z^\gamma \bar{u}_e(x_m, z_k) = {}^{RL}_{z_0} D_z^\gamma \bar{u}(x_m, z_k) = {}^{RL}_0 D_{t; [\mathcal{Z}, 1]}^\gamma u(x_m, t_k), \quad (9.6)$$

and

$$\mathcal{A}_{\tau_z, l}^\gamma \bar{u}_e(x_m, z_k) = \tau_z^{-\gamma} \sum_{j=0}^{k+l} \omega_j^\gamma \bar{u}(x_m, z_{k+l-j}) = \tau_z^{-\gamma} \sum_{j=0}^{k+l} \omega_k^\gamma u(x_m, t_{k+l-j}) = \mathcal{G}_l^\gamma u_m^k. \quad (9.7)$$

Since $u(x, 0) = 0$, the approximation (9.3) follows directly from (9.6), (9.7) and Lemma 2.2. $\square$

Remark 9.1. In practice, we take $(\hat{l}, l) = (0, -1)$ or $(-1, 0)$ for the reason that we have to solve the linear system iteratively. In this case, (9.3) becomes

$${}^C_0 D_{t; [\mathcal{Z}, 1]}^\gamma u(x_m, t_k) = \tau_z^{-\gamma} \sum_{j=0}^k \lambda_j^\gamma u_m^{k-j} + O(\tau_z^2), \quad (9.8)$$

where λ_j^γ 's are similarly defined as in (8.4)

$$\lambda_0^\gamma = \frac{\gamma+2}{2}\omega_0^\gamma, \quad j = 0, \quad \lambda_j^\gamma = \frac{\gamma+2}{2}\omega_j^\gamma - \frac{\gamma}{2}\omega_{j-1}^\gamma, \quad j \geq 1. \quad (9.9)$$

Now, we are ready to derive our numerical scheme for the problem (9.1) using approximation (9.8) which gives $O(\tau_z^2)$ in temporal and finite difference method which obtains $O(h^2)$. Considering the discretization of (9.1) at (x_m, t_k) , we shall get

$${}_0^C D_{t;[\mathcal{Z},1]}^\gamma u(x_m, t_k) = du_{xx}(x_m, t_k) + f(x_m, t_k). \quad (9.10)$$

Using formula (9.3) and the classical finite difference method

$$u_{xx}(x_m, t_k) = \delta_x^2 u_m^k + O(h^2), \quad (9.11)$$

in (9.10), we shall achieve the scheme below after omitting small terms

$$\left\{ \begin{array}{l} \tau_z^{-\gamma} \sum_{j=0}^k \lambda_j^\gamma u_m^{k-j} = d\delta_x^2 u_m^k + f_m^k, \quad 1 \leq m \leq M-1 \\ u_m^0 = 0, \quad 0 \leq m \leq M \\ u_0^k = \phi_1(t_k), \quad u_M^k = \phi_2(t_k), \quad 1 \leq k \leq K \end{array} \right. \quad (9.12)$$

where $0 < \gamma < 1$, $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{K}$, $f_m^k = f(x_m, t_k)$ and λ_j^γ is defined in (9.9).

Remark 9.2. The proposed numerical scheme (9.12) has a unique solution at each time level $t = t_k$, $1 \leq k \leq K$ since the coefficient matrix is strictly diagonally dominated.

9.2 A Priori Estimate

In this section, we shall analyze the numerical scheme (9.12) with $u_0^k = u_M^k = 0$ and then establish a priori estimate of the solution which is used to derive the stability and convergence of (9.12). To this aim, we need Lemma 8.2, Lemma 3.3 and the relation between $|u|_1$ and $\|u\|$ below.

Lemma 9.3. [57] For $u \in \mathcal{U}_P$, we have

$$\|u\| \leq \frac{L}{\sqrt{6}}|u|_1. \quad (9.13)$$

Now, we shall analyze the solution of the proposed scheme (9.12) with $u_0^k = u_M^k = 0$, that is,

$$\begin{cases} \tau_z^{-\gamma} \sum_{j=0}^k \lambda_j^\gamma u_m^{k-j} = d\delta_x^2 u_m^k + f_m^k, & 1 \leq m \leq M-1 \\ u_m^0 = 0, & 0 \leq m \leq M \\ u_0^k = 0, & u_M^k = 0, \quad 1 \leq k \leq K. \end{cases} \quad (9.14)$$

In fact, we get

Theorem 9.1. The solution $\{u_m^k\}$ of the numerical scheme (9.14) satisfies for $1 \leq k \leq K$ that

$$\tau_z \sum_{j=1}^k \|u^j\|_\infty \leq \sqrt{[\mathcal{Z}(T) - \mathcal{Z}(0)] \left[\frac{\tau_z L^3}{24d^2} \sum_{j=1}^k \|f^j\|^2 + \tau_z^{1-\gamma} \frac{\lambda_0^\gamma L}{2d} \|u^0\|^2 \right]}, \quad (9.15)$$

where $0 < \gamma < 1$, $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{K}$, $\lambda_0^\gamma = \frac{\gamma+2}{2}$ and d is the diffusion constant.

Proof. Multiplying both sides of the first equation in (9.14) $|_{k=n}$ by hu_m^n , then getting the summation for $1 \leq m \leq M-1$ and $1 \leq n \leq k$, we get

$$\tau_z^{-\gamma} \sum_{n=1}^k \sum_{j=0}^n \lambda_j^\gamma (u^{n-j}, u^n) = d \sum_{n=1}^k (\delta_x^2 u^n, u^n) + \sum_{n=1}^k (f^n, u^n), \quad (9.16)$$

or equivalently

$$\tau_z^{-\gamma} \sum_{n=0}^k \sum_{j=0}^n \lambda_j^\gamma (u^{n-j}, u^n) = d \sum_{n=1}^k (\delta_x^2 u^n, u^n) + \sum_{n=1}^k (f^n, u^n) + \tau_z^{-\gamma} \lambda_0^\gamma \|u^0\|^2. \quad (9.17)$$

Applying Lemma 8.2 to the first term in the left side of formula (9.17) gives

$$\tau_z^{-\gamma} \sum_{n=0}^k \sum_{j=0}^n \lambda_j^\gamma (u^{n-j}, u^n) \geq 0. \quad (9.18)$$

Noticing that $u_0^n = u_M^n = 0$, obviously we have $u^n \in \mathcal{U}_P$. Therefore, by simple calculation, it is found that $(\delta_x^2 u^n, u^n) = -|u^n|_1^2$. Substituting this result and (9.18) into (9.17), we have

$$d \sum_{n=1}^k |u^n|_1^2 \leq \sum_{n=1}^k (f^n, u^n) + \tau_z^{-\gamma} \lambda_0^\gamma (u^0, u^0). \quad (9.19)$$

Next, using Young's inequality with $\varepsilon > 0$ and the inequality in (9.13) of Lemma 9.3, it is found that

$$(f^n, u^n) \leq \frac{\varepsilon}{2} \|f^n\|^2 + \frac{1}{2\varepsilon} \|u^n\|^2 \leq \frac{\varepsilon}{2} \|f^n\|^2 + \frac{1}{2\varepsilon} \frac{L^2}{6} |u^n|_1^2.$$

Setting $\varepsilon = \frac{L^2}{6d}$, we shall further obtain

$$(f^n, u^n) \leq \frac{L^2}{12d} \|f^n\|^2 + \frac{d}{2} |u^n|_1^2. \quad (9.20)$$

Substituting (9.20) into (9.19) and applying the result of Lemma 3.3, it is achieved that

$$\tau_z \sum_{n=1}^k \|u^n\|_\infty^2 \leq \frac{\tau_z L^3}{24d^2} \sum_{n=1}^k \|f^n\|^2 + \tau_z^{1-\gamma} \frac{\lambda_0^\gamma L}{2d} \|u^0\|^2, \quad 1 \leq k \leq K. \quad (9.21)$$

Finally, applying Cauchy-Schwarz inequality gives

$$\begin{aligned} \left(\tau_z \sum_{n=1}^k \|u^n\|_\infty \right)^2 &\leq \left(\tau_z \sum_{n=1}^k 1 \right) \left(\tau_z \sum_{n=1}^k \|u^n\|_\infty^2 \right) \\ &\leq [\mathcal{Z}(T) - \mathcal{Z}(0)] \left[\frac{\tau_z L^3}{24d^2} \sum_{n=1}^k \|f^n\|^2 + \tau_z^{1-\gamma} \frac{\lambda_0^\gamma L}{2d} \|u^0\|^2 \right], \end{aligned} \quad (9.22)$$

which completes the proof. $\square$

9.3 Stability and Convergence

Using the priori estimate established in (9.15), we can proceed to analyze the stability and convergence of the proposed numerical scheme (9.12) rigorously in

this section. Let us start with the analysis of stability of the scheme (9.12).

Suppose $\{u_m^k\}$ is the numerical solution of the numerical scheme (9.12) while $\{v_m^k\}$ is the solution of the corresponding perturbed system

$$\begin{cases} \tau_z^{-\gamma} \sum_{j=0}^k \lambda_j^\gamma v_m^{k-j} = d\delta_x^2 v_m^k + \bar{f}_j^n, & 1 \leq m \leq M-1 \\ v_m^0 = -\theta_m, & 0 \leq m \leq M \\ v_0^k = \phi_1(t_k), \quad v_M^k = \phi_2(t_k), & 1 \leq k \leq K \end{cases} \quad (9.23)$$

where $\theta_0 = \theta_M = 0$.

We claim that the numerical scheme (9.12) is robust to perturbation to non-homogeneous data and initial data. To be specific, we have

Theorem 9.2. *Let $\epsilon_m^k = u_m^k - v_m^k$, then $\{\epsilon_m^k\}$ satisfies the following inequality for $1 \leq k \leq K$*

$$\tau_z \sum_{j=1}^k \|\epsilon^j\|_\infty \leq \sqrt{[\mathcal{Z}(T) - \mathcal{Z}(0)] \left[\frac{\tau_z L^3}{24d^2} \sum_{j=1}^k \|\hat{f}^j\|^2 + \tau_z^{1-\gamma} \frac{\lambda_0^\gamma L}{2d} \|\theta\|^2 \right]}, \quad (9.24)$$

where $0 < \gamma < 1$ and $\hat{f} = f - \bar{f}$.

Proof. From (9.12) and (9.23), it is obvious that $\{\epsilon_j^k\}$ is the solution of the linear equations below

$$\begin{cases} \tau_z^{-\gamma} \sum_{j=0}^k \lambda_j^\gamma \epsilon_m^{k-j} = d\delta_x^2 \epsilon_m^k + \hat{f}_m^k, & 1 \leq j \leq M-1 \\ \epsilon_m^0 = \theta_m, & 0 \leq m \leq M \\ \epsilon_0^k = 0, \quad \epsilon_M^k = 0, & 1 \leq k \leq K \end{cases} \quad (9.25)$$

Noticing that $\epsilon^k \in \mathcal{U}_P$, applying Theorem 9.1, we get

$$\tau_z \sum_{j=1}^k \|\epsilon^j\|_\infty \leq \sqrt{[\mathcal{Z}(T) - \mathcal{Z}(0)] \left[\frac{\tau_z L^3}{24d^2} \sum_{j=1}^k \|\hat{f}^j\|^2 + \tau_z^{1-\gamma} \frac{\lambda_0^\gamma L}{2d} \|\theta\|^2 \right]}. \quad (9.26)$$

The proof is complete. $\square$

Next, we shall present the local truncation error of the numerical scheme (9.12) that is vital to analyze the convergence. Suppose that $U(x, t)$ is the exact solution of the problem (9.1), the local truncation error will be incurred if we replace u_m^k in (9.12) by $U_m^k = U(x_m, t_k)$ directly. That is,

$$\begin{cases} \tau_z^{-\gamma} \sum_{j=0}^k \lambda_j^\gamma U_m^{k-j} = d\delta_x^2 U_m^k + f_m^k + T_m^k, & 1 \leq m \leq M-1 \\ U_m^0 = 0, & 0 \leq m \leq M \\ U_0^k = \phi_1(t_k), & U_M^k = \phi_2(t_k), & 1 \leq k \leq K \end{cases} \quad (9.27)$$

where T_m^k denotes the local truncation error at (x_m, t_k) .

Lemma 9.4. *If $U(x, \mathcal{Z}^{-1}(z)) = \bar{u}(x, z) \in C^{2,4}([0, L] \times [\mathcal{Z}(0), \mathcal{Z}(T)])$, $\frac{\partial^i \bar{u}(x, \mathcal{Z}(0))}{\partial z^i} = 0$, $i = 0, 1, 2, 3, 4$ and $\mathcal{Z}(t)$ is strictly increasing, then the local truncation error T_m^k satisfies*

$$T_m^k = O(\tau_z^2 + h^2), \quad 1 \leq m \leq M-1, \quad 1 \leq k \leq K \quad (9.28)$$

where h is the spatial step size and $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{K}$.

Proof. In view of the first equation in (9.27) and (9.10), we have

$$\begin{aligned} T_m^k &= \tau_z^{-\gamma} \sum_{j=0}^k \lambda_j^\gamma U_m^{k-j} - d\delta_x^2 U_m^k - f_m^k \\ &= \tau_z^{-\gamma} \sum_{j=0}^k \lambda_j^\gamma U_m^{k-j} - d\delta_x^2 U_m^k - f_m^k - \left[{}^C_0 D_{t;[\mathcal{Z},1]}^\gamma U(x_m, t_k) \right. \\ &\quad \left. - dU_{xx}(x_m, t_k) - f(x_m, t_k) \right] \\ &= \tau_z^{-\gamma} \sum_{j=0}^k \lambda_j^\gamma U_m^{k-j} - {}^C_0 D_{t;[\mathcal{Z},1]}^\gamma U(x_m, t_k) + d[U_{xx}(x_m, t_k) - \delta_x^2 U_m^k] \\ &= T_{mt}^k + T_{mx}^k, \end{aligned} \quad (9.29)$$

where we have used in the second equality the fact that $U(x, t)$ is the exact solution of the problem (9.1), and T_{jt}^n, T_{jx}^n are given by

$$T_{jt}^n = \tau_z^{-\gamma} \sum_{k=0}^n \lambda_j^\gamma U_j^{n-k} - {}^C_0 D_{t;[\mathcal{Z},1]}^\gamma U(x_j, t_n) \quad \text{and} \quad T_{jx}^n = d [U_{xx}(x_j, t_n) - \delta_x^2 U_j^n].$$

Applying the results (9.8) to T_{mt}^k and (9.11) to T_{mx}^k , it is easily obtained that

$$T_{mt}^k = O(\tau_z^2) \quad \text{and} \quad T_{mx}^k = O(h^2).$$

The proof is complete. $\square$

Now, we are in a position to analyze the convergence of the numerical scheme (9.12).

Theorem 9.3. *Suppose that $U(x, \mathcal{Z}^{-1}(z)) = \bar{u}(x, z) \in \mathcal{C}^{2,4}([0, L] \times [\mathcal{Z}(0), \mathcal{Z}(T)])$ and $\frac{\partial^i \bar{u}(x, \mathcal{Z}(0))}{\partial z^i} = 0$, $i = 0, 1, 2, 3, 4$ and $\mathcal{Z}(t)$ is strictly increasing. Let $e_m^k = U_m^k - u_m^k$ denote the disparity of the exact and the numerical solutions. Then it is observed that*

$$\tau_z \sum_{j=1}^k \|e^j\|_\infty \leq O(\tau_z^2 + h^2), \quad 1 \leq k \leq K. \quad (9.30)$$

where $\tau_z = \frac{\mathcal{Z}(T) - \mathcal{Z}(0)}{K}$ and h is the spatial step size.

Proof. Applying the numerical scheme (9.12) and the system (9.27), obviously, we have

$$\begin{cases} \tau_z^{-\gamma} \sum_{j=0}^k \lambda_j^\gamma e_m^{k-j} = d \delta_x^2 e_m^k + T_m^k, & 1 \leq m \leq M-1 \\ e_m^0 = 0, & 0 \leq m \leq M. \\ e_0^k = 0, & e_M^k = 0, \quad 1 \leq k \leq K \end{cases} \quad (9.31)$$

It is noted that $e^k \in \mathcal{U}_P$ and $i\tau_z \leq \mathcal{Z}(T) - \mathcal{Z}(0)$, $1 \leq k \leq K$, applying Theorem 9.1 to the system (9.31) yields

$$\begin{aligned} \tau_z \sum_{j=1}^k \|e^j\|_\infty &\leq \sqrt{\frac{\tau_z [\mathcal{Z}(T) - \mathcal{Z}(0)] L^3}{24d^2} \sum_{j=1}^k \|T^j\|^2} \\ &\leq \sqrt{\frac{k\tau_z [\mathcal{Z}(T) - \mathcal{Z}(0)] L^3}{24d^2} \max_{1 \leq k \leq K} \|T^k\|^2} \\ &\leq \sqrt{\frac{[\mathcal{Z}(T) - \mathcal{Z}(0)]^2 L^3}{24d^2} \max_{1 \leq k \leq K} \|T^k\|^2}, \quad 1 \leq k \leq K. \end{aligned} \quad (9.32)$$

Using the result (9.28) of Lemma 9.4 and $(M-1)h \leq 1$, it is found that

$$\|T^k\|^2 = h \sum_{m=1}^{M-1} (T_m^k)^2 = h(M-1) [O(\tau_z^2 + h^2)]^2 = [O(\tau_z^2 + h^2)]^2, \quad (9.33)$$

where $\tau_z = \frac{z(T)-z(0)}{K}$ and h is the spatial step size.

Therefore, (9.30) follows directly from (9.32) and (9.33). The proof is complete. $\square$

Remark 9.3. From the inequality (9.30), when $k = K$, we have established the convergence of the proposed numerical scheme in terms of average norm, namely,

$$\tau_z \sum_{k=1}^K \|e^k\|_\infty = O(\tau_z^2 + h^2),$$

that will be used in next section.

Remark 9.4. Let $\tau_1 = \max_{1 \leq k \leq K} |t_k - t_{k-1}|$. If $0 \leq \mathcal{Z}'(t) \leq C$, then we have the inequality below

$$\tau_z \sum_{j=1}^k \|e^j\|_\infty \leq O(\tau_1^2 + h^2). \quad (9.34)$$

In fact, applying mean value theorem gives

$$\tau_z = \mathcal{Z}(t_k) - \mathcal{Z}(t_{k-1}) = \mathcal{Z}'(\bar{\xi})(t_k - t_{k-1}), \quad \bar{\xi} \in (t_{k-1}, t_k),$$

and then

$$\tau_z \leq C|t_k - t_{k-1}| \leq C\tau_1$$

which yields the inequality (9.34).

9.4 Simulation

In this section, we shall use some examples to demonstrate the efficiency of the proposed numerical scheme (9.12). To this aim, the average absolute error as in Remark 9.3 will be computed and the temporal convergence order is presented accordingly.

In most cases, the exact solution of the example is unknown. Therefore, we shall compute the numerical solution $\{\tilde{u}_m^k\}$ using (9.12) for sufficiently small step size $h = \frac{L}{M}$ and sufficiently large number of intervals K as the ‘exact’ solution. In our examples, $h = \frac{1}{1000}$ and $K = 10000$ are applied. The temporal convergence order in term of average norm and maximum norm are computed respectively by

$$\mathcal{T}_{av} = \log_2 \left(\frac{e_{av}(h, K)}{e_{av}(h, 2K)} \right) \quad \text{and} \quad \mathcal{T}_{\infty} = \log_2 \left(\frac{e_{\infty}(h, K)}{e_{\infty}(h, 2K)} \right) \quad (9.35)$$

where

$$e_{av}(h, K) = \tau_z \sum_{k=1}^K \|\tilde{u}^k - u^k\|_{\infty} \quad \text{and} \quad e_{\infty}(h, K) = \|\tilde{u}^K - u^K\|_{\infty},$$

where $\{\tilde{u}_m^K\}$ is the ‘exact’ solution obtained from the scheme (9.12) when $h = \frac{1}{1000}$ and $K = 10000$ while $\{u_m^K\}$ is the approximate solution obtained from (9.12).

Example 9.1. Let $d = L = T = 1$, $\phi_1(t) = t^{\vartheta_1}$, $\phi_2(t) = et^{\vartheta_1}$, $z(t) = t^{\vartheta_2}$ and

$$f(x, t) = \exp(x) \left[\frac{\Gamma(\frac{\vartheta_1}{\vartheta_2} + 1)}{\Gamma(\frac{\vartheta_1}{\vartheta_2} + 1 - \gamma)} t^{\vartheta_1 - \vartheta_2 \gamma} - t^{\vartheta_1} \right],$$

where $\vartheta_1 \geq \vartheta_2 \gamma > 0$. The exact solution is $u(x, t) = \exp(x)t^{\vartheta_1}$.

Let $\vartheta_1 = 6 + \gamma$ and $\vartheta_2 = 0.5, 1.5$. It is easy to verify that the assumption in Theorem 9.3 are satisfied. In this example, we use the exact solution when computing the errors since it is known. We fix $h = \frac{1}{1000}$ and vary K to obtain the error $e_{av}(h, K)$ and related convergence order in Table 9.1. Obviously, the proposed numerical scheme gives second order accuracy which is consistent with the theoretical result.

Our next example is modified from Example 6.2 in [78] using the new generalized Caputo fractional derivative to replace the classical Caputo fractional derivative.

TABLE 9.1: (Example 9.1) Temporal convergence order $\mathcal{T}_{av}$ when $h = \frac{1}{1000}$

$\mathcal{Z}(t)$	K	$\gamma = 0.2$	$\mathcal{T}_{av}$	$\gamma = 0.5$	$\mathcal{T}_{av}$	$\gamma = 0.8$	$\mathcal{T}_{av}$
$t^{0.5}$	40	1.0821E-04	-	5.8926E-04	-	1.8285E-03	-
	80	2.6953E-05	2.0053	1.4871E-04	1.9864	4.6694E-04	1.9693
	160	6.7262E-06	2.0026	3.7370E-05	1.9926	1.1815E-04	1.9826
$t^{1.5}$	40	2.9129E-05	-	1.2366E-04	-	3.2860E-04	-
	80	7.2770E-06	2.0010	3.1003E-05	1.9959	8.2687E-05	1.9906
	160	1.8206E-06	1.9989	7.7636E-06	1.9976	2.0741E-05	1.9952

Example 9.2. *The equation of the new generalized fractional sub-diffusion problem is*

$${}_0^C D_{t;[\mathcal{Z},1]}^\gamma u(x,t) = u_{xx}(x,t) + f(x,t), \quad (x,t) \in (0,1) \times (0,1) \quad (9.36)$$

with $0 < \gamma < 1$ and related conditions

$$u(x,0) = u(0,t) = u(1,t) = 0, \quad f(x,t) = \left[\frac{2}{\Gamma(3-\gamma)t^{2-\gamma}} + 4\pi^2 t^2 \right] \sin 2\pi x.$$

In this example, numerical tests are carried out for fractional orders $\gamma = 0.2, 0.5$ and 0.8 and scale functions $\mathcal{Z}(t) = t^{0.5}, t, t^{1.5}$ and $\exp(2t) - 1$ when $h = \frac{1}{1000}$ and K varies as $K = 50, 100, 200$. The maximum absolute error $e_\infty(h, K)$ and corresponding temporal convergence order T_∞ are presented in Table 9.2 while the average norm error $e_{av}(h, K)$ and temporal convergence order T_{av} are displayed in Table 9.3. From these two tables, it is obvious that the proposed numerical scheme can achieve second order accuracy in temporal dimension for various fractional orders as well as scale functions.

Our third example is from [130] where only the numerical test for the typical Caputo fractional derivative is given. Here, we shall show the improvement in the temporal convergence order using the proposed scheme (9.12) in the typical setting $\mathcal{W}(t) \equiv 1$ and $\mathcal{Z}(t) = t$ as well as in generalized cases.

Example 9.3. [130] *Consider the following generalized fractional sub-diffusion problem:*

$${}_0^C D_{t;[\mathcal{Z},\mathcal{W}]}^{0.85} u(x,t) = u_{xx}(x,t) + f(x,t), \quad (x,t) \in (0,1) \times (0,1) \quad (9.37)$$

TABLE 9.2: (Example 9.2) Temporal convergence order $\mathcal{T}_\infty$ when $h = \frac{1}{1000}$

$\mathcal{Z}(t)$	K	$\gamma = 0.2$	$\mathcal{T}_\infty$	$\gamma = 0.5$	$\mathcal{T}_\infty$	$\gamma = 0.8$	$\mathcal{T}_\infty$
$t^{0.5}$	50	6.4186E-06	-	2.3100E-05	-	5.0458E-05	-
	100	1.6183E-06	1.9878	5.8258E-06	1.9874	1.2722E-05	1.9878
	200	4.0618E-07	1.9943	1.4624E-06	1.9941	3.1931E-06	1.9943
t	50	7.9791E-07	-	1.5563E-06	-	1.1350E-06	-
	100	1.9927E-07	2.0015	3.8794E-07	2.0042	2.8218E-07	2.0080
	200	4.9779E-08	2.0011	9.6822E-08	2.0024	7.0342E-08	2.0041
$t^{1.5}$	50	6.2983E-08	-	2.7791E-07	-	9.3950E-07	-
	100	1.6625E-08	1.9216	6.7502E-08	2.0416	2.3235E-07	2.0156
	200	4.3366E-09	1.9387	1.6507E-08	2.0319	5.7824E-08	2.0066
$e^{2t} - 1$	50	2.4315E-07	-	7.0911E-07	-	3.4615E-07	-
	100	6.0307E-08	2.0114	1.7473E-07	2.0209	8.2747E-08	2.0646
	200	1.5018E-08	2.0056	4.3356E-08	2.0109	2.0196E-08	2.0346

TABLE 9.3: (Example 9.2) Temporal convergence order $\mathcal{T}_{av}$ when $h = \frac{1}{1000}$

$\mathcal{Z}(t)$	K	$\gamma = 0.2$	$\mathcal{T}_{av}$	$\gamma = 0.5$	$\mathcal{T}_{av}$	$\gamma = 0.8$	$\mathcal{T}_{av}$
$t^{0.5}$	50	2.3338E-06	-	9.3045E-06	-	2.2608E-05	-
	100	5.8294E-07	2.0012	2.3305E-06	1.9973	5.6747E-06	1.9942
	200	1.4563E-07	2.0010	5.8300E-07	1.9990	1.4211E-06	1.9975
t	50	9.8573E-07	-	2.9713E-06	-	4.9237E-06	-
	100	2.4677E-07	1.9980	7.4703E-07	1.9918	1.2462E-06	1.9822
	200	6.1726E-08	1.9992	1.8744E-07	1.9947	3.1474E-07	1.9853
$t^{1.5}$	50	2.7066E-07	-	1.9492E-06	-	1.2955E-05	-
	100	7.2497E-08	1.9005	5.7110E-07	1.7711	3.8860E-06	1.7372
	200	1.9369E-08	1.9041	1.5887E-07	1.8459	1.0862E-06	1.8391
$e^{2t} - 1$	50	1.0534E-06	-	6.5793E-06	-	2.6825E-05	-
	100	2.6801E-07	1.9747	1.6846E-06	1.9655	7.0102E-06	1.9361
	200	6.7616E-08	1.9869	4.2732E-07	1.9790	1.7748E-06	1.9818

with conditions

$$u(x, 0) = \sin(\pi x), \quad u(0, t) = u(1, t) = 0,$$

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

When $\mathcal{W}(t) \equiv 1$ and $\mathcal{Z}(t) = t$, the exact solution of (9.37) is given by $u(x, t) = \sin(\pi x) + x(x - 1)t^2$.

We set $h = \frac{1}{1000}$ and $K = 50, 100$ and 200 in this example. To demonstrate the efficiency of the proposed numerical scheme (9.12), we shall present the errors

$(e_\infty(h, K), e_{av}(h, K))$ and the temporal convergence orders (T_∞, T_{av}) for four choices of $\mathcal{W}(t)$ and $\mathcal{Z}(t)$. Note that the numerical scheme (9.12) is applied directly when $\mathcal{W}(t) \equiv 1$. If $\mathcal{W}(t) \not\equiv 1$, we shall first convert the original problem to the equivalent form (9.1) and then perform the scheme (9.10) to compute the numerical solution. After that, we use the relation stated in Section 9.2 to obtain the numerical solution of the original problem. The numerical results are displayed in Table 9.4. Obviously, the expected $O(\tau_z^2)$ is achieved in temporal dimension numerically for all cases which is consistent with the theoretical result as in Remark 9.3.

TABLE 9.4: (Example 9.3) Temporal convergence order T_∞ and $\mathcal{T}_{av}$ when $h = \frac{1}{1000}$

	K	$e_\infty(h, N)$	$\mathcal{T}_\infty$	$e_{av}(h, N)$	$\mathcal{T}_{av}$
$\mathcal{W}(t) \equiv 1, \mathcal{Z}(t) = t$	50	1.0615E-06	-	5.1108E-06	-
	100	2.6378E-07	2.0088	1.2941E-06	1.9816
	200	6.5761E-08	2.0040	3.2710E-07	1.9842
$\mathcal{W}(t) \equiv 1, \mathcal{Z}(t) = t^{0.5}$	50	4.8179E-05	-	2.0669E-05	-
	100	1.2158E-05	1.9864	5.1909E-06	1.9934
	200	3.0531E-06	1.9936	1.3004E-06	1.9971
$\mathcal{W}(t) = e^t, \mathcal{Z}(t) = t$	50	1.8319E-05	-	5.3502E-05	-
	100	4.6363E-06	1.9823	1.4549E-05	1.8786
	200	1.1659E-06	1.9915	3.7716E-06	1.9477
$\mathcal{W}(t) = e^t, \mathcal{Z}(t) = t^{0.5}$	50	9.9157E-05	-	3.2865E-05	-
	100	2.6022E-05	1.9300	8.3227E-06	1.9814
	200	6.6659E-06	1.9649	2.0940E-06	1.9908

Also, we shall compare the proposed numerical scheme (9.12) with the method in [130]. The maximum absolute error at $t = 1$ when $h = \frac{1}{1000}$ and the corresponding convergence order T_∞ are presented in Table 9.5. It is observed that the proposed scheme (9.12) achieves second order accuracy in temporal as well as smaller errors for all cases except when $\mathcal{W}(t) \equiv 1, \mathcal{Z}(t) = t^{0.5}$. Since $T_\infty \approx 2$ in our numerical scheme while $T_\infty \approx 2 - \gamma = 1.15$ in [130], our method will finally give a smaller error as K becomes larger.

The last example is first used in [130] to illustrate the properties of the weight function $\mathcal{W}(t)$ and scale function $\mathcal{Z}(t)$.

Example 9.4. Consider the generalized fractional sub-diffusion

$${}_0^C D_{t;[\mathcal{Z}, \mathcal{W}]}^\gamma u(x, t) = du_{xx}(x, t) + \frac{(x-1)(t-1)}{2 + \sin(xt)}, \quad (x, t) \in (0, 1) \times (0, 1). \quad (9.38)$$

TABLE 9.5: (Example 9.3) Comparison between our scheme and scheme in [130] when $h = \frac{1}{1000}$

	K	Scheme (9.12)	$\mathcal{T}_\infty$	Scheme [130]	$\mathcal{T}_\infty$
$\mathcal{W}(t) \equiv 1, \mathcal{Z}(t) = t$	50	1.0615E-06	-	2.2467E-04	-
	100	2.6378E-07	2.0088	9.7243E-05	1.2081
	200	6.5761E-08	2.0040	3.9765E-05	1.2901
$\mathcal{W}(t) \equiv 1, \mathcal{Z}(t) = t^{0.5}$	50	4.8179E-05	-	7.2103E-06	-
	100	1.2158E-05	1.9864	3.1380E-06	1.2002
	200	3.0531E-06	1.9936	1.2866E-06	1.2863
$\mathcal{W}(t) = e^t, \mathcal{Z}(t) = t$	50	1.8319E-05	-	2.5599E-04	-
	100	4.6363E-06	1.9823	1.1217E-04	1.1903
	200	1.1659E-06	1.9915	4.6173E-05	1.2806
$\mathcal{W}(t) = e^t, \mathcal{Z}(t) = t^{0.5}$	50	9.9157E-05	-	2.6804E-04	-
	100	2.6022E-05	1.9300	1.1626E-04	1.2051
	200	6.6659E-06	1.9649	4.7601E-05	1.2883

The initial and boundary conditions are as follows:

$$u(x, 0) = x(1 - x)^3 \exp(\sin(3.5\pi x)), \quad u(0, t) = u(1, t) = 0.$$

In this example, we present illustrative figures to investigate the effects of the weight function $\mathcal{W}(t)$ and scale function $\mathcal{Z}(t)$ as well as the value of the diffusion constant d . To have proper comparisons, the parameters $h = \frac{1}{100}$, $K = 1000$ and $\gamma = 0.97$ are fixed for all cases.

We plot the numerical solutions in Figure 9.1 for four cases below:

$$(a) \mathcal{W}(t) = e^t, \mathcal{Z}(t) = t, d = 1; \quad (b) \mathcal{W}(t) = e^t, \mathcal{Z}(t) = t^5, d = 1;$$

$$(c) \mathcal{W}(t) = e^{5t}, \mathcal{Z}(t) = t, d = 1; \quad (d) \mathcal{W}(t) = e^t, \mathcal{Z}(t) = t, d = 0.5.$$

First, from Figure 9.1, it is obvious that $\mathcal{Z}(t)$ in (b) stretch the domain at the beginning which results in a coarser mesh in temporal compared to (a). Then, note that (c) gives the result using a different weight $\mathcal{W}(t) = \exp(5t)$ from (a) that applies $\mathcal{W}(t) = \exp(t)$. Typically, the solution tends to be smaller with larger weights which, unfortunately, is not easy to tell from (a) and (c) directly. Therefore, the corresponding contours with a given level list [0.0003 0.01 0.015 0.02 0.025] of diagrams (a) and (c) are plotted in Figure 9.2. From the contours in Figure 9.2, it is easily seen that the solutions of case (a) and (c) are very different. In fact, since

the weight function $\mathcal{W}(t) = \exp(5t)$ is larger than $\mathcal{W}(t) = \exp(t)$, the contour of (c) is much closer to $t = 0$ than (a) for the same level which indicates that the solution of the case (c) tends to be smaller at the same mesh point than the case (a). Finally, if a smaller diffusion constant $d = 0.5$ is used, then it is observed from (c) that the diffusion process will become slower than (a) where $d = 1$ is used.

It is noted that the weight function $\mathcal{W}(t)$ can weigh differently at different time points, the scale function $\mathcal{Z}(t)$ can stretch or contract the domain and the diffusion constant d measures the rate of the diffusion process. From above discussions, it is concluded that the proposed numerical scheme (9.12) can keep and show the properties of the weight function $\mathcal{W}(t)$, the scale function $\mathcal{Z}(t)$ and the diffusion constant d appropriately.

FIGURE 9.1: (Example 9.4) Numerical solution for: (a) (top, left); (b) (top, right); (c) (bottom, left); (d) (bottom, right).

FIGURE 9.2: (Example 9.4) Contour of (a) (left) and (c) (right) in Figure 9.1 with level list $[0.0003, 0.01, 0.015, 0.02, 0.025]$.

9.5 Summary

In this chapter, we propose an efficient numerical scheme mainly using the gWSGL technique for the new generalized fractional sub-diffusion problem. The solvability, stability and convergence have been analyzed and established rigorously. It is shown that second order accuracy is achieved in temporal and this improves the work done to date. To demonstrate the efficiency and accuracy of the proposed method, we have carried out simulation for some examples. As one can see, our method is consistent with the theoretical result which indicates a better performance in reality.

Chapter 10

New Generalized Fractional Sub-diffusion Problems II

Chapter 9 presents a high order numerical method using gWSGL method in temporal. It is noted that this method requires strong conditions to achieve high accuracy, see Theorem 9.3. In this chapter, we aim to construct a different numerical scheme that can weaken the conditions while keep the theoretical accuracy, for the problem (9.1) when $\mathcal{W}(t) \equiv 1$ due to the same consideration as in Chapter 9. In Section 10.1, we shall propose a generalized $L2 - 1_\sigma$ approximation to ${}_0^C D_{t;[z;1]}^\gamma u(x, t)$ and then develop an efficient numerical scheme for the new generalized fractional sub-diffusion problem (9.1). Then we shall establish a priori estimate in Section 10.2 and analyze the stability and convergence of the proposed numerical scheme in Section 10.3. After that, in Section 10.4, the simulation is carried out to demonstrate the efficiency as well as the accuracy of the numerical scheme. Section 10.5 summarizes the work done in this chapter.

10.1 Numerical Scheme

In this section, a high accuracy numerical scheme is constructed using generalized $L2 - 1_\sigma$ method which approximates the generalized Caputo fractional derivative in temporal dimension, and classical finite difference in spatial dimension.

Let $\mathcal{Z}(t)$ be a strictly increasing function throughout the chapter and $P, \mathcal{P}''$ be the uniform mesh of $[0, L]$ and non-uniform mesh of $[0, T]$ respectively as in Chapter 9. Once the scale function $\mathcal{Z}(t)$ is given, we have $t_k = \mathcal{Z}^{-1}(k\tau + z_0)$.

Now, let us start with the construction of a useful approximation called generalized $L2 - 1_\sigma$ for the fractional term ${}_0^C D_{t;[\mathcal{Z};1]}^\gamma u(x_m, t_{k-1+\sigma})$ where $t_{k-1+\sigma} = \mathcal{Z}^{-1}((k - 1 + \sigma)\tau + z_0)$ and $\sigma = 1 - \frac{\gamma}{2}$. From the definition (9.2), we are able to obtain the expression below

$${}_0^C D_{t;[\mathcal{Z};1]}^\gamma u(x_m, t_{k-1+\sigma}) = \frac{1}{\Gamma(1 - \gamma)} \left[\sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} + \int_{t_{k-1}}^{t_{k-1+\sigma}} \right] \frac{u_t(x_m, s)}{[\mathcal{Z}_{k-1+\sigma} - \mathcal{Z}(s)]^\gamma} ds. \quad (10.1)$$

Similar to the derivation of $L2 - 1_\sigma$ method for the Caputo fractional derivative [7], we shall apply the generalized quadratic interpolation of (z_{j-1}, u_m^{j-1}) , (z_j, u_m^j) and (z_{j+1}, u_m^{j+1})

$$\mathcal{GI}_{2,j}(t) = \sum_{i=0}^2 \prod_{n=0, n \neq i}^2 \frac{\mathcal{Z}(t) - z_{j-1+n}}{z_{j-1+i} - z_{j-1+n}} u_m^{j-1+i}, \quad (10.2)$$

to approximate $u(x_m, t)$ for $t \in [t_{j-1}, t_j]$, $1 \leq j \leq k-1$ while the generalized linear interpolation of (z_{k-1}, u_m^{k-1}) and (z_k, u_m^k)

$$\mathcal{GI}_{1,k}(t) = \frac{\mathcal{Z}(t) - z_{k-1}}{z_k - z_{k-1}} u_m^k + \frac{\mathcal{Z}(t) - z_k}{z_{k-1} - z_k} u_m^{k-1}, \quad (10.3)$$

to replace $u(x_m, t)$ when $t_{k-1} < t < t_{k-1+\sigma}$.

Using the fact $z_{j+1} - z_j = \tau_z$, $z_{k-1+\sigma} - z_{k-1} = \sigma\tau_z$, from (10.2) and (10.3), the derivatives $(\mathcal{GI}_{2,j}(t))'$ and $(\mathcal{GI}_{1,k-1}(t))'$ are explicitly given as

$$(\mathcal{GI}_{2,j}(t))' = \mathcal{Z}'(t) \left[\frac{2\mathcal{Z}(t) - 2z_{j-1} - \tau_z}{2} \tilde{\delta}_t^2 u_m^j + \tilde{\delta}_t u_m^{j-\frac{1}{2}} \right], \quad (10.4)$$

and

$$(\mathcal{GI}_{1,k}(t))' = \frac{\mathcal{Z}'(t)}{z_k - z_{k-1}} u_m^k + \frac{\mathcal{Z}'(t)}{z_{k-1} - z_k} u_m^{k-1} = \mathcal{Z}'(t) \tilde{\delta}_t u_m^{k-\frac{1}{2}}, \quad (10.5)$$

where $\tilde{\delta}_t u_m^{j-\frac{1}{2}} = (u_m^j - u_m^{j-1}) / \tau_z$ and $\tilde{\delta}_t^2 u_m^j = (\tilde{\delta}_t u_m^{j+\frac{1}{2}} - \tilde{\delta}_t u_m^{j-\frac{1}{2}}) / \tau_z$.

To get the generalized $L2 - 1_\sigma$ approximation, for simplicity, let us first calculate the following two integrals

$$\int_{t_{j-1}}^{t_j} \frac{(\mathcal{GI}_{2,j}(s))'}{[z_{k-1+\sigma} - \mathcal{Z}(s)]^\gamma} ds \quad \text{and} \quad \int_{t_{k-1}}^{t_{k-1}+\sigma} \frac{(\mathcal{GI}_{1,k}(s))'}{[z_{k-1+\sigma} - \mathcal{Z}(s)]^\gamma} ds.$$

For the former integral, it follows from (10.4) that

$$\begin{aligned} & \int_{t_{j-1}}^{t_j} \frac{(\mathcal{GI}_{2,j}(s))'}{[z_{k-1+\sigma} - \mathcal{Z}(s)]^\gamma} ds \\ &= \int_{t_{j-1}}^{t_j} [z_{k-1+\sigma} - \mathcal{Z}(s)]^{-\gamma} z'(s) \left[\frac{2\mathcal{Z}(s) - 2z_{j-1} - \tau_z}{2} \tilde{\delta}_t^2 u_m^j + \tilde{\delta}_t u_m^{j-\frac{1}{2}} \right] ds \\ &= \int_{t_{j-1}}^{t_j} [z_{k-1+\sigma} - \mathcal{Z}(s)]^{-\gamma} \left[\frac{2\mathcal{Z}(s) - 2z_{j-1} - \tau_z}{2} \tilde{\delta}_t^2 u_m^j + \tilde{\delta}_t u_m^{j-\frac{1}{2}} \right] dz(s) \\ &= P_1 \tilde{\delta}_t^2 u_m^j + P_2 \tilde{\delta}_t u_m^{j-\frac{1}{2}} \end{aligned} \tag{10.6}$$

where

$$P_1 = \int_{t_{j-1}}^{t_j} [z_{k-1+\sigma} - \mathcal{Z}(s)]^{-\gamma} \left[\frac{2\mathcal{Z}(s) - 2z_{j-1} - \tau_z}{2} \right] dz(s) = \frac{\tau_z^{2-\gamma}}{1-\gamma} b_{\sigma,k-j},$$

and

$$P_2 = \int_{t_{j-1}}^{t_j} \frac{dz(s)}{[z_{k-1+\sigma} - \mathcal{Z}(s)]^\gamma} = \frac{\tau_z^{1-\gamma}}{1-\gamma} a_{\sigma,k-j}.$$

Therefore, substituting above P_1 and P_2 into (10.6) yields

$$\int_{t_{j-1}}^{t_j} \frac{(\mathcal{GI}_{2,j}(s))'}{[z_{k-1+\sigma} - \mathcal{Z}(s)]^\gamma} ds = \frac{\tau_z^{2-\gamma}}{1-\gamma} b_{\sigma,k-j} \tilde{\delta}_t^2 u_m^j + \frac{\tau_z^{1-\gamma}}{1-\gamma} a_{\sigma,k-j} \tilde{\delta}_t u_m^{j-\frac{1}{2}}. \tag{10.7}$$

Similarly, using formula (10.5) in the second integral, it is found that

$$\int_{t_{k-1}}^{t_{k-1}+\sigma} \frac{(\mathcal{GI}_{1,k}(s))'}{[z_{k-1+\sigma} - \mathcal{Z}(s)]^\gamma} ds = \frac{\tau_z^{1-\gamma}}{1-\gamma} \sigma^{1-\gamma} \tilde{\delta}_t u_m^{k-\frac{1}{2}} = \frac{\tau_z^{1-\gamma}}{1-\gamma} a_{\sigma,0} \tilde{\delta}_t u_m^{k-\frac{1}{2}}. \tag{10.8}$$

Now, applying $\mathcal{GI}_{2,j}(t) \approx u(x_m, t)|_{[t_{j-1}, t_j]}$, $1 \leq j \leq k-1$ and $\mathcal{GI}_{1,k}(t) \approx u(x_m, t)$ for $t \in [t_{k-1}, t_{k-1}+\sigma]$ in (10.1) and then results (10.7) and (10.8), we shall get the

generalized $L2 - 1_\sigma$ approximation

$$\begin{aligned}
& {}_0^C D_{t;[\mathcal{Z};1]}^\gamma u(x_m, t_{k-1+\sigma}) \\
& \approx \frac{1}{\Gamma(1-\gamma)} \left[\sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} \frac{(\mathcal{GI}_{2,j}(s))'}{[z_{k-1+\sigma} - \mathcal{Z}(s)]^{-\gamma}} ds + \int_{t_{k-1}}^{t_{k-1+\sigma}} \frac{(\mathcal{GI}_{1,k}(s))'}{[z_{k-1+\sigma} - \mathcal{Z}(s)]^\gamma} ds \right] \\
& = \frac{\tau_z^{1-\gamma}}{\Gamma(2-\gamma)} \left[\sum_{j=1}^{k-1} b_{\sigma,k-j} \left(\tilde{\delta}_t u_m^{j+\frac{1}{2}} - \tilde{\delta}_t u_m^{j-\frac{1}{2}} \right) + \sum_{j=1}^k a_{\sigma,k-j} \tilde{\delta}_t u_m^{j-\frac{1}{2}} \right] \\
& = \frac{\tau_z^{1-\gamma}}{\Gamma(2-\gamma)} \sum_{j=0}^k r_{k-j} \tilde{\delta}_t u_m^{j+\frac{1}{2}} = \mu_z \mathcal{Q}_{m,k}(u),
\end{aligned} \tag{10.9}$$

where $\mu_z = \frac{1}{\Gamma(2-\gamma)\tau_z^\gamma}$ and

$$\mathcal{Q}_{m,k}(u) = r_0 u_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) u_j^k - r_{k-1} u_m^0.$$

Remark 10.1. Although the formulation (10.9) of generalized $L2 - 1_\sigma$ method seems to be the same as classical $L2 - 1_\sigma$ method [7], they are actually different in several aspects: i) interpolation (10.2) and (10.3) generalize the ones in [7] where $\mathcal{Z}(t) = t$ is considered; ii) non-uniform mesh is used in our case while uniform partition is taken for classical $L2 - 1_\sigma$ method.

Till now, we have derived the generalized $L2 - 1_\sigma$ method (10.9) for the new generalized Caputo fractional derivative (9.2). Next, we shall propose a more accurate numerical scheme for new generalized fractional sub-diffusion problems (9.1) using approximation (10.9) and finite difference method. To this aim, let us first discretize (9.1) at $(x_m, t_{k-1+\sigma})$ to get

$${}_0^C D_{t;[\mathcal{Z};1]}^\gamma u(x_m, t_{k-1+\sigma}) = du_{xx}(x_m, t_{k-1+\sigma}) + f(x_m, t_{k-1+\sigma}).$$

Then applying approximation (10.9) to the fractional term, finite difference

$$u_{xx}(x_m, t_{k-1+\sigma}) = \delta_x^2 u_m^{k-1+\sigma} + O(h^2) = u_m^{k-1+\sigma_k} + O(\tau_1^2 + h^2),$$

that will be demonstrated later, where $u_m^{k-1+\sigma_k} = \sigma_k u_m^k + (1 - \sigma_k) u_m^{k-1}$, $\sigma_k = \frac{t_{k-1+\sigma} - t_{k-1}}{t_k - t_{k-1}} \in (0, 1)$ and τ_1 is the same as in Remark 9.4, we obtain the following

numerical scheme

$$\begin{cases} \mu_z \left[r_0 u_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) u_m^j - r_{k-1} u_m^0 \right] = d \delta_x^2 u_m^{k-1+\sigma_k} + f_m^{k-1+\sigma}, \\ u_m^0 = \psi(x_m), \quad 1 \leq m \leq M-1 \\ u_0^k = \phi_1(t_k), \quad u_M^k = \phi_2(t_k), \quad 0 \leq k \leq K. \end{cases} \quad (10.10)$$

Remark 10.2. It is easy to verify that derived numerical scheme (10.10) is a linear system whose coefficient matrix is strictly diagonally dominated. Thus, the proposed scheme admits a unique solution at each time level $t = t_k$.

In subsequent analysis, we shall establish a priori result for the numerical scheme (10.10) with zero boundary conditions, that is, $u_0^k = u_M^k = 0$, $0 \leq k \leq K$. After that, using this priori estimate, we are able to show the proposed numerical scheme (10.10) is stable in maximum norm and convergent with accuracy $O(\tau_z^{3-\gamma} + \tau_1^2 + h^2)$.

10.2 A Priori Estimate

In this section, the proposed scheme (10.10) with zero boundary conditions will be analyzed and an estimation of the numerical solution at each time $t = t_k$ is established. To this aim, we need the following lemma which is originally proved in [7].

Lemma 10.1. [7] *For above formula, it holds that*

$$u_m^k \mathcal{Q}_{m,k}(u) \geq \frac{1}{2} \mathcal{Q}_{m,k}(u^2) + \frac{1}{2r_0} [\mathcal{Q}_{m,k}(u)]^2, \quad (10.11)$$

and

$$u_m^{k-1} \mathcal{Q}_{m,k}(u) \geq \frac{1}{2} \mathcal{Q}_{m,k}(u^2) - \frac{1}{2(r_0 - r_1)} [\mathcal{Q}_{m,k}(u)]^2. \quad (10.12)$$

Proof. Due to (4.49) in Lemma 4.6 in Chapter 4, above two inequalities follow from applying **Lemma 1** of [7] and taking $g_j = r_{k-j-1}$ there. $\square$

Through adding constraints on the increasing scale function $\mathcal{Z}(t)$ and using inequalities (10.11) and (10.12) in Lemma 10.1, we obtain an essential inequality below.

Lemma 10.2. *For any fixed $k \geq 1$, if the inverse of function $\mathcal{Z}(t)$, i.e. $\mathcal{Z}^{-1}(z)$ is concave, then it is found that*

$$(\sigma_k u_m^k + (1 - \sigma_k) u_m^{k-1}) \mathcal{Q}_{m,k}(u) \geq \frac{1}{2} \mathcal{Q}_{m,k}(u^2), \quad (10.13)$$

where $\sigma_k = \frac{t_{k-1+\sigma} - t_{k-1}}{t_k - t_{k-1}} \in (0, 1)$ and r_j 's are coefficients defined in (2.22).

Proof. Multiplying (10.11) by σ_k and (10.12) by $(1 - \sigma_k)$, after necessary manipulations, we have

$$(\sigma_k u_m^k + (1 - \sigma_k) u_m^{k-1}) \mathcal{Q}_{m,k}(u) \geq \frac{1}{2} \mathcal{Q}_{m,k}(u^2) + R_k, \quad (10.14)$$

where

$$R_k = \left[\frac{\sigma_k}{2r_0} - \frac{1 - \sigma_k}{2(r_0 - r_1)} \right] [\mathcal{Q}_{m,k}(u)]^2 = \frac{\sigma_k(2r_0 - r_1) - r_0}{2(r_0 - r_1)} [\mathcal{Q}_{m,k}(u)]^2.$$

To get (10.13), it remains to show the following inequality

$$\frac{\sigma_k(2r_0 - r_1) - r_0}{2(r_0 - r_1)} \geq 0. \quad (10.15)$$

In view of (4.49) and (4.50) in Lemma 4.6, it is obvious that

$$\frac{\sigma(2r_0 - r_1) - r_0}{2(r_0 - r_1)} = \frac{(2\sigma - 1)r_0 - \sigma r_1}{2(r_0 - r_1)} \geq 0$$

where $\sigma = 1 - \frac{\gamma}{2}$. Thus, if $\sigma_k \geq \sigma$, then obviously we have (10.15) which ends the proof.

Denote $t = \mathcal{Z}^{-1}(z)$ as the inverse function of $\mathcal{Z}(t)$. Since $t = \mathcal{Z}^{-1}(z)$ is a concave function and $z_{k-1+\sigma} = \mathcal{Z}(t_{k-1+\sigma}) = \sigma z_k + (1 - \sigma)z_{k-1}$, for $\sigma \in (0, 1)$, it is easily obtained that

$$t_{k-1+\sigma} = \mathcal{Z}^{-1}(z_{k-1+\sigma}) = \mathcal{Z}^{-1}(\sigma z_k + (1 - \sigma)z_{k-1}) \geq \sigma \mathcal{Z}^{-1}(z_k) + (1 - \sigma)\mathcal{Z}^{-1}(z_{k-1}), \quad (10.16)$$

which yields

$$t_{k-1+\sigma} \geq \sigma t_k + (1 - \sigma)t_{k-1}, \quad (10.17)$$

or equivalently

$$\sigma_k = \frac{t_{k-1+\sigma} - t_{k-1}}{t_k - t_{k-1}} \geq \sigma. \quad (10.18)$$

The proof is complete. $\square$

Next, we list the relation between norm $\|u\|_\infty$ and semi-norm $|u|_1^2$ (see Lemma 3.3) and the equivalence of $(u, \delta_x^2 v)$ and $-(u, v)_1$ which are important to establish estimation of the solution in maximum norm. In fact, for any $u, v \in \mathcal{U}_P$, it holds that

$$\|u\|_\infty^2 \leq \frac{L}{4}|u|_1^2 \quad \text{and} \quad (u, \delta_x^2 v) = -(u, v)_1. \quad (10.19)$$

Now, we are ready to present one of our main results which gives a bound of the numerical solution obtained from the proposed scheme (10.10) with zero boundary conditions: $u_0^k = u_M^k = 0$, $0 \leq k \leq K$.

Theorem 10.1. *(A priori estimate) Suppose that the inverse of scale function $\mathcal{Z}(t)$ is concave, then the solution of system (10.10) with zero boundary conditions at $t = t_k$ always satisfies*

$$\|u^k\|_\infty^2 \leq \frac{L}{4}E, \quad 1 \leq k \leq K \quad (10.20)$$

where $E = |\psi|_1^2 + \frac{\Gamma(1-\gamma)}{d} \max_{1 \leq k \leq K} \|f^{k-1+\sigma}\|^2$.

Proof. Multiplying by $-\delta_x^2 u_m^{k-1+\sigma_k} = -\sigma_k \delta_x^2 u_m^k - (1 - \sigma_k) \delta_x^2 u_m^{k-1}$ on both sides of the formula (10.10) and then summing from $m = 1$ to $j = M - 1$, we get

$$\begin{aligned} & -\mu_z \left[r_0(u^k, \delta_x^2 u^{k-1+\sigma_k}) - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j})(u^j, \delta_x^2 u^{k-1+\sigma_k}) - r_{k-1}(u^0, \delta_x^2 u^{k-1+\sigma_k}) \right] \\ & = -d \|\delta_x^2 u^{k-1+\sigma_k}\|^2 - (f^{k-1+\sigma}, \delta_x^2 u^{k-1+\sigma_k}). \end{aligned} \quad (10.21)$$

Since $u^j, u^{k-1+\sigma_k} \in \mathcal{U}_P$ due to zero boundary conditions, using the second result of (10.19) in the formula (10.21), it is achieved that

$$\begin{aligned} & \mu_z \left[r_0(u^k, u^{k-1+\sigma_k})_1 - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j})(u^j, u^{k-1+\sigma_k})_1 - r_{k-1}(u^0, u^{k-1+\sigma_k})_1 \right] \\ &= -d \|\delta_x^2 u^{k-1+\sigma_k}\|^2 - (f^{k-1+\sigma}, \delta_x^2 u^{k-1+\sigma_k}). \end{aligned} \quad (10.22)$$

Note that the inverse of function $\mathcal{Z}(t)$ is concave. Thus for the first term in (10.22), using the inequality (10.13) of Lemma 10.2, it is obvious that

$$\begin{aligned} & \mu_z \left[r_0(u^k, u^{k-1+\sigma_k})_1 - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j})(u^j, u^{k-1+\sigma_k})_1 - r_{k-1}(u^0, u^{k-1+\sigma_k})_1 \right] \\ &\geq \frac{\mu_z}{2} \left[r_0 |u^k|_1^2 - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) |u^j|_1^2 - r_{k-1} |u^0|_1^2 \right]. \end{aligned} \quad (10.23)$$

Meanwhile, using the classical inequality $\pm ab \leq \frac{a^2+b^2}{2}$, we have

$$\begin{aligned} -(f^{k-1+\sigma}, \delta_x^2 u^{k-1+\sigma_k}) &\leq \frac{1}{2} \left(\left\| \frac{f^{k-1+\sigma}}{\sqrt{2d}} \right\|^2 + \|\sqrt{2d} \delta_x^2 u^{k-1+\sigma_k}\|^2 \right) \\ &= \frac{1}{4d} \|f^{k-1+\sigma}\|^2 + d \|\delta_x^2 u^{k-1+\sigma_k}\|^2. \end{aligned} \quad (10.24)$$

Then applying the inequalities (10.23) and (10.24) to (10.22), after simple manipulations, we obtain

$$\frac{\mu_z}{2} \left[r_0 |u^k|_1^2 - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) |u^j|_1^2 - r_{k-1} |u^0|_1^2 \right] \leq \frac{1}{4d} \|f^{k-1+\sigma}\|^2. \quad (10.25)$$

Utilizing the following result

$$\frac{1}{2d\mu_z r_{k-1}} \leq \frac{\Gamma(2-\gamma)\tau_z^\gamma 2(k-1+\sigma)^\gamma}{2d(1-\gamma)} = \frac{\Gamma(1-\gamma)[(k-1+\sigma)\tau_z]^\gamma}{d} \leq \frac{\Gamma(1-\gamma)}{d},$$

into (10.25), it is found that

$$r_0|u^k|_1^2 - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j})|u^j|_1^2 \leq r_{k-1} \left[|u^0|_1^2 + \frac{1}{2d\mu_z r_{k-1}} \|f^{k-1+\sigma}\|^2 \right] \leq r_{k-1} E, \quad (10.26)$$

where E is given in the theorem.

Next, using (10.26) and mathematical induction method, we are able to get

$$|u^k|_1^2 \leq E, \quad 1 \leq k \leq K. \quad (10.27)$$

Finally, applying the first result in (10.19) to $|u^k|_1^2$ in (10.27) yields (10.20). The proof is complete. $\square$

10.3 Stability and Convergence

Applying established results in Section 10.2, we are able to show that the system (10.10) is robust to perturbations at initial condition and non-homogeneous term $f(x, t)$, and is convergent with accuracy $O(\tau_z^{3-\gamma} + \tau_1^2 + h^2)$.

Theorem 10.2. (*Stability*) *The proposed numerical scheme (10.10) is stable with respect to initial data and non-homogeneous data in $\|\cdot\|_\infty$ sense.*

Proof. Assume that v_m^k , $0 \leq m \leq M$ is the solution of the following system with perturbations at initial condition as well as non-homogeneous term

$$\begin{cases} \mu_z \left[r_0 v_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) v_m^j - r_n v_m^0 \right] = d\delta_x^2 v_m^{k-1+\sigma_k} + \bar{f}_m^{k-1+\sigma}, \\ v_m^0 = \psi(x_m) - \theta_m, \quad 1 \leq m \leq M-1 \\ v_0^k = \phi_1(t_k), \quad v_M^k = \phi_2(t_k), \quad 0 \leq k \leq K \end{cases} \quad (10.28)$$

where $\mu_z = \frac{1}{\Gamma(2-\gamma)\tau_z^\gamma}$.

Let $\epsilon_m^k = u_m^k - v_m^k$, $0 \leq m \leq M$, $0 \leq k \leq K$, from systems (10.28) and (10.10), it is found that $\{\epsilon_m^k\}$ satisfies

$$\begin{cases} \mu_z \left[r_0 \epsilon_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) \epsilon_m^j - r_{k-1} \epsilon_m^0 \right] = d \delta_x^2 \epsilon_m^{k-1+\sigma_k} + \hat{f}_m^{k-1+\sigma}, \\ \epsilon_m^0 = \theta_m, \quad 1 \leq m \leq M-1 \\ \epsilon_0^k = \epsilon_M^k = 0, \quad 0 \leq k \leq K \end{cases} \quad (10.29)$$

where $\theta_0 = \theta_M = 0$ and $\hat{f}_m^{k-1+\sigma} = f_m^{k-1+\sigma} - \bar{f}_m^{k-1+\sigma}$.

Applying Theorem 10.1 to (10.29), it is obviously achieved that

$$\|u^k\|_\infty^2 \leq \frac{L}{4} \left[|\theta|_1^2 + \frac{\Gamma(1-\gamma)}{d} \max_{1 \leq k \leq K} \|\hat{f}^{k-1+\sigma}\|^2 \right], \quad 1 \leq k \leq K \quad (10.30)$$

which gives stability of the proposed numerical scheme (10.10). $\square$

The last thing is to give the convergence order explicitly. To this aim, we shall present some lemmas before establishing the main theorem. The first lemma gives the accuracy of the approximation (10.9) for the fractional term ${}_0^C D_{t;[\mathcal{Z};1]}^\gamma u(x_m, t_{k-1+\sigma})$.

Lemma 10.3. *For any fixed $x = x_m \in [0, L]$ and $0 < \gamma < 1$, if $u(x_m, \mathcal{Z}^{-1}(z)) = \bar{u}(x_m, z) \in \mathcal{C}^3[z(0), z(1)]$ where $t = \mathcal{Z}^{-1}(z)$ is the inverse of function $\mathcal{Z}(t)$, then*

$${}_0^C D_{t;[\mathcal{Z};1]}^\gamma u(x_m, t_{k-1+\sigma}) = \mu_z \left[r_0 U_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) U_m^j - r_{k-1} U_m^0 \right] + O(\tau^{3-\gamma}) \quad (10.31)$$

where $U_m^k = u(x_m, t_k)$, $\mu_z = \frac{1}{\Gamma(2-\gamma)\tau^\gamma}$, $\tau_z = z(t_{j+1}) - z(t_j)$ and r_j 's are coefficients given in (2.22) in Chapter 2.

Proof. In view of (10.9), obviously, we have

$$\Delta = {}_0^C D_{t;[\mathcal{Z};1]}^\gamma u(x_m, t_{k-1+\sigma}) - \mu_z \left[r_0 U_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) U_m^j - r_{k-1} U_m^0 \right] = R_1 + R_2,$$

where

$$\begin{aligned}
R_1 &= \frac{1}{\Gamma(1-\gamma)} \sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} [z_{k-1+\sigma} - z(s)]^{-\gamma} [u_t(x_m, s) - (\mathcal{GI}_{2,j}(s))'] ds \\
&= \frac{1}{\Gamma(1-\gamma)} \sum_{j=1}^{k-1} \left[[z_{k-1+\sigma} - \mathcal{Z}(t)]^{-\gamma} [u(x_m, t) - \mathcal{GI}_{2,j}(t)] \Big|_{t_{j-1}}^{t_j} - \right. \\
&\quad \left. (-\gamma - 1) \int_{t_{j-1}}^{t_j} [z_{k-1+\sigma} - z(s)]^{-\gamma-1} [u(x_m, s) - \mathcal{GI}_{2,j}(z(s))] dz(s) \right] \\
&= \frac{\gamma + 1}{\Gamma(1-\gamma)} \sum_{j=1}^{k-1} \int_{z_{j-1}}^{z_j} [z_{k-1+\sigma} - z]^{-\gamma-1} [u(x_m, \mathcal{Z}^{-1}(z)) - \mathcal{GI}_{2,j}(z)] dz
\end{aligned}$$

and

$$\begin{aligned}
R_2 &= \frac{1}{\Gamma(1-\gamma)} \int_{t_{k-1}}^{t_{k-1}+\sigma} [z_{k-1+\sigma} - z(s)]^{-\gamma} [u_t(x_m, s) - (\mathcal{GI}_{1,k}(s))'] ds \\
&= \frac{1}{\Gamma(1-\gamma)} \int_{z_{k-1}}^{z_{k-1}+\sigma} [z_{k-1+\sigma} - z]^{-\gamma} \left[\frac{\partial u(x_m, \mathcal{Z}^{-1}(z))}{\partial z} - \frac{u_m^k - u_m^{k-1}}{z_k - z_{k-1}} \right] dz.
\end{aligned}$$

Since $z_{k-1+\sigma} - z_k = \sigma\tau_z$, $z_{j+1} - z_j = \tau_z$ ($\sigma = 1 - \frac{\gamma}{2}$), using the results from the proof of Lemma 2 in [7], we get

$$R_1 = O(\tau_z^{3-\gamma}), \quad R_2 = O(\tau_z^{3-\gamma})$$

which yields (10.31). □

Remark 10.3. Throughout the proof of Lemma 10.3, $u_m^k = U_m^k = u(x_m, t_k)$ has been used informally for the sake of convenience. Note that in other parts, $u_m^k \neq u(x_m, t_k)$.

Next, let us deal with the accuracy of the approximation

$$u_m^{k-1+\sigma} \approx \sigma_k u_m^k + (1 - \sigma_k) u_m^{k-1} = u_m^{k-1+\sigma_k}$$

that used in deriving numerical scheme (10.10). Generally speaking, the following result is true

Lemma 10.4. For any function $\mathcal{Y}(t) \in \mathcal{C}^2[0, T]$ with the mesh $\mathcal{P}''$, we find

$$\sigma_k \mathcal{Y}(t_k) + (1 - \sigma_k) \mathcal{Y}(t_{k-1}) = \mathcal{Y}(t_{k-1+\sigma}) + O(\tau_1^2), \quad (10.32)$$

where $\sigma = 1 - \frac{\gamma}{2}$, $\sigma_k = \frac{t_{k-1+\sigma} - t_{k-1}}{t_k - t_{k-1}}$ and $\tau_1 = \max_{0 \leq k \leq K-1} (t_{k+1} - t_k)$.

Proof. Applying Taylor expansion to $\mathcal{Y}(t_k)$ and $\mathcal{Y}(t_{k-1})$ at $t = t_{k-1+\sigma}$ gives

$$\mathcal{Y}(t_k) = \mathcal{Y}_{k-1+\sigma} + (t_k - t_{k-1+\sigma}) \mathcal{Y}'(t_{k-1+\sigma}) + \frac{(t_k - t_{k-1+\sigma})^2}{2} \mathcal{Y}''(\zeta_1), \quad (10.33)$$

for $t_{k-1+\sigma} < \zeta_1 < t_k$ and

$$\mathcal{Y}(t_{k-1}) = \mathcal{Y}_{k-1+\sigma} + (t_{k-1} - t_{k-1+\sigma}) \mathcal{Y}'(t_{k-1+\sigma}) + \frac{(t_{k-1} - t_{k-1+\sigma})^2}{2} \mathcal{Y}''(\zeta_2) \quad (10.34)$$

for $t_{k-1} < \zeta_2 < t_{k-1+\sigma}$.

Since $\sigma_k = \frac{t_{k-1+\sigma} - t_{k-1}}{t_k - t_{k-1}}$ leads to $t_k - t_{k-1+\sigma} = (1 - \sigma_k)(t_k - t_{k-1})$ and $t_{k-1} - t_{k-1+\sigma} = -\sigma_k(t_k - t_{k-1})$, this together with equations (10.33) and (10.34) yields

$$\begin{aligned} |\sigma_k \mathcal{Y}(t_k) + (1 - \sigma_k) \mathcal{Y}(t_{k-1}) - \mathcal{Y}_{k-1+\sigma}| &\leq \frac{\sigma_k(1 - \sigma_k)}{2} \max_{t \in [0, T]} |\mathcal{Y}''(t)| (t_k - t_{k-1})^2 \\ &\leq \frac{1}{8} \max_{t \in [0, T]} |\mathcal{Y}''(t)| \tau_1^2, \end{aligned} \quad (10.35)$$

that ends the proof. $\square$

Remark 10.4. If $\mathcal{Z}'(t) \geq c > 0$ where c is a constant, then using Langrange mean value theorem, we get

$$\frac{\mathcal{Z}(t_k) - \mathcal{Z}(t_{k-1})}{t_k - t_{k-1}} = \mathcal{Z}'(\xi) \geq c, \quad 1 \leq k \leq K.$$

Therefore, τ_z and τ_1 can be related by

$$\tau_1 = \max_{0 \leq k \leq K-1} (t_k - t_{k-1}) \leq \frac{\mathcal{Z}(t_k) - \mathcal{Z}(t_{k-1})}{c} = \frac{\tau_z}{c}. \quad (10.36)$$

The next essential result is about the local truncation error T_m^k which is the residual generated by substituting exact solutions $\{U_m^k = u(x_m, t_k)\}$ into scheme (10.10),

namely,

$$\mu_z \left[r_0 U_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) U_m^j - r_{k-1} U_m^0 \right] = d \delta_x^2 U_m^{k-1+\sigma_k} + f_m^{k-1+\sigma} + T_m^k. \quad (10.37)$$

Lemma 10.5. *Suppose that the exact solution $u(x, t) \in \mathcal{C}^{2,2}([0, L] \times [0, T])$ and $u(x, \mathcal{Z}^{-1}(z)) = \bar{u}(x, z) \in \mathcal{C}^3[z(0), z(T)]$ for any fixed x where $\mathcal{Z}^{-1}(z)$ is the inverse of increasing scale function $\mathcal{Z}(t)$. Then it holds that*

$$T_m^k = O(\tau_z^{3-\gamma} + \tau_1^2 + h^2), \quad 1 \leq m \leq M-1, \quad 1 \leq k \leq K \quad (10.38)$$

where $\tau_z = z(t_k) - z(t_{k-1})$, $\tau_1 = \max_{0 \leq k \leq K-1} |t_{k+1} - t_k|$ and $h = \frac{L}{M}$.

Proof. Considering the problem (9.1) at $(x_m, t_{k-1+\sigma})$ and the equation (10.37), it is obvious that

$$\begin{aligned} T_m^k &= \mu_z \left[r_0 U_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) U_m^j - r_{k-1} U_m^0 \right] - d \delta_x^2 U_m^{k-1+\sigma_k} - f_m^{k-1+\sigma} \\ &\quad - \left[{}^C_0 D_{t;[\mathcal{Z};1]}^\gamma u(x_m, t_{k-1+\sigma}) - du_{xx}(x_m, t_{k-1+\sigma}) - f(x_m, t_{k-1+\sigma}) \right] \\ &= \left\{ \mu_z \left[r_0 U_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) U_m^j - r_{k-1} U_m^0 \right] - {}^C_0 D_{t;[\mathcal{Z};1]}^\gamma u(x_m, t_{k-1+\sigma}) \right\} \\ &\quad - d (\delta_x^2 U_m^{k-1+\sigma_k} - \delta_x^2 U_m^{k-1+\sigma}) - d (\delta_x^2 U_m^{k-1+\sigma} - u_{xx}(x_m, t_{k-1+\sigma})) \end{aligned}$$

Applying Lemma 10.3 to the first term, Lemma 10.4 to the second term and taking Taylor expansion at $x = x_m$ for the last term, we then get (10.38). $\square$

Now we are in a position to analyze the convergence of the developed numerical scheme (10.10).

Theorem 10.3. *Assume that the exact solution $u(x, t) \in \mathcal{C}^{2,2}([0, L] \times [0, T])$ and $u(x, \mathcal{Z}^{-1}(z)) = \bar{u}_x(z) \in \mathcal{C}^3[z(0), z(T)]$, where $\mathcal{Z}^{-1}(z)$ is the inverse of increasing scale function $\mathcal{Z}(t)$ and is concave. Let $\{U_m^k = u(x_m, t_k)\}$ be the exact solution at mesh points and $\{u_m^k\}$ be the numerical solution obtained from the scheme (10.10). Denote $e_m^k = U_m^k - u_m^k$, $0 \leq m \leq M$, $0 \leq k \leq K$ as the error at (x_m, t_k) , then*

$$\|e^k\|_\infty \leq O(\tau_z^{3-\gamma} + \tau_1^2 + h^2), \quad 0 \leq k \leq K-1 \quad (10.39)$$

where $0 < \gamma < 1$.

Proof. From systems (10.10) and (10.37) with conditions

$$U_m^0 = \psi(x_m), \quad 1 \leq m \leq M-1 \quad U_0^k = \phi_1(t_k), \quad U_M^k = \phi_2(t_k), \quad 0 \leq k \leq K$$

it is easily seen that $\{e_m^k\}$ is the solution of the following system

$$\begin{cases} \mu_z \left[r_0 e_m^k - \sum_{j=1}^{k-1} (r_{k-j-1} - r_{k-j}) e_m^j - r_{k-1} e_m^0 \right] = d \delta_x^2 e_m^{k-1+\sigma_k} + T_m^k, \\ e_m^0 = 0, \quad 1 \leq m \leq M-1 \\ e_0^k = e_M^k = 0, \quad 0 \leq k \leq K \end{cases} \quad (10.40)$$

where $\mu_z = \frac{1}{\Gamma(2-\gamma)\tau_z^\gamma}$ and $\sigma_k = \frac{t_{k-1}+\sigma-t_{k-1}}{t_k-t_{k-1}}$.

Applying Theorem 10.1 to above system (10.40), we shall get an analog result as in (10.20) given by

$$\|e^k\|_\infty^2 \leq \frac{L}{4} \left[|e^0|_1^2 + \frac{\Gamma(1-\gamma)}{d} \max_{1 \leq k \leq K} \|T^k\|^2 \right], \quad 1 \leq k \leq K. \quad (10.41)$$

Since $e_m^0 = 0$, $0 \leq m \leq M$, we have $|e^0|_1^2 = 0$. Using (10.38) and $(M-1)h \leq L$, we are able to achieve

$$\|T^k\| = \sqrt{h \sum_{m=1}^{M-1} (T_m^k)^2} \leq \sqrt{h(M-1)} O(\tau_z^{3-\gamma} + \tau_1^2 + h^2) \leq O(\tau_z^{3-\gamma} + \tau_1^2 + h^2). \quad (10.42)$$

Hence, (10.39) follows directly from (10.41) and (10.42). $\square$

Remark 10.5. If $\mathcal{Z}'(t) \geq c > 0$ where c is constant, then using (10.36) in (10.39), the bound of maximum absolute error becomes

$$\|e^k\|_\infty \leq O(\tau_z^2 + h^2), \quad 0 \leq n \leq N-1 \quad (10.43)$$

that will be used in examples in next section.

10.4 Simulation

In this section, we shall present two examples to demonstrate the efficiency of our proposed numerical scheme (10.10) as well as verify the established theoretical result (10.39). For this purpose, we shall compute the maximum absolute error at $t = T$ in and the temporal convergence order.

Example 10.1. *Consider Example 9.1.*

Let $\vartheta_2 = 1.1$ and $\vartheta_1 = \gamma + 3.3$. It is easy to verify that the conditions in Theorem 10.3 are satisfied and somehow weaker than in Chapter 9. In this case, we fix $h = \frac{1}{1000}$ and vary K to compute the maximum absolute error at $t = 1$ and corresponding temporal convergence order $\mathcal{O}_{\infty,t}$. The result is displayed in Table 10.1. As one can see, we obtain approximately second order accuracy in the temporal dimension which is consistent with our theoretical result.

TABLE 10.1: (Example 10.1) Temporal convergence order when $h = \frac{1}{1000}$

K	$\gamma = 0.2$	$\mathcal{O}_{\infty,t}$	$\gamma = 0.5$	$\mathcal{O}_{\infty,t}$	$\gamma = 0.8$	$\mathcal{O}_{\infty,t}$
10	5.2935E-04	-	1.1990E-03	-	1.3303E-03	-
20	1.3853E-04	1.9341	3.1864E-04	1.9119	3.5792E-04	1.8941
40	3.5618E-05	1.9595	8.3180E-05	1.9376	9.5197E-05	1.9106

Also, for visualization purpose, we plot the numerical solution obtained from the proposed scheme (10.10), the exact solution and the absolute error in Figures 10.1 and 10.2 when $\gamma = 0.2$. From these two figures, it is easily seen that the proposed numerical scheme (10.10) can give a very good and accurate approximation to the exact solution.

Our next example is a generalized fractional sub-diffusion problem from [130] where the exact solution is not available.

Example 10.2. [130] *The generalized fractional sub-diffusion problem is as follows:*

$$\left\{ \begin{array}{l} {}^C_0 D_{t;[Z;1]}^\gamma u(x, t) = u_{xx}(x, t) + f(x, t), \quad x \in [0, 1], \quad t \in [0, 1] \\ u(x, 0) = \sin(\pi x), \\ u(0, t) = 0, \quad u(1, t) = 0 \end{array} \right. \quad (10.44)$$

FIGURE 10.1: (Example 10.1) Approximate solution obtained from (10.10) and exact solution when $\gamma = 0.2$, $h = \frac{1}{1000}$, $K = 40$.

FIGURE 10.2: (Example 10.1) Absolute error when $\gamma = 0.2$, $h = \frac{1}{1000}$, $K = 40$.

where $0 < \gamma < 1$ and

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

In this example, we shall use sufficiently small h and τ_z (e.g. $h = \frac{1}{1000}$, $\tau_z = \frac{1}{1000}$) to obtain an approximate solution $\{\tilde{U}_m^k\}$ from the numerical scheme (10.10). When computing the absolute error, this $\{\tilde{U}_m^k\}$ will be used to replace the exact value $\{U_m^k\}$.

Let $h = \frac{1}{1000}$ be fixed and τ_z vary as $\frac{1}{10}$, $\frac{1}{20}$, $\frac{1}{40}$ to obtain temporal convergence order. The maximum absolute error at $t = 1$ and the temporal convergence order

for $\mathcal{Z}(t) = e^{2t} - 1$, $t^{1.1}$ and $t^{0.9}$ are presented in Tables 10.2, 10.3 and 10.4. It is shown that the second order accuracy in the temporal dimension is achieved for the given scale functions $\mathcal{Z}(t) = e^{2t} - 1$ and $\mathcal{Z}(t) = t^{1.1}$. Even though the inverse of the scale function $\mathcal{Z}(t) = t^{0.9}$ is not concave which somehow violates the assumption in Theorem 10.3, it is good to see that we can still get second accuracy.

The numerical results from implementing the method in [130] are also given for various scale functions $\mathcal{Z}(t) = e^{2t} - 1$, $t^{1.1}$ and $t^{0.9}$ in Tables 10.2, 10.3 and 10.4 respectively. Obviously, the proposed numerical method (10.10) can achieve second order accuracy in temporal dimension in general which improves the work done in [130] where they have $(2 - \gamma)$ order accuracy in general. Though in some cases, the numerical scheme (10.10) do not give smaller error, this will not be a big problem since a high temporal convergence order is obtained. As $K \rightarrow \infty$ and $h \rightarrow 0$, our scheme (10.10) will converge faster to the exact solution than method in [130] and thus give a smaller error in the end.

TABLE 10.2: (Example 10.2) Temporal convergence order when $\mathcal{Z}(t) = e^{2t} - 1$,
 $h = \frac{1}{1000}$

	K	$\gamma = 0.2$	$\mathcal{O}_{\infty,t}$	$\gamma = 0.5$	$\mathcal{O}_{\infty,t}$	$\gamma = 0.8$	$\mathcal{O}_{\infty,t}$
Scheme (10.10)	10	4.2633E-05	-	8.6927E-05	-	1.2463E-04	-
	20	1.0356E-05	2.0415	2.1168E-05	2.0379	3.0721E-05	2.0203
	40	2.5363E-06	2.0297	5.1956E-06	2.0265	7.6096E-06	2.0134
Method in [130]	10	3.0844E-05	-	8.8251E-05	-	1.5905E-04	-
	20	1.0138E-05	1.6052	3.3548E-05	1.3954	7.1223E-05	1.1591
	40	3.2180E-06	1.6556	1.2375E-05	1.4388	3.1179E-05	1.1917

TABLE 10.3: (Example 10.2) Temporal convergence order when $\mathcal{Z}(t) = t^{1.1}$,
 $h = \frac{1}{1000}$

	K	$\gamma = 0.2$	$\mathcal{O}_{\infty,t}$	$\gamma = 0.5$	$\mathcal{O}_{\infty,t}$	$\gamma = 0.8$	$\mathcal{O}_{\infty,t}$
Scheme (10.10)	10	1.4387E-04	-	3.2093E-04	-	4.4405E-04	-
	20	3.5921E-05	2.0019	8.0203E-05	2.0005	1.1101E-04	2.0001
	40	8.9669E-06	2.0021	2.0032E-05	2.0013	2.7730E-05	2.0011
Method in [130]	10	6.8784E-05	-	3.7115E-04	-	1.3757E-03	-
	20	2.1053E-05	1.7081	1.3372E-04	1.4728	5.9882E-04	1.2000
	40	6.3583E-06	1.7273	4.7702E-05	1.4871	2.5826E-04	1.2133

Next, in Figure 10.3, we plot the numerical solution $\{u_m^k\}$ and $\{\tilde{U}_m^k\}$ for visualization purpose. We can not draw the absolute error between $\{u_m^k\}$ and $\{\tilde{U}_m^k\}$ as the

TABLE 10.4: (Example 10.2) Temporal convergence order when $\mathcal{Z}(t) = t^{0.9}$,
 $h = \frac{1}{1000}$

	K	$\gamma = 0.2$	$\mathcal{O}_{\infty,t}$	$\gamma = 0.5$	$\mathcal{O}_{\infty,t}$	$\gamma = 0.8$	$\mathcal{O}_{\infty,t}$
Scheme (10.10)	10	2.5975E-04	-	5.6279E-04	-	7.6311E-04	-
	20	6.5074E-05	1.9970	1.4082E-04	1.9988	1.9069E-04	2.0007
	40	1.6267E-05	2.0001	3.5176E-05	2.0012	4.7598E-05	2.0022
Method in [130]	10	5.2005E-05	-	2.7657E-04	-	9.9880E-04	-
	20	1.5991E-05	1.7014	9.9812E-05	1.4704	4.3410E-04	1.2022
	40	4.8464E-06	1.7222	3.5649E-05	1.4853	1.8708E-04	1.2144

mesh is non-uniform and different. However, from Figure 10.3, it is obvious that these diagrams have similar shape which implies the convergence of the proposed numerical scheme (10.10) and the reasonable usage of $\{\tilde{U}_m^k\}$.

FIGURE 10.3: (Example 10.2) Numerical solution $\{u^k\}$ when $\gamma = 0.2$, $h = \frac{1}{1000}$, $K = 40$ and $\mathcal{Z}(t) = e^{2t} - 1$, and solution $\{\tilde{U}^k\}$.

10.5 Summary

This chapter constructs a generalized $L2 - 1_\sigma$ approximation for a new generalized Caputo fractional derivative with order $0 < \gamma < 1$, and then apply this new approximation and finite difference method to a new generalized fractional sub-diffusion problem. Under proper assumptions, it is shown that the proposed numerical scheme is uniquely solvable, stable and convergent. The convergence order is proven to be $O(\tau_z^{3-\gamma} + \tau_1^2 + h^2)$. In the end, two examples (one with exact solution and the other one without exact solution) are used to demonstrate the efficiency and accuracy of the proposed method. It is found that the numerical

result is consistent with the theoretical one and more importantly, the scheme can work well even if some assumptions in Theorem [10.3](#) are not satisfied which is a good sign in practice.

Chapter 11

Conclusion and Future Research

11.1 Conclusion

Fractional problems have gained sufficient attention in recent decades as they are more accurate in modeling memory process than integer order models. However, it is extremely difficult to get the explicit expression of the exact solution for most fractional problems if it is not impossible. Therefore, in reality, efficient and effective numerical methods are very important. To this aim, we have investigated typical fractional problems in Chapters 3-8 using parametric quintic spline method and new generalized fractional problems in Chapters 9 and 10 through non-uniform mesh method. The contributions and main results are summarized in two aspects below.

- In Chapters 3-8, we have considered various typical fractional problems: second-order one and two dimensional fractional sub-diffusion equations, fourth-order fractional sub-diffusion equation, fourth-order diffusion-wave model and distributed order fractional sub-diffusion model. In all these problems, parametric quintic spline method that involves a parameter $\xi > 0$ has been explored. By selecting the parameter based on the local truncation error, we can get various numerical schemes with different accuracy. In these chapters, we actually analyze cases that can yield the best spatial convergence order, i.e. $O(h^{4.5})$. It is noted that the attained result improves the compact finite difference method ($O(h^4)$) and finite difference method ($O(h^2)$) while

requires acceptable computation cost. Another major contribution in these chapters is, of course, the theoretical analysis including solvability, stability and convergence of the proposed numerical scheme through discrete energy methodology. We are confident that the proposed numerical schemes can work well for a large class of the fractional problems based on the theoretical results established in Chapters 3-8. In fact, it is true and easily observed from the related simulation results.

- The objective of Chapter 9 and Chapter 10 is to improve performance of the numerical methods of new generalized fractional sub-diffusion problems, especially the performance in temporal dimension. To this aim, we generalize the WSGL approximation to gWSGL and $L2-1_\sigma$ approximation to $gL2-1_\sigma$. These two generalized approximations are actually based on a particular non-uniform mesh in temporal which are totally different from WSGL and $L2-1_\sigma$ methods. In this case, we have established the stability and convergence of the proposed numerical scheme. It is shown that both methods can obtain better performance theoretically and numerically. We note that gWSGL based method can work for a larger class of scale function $\mathcal{Z}(t)$ than $gL2-1_\sigma$ method, whereas the latter one has weakened regularities of the exact solution required by the former method. In reality, one needs to choose the one that is suitable and can be well applied.

11.2 Future Research

In the future, we may conduct research on a few aspects that include but not limited to:

- The parametric quintic spline method has achieved better results comparing to previous work done to date. In fact, the method itself can achieve $O(h^6)$ which can be easily seen from the local truncation error there. Due to two extra conditions that give $O(h^4)$, globally, we only get $O(h^{4.5})$. In the future, appropriate high accuracy extra conditions will be developed or periodic boundary conditions that can somehow avoid the extra conditions will be considered.

- For the typical fractional sub-diffusion or diffusion-wave problems, we have used high order method in time that require the solution to be sufficiently smooth. However, it is well known that the exact solution is singular at the origin in time. It means that the solution is not smooth and may have a weak singularity at the initial time $t = 0$ in the sense that the derivatives of the solution may become unbounded near that point, see [60–62, 93, 132]. However, the best result in these papers can achieve at most $O(\tau^2)$. Therefore, it is still challenging to propose high order approximate methods under limited regularity and that will be our future topic.
- Besides the fractional derivatives that we have discussed here, namely, RL fractional derivative, Caputo fractional derivative, distributed order fractional derivative and new generalized Caputo fractional derivative, there are other fractional derivatives that have shown to be useful in applications, e.g. Risez fractional derivative [137] and tempered fractional derivative [111]. Research on both well-posedness of the problem which is rare in the literature and the high order numerical schemes of these topics is no doubt necessary and important.
- In this thesis, only one work is about high dimensional fractional problems. As one can see, the theoretical results may be similarly analyzed for two dimensional problems as in one dimensional problems. But the computation incurred in high dimensional problems is far more than low dimensional cases unless particular techniques are used. Besides this, the partition of the domain can be very flexible and complex for high dimensional problems. In the future, we will also focus on the numerical treatment on the high dimensional problems from the following two aspects:
 - Mathematical methods: decomposition of matrix or alternating direction techniques which convert the original problem into a series of sub-problems that can be efficiently solved.
 - Artificial neural network or deep neural network. Artificial neural network has been successfully used for (integer order) ordinary differential equations and partial differential equations, especially for large systems or high dimension problems, see [75, 92, 108, 109]. Recently, deep neural network [49, 126] has been applied to high dimensional parabolic partial differential equations and gained a great success. However, there is no

work about fractional problems in the literature. Since we can use GPU to speed up the computation in neural network, we believe that it is meaningful to conduct this potential research.

- Chapters 3-10 all deal with linear fractional problems which have good properties comparing with non-linear ones. In fact, due to the complexity of the real world problems, it seems that non-linear fractional equations, like [107], are more practical and useful. Therefore, the numerical consideration on this kind of fractional problems is worthwhile. This will of course be the main topic in the future research.

Author's Publications

Journal Articles

- **Xuhao Li** and Patricia Jia Yiing Wong, “A higher order non-polynomial spline method for fractional sub-diffusion problems,” *J. Comput. Phys.*, 328(2017), 46–65.
- **Xuhao Li** and Patricia Jia Yiing Wong, “A non-polynomial numerical scheme for fourth-order fractional diffusion-wave model,” *Appl. Math. Comput.*, 331(2018), 80-95.
- **Xuhao Li** and Patricia Jia Yiing Wong, “An efficient numerical treatment of fourth-order fractional diffusion-wave problems,” *Numer. Methods Partial Differential Equations*, 2018.
- **Xuhao Li** and Patricia Jia Yiing Wong, “An efficient non-polynomial spline method for distributed order fractional sub-diffusion equations,” *Math. Methods Appl. Sci.*, 2018.
- **Xuhao Li** and Patricia Jia Yiing Wong, “Numerical solutions of fourth-order fractional sub-diffusion problems via parametric quintic spline.” (Submitted)
- **Xuhao Li** and Patricia Jia Yiing Wong, “Non-polynomial spline approach in two-dimensional fractional sub-diffusion problems.” (Submitted)

Conference Proceedings

- **Xuhao Li** and Patricia Jia Yiing Wong, “A new implicit numerical scheme for fractional sub-diffusion equation,” In *2016 14th International Conference on Control, Automation, Robotics and Vision (ICARCV)*, 2016, 1-6.

- **Xuhao Li** and Patricia Jia Yiing Wong, “Nonpolynomial numerical scheme for fourth-order fractional sub-diffusion equations,” *Proceedings of the International Conference on Numerical Analysis and Applied Mathematics 2016 (ICNAAM-2016)*, *AIP Conference Proceedings* 1863, 190002 (2017).
- **Xuhao Li** and Patricia Jia Yiing Wong, “Numerical solution of fourth-order fractional diffusion wave model,” *ICNAAM 2017* (Accepted).
- **Xuhao Li** and Patricia Jia Yiing Wong, “High order approximation to new generalized fractional Caputo derivatives and its applications,” *ICNAAM 2017* (Accepted).
- **Xuhao Li** and Patricia Jia Yiing Wong, “Parametric quintic spline approach for two-dimensional fractional sub-diffusion equation,” *ICNAAM 2017* (Accepted).

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