INVERSE PROBLEMS OF TIME-FRACTIONAL DIFFERENTIAL EQUATIONS: ANALYSIS AND NUMERICAL METHODS

ZHENGQI ZHANG

PhD

The Hong Kong Polytechnic University

2023

The Hong Kong Polytechnic University

Department of Applied Mathematics

Inverse Problems of Time-Fractional Differential Equations: Analysis and Numerical Methods

Zhengqi Zhang

A thesis submitted in partial fulfilment of the requirements for the degree of Doctor of Philosophy

April 2023

CERTIFICATE OF ORIGINALITY

I hereby declare that this thesis is my own work and that, to the best of my knowledge and belief, it reproduces no material previously published or written, nor material that has been accepted for the award of any other degree or diploma, except where due acknowledgement has been made in the text.

____________________ (Signed)

Zhengqi Zhang (Name of student)

Abstract

This thesis is devoted to theoretical and numerical analysis of inverse problems of fractional differential equations, which have drawn much attention over the past decades due to the maybe ”mild” ill-posedness of fractional derivatives.

In recent years, some numerical algorithms and mathematical analysis are provided and tested. However, in most of these works, only some convergence results and semidiscrete numerical analysis are analyzed. Then our aim is to give a thorough numerical analysis of inverse problems, where numerical estimates are provided including noise level, regularization and discretization parameters. The numerical estimates provide a balancing way to choose regularization and discretization parameter from the noise level. Therefore, we could use a relevant coarser grid to obtain some optimal convergent results.

After a background and preliminary introduction in Chapter 1 and Chapter 2, firstly in Chapter 3 we focus on the backward subdiffusion problem, with the application of quasi-boundary regularization method, piecewise-linear finite element method and convolution quadrature, we show a total error estimate based on smoothing properties of (discrete) solution operators, and nonstandard error estimate for the direct problem in terms of problem data regularity. Next in Chapter 4 when the backward subdffision model includes a time-dependent coefficient, we use a perturbation argument of freezing the diffusion coefficients. Similarly, we apply a quasi-boundary value method and a fully discrete method consisting of finite element method in space and backward Euler convolution quadrature in time. An *a priori* error estimate is established. Based on the motivation in subdiffusion we extend our idea to fractional-wave equation in Chapter 5 where we want to simultaneously determine two initial conditions based on two different observations. After a new proposed quasi-boundary value method and a classical fully discrete method in space and time, a conditional *a priori* error estimate is shown. On the other hand, we focus on the inverse potential problem in Chapter 6, to recover potential in a fractional differential equation, with the severely ill posed nature, we construct a monotone operator one of whose fixed points is the unknown potential. The uniqueness of the identification is theoretically verified. Moreover, we show a conditional stability in Hilbert spaces under some suitable conditions on the problem data. Next, a completely discrete scheme is developed by using Galerkin finite method in space and finite difference method in time. A discrete fixed point iteration is constructed and a thorough numerical analysis is given. Lastly in Chapter 7, we summarize our work and mention possible future research topics.

In each chapter, various numerical experiments are provided to support our obtained numerical error estimates. By a balancing choice of parameters, we would obtain an optimal convergence rates,

which is strongly supported by our numerical experiments.

Acknowledgements

First and foremost, I would like to express my sincere gratitude to my supervisor, Dr. Zhi Zhou, for his invaluable guidance, unwavering support, and insightful suggestions throughout my research journey. Dr. Zhi Zhou's mentorship and expertise have been instrumental in shaping my research skills and professional development. I feel truly fortunate to have met Dr. Zhi Zhou during my time at the Hong Kong Polytechnic University. He not only taught me how to conduct scientific research but also how to approach problems and think critically like a professional scientist. I am deeply grateful for his support and encouragement, which have been essential to the successful completion of this thesis.

Dr. Philippe G. Ciarlet taught me mathematical analysis on linear and nonlinear partial differential equations. Dr. Zhonghua Qiao taught me the numerical methods. Dr. Xiaojun Chen taught me how to give a research talk. I would like to thank them and all the professors who taught me at Hong Kong. I would also thank Dr. Buyang Li and Dr. Bangti Jin, for their suggestions for my study and research. I thank Dr. Zhidong Zhang for his collaboration. I thank Dr. Defeng Sun, Dr. Xingqiu Zhao, Dr. Yanping Lin, Miss. Natalie Cheung Ting-ting and all other staffs at the Department of applied mathematics for their appropriate support.

Finally, I would also be grateful to Dr. Shin Kwancheol, Dr. Qimeng Quan, Dr. Shu Ma, Dr. Chaoyu Liu, Mr. Run Zheng, Mr. Zhaoming Yuan, Mr. Siyu Cen, Mr. Yongcheng Dai and all my friends at our math department for their help and collaboration. I have to express my deep gratitude to my parents and family for their love and patience.

Contents

List of Figures

List of Tables

CHAPTER 1.
INTRODUCTION

In this chapter, we will introduce anomalous diffusion and mathematical foundations on non-integer order calculus in section 1.1. The development of inverse problems for systems with non-integer order, would be presented in section 1.2. This dissertation's contributions and organizational structure, are then described in section 1.3.

1.1 Introduction to anomalous diffusion

In 1855, Adolf Fick introduced Fick's first law of diffusion, which describes how the diffusive flux travels from areas of high concentration to areas of low concentration.(see Figure 1.1[1]) The magnitude of the flux is proportional to the concentration gradient. Applying this law to mass concentration leads to the classical diffusion equation, which characterizes the evolution of concentration over time:

$$\partial_t u(x,t) - D\Delta u(x,t) = 0,$$

where u represents the concentration of substances and D is the diffusion coefficient.

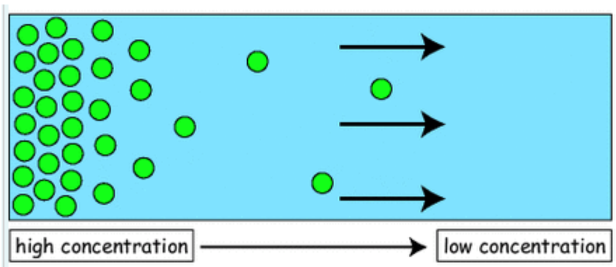


Figure 1.1: Figure of diffusion

Moreover, in 1905, Einstein [14] derived the classical diffusion equation from a microscopic level, assuming a Brownian motion of the concentration movement and applying a stochastic process. The probability density function of the particle then follows the classical diffusion equation in the macroscopic level.

In recent decades, many experiments and studies have reported that the diffusion observed in complex systems no longer follows Brownian motion, but rather Lévy processes. This type of diffusion is known as anomalous diffusion, and its main characteristic is that the mean square displacement of particles varies superlinearly (superdiffusion) or sublinearly (subdiffusion) with time. Applying

[1]The figure is from https://quizlet.com/gb/519036925/diffusion-scaling-up-biology-gcse-91-flash-cards/

anomalous diffusion models provides a better fit to experimental data observed in many significant practical applications. Specifically, subdiffusion models are often used to describe media with highly heterogeneous aquifers [2, 29, 22] and fractal geometry [85]. For example in figure 1.2 the subdiffusive motion is showed in RNA molecules in the cell, and we could see that the mean square displacement is proportional to the fractional power($\alpha = 0.7$) of time. While superdiffusion models, also known as diffusion-wave models, are frequently used to describe the propagation of mechanical waves in viscoelastic media [74, 75]. Interested readers can refer to [80, 81, 109] for a long list of applications of fractional models in biology and physics.

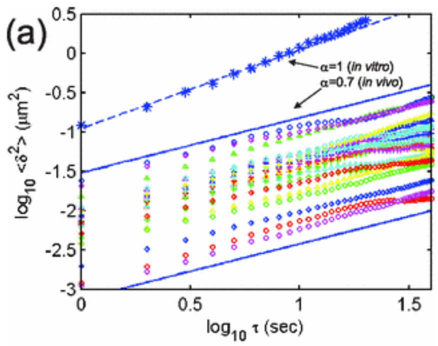


Figure 1.2: Subdiffusive motion of RNA molecules in the cell. Figure is from [22, Fig2(a)]

In this thesis, we will only consider the anomalous diffusion in time. The anomalous diffusion can be represented by an equation of the form:

$$\partial_t^\alpha u = D(-\Delta)u$$

where ∂_t^α represents a fractional derivative related to time and α is the order. We can say that $\alpha \in (0, 1)$ represents the subdiffusion model, $\alpha = 1$ represents the classical diffusion model, and $\alpha \in (1, 2)$ belongs to the diffusion-wave model.

From a mathematical point of view, fractional-order derivatives, and more generally, non-integer calculus, can be traced back to Leibniz's notes in 1695. The development of the theory of arbitrary order derivatives and integrals originated from Leibniz and evolved over three hundred years in the pure theoretical field of mathematics, primarily through the work of Liouville, Grünwald, Letnikov, and Riemann, among others. The advantage of fractional derivatives is that they provide an excellent explanation for the memory and hereditary properties of varying quantities in complex environments. There is a large amount of mathematical background literature about fractional order calculus [87, 60, 57, 38].

1.2 Introduction to inverse problems

1.2.1 Inverse problems: derivation and applications

Assume that a direct problem is well-posed in the meaning of mathematical physics, that is, if we completely know a "physical device", then we could describe this device with a classical mathematical model including the existence, uniqueness and stability of a solution state of the model. The inverse problems come from a trivial question that, given some measurement data of this device, could we find one of the parameters describing this device.

The inverse problem exists very long in our daily life. In science, a historical example may come from the discovery of Neptune from the perturbed trajectory of Uranus from Adams and Le Verrier. However, the thorough study of inverse problems may initiate from 20th century to give a comprehensive understanding of practical problems. For example, the medical imaging [32, 79] is to seek the hidden structure under skin and bones without any penetration and damage to our body. The method of weather prediction [105] uses the identification and prediction to help better industry manufacture. Oil detection [33, 7] is based on the inverse problem of diffusion in porous media. The extensive practical applications of inverse problems happens in gravimetry, computer vision, geophysics, machine learning, etc.

1.2.2 Inverse problem in differential equations

Due to various kinds of inverse problems, there are many mathematical models describing them. The difficulties of solving these models including differential equations mainly come from the ill-posedness in the Hadamard sense [25]. Given the abstract equation

$$Ax = y,$$

the well-posedness of the equation is to require A has a continuous inverse A^{-1}, in other words, the solution x must enhance the uniqueness, stability and existence. If one of them violates, we call this equation "ill-posed" (in the sense of Hadamard).

It is very essential to seek the uniqueness in inverse problem which makes much sense in practical applications. However, the existence condition would not be necessary, for even if there is no existence, we could find an "approximate" unique solution. The stability would imply the level of ill-posedness of inverse problems, but it is very challenging to obtain. The importance of stability is to derived from the noise from data measured and computed from reality. We introduce interesting readers to some literatures like [34, 25, 12, 84, 28, 36, 92, 90, 35, 97, 94, 15].

The noisy observation data in inverse problems are unavoidable, without any preprocessing we may arrive results at opposite parts. The most popular processing dealing with noisy data is regularization, the main idea is to find the solution into another correct class [34, section 2.2], guaranteeing the uniqueness and "conditional stability". It is very essential in numerical methods for inverse problems to obtain stability. Tikhonov in 1943 firstly promotes this observation in his work, initiating the theory of stable recovery of linear or nonlinear ill-posed problems. The general idea is to add an extra penalty term to find minimizers of the functional [94], i.e.

$$x \mapsto \|Ax - y^\delta\|^2 + \alpha\|x - x_0\|^2$$

where α, called regularization parameter, states the level of penalty and x_0 includes *a priori* information about solutions. Tikhonov regularization has been investigated extensively in linear and nonlinear ill-posed problems. By additional assumptions on operator A and initial setting for solutions, we would arrive a stability of minimizer x_α^δ corresponding to the noisy data y^δ. Even some convergence rates have been showed upon some more conditions on operators and solution. To solve Tikhonov regularization method in nonlinear ill-posed problems, we always use iterative methods in optimization which guarantee the convergence of iterative solutions and are easy to program on electrical device. We recommend the following literatures of regularization and inverse problems [36, 94, 52, 95, 15].

For linear ill-posed problems, there are many direct regularization methods. For example, the backward parabolic problems could use truncation regularization, quasi reversibility, pseudo-parabolic, etc. [31]. The computerized tomography (cf., e.g., [84]) is also a linear problem, including the Radon transform which is basis of CT scan.

1.2.3 Inverse problems consist of anomalous diffusion in time

Following the rising interest in anomalous diffusion, it is trivial to study the inverse problem from anomalous diffusions. The inverse problems for classical diffusion could consist of recover diffusion and potential coefficients, initial condition, source term, boundary conditions and domain geometry. Not only the inverse problems for anomalous diffusion inherits these parameters, but the recovery of non-integer order (fractional order) is more important. The second interest is to compare the impact of new physics on the behavior of inverse problems with classical results.

The last aspect plays a more important role in our practical point, since it could infer the more or less reconstruction of quantities of interest. Here we briefly introduce some inverse problems related to anomalous diffusion which we use in the following chapters.

Backward diffusion Firstly let $\Omega \subset \mathbb{R}^d$ $(d \geq 1)$ be a bounded and convex domain with smooth boundary $\partial\Omega$, and consider the following backward subdiffusion equation

$$\begin{aligned} \partial_t^\alpha u - \Delta u &= f && \text{in } \Omega \times (0,T), \\ u &= 0 && \text{on } \partial\Omega \times (0,T), \\ u(0) &= u_0 && \text{in } \Omega \end{aligned} \tag{1.1}$$

where $0 < \alpha < 1$ and Δ is the Laplace operator in space. Here $\partial_t^\alpha u(t)$ denotes the Caputo fractional derivative introduced in Section 2.1.

Inverse problems for fractional diffusion have attracted much interest, and there has already been a vast literature; see e.g., review papers [48, 66, 67, 70] and references therein. Firstly we aim at the **classical backward problem**: determining the function $u(x,t)$ with $(x,t) \in \Omega \times [0,T)$ from a terminal observation $u(x,T) = g(x)$.

The smoothing property

$$c_1 \|u_0\|_{L^2(\Omega)} \leq \|u(T)\|_{L^2(\Omega)} \leq c_2 \|u_0\|_{L^2(\Omega)} \tag{1.2}$$

given by [89, Theorem 2.1] contrasts sharply with the classical parabolic counterpart ($\alpha = 1$), whose solution is infinitely differentiable in space for all $t > 0$. Thus, the backward problem of subdiffusion is far "less" ill-posed than that of normal diffusion. The existence, uniqueness and stability of the time-fractional backward problem were analyzed by Sakamoto and Yamamoto in [89]. This work motivates many subsequent developments of regularized algorithms. In [69], Liu and Yamamoto proposed a numerical method based on the quasi-reversibility method, and analyze the approximation error (in terms of noise level) under *a priori* smoothness assumption on u_0. Then a total variation regularization method was proposed and studied by Wang and Liu in [102]. In [100], Wang and Wei developed and analyzed an iteration method to regularize the backward problem. The quasi-boundary value method for solving the fractional backward problem was firstly studied in [108] for a one-dimensional subdiffusion model, and then extended in [103] to the general case by modifying the regularization term. See also [27] for a novel Hölder type estimate of the quasi-boundary value methods.

To solve the regularized system, people applied different numerical approaches, e.g., finite element method, finite different method, etc. Then some discretization error will be introduced into the system. Therefore, it is necessary to establish an estimate to balance discretization parameter, regularization parameter and noise level.

As Section 1.2 points out, we need to regularize the ill-posed problem. For the backward problem, there are many popular regularization methods such as quasi-reversibility [63], pseudo-parabolic method [18] and quasi-boundary value method [31]. In this thesis we apply quasi-boundary value method at time boundary $t = T$, which is

However, when the operator $-\Delta$ in (1.1) be more general, i.e. be time dependent operator $A(t)$: $H_0^1(\Omega) \cap H^2(\Omega) \to L^2(\Omega)$ defined by

$$A(t)\phi = -\nabla \cdot (a(x,t)\nabla\phi) \tag{1.3}$$

satisfying Elliptic conditions, the PDE of (1.1) becomes

$$\begin{aligned} \partial_t^\alpha u + A(t)u = f \qquad & \text{in } \Omega \times (0,T), \\ u = 0 \qquad & \text{on } \partial\Omega \times (0,T), \\ u(0) = u_0 \qquad & \text{in } \Omega \end{aligned} \tag{1.4}$$

the analysis of backward subdiffusion used in Chapter 3 may be not directly applicable for subdiffusion models with time dependent coefficients since it heavily relies on the asymptotic behaviors of Mittag-Leffler functions. Unfortunately, this strategy is Moreover, for fractional model, the analysis is much more challenging since many useful mathematical tools, including product rule and chain rule, are not directly applicable.

For time-dependent elliptic operators or nonlinear problems, energy arguments [99] or perturbation arguments [58] can be used to show existence and uniqueness of the solution. However, more refined stability estimates, needed for numerical analysis of nonsmooth problem data, often have to be derived separately. Mustapha [83] analyzed the spatially semidiscrete Galerkin FEM approximation of problem (1.4) using a novel energy argument, and established optimal-order convergence rates for both smooth and nonsmooth initial data. See also [76, 77, 78] for time-fractional advection diffusion equation. In [45], a perturbation argument of freezing the diffusion coefficients was proposed to analyze the PDE (1.4) and its numerical treatment. The argument was then modified and adapted to the error analysis of high-order discretization scheme in [46]. However, the analysis for the uniqueness and stability of backward problem is still missing in the literature. We also refer interested readers to [30, 6] for the inverse source problem with time-dependent coefficients, where the uniqueness was proved using some nonstandard energy argument.

After dealing cases for subdiffusion model, i.e. $0 < \alpha < 1$, there are cases related to fractional wave case of $1 < \alpha < 2$. We consider

$$\begin{aligned} \partial_t^\alpha u - \Delta u = f \qquad & \text{in } \Omega \times (0,T), \\ u = 0 \qquad & \text{on } \partial\Omega \times (0,T), \\ u(0) = a, \quad \partial_t u(0) = b \quad & \text{in}\Omega. \end{aligned} \tag{1.5}$$

It is interesting to investigate the backward problem for the diffusion-wave model (1.5): we want to simultaneously determine the initial data $u(x,0)$ and $u_t(x,0)$ with $x \in \Omega$ (and hence the function $u(x,t)$ for all $(x,t) \in \Omega \times (0,T)$) from two terminal observations

$$u(x,T_1) = g_1(x), \quad u(x,T_2) = g_2(x) \quad \text{for all } \ x \in \Omega, \tag{1.6}$$

where $T_1, T_2 \in (0, T]$ and $T_1 < T_2$.

The study on the backward problem for the diffusion-wave model remains fairly scarce. In [104] Wei and Zhang studied the backward problem to recover a single initial condition $u(0)$ or $u_t(0)$ (with the other one known) from the single terminal data $u(T)$. Floridia and Yamamoto analyzed the simultaneous recovery of two initial data from two terminal observations $u(T)$ and $u_t(T)$, and established a Lipschitz stability in [20]. In the setting of current paper, we consider two observations $u(T_1)$ and $u(T_2)$, which are practical in many empirical experiments. As far as we know, there is no rigorous analysis of the discretized (numerical) scheme for solving the backward problem where some regularization error and discretization error(s) will be introduced into the system. Then there arises a natural question: is it possible to derive an a priori error estimate, showing the way to balance discretization error, regularization parameter and the noise.

Inverse potential problems Here we consider the following initial-boundary value problem for the diffusion model with $\alpha \in (0, 1]$:

$$\begin{aligned} \partial_t^\alpha u(x,t) - \Delta u(x,t) + q(x)u(x,t) &= f(x), \quad (x,t) \in \Omega \times (0,T], \\ u(x,t) &= b(x), \quad (x,t) \in \partial\Omega \times (0,T], \\ u(x,0) &= v(x), \quad x \in \Omega, \end{aligned} \tag{1.7}$$

The notation $\partial_t^\alpha u$ denotes the conventional first-order derivative when $\alpha = 1$, and the Djrbashian-Caputo fractional derivative in time t for $\alpha \in (0, 1)$.

For the inverse potential problem, we study the following **inverse potential problem** for the (sub)diffusion model (1.7): setting appropriate problem data v, f, b and measuring the final time data $g(x) := u(x, T; q^\dagger)$, then we aim to recover the unknown potential term $q^\dagger(x) \in L^\infty(\Omega)$ such that

$$u(x, T; q^\dagger) = g(x) \quad \text{in } \Omega.$$

This inverse potential problem arises in many practical applications, where $q^\dagger$ represents the radiativity coefficient in heat conduction [106] and perfusion coefficient in Pennes' bio-heat equation in human physiology [86].

The theoretical analysis of inverse potential problem in diffusion equation from final time observational data has a long history, see e.g, [34, 9, 10, 8, 59] and the references therein. In [34] Isakov showed the uniqueness and (conditional) existence of the inverse potential problem for parabolic equations, by developing a unique continuation principle and a constructive fixed point iteration. A similar strategy was then adopted in [113] by Zhang and Zhou for a one-dimensional time-fractional subdiffusion model. Using the spectrum perturbation argument ([113, Lemma 2.2] and [88]) they proved that the fixed point iteration is a contraction, from which the uniqueness and existence followed immediately.

Choulli and Yamamoto proved a generic well-posedness result in a Hölder space [9], and then proved a conditional stability result in a Hilbert space setting [10] for sufficiently small T. By using refined properties of two-parameter Mittag-Leffler functions, e.g., complete monotonicity and asymptotics, a similar result was proved in [50] for the case that $\alpha \in (0,1)$. Kaltenbacher and Rundell [53] proved the invertibility of the linearized map (of the direct problem) from the space $L^2(\Omega)$ to $H^2(\Omega)$ under the condition $u_0 > 0$ in Ω and $q \in L^\infty(\Omega)$ using a Paley-Wiener type result and a type of strong maximum principle. In [55], they studied the recovery of several parameters simultaneously from overposed data consisting of $u(T)$. Chen et al. [8] considered the observational data in $[T_0, T_1] \times \Omega$ for the parabolic equation, and proved conditional stability of the inverse problem in negative Sobolev spaces. Most recently, Jin et al. [47] used the same observational data and showed a weighted L^2 stability which leads to a Hölder type stability in the standard L^2 norm under a positivity condition. We also refer interested readers to [56, 82, 54] and references therein for the inverse potential problem for (sub)diffusion models from different types of observational data.

The ill-posed nature of inverse potential problems usually poses big challenges to construct accurate and stable numerical approximations. Regularization, especially Tikhonov regularization, is designed to overcome the ill-posed nature [16, 106, 13, 107]. In practical computation, one still needs to discretize the continuous regularized formulation and hence introduces the discretization error. See [106] for the convergence of the discrete approximations in the parabolic case. However, the convergence rates of discrete approximations are generally very challenging to obtain, due to the strong non-convexity of the regularized functional, which itself stems from the high degree nonlinearity of the parameter-to-state map. So far there have been only very few error bounds on discrete approximations, even though an optimal *a priori* estimate provides a useful guideline to choose suitable discretization parameters according to the noise level. See [47] for an L^2 estimate under a positivity condition, where the observational data is required to be known in $[T-\sigma, T] \times \Omega$ for some positive parameter σ. Moreover, in case that $\alpha \in (0,1)$, due to the presence of the nonlocal fractional differential operator, the subdiffusion model (6.1) differs considerably from the normal diffusion problem. For example, many powerful tools, e.g. energy argument and product rule, are not directly applicable, and the solution has only limited spatial and temporal regularity, even for smooth problem data. Both of them often result in additional difficulties to the mathematical and numerical analysis for both direct and inverse problems. See a related inverse conductivity problem in [101] and [51] respectively for normal diffusion and subdiffusion model, where the error estimate requires the observational data in $(0, T] \times \Omega$.

1.3 Contributions and organizations of the thesis

In this thesis, we provide mathematical and numerical analysis for approximately solving the backward problem and inverse potential problem of time anomalous diffusion equation. The analysis cover backward subdiffusion with time dependent or independent coefficients, backward diffuion-wave problem with two unknown initial conditions and inverse potential problem. The error estimates from numerical algorithms are very useful to choose discretization parameters and regularization parameters according to the noise level.

In Chapter 2, we provide some necessary preliminaries needed for the analysis of fractional partial differential equations. Firstly we list some fractional calculus including integral and derivative. The Mittag-Leffler functions which play an essential role in fractional PDEs, is clearly introduced, and its asymptotic behavior is given in Lemma 2.1. The solution representations are also given based on the spectral expansion and Mittag-Leffler functions. Some numerical methods including finite element methods and convolution quadrature are illustrated. All these preliminaries form basis for the following mathematical analysis and numerical algorithms

In Chapter 3 we provide a complete numerical analysis to the backward subdiffusion problem of fractional order $\alpha \in (0,1)$. After using quasi-boundary value method to regularize the problem, we propose a fully discrete scheme by applying finite element method (FEM) in space and convolution quadrature (CQ) in time. The analysis relies heavily on smoothing properties of (discrete) solution operators directly from Mittag-Leffler functions and nonstandard error estimate for the direct problem.

In the past, the backward diffusion problem for a standard parabolic equation, i.e., $\alpha = 1$, is intensively studied. Due to the strong smoothing properties of solution operators $E(t) = \exp(-\Delta t)$, the backward stability is at most log type. However, the limited smoothing properties of solution operator from subdiffusion would infer the far "less" ill-posedness of the backward stability.

Specifically, if the observation data is noisy in level $\delta > 0$ in L^2 sense. Given the regularization parameter $\gamma > 0$, the space and time discretization h and τ. Firstly for smooth data, there holds (Theorem 3.3 (i))

$$\|\tilde{U}_n^\delta - u(t_n)\|_{L^2(\Omega)} \le c \begin{cases} \gamma + (h^2 + \tau + \delta)\min(\gamma^{-1}, t_n^{-\alpha}) + \tau t_n^{\alpha-1}, n \ge 1; \\ \gamma + (h^2 + \tau + \delta)\gamma^{-1}, \qquad n = 0. \end{cases}$$

As for nonsmooth data we could have a convergence at $n = 0$ and even a convergence rate for $n \ge 1$. And this is the first work providing rigorous error analysis of numerical methods for solving the time-fractional backward problem.

In Chapter 4, we study the backward subdiffusion problem with time dependent coefficients, i.e. the spatial differential operator $A = A(t)$. Since the method of Mittag-Leffler function could not be used, we apply a perturbation argument [44, 45] and show some smoothing properties of solution operators. The quasi boundary regularization method is applied, then after some numerical designs we establish a thorough error analysis.

The main contribution of this chapter is firstly to develop a conditional stability in Sobolev spaces (Cf. Theorems 4.2 and 4.4). Next we apply piecewise linear FEM in space and CQ-BE in time, then the complete error analysis is given for smooth (Theorem 4.7)

$$\|\tilde{U}_0^\delta - u_0\|_{L^2(\Omega)} \leq c\Big(\gamma^{\frac{q}{2}} + \delta\gamma^{-1} + h^2\gamma^{-1} + \tau|\log\tau|(h^2\gamma^{-1}+1)\Big),$$

and for nonsmooth data in $L^2(\Omega)$, we also show a convergence following $\delta \to 0$.

In Chapter 5 we introduce simultaneous recovery of two initial conditions from backward diffusion-wave problem. Firstly the existence, uniqueness and Lipschitz stability are established. Moreover, we apply regularized quasi-boundary value method and piecewise linear FEM in space and CQ-BE in time. Then we could derive a comprehensive numerical analysis to the simultaneous recovery problem.

The simultaneous recovery is to recover initial state $u_0 = a$ and velocity $\partial_t u(0) = b$ from different time T_1, T_2 In particular, using the asymptotic behavior of Mittag-Leffler functions, we show a two-sided Lipschitz stability (Theorem 5.1) under some conditions on T_1 and T_2 (depending on the spectrum of $-\Delta$). In the second part, total analyzed numerical schemes are promoted and imply the main results in Theorem (Theorem 6.5) of

$$\|\tilde{a}_{h,\tau}^\delta - a\|_{L^2(\Omega)} + \|\tilde{b}_{h,\tau}^\delta - b\|_{L^2(\Omega)} \leq c\big(\gamma^{\frac{q}{2}} + \tau + (h^2+\delta)\gamma^{-1}\big),$$

if $a, b \in \dot{H}^q(\Omega)$ with $q \in (0, 2]$, and for $n \geq 1$

$$\|\tilde{U}_n^\delta - u(t_n)\|_{L^2(\Omega)} \leq c\Big[\gamma\min(\gamma^{-(1-\frac{q}{2})}, t_n^{-(1-\frac{q}{2})\alpha}) + (\tau t_n^{\alpha-1} + h^2 + \delta)\min(\gamma^{-1}, t_n^{-\alpha})\Big].$$

And for L^2 constraints we also could obtain a convergence.

In Chapter 6, we move our focus to inverse potential problem, i.e. to recover a spatially dependent potential in a (sub)diffusion equation from overposed final time data. We construct a monotone operator one of whose fixed points is the unknown potential. We verify the uniqueness of the identification via the operator monotonicity and a fixed point argument. Based on an extra proved stability, we propose a completely discrete scheme by using FEM in space and finite difference method in time and a fixed point iteration is applied to reconstruct the potential.

Motivated by [113] for a one-dimensional time-fractional subdiffusion model, we apply a totally different idea for high dimensional cases of inverse potential problem. To recover the potential q firstly we construct an operator K and show its monotonicity, which is used to prove that there at most one fixed point (Theorem 6.2). Besides under some conditions for final time T, we show a Lipschitz-type stability in Hilbert spaces (Theorem 6.3). Based on this stability, we apply a fully discrete scheme by Galerkin finite element method with conforming piecewise bilinear finite elements in space and backward Euler method in time for $\alpha = 1$, and BE-CQ for $\alpha \in (0, 1)$. Under some clear numerical analysis we obtain *a priori* error estimate for any parameter $\epsilon \in (0, \min(1, 2 - \frac{d}{2}))$ (Theorem 6.5)

$$\|q^\dagger - q^*\|_{L^2(\Omega)} \le \frac{c}{1 - cT^{-(1-\epsilon)\alpha}} \Big(\frac{\delta}{h^2} + h + \tau \Big) \le c\Big(\frac{\delta}{h^2} + h + \tau \Big)$$

if $cT^{-(1-\epsilon)\alpha} \le c_0 < 1$ for some constant c_0.

Finally, we summarize the main results in the thesis and try to discuss possible future work in Chapter 7. In each chapter various numerical experiments are provided to support theoretical results.

CHAPTER 2.

Preliminary

In this Chapter, some preliminaries are introduced related to the fractional differential equations. Firstly, in Sections 2.1 and 2.2 the basis of fractional calculus is presented followed by the corresponding Mittag-Leffler functions arising from fractional ODEs. Next, in Section 2.3 and 2.4 the representation of solution in fractional PDEs are given from Mittag-Leffler functions and semigroup approaches, also some smoothing properties of solution operators are given. And finally in Section 2.5 we introduce some numerical algorithms considering the fractional PDEs, including discretization in space and time.

2.1 Fractional calculus

In this section we would briefly introduce some basis definitions of fractional calculus. Let $D = (a, b)$, extending Cauchy iterative integral formula for integers to fractions, the left-sided Riemann-Liouville's fractional integer of order $\beta > 0$ based at $t = a$, for any $u \in L^1(D)$, is defined as ([38, Definition 2.1])

$$({}_aI_t^\beta u)(t) = \frac{1}{\Gamma(\beta)} \int_a^t (t-s)^{\beta-1} u(s)\mathrm{d}s \tag{2.1}$$

and the right-sided Riemann-Liouville fractional integral with order $\beta > 0$ at $t = b$ is defined by

$$({}_tI_b^\beta u)(t) = \frac{1}{\Gamma(\beta)} \int_t^b (s-t)^{\beta-1} u(s)\mathrm{d}s$$

here $\Gamma(\beta)$ stands for the Gamma function. And if $\beta = k \in \mathbb{N}$, we would arrive the regular k-fold integral of u.

Moreover, based on this fractional integral we could obtain the fractional derivative. The left-sided and right-sided Riemann-Liouville fractional derivative are defined as

$$\begin{aligned} {}_a^RD_t^\alpha u(t) &= \frac{d^n}{dt^n}({}_aI_t^\alpha u), \\ {}_t^RD_b^\alpha u(t) &= (-1)^n \frac{d^n}{dt^n}({}_tI_b^\alpha u), \end{aligned} \tag{2.2}$$

where the fractional order $n-1 < \alpha < n$ for any $n \in \mathbb{N}$. However, the existence of the fractional derivative is guaranteed by $u \in L^1(D)$ and u has n-th continuous derivative for $t \geq a$.

Moreover, the derivative could take inside the integral, after which we could obtain the Djrbashian-Caputo fractional derivate, i.e., [38, Definition 2.3]

$$\begin{aligned} {}_a^CD_t^\alpha u(t) &= ({}_aI_t^\alpha u^{(n)})(t), \\ {}_t^CD_b^\alpha u(t) &= (-1)^n({}_tI_b^\alpha u^{(n)})(t), \end{aligned} \tag{2.3}$$

in left and right-hand sense and here $u^{(n)}$ means the $n-th$ derivative of u. The existence of such fractional derivatives is guaranteed by $u \in L^1(D)$ and $u \in AC^n(\bar{D})$, where $AC(\bar{D})$ denotes the absolutely continuous function on $\bar{D}$ [38, Appendix 1].

It is very important to state the relation between Riemann-Liouville and Caputo fractional derivatives [57, p. 91]:

$$({}_a^C D_t^\alpha u)(t) = ({}_a^R D_t^\alpha u)(t) - \sum_{k=0}^{n-1} \frac{u^{(k)}(a)}{\Gamma(k-\alpha+1)}(t-a)^{k-\alpha}. \tag{2.4}$$

In this thesis we apply left-sided Djrbashian-Caputo derivative $\partial_t^\alpha := {}_0^C D_t^\alpha$ (2.3) and Riemann-Liouville as ${}^R\partial_t^\alpha := {}_0^R D_t^\alpha$ in our differential equation models from $a = 0$ due to its better explanation to physical technology ([87, p. 78-79], [60, p. 10-11]).

Some properties of fractional derivatives are well-studied recently(e.g. [38, 87]). For examples, if $u \in L^1(D)$ with $({}_aI_t^{\alpha-n+1}u)(t)$ and $({}_aI_t^{\alpha-n+1}u)(a) = 0$ then [38, Theorem 2.13]

$${}_a^C D_t^\alpha \, {}_aI_t^u = u, \quad \text{a.e. in } D.$$

Also, the Caputo fractional derivatives can commute under some conditions see more detail in [38, Proposition 2.3]. However, the chain rule and product rule may fail which bring obstacles in applying some classical powerful tools like energy arguments.
The Laplace transforms for fractional derivatives are well-known(e.g. [38, 87, 60]). Applying the Laplace transform to Caputo derivative we would obtain([38, Lemma 2.9]):

$$\mathcal{L}[{}_0^C D_t^\alpha u](z) = z^\alpha \hat{u}(z) - \sum_{k=0}^{n-1} z^{\alpha-k-1} u^{(k)}(0)$$

where $n-1 < \alpha < n$ and $\hat{u}$ means the Laplace transform of u.

2.2 Mittag-Leffler functions

In this section, we would introduce the Mittag-Leffler functions, which is a basis for fractional differential equations.

2.2.1 Basic definitions and properties of Mittag-Leffler functions

The two parameter Mittag-Leffler function is defined as ([87, equation (1.56)])

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k\alpha+\beta)}, \quad \alpha > 0, \quad \beta > 0, \quad \forall z \in \mathbb{C}. \tag{2.5}$$

The connection between Mittag-Leffler function and some well-known functions is given in various materials ([87, 60]). For example,

$$E_{1,1}(z) = e^z, \quad E_{2,1}(z^2) = \cosh(z), \quad E_{2,2}(z^2) = \frac{\sinh(z)}{z}$$

The Mittag-Leffler function $E_{\alpha,\beta}(z)$ is a generalization of the familiar exponential function e^z appearing in normal diffusion. The next lemma provides the upper and lower bounds of Mittag-Leffler functions. See [87, Theorem 1.4], [38, Theorem 3.2] for detailed proof.

Lemma 2.1. *If $0 < \alpha < 2$, β is an arbitrary complex number and μ is an arbitrary real number such that*

$$\frac{\pi\alpha}{2} < \mu < \min\{\pi, \pi\alpha\},$$

then there exists a constant C only dependent on α, β, μ such that

$$|E_{\alpha,\beta}(z)| \leq \frac{C}{1+|z|}, \quad \mu \leq |\arg(z)| \leq \pi.$$

Moreover, for large z, there holds the following asymptotic behaviors

$$E_{\alpha,1} = \frac{1}{\Gamma(1-\alpha)}\frac{1}{z} + O(\frac{1}{z^2}) \text{ and } E_{\alpha,2} = \frac{1}{\Gamma(2-\alpha)}\frac{1}{z} + O(\frac{1}{z^2}), \quad \forall z \to \infty. \tag{2.6}$$

The function $E_{\alpha,\beta}(-\lambda t^\alpha)$ decays only polynomially like $t^{-\alpha}$ as $t \to \infty$ (cf. Lemma 2.1), which contrasts sharply with the exponential decay for $e^{-\lambda t}$ appearing in normal diffusion.

Note that the Mittag-Leffler functions appear in some fractional ordinary differential equations ([38, Proposition 4.5]), simply let $w(t) = E_{\alpha,1}(-\lambda t^\alpha)$ be the solution to the initial value problem

$$\partial_t^\alpha w(t) + \lambda w(t) = 0, \quad \text{with} \quad w(0) = 1.$$

By means of Laplace transform, it can be written as

$$w(t) = E_{\alpha,1}(-\lambda t^\alpha) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}} e^{zt} z^{\alpha-1}(z^\alpha + \lambda)^{-1}\, dz \tag{2.7}$$

with integration over a contour $\Gamma_{\theta,\sigma}$ in the complex plane $\mathbb{C}$ (oriented counterclockwise), defined by

$$\Gamma_{\theta,\sigma} = \{z \in \mathbb{C} : |z| = \delta, |\arg z| \leq \theta\} \cup \{z \in \mathbb{C} : z = \rho e^{\pm \mathrm{i}\theta}, \rho \geq \sigma\}. \tag{2.8}$$

Throughout, we fix $\theta \in (\frac{\pi}{2}, \pi)$ so that $z^\alpha \in \Sigma_{\alpha,\theta} \subset \Sigma_\theta := \{0 \neq z \in \mathbb{C} : \arg(z) \leq \theta\}$, for all $z \in \Sigma_\theta$.

Computing the value of Mittag-Leffler functions is well-studied in [91], they give a detailed algorithm to numerically approximate generalized Mittag-Leffler functions.

2.3 Fractional subdiffusion model

In this section, we introduce the representation of the solution to the subdiffusion problem:

$$\begin{aligned} \partial_t^\alpha u - \Delta u &= f \qquad \text{in } \Omega \times (0,T), \\ u &= 0 \qquad \text{on } \partial\Omega \times (0,T), \\ u(0) &= u_0 \qquad \text{in } \Omega \end{aligned} \tag{2.9}$$

Here $0 < \alpha < 1$, this model coincides with classical diffusion with $\alpha = 1$. And solution regularities of the subdiffusion model may differ with classical models.

To begin with, we introduce some notation. For $q \geq 0$, we denote by $\dot{H}^q(\Omega)$ the Hilbert space induced by the norm:

$$\|v\|^2_{\dot{H}^q(\Omega)} = \sum_{j=1}^{\infty} \lambda_j^q (v, \varphi_j)^2$$

with $\{\lambda_j\}_{j=1}^{\infty}$ and $\{\varphi_j\}_{j=1}^{\infty}$ being respectively the eigenvalues and the $L^2(\Omega)$-orthonormal eigenfunctions of the negative Laplacian $-\Delta$ on the domain Ω with a homogeneous Dirichlet boundary condition. Then $\{\varphi_j\}_{j=1}^{\infty}$ forms orthonormal basis in $L^2(\Omega)$. Further, $\|v\|_{\dot{H}^0(\Omega)} = \|v\|_{L^2(\Omega)} = (v,v)^{1/2}$ is the norm in $L^2(\Omega)$. Besides, it is easy to verify that $\|v\|_{\dot{H}^1(\Omega)} = \|\nabla v\|_{L^2(\Omega)}$ is equivalent to the norm in $H_0^1(\Omega)$ and $\|v\|_{\dot{H}^2(\Omega)} = \|\Delta v\|_{L^2(\Omega)}$ is equivalent to the norm in $H^2(\Omega) \cap H_0^1(\Omega)$ [93, Section 3.1]. By the complex interpolation method [96], this implies

$$\dot{H}^q(\Omega) = (L^2(\Omega), H_0^1(\Omega) \cap H^2(\Omega))_{[\frac{q}{2}]}, \quad \forall\, t \in [0,T], \;\; \forall\, \gamma \in [0,1],$$

Then the solution of the forward problem (2.9) could be written as [40]

$$u(t) = F(t)u_0 + \int_0^t E(t-s) f(s) ds \tag{2.10}$$

where the solution operators are defined as

$$F(t)\chi = \sum_{j=1}^{\infty} E_{\alpha,1}(-\lambda_j t^\alpha)(\chi, \varphi_j)\varphi_j \quad \text{and} \quad E(t)\chi = \sum_{j=1}^{\infty} t^{\alpha-1} E_{\alpha,\alpha}(-\lambda_j t^\alpha)(\chi,\varphi_j)\varphi_j. \tag{2.11}$$

Next, we state a few regularity results. The proof of these results can be found in, e.g., [5, 89, 45]

Lemma 2.2. *Let $u(t)$ be defined in* (2.10). *Then the following statements hold.*

(i) *If $u_0 \in \dot{H}^q(\Omega)$ with $s \in [0,2]$ and $f = 0$, then $u(t)$ is the solution to problem* (2.9), *and $u(t)$ satisfies*

$$\|\partial_t^{(m)} u(t)\|_{\dot{H}^p(\Omega)} \leq c t^{\frac{(s-p)\alpha}{2} - m} \|u_0\|_{\dot{H}^q(\Omega)}$$

with $0 \leq p - q \leq 2$ and any integer $m \geq 0$.

(ii) *If $u_0 = 0$ and $f \in L^p(0,T;L^2(\Omega))$ with $1 < p < \infty$, then there holds*

$$\|u\|_{L^p(0,T;\dot{H}^2(\Omega))} + \|\partial_t^\alpha u\|_{L^p(0,T;L^2(\Omega))} \leq c\|f\|_{L^p(0,T;L^2(\Omega))}.$$

Moreover, if $f \in L^p(0,T;L^2(\Omega))$ with $1/\alpha < p < \infty$, then $u(t)$ is the solution to problem (2.9) *such that $u \in C([0,T];L^2(\Omega))$.*

2.4 Fractional diffusion-wave model

In this section we consider the following initial-boundary value problem of diffusion-wave equation with $\alpha \in (1,2)$

$$\begin{aligned} \partial_t^\alpha u - \Delta u &= f, \quad \text{in } \Omega \times (0,T], \\ u &= 0, \quad \text{on } \partial\Omega, \\ u(0) = a,\ \partial_t u(0) &= b, \quad \text{in } \Omega, \end{aligned} \tag{2.12}$$

where $T > 0$ is a fixed final time, $f \in L^\infty(0,T;L^2(\Omega))$ and $a, b \in L^2(\Omega)$ are given source term and initial data, respectively.

Then the solution of the diffusion-wave problem (2.12) could be written as

$$u(t) = \mathcal{F}(t)\begin{bmatrix} a \\ b \end{bmatrix} + \int_0^t E(t-s)f(s)\,\mathrm{d}s = F(t)a + \bar{F}(t)b + \int_0^t E(t-s)f(s)\,\mathrm{d}s \tag{2.13}$$

where the solution operators $F(t)$, $E(t)$ are the same in (2.11), the new operator $\bar{F}(t)$ is defined by

$$\bar{F}(t)v = \sum_{j=1}^{\infty} tE_{\alpha,2}(-\lambda_j t^\alpha)(v,\varphi_j)\varphi_j, \tag{2.14}$$

for any $v \in L^2(\Omega)$. By Laplace Transform, we have the following integral representations of the solution operators:

$$\begin{aligned} F(t) &= \frac{1}{2\pi i}\int_{\Gamma_{\theta,\sigma}} e^{zt}z^{\alpha-1}(z^\alpha - \Delta)^{-1}dz, \quad \bar{F}(t) = \frac{1}{2\pi i}\int_{\Gamma_{\theta,\sigma}} e^{zt}z^{\alpha-2}(z^\alpha - \Delta)^{-1}dz, \\ E(t) &= \frac{1}{2\pi i}\int_{\Gamma_{\theta,\sigma}} e^{zt}(z^\alpha - \Delta)^{-1}dz. \end{aligned} \tag{2.15}$$

Here $\Gamma_{\theta,\sigma}$ denotes the integral contour in (2.8).

The important bounds in Lemma 2.1 are directly translated into the limited smoothing property in both space and time for the solution operators $F(t)$, $\bar{F}(t)$ and $E(t)$. Next, we state a few regularity results. See more details in [5, 41, 38, 89].

Lemma 2.3. *Let $u(t)$ be defined in (2.12). Then the following statements hold.*

(i) *If $a, b \in \dot{H}^q(\Omega)$ with $q \in [0,2]$ and $f = 0$, then $u(t)$ is the solution to problem (2.12), and $u(t)$ satisfies for any integer $m \geq 0$ and $q \leq p \leq 2+q$*

$$\|\partial_t^{(m)} u(t)\|_{\dot{H}^p(\Omega)} \leq c\left(t^{-m-\alpha(p-q)/2}\|a\|_{\dot{H}^q(\Omega)} + t^{1-m-\alpha(p-q)/2}\|b\|_{\dot{H}^q(\Omega)}\right).$$

(ii) *If $a = b = 0$ and $f \in L^p(0,T;L^2(\Omega))$ with $1/\alpha < p < \infty$, then $u(t)$ is the solution to problem (2.12) such that $u \in C([0,T];L^2(\Omega))$ and*

$$\|u\|_{L^p(0,T;\dot{H}^2(\Omega))} + \|\partial_t^\alpha u\|_{L^p(0,T;L^2(\Omega))} \leq c\|f\|_{L^p(0,T;L^2(\Omega))}.$$

2.5 Numerics

In this section, we shall briefly introduce the existing results of some discretization methods we use in the following inverse problem, including finite element method(FEM) in space and backward Euler convolution quadrature(BE-CQ) in time.

2.5.1 Triangular finite element method in space

Now we describe the spatial discretization by finite element method. For $h \in (0, h_0]$, we denote by $\mathcal{T}_h = \{K_j\}$ a triangulation of $\Omega_h = \mathrm{Int}(\cup \overline{K}_j)$ into mutually disjoint open face-to-face simplices K_j. Assume that all boundary vertices of Ω_h locate on $\partial\Omega$. We also assume that $\{\mathcal{T}_h\}$ is globally quasi-uniform, i.e., $|K_j| \geq ch^d$ with a given $c > 0$. Let X_h be the finite dimensional space of continuous piecewise linear functions associated with $\mathcal{T}_h$, that vanish outside Ω_h, i.e.

$$X_h = \left\{\chi \in C(\bar{\Omega}) \cap H_0^1 : \ \chi|_K \in P_1(K), \ \ \forall K \in \mathcal{T}_h\right\}. \tag{2.16}$$

We need the $L^2(\Omega)$ projection $P_h : L^2(\Omega) \to X_h$ and Ritz projection $R_h : \dot{H}^1(\Omega) \to X_h$, respectively, defined by (recall that $(\cdot,\cdot)$ denotes the $L^2(\Omega)$ inner product)

$$\begin{aligned} (P_h\psi, \chi) \quad &= (\psi, \chi) \qquad \forall\ \chi \in X_h, \psi \in L^2(\Omega), \\ (\nabla R_h\psi, \nabla\chi) \ &= (\nabla\psi, \nabla\chi) \qquad \forall\ \chi \in X_h, \psi \in \dot{H}^1(\Omega). \end{aligned}$$

The following approximation properties of R_h and P_h are well known [93, Chapter 1]:

$$\|P_h\psi - \psi\|_{L^2(\Omega)} + h\|\nabla(P_h\psi - \psi)\|_{L^2(\Omega)} \ \leq ch^q\|\psi\|_{H^q(\Omega)} \qquad \forall\psi \in \dot{H}^q(\Omega), q = 1, 2, \tag{2.17}$$

$$\|R_h\psi - \psi\|_{L^2(\Omega)} + h\|\nabla(R_h\psi - \psi)\|_{L^2(\Omega)} \ \leq ch^q\|\psi\|_{H^q(\Omega)} \qquad \forall\psi \in \dot{H}^q(\Omega), q = 1, 2. \tag{2.18}$$

Upon introducing the discrete Laplacian Δ_h: $X_h \to X_h$ defined by

$$-(\Delta_h\psi, \chi) = (\nabla\psi, \nabla\chi), \ \ \forall\psi, \chi \in X_h.$$

2.5.2 Backward Euler convolution quadrature

Here we briefly introduce the concept of convolution quadratures proposed in [71, 43]. Applying the Laplace transform to Riemann-Liouville type fractional derivative in (2.2) with $0 < \alpha < 1$, we obtain

$$(\mathcal{L}\,{}^R\partial_t^\alpha\varphi(t))(z) = z^\alpha(\mathcal{L}\varphi)(z),$$

where $\mathcal{L}$ stands for the Laplace transform where $\mathcal{L}u = \int_0^\infty e^{-zs}u(s)\mathrm{d}s$. Suppose $\alpha = 1$, there are many stable linear multistep methods to approximate z with the characteristic polynomial $\delta_\tau(\zeta)$, including backward differentiation formula(BDF), trapezoidal rule, Runge-Kutta methods (see more details in

[26]). The most popular one is backward differentiation formula of order k (BDF-k), $k = 1, 2, \cdots, 6$, where the characteristic polynomial is given

$$\delta_\tau(\zeta) := \frac{1}{\tau}\sum_{j=1}^{k}\frac{1}{j}(1-\zeta)^j. \tag{2.19}$$

In this thesis, we would only use the BDF-1 method with $\delta_\tau(\zeta) = (1-\zeta)/\tau$, where we call it backward Euler convolution quadrature (BE-CQ), to approximate z^α with the power series expansion

$$\delta_\tau(\zeta)^\alpha = \frac{1}{\tau^\alpha}\sum_{j=0}^{\infty} b_j\zeta^j.$$

Therefore, we could approximate the Riemann-Liouville fractional derivative as (with $\varphi_j = \varphi(t_j)$)

$${}^R\partial_t^\alpha\varphi(t_n) \approx \tau^{-\alpha}\sum_{j=0}^{n} b_j\varphi_{n-j} := \bar\partial_\tau^\alpha\varphi_n.$$

Then using the relation between Riemann-Liouville and Caputo fractional derivative (2.4) to approximate Caputo type:

$$\partial_t^\alpha\varphi(t_n) = \partial_t^\alpha(\varphi(t_n)-\varphi(0)) = {}^R\partial_t^\alpha(\varphi(t_n)-\varphi(0)) \approx \bar\partial_\tau^\alpha(\varphi(t_n)-\varphi(0)).$$

The next lemma gives elementary properties of the kernel $\delta_\tau(e^{-z\tau})$ [43, Lemma B.1].

Lemma 2.4. *For any $\theta \in (\pi/2, \pi)$, there exists $\theta' \in (\pi/2, \pi)$ and positive constants c, c_1, c_2 which is independent of τ such that for all $z \in \Gamma_{\theta,\sigma}^\tau$*

$$\begin{aligned} &c_1|z| \le |\delta_\tau(e^{-z\tau})| \le c_2|z|, \qquad \delta_\tau(e^{-z\tau}) \in \Sigma_{\theta'}.\\ &|\delta_\tau(e^{-z\tau}) - z| \le c\tau|z|^2, \qquad |\delta_\tau(e^{-z\tau})^\alpha - z^\alpha| \le c\tau|z|^{1+\alpha}.\end{aligned}$$

For $1 < \alpha < 2$, the convolution quadrature could be extended into diffusion-wave case similarly, which is deeply studied in Section 5.3.

CHAPTER 3.

Numerical Analysis of Backward Subdiffusion Problems

We consider $\Omega \subset \mathbb{R}^d$ $(d \geq 1)$ be a bounded and convex domain with smooth boundary $\partial\Omega$, and consider the following subdiffusion equation

$$\begin{aligned} \partial_t^\alpha u - \Delta u &= f \qquad \text{in } \Omega \times (0,T), \\ u &= 0 \qquad \text{on } \partial\Omega \times (0,T), \\ u(0) &= u_0 \qquad \text{in } \Omega \end{aligned} \tag{3.1}$$

where $T > 0$ is a fixed terminal time, $f \in L^\infty(0,T; L^2(\Omega))$ and $u_0 \in L^2(\Omega)$ are given source term and initial data, respectively, and Δ is the Laplace operator in space.

In this chapter want to determine the function $u(x,t)$ with $(x,t) \in \Omega \times [0,T)$ from a terminal observation

$$u(x,T) = g(x), \qquad \text{for all} \quad x \in \Omega.$$

Specifically, we assume that the observation data g^δ is noisy such that

$$\|g^\delta - g\|_{L^2(\Omega)} \leq \delta.$$

To regularize the ill-posed problem, we apply the quasi-boundary value method [27, 108] and consider

$$\begin{aligned} \partial_t^\alpha \tilde{u}^\delta - \Delta \tilde{u}^\delta &= f. \qquad \text{in } \Omega \times (0,T), \\ \tilde{u}^\delta &= 0 \qquad \text{on } \partial\Omega \times (0,T), \\ \gamma \tilde{u}^\delta(0) + \tilde{u}^\delta(T) &= g_\delta \qquad \text{in } \Omega, \end{aligned} \tag{3.2}$$

where $\gamma > 0$ denotes the regularization parameter. In [108], Yang and Liu considered the homogeneous problem $(f \equiv 0)$. It was proved that the regularized problem (3.2) has a unique solution, and if $u_0 \in L^2(\Omega)$, then for all $t \in [0,T]$ there holds

$$\|(\tilde{u}^\delta - u)(t)\|_{L^2(\Omega)} \to 0, \quad \text{as} \quad \gamma, \delta \to 0 \ \text{ and } \ \frac{\delta}{\gamma} \to 0. \tag{3.3}$$

Moreover, if $u_0 \in \mathrm{Dom}(A) = H^2(\Omega) \cap H_0^1(\Omega)$, there holds

$$\|(\tilde{u}^\delta - u)(t)\|_{C([0,T];L^2(\Omega))} \leq c\delta\gamma^{-1} + \gamma,$$

where the constant c depends only on u_0, g, g_δ, but is independent of δ and γ. By choosing $\gamma = O(\sqrt{\delta})$ *a priori*, one obtains an approximation with accuracy $O(\sqrt{\delta})$. The result contrasts sharply with that for normal diffusion, and the proof relies on the linear-decay property of the Mittag-Leffler function $E_{\alpha,1}(-x)$.

The rest of this Chapter is organized as follows. In Section 3.1, we provide some preliminary results about the regularization at the continuous level, which will be intensively used in error estimation. Then in Section 3.2 and Section 3.3, we describe and analyze spatially semi-discrete scheme and fully discrete scheme, respectively. Finally, in Section 3.4, we present illustrative numerical examples to illustrate the theoretical analysis. Throughout, the notation c denotes a generic constant, which may change at each occurrence, but it is always independent of the noise level δ, the regularization parameter γ, the mesh size h and time step size τ etc.

3.1 Regularization algorithm

3.1.1 Reformulation of original problem

In this chapter, we shall study an equivalent reformulation of the original backward subdiffusion problem (2.9). We let $w(t) = u(t) - \int_0^t E(t-s)f(s)\,ds$, then w satisfies the subdiffusion problem (2.9) with trivial source term, and the terminal data is

$$w(T) = u(T) - \int_0^T E(T-s)f(s)\,ds.$$

Meanwhile, in case that $f \in L^p(0,T;L^2(\Omega))$ with $1/\alpha < p < \infty$, then by Lemma 2.2 we have $w(0) = u(0) = u_0$. Then without loss of generality, we only consider the following backward subdiffusion problem with trivial source data:

$$\begin{aligned} \partial_t^\alpha u - \Delta u &= 0 && \text{in } \Omega \times (0,T), \\ u &= 0 && \text{on } \partial\Omega \times (0,T), \\ u(T) &= g && \text{in } \Omega. \end{aligned} \tag{3.4}$$

The solution u has the representation that

$$u(t) = F(t)u(0) = F(t)(F(T)^{-1}g). \tag{3.5}$$

Inspired by the estimate in [108], we defined an axillary function $\tilde{u}(t)$, which satisfies the regularized problem (without noise):

$$\begin{aligned} \partial_t^\alpha \tilde{u}(t) - \Delta \tilde{u}(t) &= 0, && \text{in } \Omega \times (0,T), \\ \tilde{u} &= 0 && \text{on } \partial\Omega \times (0,T), \\ \gamma\tilde{u}(0) + \tilde{u}(T) &= g, && \text{in } \Omega. \end{aligned} \tag{3.6}$$

Here γ denotes the regularization parameter. The appearance of regularization term essentially improves the regularity of the backward problem.

Analogue to (3.5), the function $\tilde{u}$ can be represented by

$$\tilde{u}(t) = F(t)\tilde{u}(0) = F(t)\big(\gamma I + F(T)\big)^{-1} g = F(t)\big(\gamma I + F(T)\big)^{-1}\big(F(T)u_0\big), \tag{3.7}$$

where I denotes the identity operator.

The next lemma provides an estimate of the operator $F(t)\big(\gamma I + F(T)\big)^{-1}$.

Lemma 3.1. *Let $F(t)$ be operator defined in* (2.11), *then*

$$\|F(t)\big(\gamma I + F(T)\big)^{-1} v\|_{\dot{H}^q(\Omega)} \leq c \min(\gamma^{-1}, t^{-\alpha}) \|v\|_{\dot{H}^q(\Omega)} \quad \forall\ q \geq 0,$$

where the generic constant c may depend on T, but is always independent of γ and t.

Proof. From Lemma 2.1 we have $E_{\alpha,1}(-z) > 0$ for any $z \geq 0$, then

$$\|F(t)\big(\gamma I + F(T)\big)^{-1} v\|^2_{\dot{H}^q(\Omega)} = \sum_{j=1}^{\infty} \left[\frac{E_{\alpha,1}(-\lambda_j t^\alpha)}{\gamma + E_{\alpha,1}(-\lambda_j T^\alpha)}\right]^2 \lambda_j^q (v, \varphi_j)^2.$$

By applying the fact that $0 \leq E_{\alpha,1}(-z) \leq 1$ with $z \geq 0$, we arrive at

$$\|F(t)\big(\gamma I + F(T)\big)^{-1} v\|^2_{\dot{H}^q(\Omega)} \leq \gamma^{-1} \|v\|^2_{\dot{H}^q(\Omega)}.$$

On the other hand, we apply Lemma 2.1 again to obtain for any $t \in (0, T]$

$$\begin{aligned} \frac{E_{\alpha,1}(-\lambda_j t^\alpha)}{\gamma + E_{\alpha,1}(-\lambda_j T^\alpha)} &\leq \tfrac{E_{\alpha,1}(-\lambda_j t^\alpha)}{E_{\alpha,1}(-\lambda_j T^\alpha)} \leq \tfrac{1+\Gamma(1-\alpha)(\lambda_j T^\alpha)}{1+\Gamma(1+\alpha)^{-1}(\lambda_j t^\alpha)} \\ &\leq 1 + \tfrac{\Gamma(1-\alpha)(\lambda_j T^\alpha)}{\Gamma(1+\alpha)^{-1}(\lambda_j t^\alpha)} \leq c_T t^{-\alpha} \end{aligned}$$

and hence

$$\|F(t)\big(\gamma I + F(T)\big)^{-1} v\|_{\dot{H}^q(\Omega)} \leq c t^{-\alpha} \|v\|_{\dot{H}^q(\Omega)}.$$

This completes the proof of the lemma. □

Using this lemma, we can derive the following estimate of $\tilde{u}(t) - u(t)$ with $t \in [0, T)$.

Lemma 3.2. *Let u and $\tilde{u}$ be solutions to problems* (3.4) *and* (3.6), *respectively. Then there holds*

$$\|\tilde{u}(0) - u(0)\|_{L^2(\Omega)} \leq c\gamma^{\frac{q}{2}} \|u_0\|_{\dot{H}^q(\Omega)} \qquad \forall\ q \in [0, 2].$$

Meanwhile, for any $t \in (0, T)$, there holds

$$\|\tilde{u}(t) - u(t)\|_{L^2(\Omega)} \leq c\gamma t^{-(1-\frac{q}{2})\alpha} \|u_0\|_{\dot{H}^q(\Omega)} \qquad \forall\ q \in [0, 2].$$

where the generic constant c may depends on T, but is always independent of γ and t.

Proof. By (3.5) and (3.7) we obtain

$$\tilde{u}(0) - u(0) = -\big(\gamma I + F(T)\big)^{-1}\gamma u_0.$$

Now applying (2.11) and positivity of $E_{\alpha,1}(z)$ with $z \le 0$, we derive that for any $q \in [0,2]$,

$$\begin{aligned}
\|\tilde{u}(0) - u(0)\|_{L^2(\Omega)}^2 &= \|(\gamma I + F(T))^{-1}\gamma u_0\|_{L^2(\Omega)}^2 \\
&= \sum_{j=1}^{\infty} \Big(\frac{\gamma}{\gamma + E_{\alpha,1}(-\lambda_j T^\alpha)}\Big)^2 (u_0, \varphi_j)^2 \\
&\le \sum_{j=1}^{\infty} \frac{\gamma^q}{\lambda_j^q |E_{\alpha,1}(-\lambda_j T^\alpha)|^q} \lambda_j^q (u_0, \varphi_j)^2.
\end{aligned}$$

The property of Mittag-Leffler functions in Lemma 2.1 implies that

$$\frac{\gamma^q}{\lambda_j^q |E_{\alpha,1}(-\lambda_j T^\alpha)|^q} \le \frac{c\gamma^q(1+\lambda_j T)^q}{\lambda_j^q} \le c_T \gamma^q.$$

and hence

$$\|\tilde{u}(0) - u(0)\|_{L^2(\Omega)}^2 \le c\gamma^q \|u_0\|_{\dot{H}^q(\Omega)}^2.$$

Now we turn to the second estimate, which follows from the representation

$$\tilde{u}(t) - u(t) = -F(t)\big(\gamma I + F(T)\big)^{-1}\gamma u_0.$$

Here we apply the definition of the solution operator and obtain

$$\begin{aligned}
\|\tilde{u}(t) - u(t)\|_{L^2(\Omega)}^2 &= \|F(t)(\gamma I + F(T))^{-1}\gamma u_0\|_{L^2(\Omega)}^2 \\
&= \sum_{j=1}^{\infty} \left(\frac{\gamma E_{\alpha,1}(-\lambda_j t^\alpha)}{\gamma + E_{\alpha,1}(-\lambda_j T^\alpha)}\right)^2 (u_0, \varphi_j)^2 \\
&\le \gamma^2 \sum_{j=1}^{\infty} \left(\frac{E_{\alpha,1}(-\lambda_j t^\alpha)}{\lambda_j^{q/2} E_{\alpha,1}(-\lambda_j T^\alpha)}\right)^2 \lambda_j^q (u_0, \varphi_j)^2
\end{aligned}$$

Then Lemma 2.1 leads to the estimate

$$\frac{E_{\alpha,1}(-\lambda_j t^\alpha)}{\lambda_j^{q/2} E_{\alpha,1}(-\lambda_j T^\alpha)} \le \frac{c(1+\lambda_j T^\alpha)}{\lambda_j^{q/2}(1+\lambda_j t^\alpha)} \le c_T \frac{\lambda_j^{1-q/2}}{1+\lambda_j t^\alpha} \le c_T t^{-(1-q/2)\alpha},$$

and therefore there holds

$$\|\tilde{u}(t) - u(t)\|_{L^2(\Omega)}^2 \le c\gamma^2 t^{-(2-q)\alpha} \|u_0\|_{\dot{H}^q(\Omega)}^2.$$

This completes the proof of the lemma. $\square$

If $u_0 \in L^2(\Omega) = \dot{H}^0(\Omega)$, the preceding lemma does not imply a convergence rate. However, one can still show the convergence in case of nonsmooth data.

Corollary 3.1. *Assume that* $u_0 \in L^2(\Omega)$. *Let* u *and* $\tilde{u}$ *be solutions to problems* (3.4) *and* (3.6), *respectively. Then there holds that*

$$\lim_{\gamma \to 0} \|\tilde{u}(0) - u(0)\|_{L^2(\Omega)} = 0.$$

Proof. In case that $u_0 \in L^2(\Omega)$, we know that $\tilde{u}, u \in C([0,T]; L^2(\Omega))$. Then for any small ϵ, we choose t_0 small enough such that

$$\|\tilde{u}(t_0) - \tilde{u}(0)\|_{L^2(\Omega)} + \|u(t_0) - u(0)\|_{L^2(\Omega)} < \epsilon/2.$$

Then by Lemma 3.2, we may find γ_0 small enough such that

$$\|\tilde{u}(t_0) - u(t_0)\|_{L^2(\Omega)} < \epsilon/2 \quad \text{for all } \gamma < \gamma_0.$$

By triangle inequality , we obtain that for any $\gamma < \gamma_0$

$$\|\tilde{u}(0) - u(0)\|_{L^2(\Omega)} < \epsilon.$$

Therefore, $\tilde{u}(0)$ converges to $u(0)$ in L^2-sense, as $\gamma \to 0$. □

3.2 Spatial semidiscrete method by finite element method

In this section, we shall propose and analyze a spatially semidiscrete scheme for solving the backward subdiffusion problem (3.4). Even though the semidiscrete scheme is not directly implementable and rarely used in practical computation, it is important for understanding the role of the regularity of problem data and also for the analysis of fully discrete schemes.

3.2.1 Semidiscrete scheme for solving direct problem.

Now we let the triangulation $\mathcal{T}_h$, piecewise-linear finite element space X_h, L^2 projection P_h, Ritz projection R_h and the discrete Laplacian Δ_h defined in Section 2.5.

The semidiscrete Galerkin FEM for problem (2.9) is: find $u_h(t) \in X_h$ such that

$$\begin{aligned} (\partial_t^\alpha u_h, \chi) + (\nabla u_h, \nabla \chi) &= (f, \chi), \qquad \forall\, \chi \in X_h,\ T \geq t > 0, \\ u_h(0) &= P_h u_0. \end{aligned} \tag{3.8}$$

Let $f_h = P_h f$, we may write the spatially semidiscrete problem (3.8) as

$$\partial_t^\alpha u_h(t) - \Delta_h u_h(t) = f_h(t) \text{ for } t \geq 0 \quad \text{with} \quad u_h(0) = P_h u_h. \tag{3.9}$$

Now we give a representation of the solution of (3.9) using the eigenvalues and eigenfunctions $\{\lambda_j^h\}_{j=1}^K$ and $\{\varphi_j^h\}_{j=1}^K$ of the discrete Laplacian $-\Delta_h$. Here we introduce the discrete analogue of (2.11) for

$t > 0$:

$$F_h(t)\chi = \sum_{j=1}^{K} E_{\alpha,1}(-\lambda_j^h t^\alpha)(\chi,\varphi_j^h)\varphi_j^h \quad \text{and} \quad E_h(t)\chi = \sum_{j=1}^{K} t^{\alpha-1}E_{\alpha,\alpha}(-\lambda_j^h t^\alpha)(\chi,\varphi_j^h)\varphi_j^h, \tag{3.10}$$

Then the solution $u_h(t)$ of the semidiscrete problem (3.9) can be expressed by:

$$u_h(t) = F_h(t)u_h(0) + \int_0^t E_h(t-s)f_h(s)\,\mathrm{d}s. \tag{3.11}$$

The discrete solution operator $E_h(t)$ satisfies the following smoothing property. See [40, Lemma 3.2] for proof.

Lemma 3.3. *We have $E_h(t)$ and $\psi \in X_h$. Then we have for all $t > 0$ and $q \in [0,1]$*

$$\|\Delta_h^q E_h(t)\psi\|_{L^2(\Omega)} \le ct^{(1-q)\alpha-1}\|\psi\|_{L^2(\Omega)}.$$

3.2.2 Semidiscrete scheme for solving backward problem.

In this part, we consider the semidiscrete solution $\tilde{u}_h^\delta(t) \in X_h$ such that

$$\begin{aligned} \partial_t^\alpha \tilde{u}_h^\delta(t) - \Delta_h \tilde{u}_h^\delta(t) &= 0, \quad \forall t \in (0,T] \\ \gamma\tilde{u}_h^\delta(0) + \tilde{u}_h^\delta(T) &= P_h g_\delta. \end{aligned} \tag{3.12}$$

Then the function $\tilde{u}_h^\delta$ can be written as

$$\tilde{u}_h^\delta(t) = F_h(t)\tilde{u}_h^\delta(0) = F_h(t)(\gamma + F_h(T))^{-1}P_h g_\delta. \tag{3.13}$$

Meanwhile, we shall use an axillary function $\tilde{u}_h(t)$, which is the semidiscrete solution to (3.6), i.e., satisfying

$$\begin{aligned} \partial_t^\alpha \tilde{u}_h(t) - \Delta_h \tilde{u}_h(t) &= 0, \quad \forall t \in (0,T] \\ \gamma\tilde{u}_h(0) + \tilde{u}_h(T) &= P_h g, \end{aligned} \tag{3.14}$$

Similarly, we have the representation

$$\tilde{u}_h(t) = F_h(t)\tilde{u}_h(0) = F_h(t)(\gamma I + F_h(T))^{-1}P_h g. \tag{3.15}$$

Analogue to Lemma 3.1, we have the following estimate of the operator $F_h(t)(\gamma I + F_h(T))^{-1}$. Note that the error is independent of the mesh size h.

Lemma 3.4. *Let $F_h(t)$ be operator defined in* (3.10)*, then there holds that*

$$\|F_h(t)\big(\gamma I + F_h(T)\big)^{-1}v\|_{L^2(\Omega)} \le c\min(\gamma^{-1}, t^{-\alpha})\|v\|_{L^2(\Omega)} \quad \forall\ v \in X_h,$$

where the constant c may depend on T, but is always independent of h, γ and t.

This Lemma together with (3.13) and (3.15) immediately leads to the following estimate of $\tilde{u}_h^\delta(t) - \tilde{u}_h(t)$.

Corollary 3.2. *Let $\tilde{u}_h^\delta$ and $\tilde{u}_h$ be the solution to the semidiscrete problems* (3.12) *and* (3.14)*, respectively. Then, there holds that*

$$\|(\tilde{u}_h^\delta - \tilde{u}_h)(t)\|_{L^2(\Omega)} \le c\delta \min(\gamma^{-1}, t^{-\alpha}) \quad \forall\, t \in [0, T],$$

where the generic constant c is independent of γ, δ, h and t.

Next, we shall derive a bound of $\tilde{u}_h - \tilde{u}$.

Lemma 3.5. *Assume that $u_0 \in \dot{H}^2(\Omega)$. Let $\tilde{u}$ be the solution to the regularized backward subdiffusion problem* (3.6)*, and $\tilde{u}_h$ be the solution to the corresponding semidiscrete problem* (3.14)*. Then there holds*

$$\|(\tilde{u}_h - \tilde{u})(t)\|_{L^2(\Omega)} \le ch^2 \min(\gamma^{-1}, t^{-\alpha}) \|u_0\|_{\dot{H}^2(\Omega)} \quad \forall\, t \in [0, T],$$

where c might depend on T, but is always independent of h, γ and t.

Proof. We split $\tilde{u}_h(t) - \tilde{u}(t)$ into two components such that

$$\tilde{u}_h(t) - \tilde{u}(t) = (\tilde{u}_h(t) - R_h\tilde{u}(t)) + (R_h\tilde{u}(t) - \tilde{u}(t)) =: \zeta(t) + \rho(t),$$

By the approximation property of the Ritz projection in (2.18), we have

$$\|\rho(t)\|_{L^2(\Omega)} \le ch^2 \|\tilde{u}(t)\|_{\dot{H}^2(\Omega)} \le ch^2 \|u_0\|_{\dot{H}^2(\Omega)} \tag{3.16}$$

where the last inequality follows from (3.7) and Lemma 3.1 (with $t = T$).

Now we turn to the bound of $\zeta = \tilde{u}_h - R_h\tilde{u}$, where $\tilde{u}_h$ and $R_h\tilde{u}$ satisfy

$$\gamma\tilde{u}_h(0) + \tilde{u}_h(T) = P_h g \qquad \text{and} \qquad \gamma R_h\tilde{u}(0) + R_h\tilde{u}(T) = R_h g,$$

respectively. By noting the fact $\Delta_h R_h = P_h\Delta$, we have

$$\partial_t^\alpha \zeta(t) - \Delta_h\zeta(t) = -P_h\partial_t^\alpha\rho(t) \quad \text{with} \quad \gamma\zeta(0) + \zeta(T) = (P_h - R_h)g. \tag{3.17}$$

Then we arrive at

$$\zeta(T) = F_h(T)\zeta(0) - \int_0^T E_h(T-s)P_h\partial_s^\alpha\rho(s)ds.$$

We add $\gamma\zeta(0)$ at both sides of the equation and use (3.17) to derive that

$$P_h g - R_h g = (\gamma I + F_h(T))\zeta(0) - \int_0^T E_h(T-s)P_h\partial_s^\alpha\rho(s)ds,$$

and therefore

$$\begin{aligned}\zeta(t) &= F_h(t)\big(\gamma I + F_h(T)\big)^{-1}\Big[(P_h - R_h)g + \int_0^T E_h(T-s)P_h\partial_s^\alpha \rho(s)ds\Big]\\ &\quad - \int_0^t E_h(t-s)P_h\partial_s^\alpha\rho(s)ds\\ &=: I_1 + I_2 + I_3.\end{aligned}$$

The properties (2.17) and (2.18), and Lemma 3.4 lead to the estimate that

$$\begin{aligned}\|I_1\|_{L^2(\Omega)} &\le c\min(\gamma^{-1}, t^{-\alpha})\|(P_h - R_h)g\|_{L^2(\Omega)} \le ch^2\min(\gamma^{-1}, t^{-\alpha})\|g\|_{\dot H^2(\Omega)}\\ &\le ch^2\min(\gamma^{-1}, t^{-\alpha})\|u_0\|_{\dot H^2(\Omega)}.\end{aligned}$$

The last inequality is the direct result of the solution regularity in Lemma 2.2. Similarly, we apply Lemmas 3.3 and 3.4, and stability of L^2 projection P_h to arrive at

$$\|I_2\|_{L^2(\Omega)} \le c\min(\gamma^{-1}, t^{-\alpha})\int_0^T (T-s)^{\alpha-1}\|\partial_s^\alpha\rho(s)\|_{L^2(\Omega)}ds.$$

Then (2.18) and the solution regularity in Lemma 2.2 immediately imply that

$$\begin{aligned}\|I_2\|_{L^2(\Omega)} &\le ch^2\min(\gamma^{-1}, t^{-\alpha})\int_0^T (T-s)^{\alpha-1}\|\partial_s^\alpha u(s)\|_{\dot H^2(\Omega)}\,ds\\ &\le ch^2\min(\gamma^{-1}, t^{-\alpha})\int_0^T (T-s)^{\alpha-1}s^{-\alpha}\,ds\|u_0\|_{\dot H^2(\Omega)}\\ &\le ch^2\min(\gamma^{-1}, t^{-\alpha})\|u_0\|_{\dot H^2(\Omega)}.\end{aligned}$$

Similar argument also leads to a bound of the term I_3:

$$\begin{aligned}\|I_3\|_{L^2(\Omega)} &\le ch^2\int_0^T (T-s)^{\alpha-1}\|\partial_s^\alpha u(s)\|_{\dot H^2(\Omega)}\,ds\\ &\le ch^2\int_0^T (T-s)^{\alpha-1}s^{-\alpha}\,ds\|u_0\|_{\dot H^2(\Omega)} \le ch^2\|u_0\|_{\dot H^2(\Omega)}.\end{aligned}$$

As a result, we arrive at the desired estimate. □

Then, Lemmas 3.2 and 3.5 and Corollary 3.2 together lead to the following theorem which providing an error estimate of the numerical solution $\widetilde{u}_h^\delta$, in case of smooth initial data, i.e., $u_0 \in D(\Delta) = \dot H^2(\Omega)$.

Theorem 3.1. *Assume that $u_0 \in \dot H^2(\Omega)$. Let u be the solution to the problem* (3.4) *and $\widetilde{u}_h^\delta$ be the solution to the (regularized) semidiscrete problem* (3.12). *Then there holds*

$$\|\tilde u_h^\delta(t) - u(t)\|_{L^2(\Omega)} \le c\big(\gamma + (h^2+\delta)\min(\gamma^{-1}, t^{-\alpha})\big) \quad \forall\ t \in [0,T],$$

where c might depend on T and u_0, but is always independent of h, γ, δ and t.

Remark 3.1. *The error estimate in Theorem 3.1 is useful, since it specifies the scale to balance the discretization error, regularization parameter and noise level. For example, if we decide the a priori choice of parameters:* $h = O(\sqrt{\delta})$ *and* $\gamma = O(\sqrt{\delta})$, *then there holds*

$$\|\tilde{u}_h^\delta(0) - u_0\|_{L^2(\Omega)} \le c\sqrt{\delta}.$$

On the other hand, for any $t > 0$, *we have*

$$\|\tilde{u}_h^\delta(t) - u(t)\|_{L^2(\Omega)} \le c\delta t^{-\alpha},$$

by the a priori choice of parameters: $h = O(\sqrt{\delta})$ *and* $\gamma = O(\delta)$. *This is the first study of the discretized problem, and the result is consistent with the estimate in the continuous level, see e.g. [108, Theorem 3.4]. The analysis relies heavily on the nonstandard error estimate for the direct problem in terms of problem data regularity [40].*

Next, we shall consider the worse case that $u_0 \in L^2(\Omega)$.

Lemma 3.6. *Assume that* $u_0 \in L^2(\Omega)$. *Let* $\tilde{u}$ *be the solution to the regularized backward subdiffusion problem* (3.6), *and* $\tilde{u}_h$ *be the solution to the corresponding semidiscrete problem* (3.14). *Then there holds for all* $t \in [0, T]$ *and* $\ell_h = \max(1, |\ln h|)$

$$\|(\tilde{u}_h - \tilde{u})(t)\|_{L^2(\Omega)} \le c\gamma^{-1} \min(\gamma^{-1}, t^{-\alpha}) h^2 \ell_h \|u_0\|_{L^2(\Omega)},$$

where the constant c *might depend on* T, *but is always independent of* h, γ *and* t.

Proof. By using the L^2-projection P_h, we split $\tilde{u}_h(t) - \tilde{u}(t)$ into two components:

$$\tilde{u}_h(t) - \tilde{u}(t) = (\tilde{u}_h(t) - P_h\tilde{u}(t)) + (P_h\tilde{u}(t) - \tilde{u}(t)) =: \zeta(t) + \rho(t),$$

By the approximation property of the L^2-projection in (2.18), we have

$$\|\rho(t)\|_{L^2(\Omega)} \le ch^2 \|\tilde{u}(t)\|_{\dot{H}^2(\Omega)} \le c_T h^2 \gamma^{-1} \|u_0\|_{L^2(\Omega)},$$

where the last inequality follows from the solution representation (3.7), Lemma 3.1 and Lemma 2.2, such that

$$\|\tilde{u}(t)\|_{\dot{H}^2(\Omega)} \le c\gamma^{-1} \|F(T)u_0\|_{\dot{H}^2(\Omega)} \le c\gamma^{-1} T^{-\alpha} \|u_0\|_{L^2(\Omega)}. \tag{3.18}$$

Now we turn to the bound of $\zeta = \tilde{u}_h - P_h\tilde{u}$, where $\tilde{u}_h$ and $P_h\tilde{u}$ satisfy

$$\gamma\tilde{u}_h(0) + \tilde{u}_h(T) = P_h g \qquad \text{and} \qquad \gamma P_h\tilde{u}(0) + P_h\tilde{u}(T) = P_h g,$$

respectively. By noting the fact $\Delta_h R_h = P_h \Delta$, we have

$$\partial_t^\alpha \zeta(t) - \Delta_h \zeta(t) = \Delta_h (P_h - R_h)\widetilde{u}(t) \quad \text{with} \quad \gamma\zeta(0) + \zeta(T) = 0. \tag{3.19}$$

Then we arrive at

$$\zeta(T) = F_h(T)\zeta(0) + \int_0^T E_h(T-s)\Delta_h(P_h - R_h)\widetilde{u}(s)ds.$$

We add $\gamma\zeta(0)$ at both sides of the equation and derive that

$$\zeta(0) = -(\gamma I + F_h(T))^{-1} \int_0^T E_h(T-s)\Delta_h(P_h - R_h)\widetilde{u}(s)ds,$$

and hence

$$\begin{aligned}\zeta(t) &= F_h(t)\zeta(0) + \int_0^t E_h(t-s)\Delta_h(P_h - R_h)\widetilde{u}(s)ds \\ &= -F_h(t)\big(\gamma I + F_h(T)\big)^{-1} \int_0^T E_h(T-s)\Delta_h(P_h - R_h)\widetilde{u}(s)ds \\ &\quad + \int_0^t E_h(t-s)\Delta_h(P_h - R_h)\widetilde{u}(s)ds \\ &=: I_1 + I_2.\end{aligned}$$

Similarly, we apply Lemmas 3.3 and 3.4, to arrive at

$$\begin{aligned}\|I_1\|_{L^2(\Omega)} &\le c\min(\gamma^{-1}, t^{-\alpha}) \textstyle\int_0^T (T-s)^{\alpha\epsilon-1}\|\Delta_h^\epsilon(P_h - R_h)\widetilde{u}(s)\|_{L^2(\Omega)}ds \\ &\le c\min(\gamma^{-1}, t^{-\alpha})h^{-2\epsilon} \textstyle\int_0^T (T-s)^{\alpha\epsilon-1}\|(P_h - R_h)\widetilde{u}(s)\|_{L^2(\Omega)}ds\end{aligned}$$

where we apply the inverse estimate for FEM functions in the second inequality. The approximation properties (2.18) and (2.17) lead to

$$\|I_1\|_{L^2(\Omega)} \le c\min(\gamma^{-1}, t^{-\alpha})h^{2-2\epsilon} \int_0^T (T-s)^{\alpha\epsilon-1}\|\widetilde{u}(s)\|_{\dot{H}^2(\Omega)}ds,$$

and then the regularity estimate of $\widetilde{u}$ in (3.18) implies that

$$\begin{aligned}\|I_1\|_{L^2(\Omega)} &\le c\gamma^{-1}\min(\gamma^{-1}, t^{-\alpha})h^{2-2\epsilon} \textstyle\int_0^T (T-s)^{\alpha\epsilon-1}T^{-\alpha}ds\|u_0\|_{L^2(\Omega)} \\ &\le c\gamma^{-1}\min(\gamma^{-1}, t^{-\alpha})h^{2-2\epsilon}\epsilon^{-1}\|u_0\|_{L^2(\Omega)}.\end{aligned}$$

Similar argument also leads to a bound of the term I_2:

$$\|I_2\|_{L^2(\Omega)} \le ch^{2-2\epsilon}\epsilon^{-1}\|u_0\|_{L^2(\Omega)}.$$

Then the desired assertion follows immediately by choosing $\epsilon = 1/\ell_h$. □

Then, Lemmas 3.2 and 3.6 and Corollary 3.2 together lead to the following error estimate, in case of nonsmooth initial data.

Theorem 3.2. *Assume that $u_0 \in \dot{H}^q(\Omega)$ with $q \in [0,2]$. Let u be the solution to the problem (3.4) and $\widetilde{u}_h^\delta$ be the solution to the (regularized) semidiscrete problem (3.12). Then there holds for all $t \in [0,T]$ and $\ell_h = \max(1, |\ln h|)$*

$$\|\tilde{u}_h^\delta(t) - u(t)\|_{L^2(\Omega)} \le c\Big(\min(\gamma^{q/2}, \gamma t^{-(1-q/2)\alpha}) + (\gamma^{-(1-q/2)}h^2\ell_h^{1-q/2} + \delta)\min(\gamma^{-1}, t^{-\alpha})\Big)$$

where the constant c depends on T and u_0, but is always independent of h, γ, δ and t.

Remark 3.2. *In case that $u_0 \in L^2(\Omega)$, the above estimate does not imply a convergence rate of $\tilde{u}_h^\delta(0)$. However, we can still show the convergence, provided suitable scales of parameters. The proof is a direct result of Corollaries 3.1 and 3.2, and Lemma 3.6.*

Let u be the solution to the problem (3.4) *and $\widetilde{u}_h^\delta$ be the solution to the semidiscrete problem* (3.12)*. Then there holds*

$$\|\tilde{u}_h^\delta(0) - u(0)\|_{L^2(\Omega)} \to 0, \quad \text{as } \gamma \to 0, \ \frac{\delta}{\gamma} \to 0 \text{ and } \frac{h\ell_h^{1/2}}{\gamma} \to 0.$$

3.3 Fully discrete solution and error estimate

3.3.1 Fully discrete scheme and solution operators.

From Section 2.5, we apply backward Euler convolution quadrature(BE-CQ) here for $0 < \alpha < 1$. The fully discrete scheme for problem (2.9) reads: find $U_n \in X_h$ such that

$$\bar{\partial}_\tau(U_n - U_0) - \Delta_h U_n = P_h f(t_n), \quad n = 1, 2, \ldots, N, \tag{3.20}$$

with the initial condition $U_0 = P_h u_0 \in X_h$.

By means of discrete Laplace transform, the fully discrete solution $U_n \in X_h$ is given by

$$U_n = F_{h,\tau}^n U_0 + \tau \sum_{k=1}^{n} E_{h,\tau}^{n-k} P_h f(t_k), \quad n = 1, 2, \ldots, N, \tag{3.21}$$

where the fully discrete operators $F_{h,\tau}^n$ and $E_{h,\tau}^n$ are respectively defined by (see e.g., [43])

$$F_{h,\tau}^n = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} \delta_\tau(e^{-z\tau})^{\alpha-1} (\delta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1} \, \mathrm{d}z, \tag{3.22}$$

$$E_{h,\tau}^n = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} (\delta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1} \, \mathrm{d}z, \tag{3.23}$$

with $\delta_\tau(\xi) = (1-\xi)/\tau$ and the contour $\Gamma_{\theta,\sigma}^\tau := \{z \in \Gamma_{\theta,\sigma} : |\Im(z)| \le \pi/\tau\}$ (oriented with an increasing imaginary part).

The fully discrete solution operators have been fully understood in [43], by using the expression (3.22) and (3.23), resolvent estimate and properties of the kernel $\delta_\tau(e^{-z\tau})$ in Lemma 2.4. With the spectral decomposition, we can write

$$U_n = F_{h,\tau}^n U_0 = \sum_{j=1}^{K} F_\tau^n(\lambda_j^h)(u_0, \varphi_j^h)\varphi_j^h \tag{3.24}$$

where $F_\tau^n(\lambda_j^h)$ is the solution to the discrete initial value problem

$$\bar{\partial}_\tau[F_\tau^n(\lambda_j^h) - F_\tau^0(\lambda_j^h)] + \lambda_j^h F_\tau^n(\lambda_j^h) = 0, \quad \text{with} \quad F_\tau^0(\lambda_j^h) = 1.$$

From (3.22), we know that $F_\tau^n(\lambda_j^h)$ could be written as

$$F_\tau^n(\lambda_j^h) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} \delta_\tau(e^{-z\tau})^{\alpha-1} (\delta_\tau(e^{-z\tau})^\alpha + \lambda_j^h)^{-1} \, \mathrm{d}z. \tag{3.25}$$

Lemma 3.7. *Let $F_\tau^n(\lambda)$ be defined as in (3.25). Then for $\lambda > 0$, there holds*

$$\big|E_{\alpha,1}(-\lambda t_n^\alpha) - F_\tau^n(\lambda)\big| \le \frac{c}{(1+\lambda t_n^\alpha)} n^{-1}. \tag{3.26}$$

Meanwhile, there holds

$$\lambda^{-1}\big|E_{\alpha,1}(-\lambda t_n^\alpha) - F_\tau^n(\lambda)\big| \le c\tau t_n^{\alpha-1} \tag{3.27}$$

where c is a generic number independent of λ, t and τ.

Proof. It has been proved in [39] that

$$\big|E_{\alpha,1}(-\lambda t_n^\alpha) - F_\tau^n(\lambda)\big| \le cn^{-1}.$$

Therefore, it suffices to show that

$$\big|E_{\alpha,1}(-\lambda t_n^\alpha) - F_\tau^n(\lambda)\big| \le c\lambda^{-1} t_n^{-\alpha} n^{-1}.$$

From (3.25) and (2.7), we know

$$\begin{aligned}
&\big|E_{\alpha,1}(-\lambda_j^h t^\alpha) - F_\tau^n(\lambda_j^h)\big| \le \Big|\frac{1}{2\pi i}\int_{\Gamma_{\theta,\sigma}\backslash\Gamma_{\theta,\sigma}^\tau} e^{zt_n} z^{\alpha-1}(z^\alpha+\lambda)^{-1} dz\Big| \\
&+ \Big|\frac{1}{2\pi i}\int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n}\left[z^{\alpha-1}(z^\alpha+\lambda)^{-1} - \delta_\tau(e^{-z\tau})^{\alpha-1}(\delta_\tau(e^{-z\tau})^\alpha+\lambda)^{-1}\right] dz\Big| \\
&=: I_1 + I_2.
\end{aligned}$$

First of all, we shall establish a bound of I_1, which follows from the direct calculation:

$$\begin{aligned}
I_1 &\le c\int_{\Gamma_{\theta,\sigma}\backslash\Gamma_{\theta,\sigma}^\tau} |e^{zt_n}||z|^{\alpha-1}|z^\alpha+\lambda|^{-1}\,|dz| \le c\lambda^{-1}\int_{\pi/\tau\sin\theta}^\infty e^{\rho(\cos\theta)t_n}\rho^{\alpha-1}d\rho \\
&\le c\lambda^{-1}t_n^{-\alpha}\int_{cn}^\infty e^{-c\rho}\rho^{\alpha-1}d\rho \le c\lambda^{-1}t_n^{-\alpha}n^{-1}\int_{cn}^\infty e^{-c\rho}\rho^{\alpha}d\rho \le c\lambda^{-1}t_n^{-\alpha}n^{-1}.
\end{aligned}$$

Next we turn to I_2. By lemma 2.4, we have for all $z \in \Gamma_{\theta,\sigma}^\tau$

$$\begin{aligned}
&\Big|\frac{z^{\alpha-1}}{z^\alpha+\lambda} - \frac{\delta_\tau(e^{-z\tau})^{\alpha-1}}{\delta_\tau(e^{-z\tau})^\alpha+\lambda}\Big| \\
=&\Big|\frac{z^{\alpha-1}\delta_\tau(e^{-z\tau})^{\alpha-1}(\delta_\tau(e^{-z\tau})-z)}{(z^\alpha+\lambda)(\delta_\tau(e^{-z\tau})^\alpha+\lambda)}\Big| + \Big|\frac{(z^{\alpha-1}-\delta_\tau(e^{-z\tau})^{\alpha-1})\lambda}{(z^\alpha+\lambda)(\delta_\tau(e^{-z\tau})^\alpha+\lambda)}\Big| \\
\le& c\tau\lambda^{-1}|z|^\alpha.
\end{aligned}$$

Therefore, with $\sigma = t_n^{-1}$, the term I_2 can be bounded as

$$\begin{aligned}
I_2 &\le c\tau\lambda^{-1}\int_{\Gamma_{\theta,\sigma}^\tau} |e^{zt_n}||z|^\alpha\,|dz| \\
&\le c\tau\lambda^{-1}\Big(\int_\sigma^\infty e^{-c\rho t_n}\rho^\alpha\,d\rho + \sigma^{1+\alpha}\int_{-\theta}^\theta d\psi\Big) \\
&\le c\tau\lambda^{-1}t_n^{-\alpha-1} \le c\lambda^{-1}t_n^{-\alpha}n^{-1}.
\end{aligned}$$

Next, we turn to the estimate (3.27), which can be derived from the expressions:

$$E_{\alpha,1}(-\lambda t_n^\alpha) = 1 - \frac{\lambda}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}} e^{zt_n} z^{-1}(z^\alpha + \lambda)^{-1} \,\mathrm{d}z,$$
$$F_\tau^n(\lambda) = 1 - \frac{\lambda}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} \delta_\tau(e^{-z\tau})^{-1}(\delta_\tau(e^{-z\tau})^\alpha + \lambda)^{-1} \,\mathrm{d}z,$$

with $n \geq 1$. Then we arrive at

$$\begin{aligned}
&\lambda^{-1}\big|E_{\alpha,1}(-\lambda t_n^\alpha) - F_\tau^n(\lambda)\big| \\
\leq& \Big|\frac{1}{2\pi i}\int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n}\left[z^{-1}(z^\alpha+\lambda)^{-1} - \delta_\tau(e^{-z\tau})^{-1}(\delta_\tau(e^{-z\tau})^\alpha + \lambda)^{-1}\right] dz\Big| \\
\leq& \Big|\frac{1}{2\pi i}\int_{\Gamma_{\theta,\sigma}\backslash\Gamma_{\theta,\sigma}^\tau} e^{zt_n} z^{-1}(z^\alpha+\lambda)^{-1} dz\Big| =: II_1 + II_2.
\end{aligned}$$

By Lemma 2.4, we have for all $z \in \Gamma_{\theta,\sigma}^\tau$

$$\big|z^{-1}(z^\alpha+\lambda)^{-1} - \delta_\tau(e^{-z\tau})^{-1}(\delta_\tau(e^{-z\tau})^\alpha+\lambda)^{-1}\big| \leq c\tau|z|^{-\alpha},$$

and therefore with the setting $\sigma = t_n^{-1}$ we have the bound for $n \geq 1$

$$II_1 \leq c\tau \int_{\Gamma_{\theta,\sigma}^\tau} |e^{zt_n}||z|^{-\alpha}\,|dz| \leq c\tau\Big(\int_\sigma^\infty e^{-c\rho t_n}\rho^{-\alpha}\,d\rho + \sigma^{1-\alpha}\int_{-\theta}^{\theta} d\psi\Big) \leq c\tau t_n^{\alpha-1}.$$

Similarly, to bound II_2, we apply Lemma 2.4 to derive that for $n \geq 1$

$$\begin{aligned}
II_2 &\leq c\int_{\Gamma_{\theta,\sigma}\backslash\Gamma_{\theta,\sigma}^\tau} |e^{zt_n}||z|^{-\alpha-1}\,|dz| \leq c\int_{\pi/\tau\sin\theta}^\infty e^{\rho(\cos\theta)t_n}\rho^{-\alpha-1}d\rho \\
&\leq ct_n^\alpha \int_{cn}^\infty e^{-c\rho}\rho^{-\alpha-1}d\rho \leq ct_n^\alpha n^{-1}\int_0^\infty e^{-c\rho}\rho^{-\alpha}d\rho \leq ct_n^\alpha n^{-1} \leq c\tau t_n^{\alpha-1}.
\end{aligned}$$

Both the estimates together with the fact that $E_{\alpha,1}(0) = F_\tau^0(\lambda) = 1$ lead to the desired result. □

The above lemma and Lemma 2.1 lead to the following corollary.

Corollary 3.3. *For any $1 \leq n \leq N$, $F_{h,\tau}^n(\lambda)$ is positive, and there exist positive constants c_0, c_1 such that*

$$\frac{c_0}{1+\lambda t_n^\alpha} \leq F_\tau^n(\lambda_j^h) \leq \frac{c_1}{1+\lambda t_n^\alpha},$$

Then the next corollary follows immediately.

Corollary 3.4. *Let $F_{h,\tau}^n(\lambda)$ be defined as (3.25), then there holds*

$$|F_{h,\tau}^n(\lambda)\big(\gamma + F_{h,\tau}^N(\lambda)\big)^{-1}| \leq c\min(\gamma^{-1}, t_n^{-\alpha}),$$

where the generic constant c may depend on T, but is always independent of γ, λ, τ, n and h.

Proof. By Corollary 3.3, we know that $0 \le F_\tau^n(\lambda) \le c_1$, we arrive at

$$|F_{h,\tau}^n(\lambda)\big(\gamma + F_{h,\tau}^N(\lambda)\big)^{-1}| \le c\gamma^{-1}.$$

On the other hand, we apply Corollary 3.3 again to obtain

$$\frac{F_{h,\tau}^n(\lambda)}{\gamma + F_{h,\tau}^N(\lambda)} \le \frac{F_{h,\tau}^n(\lambda)}{F_{h,\tau}^N(\lambda)} \le \frac{c(1+\lambda T^\alpha)}{1+\lambda t_n^\alpha} \le c_T t_n^{-\alpha}.$$

This completes the proof of the corollary. □

3.3.2 Fully discrete scheme for backward problem and error estimate.

Now we shall propose a fully discrete scheme for solving the backward subdiffusion problem. Here we apply the semidiscrete scheme and the convolution quadrature generated by backward Euler scheme. Then the fully discrete scheme reads: find $\tilde U_n^\delta \in X_h$, $n = 1, 2, \ldots, N$, such that

$$\begin{aligned} \bar\partial_\tau(\tilde U_n^\delta - \tilde U_0^\delta) - \Delta_h \tilde U_n^\delta = 0, \quad \forall\ n = 1, 2, \ldots, N. \\ \gamma \tilde U_0^\delta + \tilde U_N^\delta = P_h g_\delta. \end{aligned} \tag{3.28}$$

Then the solution could be written as

$$\tilde U_n^\delta = F_{h,\tau}^n \tilde U_0^\delta = F_{h,\tau}^n(\gamma I + F_{h,\tau}^N)^{-1} P_h g_\delta = \sum_{j=1}^K \frac{F_\tau^n(\lambda_j^h)}{\gamma + F_\tau^N(\lambda_j^h)} (P_h g_\delta, \varphi_j^h)\varphi_j^h. \tag{3.29}$$

Similarly, we shall use the auxiliary solution $\tilde U_n$ satisfying

$$\begin{aligned} \bar\partial_\tau(\tilde U_n - \tilde U_0) - \Delta_h \tilde U_n = 0, \quad \forall\ n = 1, 2, \ldots, N. \\ \gamma \tilde U_0 + \tilde U_N = P_h g. \end{aligned} \tag{3.30}$$

Then $\tilde U_n$ could be written as

$$\tilde U_n = F_{h,\tau}^n(\gamma I + F_{h,\tau}^N)^{-1} P_h g = \sum_{j=1}^K \frac{F_\tau^n(\lambda_j^h)}{\gamma + F_\tau^N(\lambda_j^h)} (P_h g, \varphi_j^h)\varphi_j^h. \tag{3.31}$$

The same as Corollary 3.2, we may show the following estimate of $\tilde U_n^\delta - \tilde U_n$.

Lemma 3.8. *Let $\tilde U_n^\delta$ and $\tilde U_n$ be solutions to* (3.28) *and* (3.30)*, respectively. Then there holds that*

$$\|\tilde U_n^\delta - \tilde U_n\|_{L^2(\Omega)} \le c\delta \min(\gamma^{-1}, t_n^{-\alpha}), \quad \textit{for all } 0 \le n \le N$$

where the generic constant c is independent of γ, δ, τ, n and h.

Proof. From Corollary 3.4, we have ($\forall v \in X_h$)

$$\|F_{h,\tau}^n\big(\gamma + F_{h,\tau}^N(T)\big)^{-1} v\|_{L^2(\Omega)}^2 = \sum_{j=1}^K \left[\frac{F_\tau^n(-\lambda_j^h)}{\gamma + F_\tau^N(-\lambda_j^h)}\right]^2 (v, \varphi_j)^2 \le c \min(\gamma^{-1}, t_n^{-\alpha})\|v\|_{L^2(\Omega)}$$

Therefore for all $0 \le n \le N$

$$\|\tilde{U}_n^\delta - \tilde{U}_n\|_{L^2(\Omega)} \le c\min(\gamma^{-1}, t_n^{-\alpha})\|g-g^\delta\| \le c\delta\min(\gamma^{-1}, t_n^{-\alpha}).$$

□

Lemma 3.9. *Let $\tilde{U}_n$ and $\tilde{u}_h(t)$ be solutions to* (3.30) *and* (3.14), *respectively. Then there holds that*

$$\|\tilde{U}_0 - \tilde{u}_h(0)\|_{L^2(\Omega)} \le c\Big(\tau\gamma^{-1-(1-q/2)}\|u_0\|_{\dot{H}^q(\Omega)} + h^2\gamma^{-1}\|u_0\|_{L^2(\Omega)}\Big)$$

where the generic constant c is independent of γ, δ, τ, n and h.

Proof. By (3.15), we know the semidiscrete function $\tilde{u}_h(t)$ can be represented as

$$\tilde{u}_h(0) = (\gamma I + F_h(T))^{-1}P_h g = \sum_{j=1}^K \frac{(g,\varphi_j^h)}{\gamma + E_{\alpha,1}(-\lambda_j^h T^\alpha)}\varphi_j^h.$$

This combined with (3.31) results in the splitting

$$\begin{aligned}\tilde{U}_0 - \tilde{u}_h(0) &= \Big((\gamma I + F_{h,\tau}^N)^{-1}(P_h - R_h)g + (\gamma I + F_h(T))^{-1}(R_h - P_h)g\Big)\\ &\quad + \Big((\gamma I + F_{h,\tau}^N)^{-1} - (\gamma I + F_h(T))^{-1}\Big)R_h g\\ &= I_1 + I_2.\end{aligned}$$

Using the approximation property of P_h and R_h, Lemma 3.4, Corollary 3.4, and the regularity result in Lemma 2.2, we have an estimate of the term I_1:

$$\|I_1\|_{L^2(\Omega)} \le ch^2\gamma^{-1}\|u_0\|_{L^2(\Omega)}.$$

To bound the term I_2, we note that

$$\begin{aligned}\|I_2\|_{L^2(\Omega)}^2 &= \sum_{j=1}^K \left[\frac{1}{\gamma + F_\tau^N(\lambda_j^h)} - \frac{1}{\gamma + E_{\alpha,1}(-\lambda_j^h T^\alpha)}\right]^2 (R_h g, \varphi_j^h)^2\\ &= \sum_{j=1}^K \left|\frac{[E_{\alpha,1}(-\lambda_j^h T^\alpha) - F_\tau^N(\lambda_j^h)](\lambda_j^h)^{-1}}{(\gamma + F_\tau^N(\lambda_j^h))(\gamma + E_{\alpha,1}(-\lambda_j^h T^\alpha))}\right|^2 (\lambda_j^h)^2 (R_h g, \varphi_j^h)^2.\end{aligned}$$

Then we apply Lemma 3.7 to obtain

$$\|I_2\|_{L^2(\Omega)}^2 \le c\tau^2\gamma^{-2}\sum_{j=1}^K \left|\frac{1}{(\gamma + E_{\alpha,1}(-\lambda_j^h T^\alpha))(\lambda_j^h)^{q/2}}\right|^2 (\lambda_j^h)^{2+q}(R_h g, \varphi_j^h)^2. \tag{3.32}$$

For $q = 0$, we use Lemma 2.1 to deduce that

$$\|I_2\|_{L^2(\Omega)}^2 \le c\tau^2\gamma^{-4}\sum_{j=1}^K (\lambda_j^h)^2 (R_h g, \varphi_j^h)^2 = c\tau^2\gamma^{-4}\|\Delta_h R_h g\|_{L^2(\Omega)}^2.$$

Using fact that $P_h\Delta = \Delta_h R_h$ and applying Lemma 2.2, we obtain

$$\|I_2\|_{L^2(\Omega)}^2 = c\tau^2\gamma^{-4}\|P_h\Delta g\|_{L^2(\Omega)}^2 = c\tau^2\gamma^{-4}\|\Delta g\|_{L^2(\Omega)}^2 \le c\tau^2\gamma^{-4}T^{-\alpha}\|u_0\|_{L^2(\Omega)}.$$

Next we turn to the case that $q = 2$. The estimate (3.32) and Lemma 2.1 imply that

$$\begin{aligned}\|I_2\|^2_{L^2(\Omega)} &\le c\tau^2\gamma^{-2}\sum_{j=1}^K \left|\frac{1}{E_{\alpha,1}(-\lambda_j^h T^\alpha)\lambda_j^h}\right|^2 (\lambda_j^h)^4 (R_h g, \varphi_j^h)^2 \\ &\le c\tau^2\gamma^{-2}\sum_{j=1}^K (\lambda_j^h)^4 (R_h g, \varphi_j^h)^2 = c\tau^2\gamma^{-2}\|\Delta_h^2 R_h g\|_{L^2(\Omega)}.\end{aligned}$$

Now we use the fact that $P_h\Delta = \Delta_h R_h$ and triangle's inequality to derive

$$\begin{aligned}\|\Delta_h^2 R_h g\|_{L^2(\Omega)} &= \|\Delta_h P_h \Delta g\|_{L^2(\Omega)} \\ &\le \|\Delta_h(P_h - R_h)\Delta g\|_{L^2(\Omega)} + \|\Delta_h R_h \Delta g\|_{L^2(\Omega)}.\end{aligned} \tag{3.33}$$

The second term in (3.33) can be bounded by

$$\begin{aligned}\|\Delta_h R_h \Delta g\|_{L^2(\Omega)} &= \|P_h \Delta^2 g\|_{L^2(\Omega)} \\ &= \|\Delta^2 g\|_{L^2(\Omega)} = \|g\|_{\dot H^4(\Omega)} \le cT^{-\alpha}\|u_0\|_{\dot H^2(\Omega)}\end{aligned} \tag{3.34}$$

while the first term in (3.33) can be bounded by using the standard inverse inequality and the approximation properties (2.17) and (2.18) as

$$\begin{aligned}\|\Delta_h(P_h - R_h)\Delta g\|_{L^2(\Omega)} &\le ch^{-2}\|(P_h - R_h)\Delta g\|_{L^2(\Omega)} \\ &\le c\|\Delta g\|_{H^2(\Omega)} \le cT^{-\alpha}\|u_0\|_{\dot H^2(\Omega)}.\end{aligned} \tag{3.35}$$

This leads to the desired estimate with $q = 2$. Finally, the estimate for $q \in (0, 2)$ follows immediately from interpolation. $\square$

Using the similar argument, one can also derive an estimate of $\tilde U_n - \tilde u_h(t_n)$ for $n \ge 1$.

Lemma 3.10. *Let $\tilde U_n$ and $\tilde u_h(t)$ be solutions to* (3.30) *and* (3.14)*, respectively. Then there holds that*

$$\begin{aligned}\|\tilde U_n - \tilde u_h(t_n)\|_{L^2(\Omega)} \le c\Big(&\gamma^{-(1-q/2)}(\tau t_n^{\alpha-1} + \tau\min(\gamma^{-1}, t_n^{-\alpha}))\|u_0\|_{\dot H^q(\Omega)} \\ &+ h^2\min(\gamma^{-1}, t_n^{-\alpha})\|u_0\|_{L^2(\Omega)}\Big)\end{aligned}$$

where the generic constant c is independent of γ, δ, τ, n and h.

Proof. First of all, we split $\tilde U_n - \tilde u_h(t_n)$ into two terms

$$\begin{aligned}\tilde U_0 - \tilde u_h(0) &= \Big(F_{h,\tau}^n(\gamma I + F_{h,\tau}^N)^{-1}(P_h - R_h)g + F_h(t_n)(\gamma I + F_h(T))^{-1}(R_h - P_h)g\Big) \\ &\quad + \Big(F_{h,\tau}^n(\gamma I + F_{h,\tau}^N)^{-1} - F_h(t_n)(\gamma I + F_h(T))^{-1}\Big)R_h g \\ &= I_1 + I_2.\end{aligned}$$

The approximation property of P_h and R_h, Lemma 2.2, Lemma 3.4 and Corollary 3.4 lead to an estimate of the term I_1:

$$\|I_1\|_{L^2(\Omega)} \le ch^2\min(\gamma^{-1}, t_n^{-\alpha})\|u_0\|_{L^2(\Omega)}.$$

Next, we turn to the I_2, which can be split into three components:

$$\begin{aligned}\|I_2\|^2_{L^2(\Omega)} &= \sum_{j=1}^{K}\Big[\frac{F_\tau^n(\lambda_j^h)}{\gamma+F_\tau^N(\lambda_j^h)} - \frac{E_{\alpha,1}(-\lambda_j^h t_n^\alpha)}{\gamma+E_{\alpha,1}(-\lambda_j^h T^\alpha)}\Big]^2 (R_h g,\varphi_j^h)^2\\
&\le c\sum_{j=1}^{K}\Big|\frac{\gamma[F_\tau^n(\lambda_j^h)-E_{\alpha,1}(-\lambda_j^h t_n^\alpha)](\lambda_j^h)^{-1}}{(\gamma+F_\tau^N(\lambda_j^h))(\gamma+E_{\alpha,1}(-\lambda_j^h T^\alpha))}\Big|^2(\lambda_j^h)^2(R_h g,\varphi_j^h)^2\\
&+c\sum_{j=1}^{K}\Big|\frac{F_\tau^N(\lambda_j^h)[F_\tau^n(\lambda_j^h)-E_{\alpha,1}(-\lambda_j^h t_n^\alpha)](\lambda_j^h)^{-1}}{(\gamma+F_\tau^N(\lambda_j^h))(\gamma+E_{\alpha,1}(-\lambda_j^h T^\alpha)}\Big|^2(\lambda_j^h)^2(R_h g,\varphi_j^h)^2\\
&+c\sum_{j=1}^{K}\Big|\frac{F_\tau^n(\lambda_j^h)[(E_{\alpha,1}(-\lambda_j^h T^\alpha)-F_\tau^N(\lambda_j^h)](\lambda_j^h)^{-1}}{(\gamma+F_\tau^N(\lambda_j^h))(\gamma+E_{\alpha,1}(-\lambda_j^h T^\alpha)}\Big|^2(\lambda_j^h)^2(R_h g,\varphi_j^h)^2\\
&=: \sum_{k=1}^{3} I_{2,k}.\end{aligned}$$

The estimates of $I_{2,1}$ and $I_{2,2}$ follows directly from the proof of Lemma 3.9, i.e.,

$$I_{2,1}+I_{2,2}\le c\tau^2 t_n^{2\alpha-2}\gamma^{-(2-q)}\|u_0\|_{\dot H^q(\Omega)}.$$

Now it remains to bound I_3. Here we apply Lemma 3.7 and Corollary 3.4, and obtain

$$I_{2,3}\le c\tau^2 T^{2\alpha-2}\min\{\gamma^{-2},t_n^{-2\alpha}\}\sum_{j=1}^{K}\Big|\frac{1}{(\gamma+E_{\alpha,1}(-\lambda_j^h T^\alpha))(\lambda_j^h)^{q/2}}\Big|^2(\lambda_j^h)^{2+q}(R_h g,\varphi_j^h)^2.$$

Then the estimates (3.32)–(3.35) imply

$$I_{2,3}\le c\tau^2\gamma^{-(2-q)}\min\{\gamma^{-2},t_n^{-2\alpha}\}\|u_0\|^2_{\dot H^q(\Omega)}.$$

This completes the proof of the lemma. □

Then Lemmas 3.8–3.10 together with Theorem 3.2 and Corollary 3.1 result in the main theorem of this section.

Theorem 3.3. *Let u be the solution to the backward subdiffusion problem* (3.4), *and $\tilde U_n^\delta$ be the solution to the (regularized) fully discrete scheme* (3.28). *Then we have the following error estimate:*

(a) In case that $u_0\in\dot H^2(\Omega)$, there holds

$$\|\tilde U_n^\delta-u(t_n)\|_{L^2(\Omega)}\le c\begin{cases}\gamma+(h^2+\tau+\delta)\min(\gamma^{-1},t_n^{-\alpha})+\tau t_n^{\alpha-1}, n\ge 1;\\ \gamma+(h^2+\tau+\delta)\gamma^{-1}, \qquad n=0.\end{cases}$$

(b) In case that $u_0\in L^2(\Omega)$, there holds for $n\ge1$

$$\|\tilde U_n^\delta-u(t_n)\|_{L^2(\Omega)}\le c\Big(\gamma t_n^{-\alpha}+\big(\delta+\gamma^{-1}(h^2\ell_h+\tau)\big)\min(\gamma^{-1},t_n^{-\alpha})+\gamma^{-1}\tau t_n^{\alpha-1}\Big).$$

Meanwhile, for $n=0$, there holds

$$\|\tilde U_0^\delta-u(0)\|_{L^2(\Omega)}\to 0,\quad \textit{as}\ \ \gamma\to0,\ \frac{\delta}{\gamma}\to0,\ \frac{h\ell_h^{\frac12}}{\gamma}\to 0\ \textit{and}\ \frac{\tau^{\frac12}}{\gamma}\to0.$$

Remark 3.3. *For the intermediate case that* $u_0 \in \dot H^q(\Omega)$, $q \in (0,2)$, *the error estimate follows from Lemma 3.8–3.10, Theorem 3.2, and the real interpolation. In particular, for* $n = 0$, *we have*

$$\|\tilde U_0^\delta - u(0)\|_{L^2(\Omega)} \le c\Big(\gamma^{q/2} + \delta\gamma^{-1} + \gamma^{-2+q/2}(h^2\ell_h^{1-q/2} + \tau)\Big).$$

Then one may obtain the optimal convergence rate $O(\delta^{\frac{q}{q+2}})$ *by the a priori choices:*

$$\gamma = O(\delta^{\frac{2}{q+2}}), \quad h\ell_h^{\frac12-\frac q4} = O(\delta^{\frac{2}{q+2}}) \quad \text{and} \quad \tau = O(\delta^{\frac{2}{q+2}}).$$

Meanwhile, for $n \ge 1$, *there holds the estimate*

$$\begin{aligned}\|\tilde U_n^\delta - u(t_n)\|_{L^2(\Omega)} \quad &\le c\Big(\min(\gamma^{q/2}, \gamma t_n^{-(1-q/2)\alpha}) + \Big(\gamma^{-(1-q/2)}(h^2\ell_h^{1-q/2} + \tau) + \delta\Big)\min(\gamma^{-1}, t_n^{-\alpha}) \\ &\qquad + \gamma^{-(1-q/2)}\tau t_n^{\alpha-1}\Big).\end{aligned}$$

Asymptotically, the a priori choice, that $\gamma = O(\delta)$, $h\ell_h^{\frac12-\frac q4} = O(\delta^{1-\frac q4})$ *and* $\tau = O(\delta^{2-\frac q2})$, *leads to the optimal convergence rate* $O(\delta)$.

Remark 3.4. *Theorem 3.3 and Remark 3.3 indicates the correct way to scale noise level* δ, *regularization parameter* γ, *and mesh sizes* h *and* τ, *with different types of problem data. The novel argument uses the smoothing properties of fully discrete solution operators, and the nonstandard error estimate for the direct problem [43, 45].*

3.4 Numerical results

In this section, we shall illustrate the theoretical results by presenting some 1-D and 2-D examples. Throughout, we consider the observation data

$$g_\delta = u(T) + \varepsilon\delta \sup_{x\in\Omega} u(x,T),$$

ε is generated following the standard Gaussian distribution and δ denotes the (relative) noise level. Throughout this section, we fix $T = 1$.

We consider the one-dimensional subdiffusion problem in the unit interval $\Omega = (0,1)$. We use the standard piecewise linear FEM with uniform mesh size $h = 1/(K+1)$ for the space discretization, and the BE-CQ method with uniform step size $\tau = T/N$ for the time discretization. Although the fully discrete solution can be efficiently computed by using conjugate gradient method, in 1-D example we apply the following direct method by spectral decomposition to avoid any iteration error.

For the uniform mesh size $h = 1/(K+1)$, the eigenpairs of $-\Delta_h$ has the closed form:

$$\lambda_j^h = \frac{6}{h^2}\frac{1-\cos(j\pi h)}{2+\cos(j\pi h)}, \quad \varphi_j^h(x_i) = \sqrt2\sin(j\pi x_i), \quad i,j = 1,2,\cdots,K. \tag{3.36}$$

The semidiscrete solution of the forward problem can be computed by using the solution representation (3.11) involving the Mittag-Leffler function (2.5), which could be evaluated by the algorithm developed in [91]. We compute the observation data $u(T)$ and reference solution $u(t)$ with $t \in [0, T)$ by using the semidiscrete scheme with a very fine mesh size, i.e., $h = 1/2000$.

For each example, we measure the accuracy of the approximation $\tilde{u}_h^\delta(t)$ and $\tilde{U}_n^\delta$ by the normalized error $\|u(t) - \tilde{u}_h^\delta(t)\|_{L^2(\Omega)}/\|u(t)\|_{L^2(\Omega)}$ and $\|u(t_n) - \tilde{U}_n^\delta\|_{L^2(\Omega)}/\|u(t_n)\|_{L^2(\Omega)}$. The normalization enables us to observe the behaviour of the error with respect to α and t.

Example (a): Smooth initial data. We start with the smooth initial condition

$$u_0(x) = x(1-x) \in \dot{H}^2(\Omega) = H^2(\Omega) \cap H_0^1(\Omega),$$

and source term $f \equiv 0$. We compute the solution of the (regularized) semidiscrete scheme (3.12) by

$$\tilde{u}_h^\delta(t) = \sum_{j=1}^{K} \frac{E_{\alpha,1}(\lambda_j^h t^\alpha)}{\gamma + E_{\alpha,1}(\lambda_j^h T^\alpha)} (g_\delta, \varphi_j^h)\varphi_j^h, \tag{3.37}$$

where the eigenpairs $(\lambda_j^h, \varphi_j^h)$, for $j = 1, \ldots, K-1$, are given by (3.36). In Figure 3.1, we plot the error of numerical solution (3.37), with different fractional order α and at different time. By Theorem 3.1 and Remark 3.1, we compute the $\tilde{u}_h^\delta(0)$ with $h = \sqrt{\delta}$, $\gamma = \sqrt{\delta}$ for a given δ; and compute the $\tilde{u}_h^\delta(t)$ for $t > 0$ with $h = \sqrt{\delta}$, $\gamma = \delta$ for a given δ. Numerical experiments show an empirical convergence rate of $O(\sqrt{\delta})$ for $t = 0$, and $O(\delta)$ for $t > 0$. This coincides with our theoretical result (Theorem 3.1).

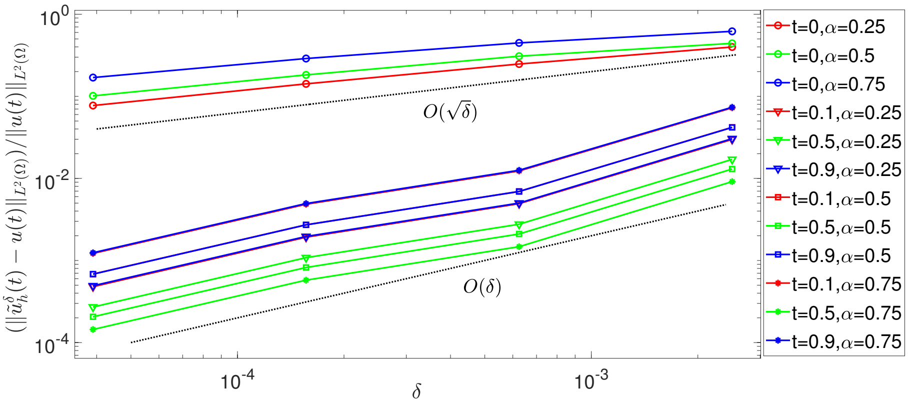


Figure 3.1: Plot of $\|u(t) - \tilde{u}_h^\delta(t)\|_{L^2(\Omega)}/\|u(t)\|_{L^2(\Omega)}$ with $h = \gamma = \sqrt{\delta}$ for $t = 0$; and $h = \sqrt{\delta}$, $\gamma = \delta$ for $t_n > 0$.

In Figure 3.2, we plot the error of numerical reconstruction by the fully scheme (3.28), with different α and at different time. In our experiments, we compute fully discrete solution $\tilde{U}_n^\delta$ by

$$\tilde{U}_n^\delta = \sum_{j=1}^{K} \frac{F_\tau^n(\lambda_j^h)}{\gamma + F_\tau^N(\lambda_j^h)} (P_h g_\delta, \varphi_j^h)\varphi_j^h.$$

Then Theorem 3.3 (i) implies for $u_0 \in \dot H^2(\Omega)$

$$\|\tilde U_n^\delta - u(t_n)\|_{L^2(\Omega)} \le c \begin{cases} \gamma + (h^2+\tau+\delta)\min(\gamma^{-1}, t_n^{-\alpha}) + \tau t_n^{\alpha-1}, n \ge 1; \\ \gamma + (h^2+\tau+\delta)\gamma^{-1}, \qquad n = 0. \end{cases}$$

For $t=0$, we let $h=\gamma=\sqrt{\delta}$ and $\tau=\delta$, and then we observe that the empirical convergence rate is $O(\sqrt{\delta})$. Meanwhile, for $t>0$, and we let $h=\sqrt{\gamma}=\sqrt{\delta}=\sqrt{\tau}$. The empirical convergence rate is $O(\delta)$. These observation agrees well with our theoretical results in Theorem 3.3 (i).

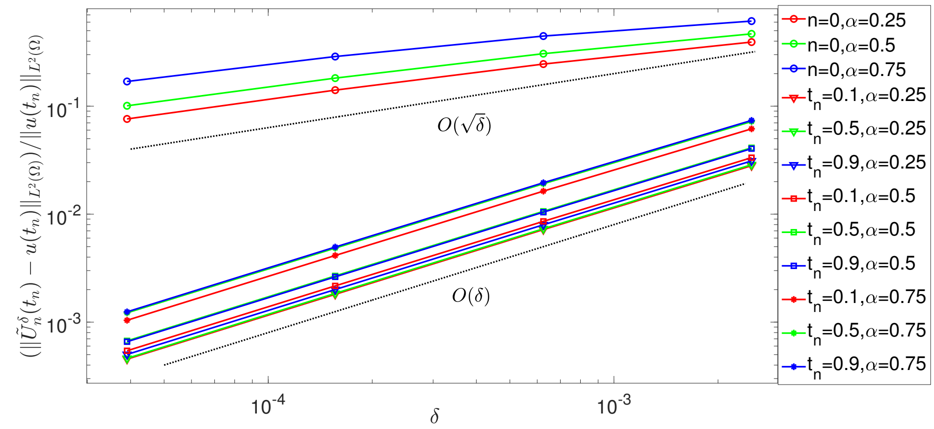


Figure 3.2: Plot of $\|u(t_n) - \tilde U_n^\delta(t_n)\|_{L^2(\Omega)}/\|u(t_n)\|_{L^2(\Omega)}$ with $h=\sqrt{\delta}$, $\tau=\delta$ and $\gamma=\sqrt{\delta}$ for $t_n=0$; and $h=\sqrt{\delta}$, $\tau=\delta$, $\gamma=\delta$ for $t_n>0$.

Example (b): Nonsmooth initial data. Now we test numerical experiments with a step initial condition:

$$u_0(x) = \begin{cases} 0, & 0 \le x \le \frac{1}{2}, \\ 1, & \frac{1}{2} < x < 1. \end{cases}$$

Since u_0 is discontinuous and piecewise smooth, it is easy to see that $u_0 \in H^{\frac12-\epsilon}(\Omega)$ for any $\epsilon \in (0, \frac12]$.

According to Theorem 3.2, we have the error estimate of the semidiscrete solution at $t=0$:

$$\|\tilde u_h^\delta(t) - u(t)\|_{L^2(\Omega)} \le c\big(\gamma^{q/2} + h^2 \ell_h^{1-q/2}\gamma^{-(2-q/2)} + \delta\gamma^{-1}\big), \quad \text{with} \;\; u_0 \in \dot H^q(\Omega).$$

This implies that the convergence rate may deteriorate when the initial data gets worse. This is fully supported by empirical results showed in Table 3.1, where we present the L^2-error of the semidiscrete solution at $t=0$. In the computation, we let $h=O(\delta^{\frac45})$ and $\gamma=O(\delta^{\frac45})$ in order to balance to noise level, regularization parameter and the discretization error. Then the empirical convergence rate is $O(\delta^{\frac15})$, which is consistent with the theoretical results.

Meanwhile, for a fixed $t>0$, we have the error estimate (cf. Theorem 3.2)

$$\|\tilde u_h^\delta(t) - u(t)\|_{L^2(\Omega)} \le c\big(\gamma\, t^{q\alpha/2} + \gamma^{-(1-q/2)} h^2 \ell_h^{1-q/2} + \delta\big)t^{-\alpha}.$$

This implies the almost optimal scaling $h = O(\delta^{\frac{7}{8}})$ and $\gamma = O(\delta)$, and the resulting optimal convergence rate $O(\delta)$. This is supported by the numerical results shown in Table 3.2.

For the numerical reconstruction by the fully discrete scheme (3.28), we recall the result in Remark 3.3. To compute $\tilde{U}_0^\delta$, we let $\gamma = O(\delta^{\frac{4}{5}})$, $h = O(\delta^{\frac{4}{5}})$ and $\tau = O(\delta^{\frac{8}{5}})$, for a given δ. Then our theory indicates a convergence rate of $O(\delta^{\frac{1}{5}})$, which agrees well with the numerical results in Table 3.3. On the other hand, to compute $\tilde{U}_n^\delta$ for a fixed $t_n > 0$ and $\delta > 0$, we let $h = \delta^{\frac{7}{4}}$, $\tau = O(\delta^{\frac{7}{8}})$ and $\gamma = O(\delta)$. Then the empirical convergence rate is close to $O(\delta)$, which fully supports our theoretical estimates in Table 3.4.

Table 3.1: Example (b): error of $\tilde{u}_h^\delta(0)$, with $\delta = 1/M$, $h = \gamma = \delta^{\frac{4}{5}}$.

$\alpha\backslash M$	40	80	160	320	Rate(δ)
0.25	4.68e-1	4.07e-1	3.48e-1	2.95e-1	0.22(0.20)
0.5	5.07e-1	4.46e-1	3.84e-1	3.27e-1	0.21(0.20)
0.75	5.70e-1	5.18e-1	4.59e-1	3.98e-1	0.17(0.20)

Table 3.2: Example (b): error of $\tilde{u}_h^\delta(t)$ at different t with $\delta = 1/M$, $h = \delta^{\frac{7}{8}}$, $\gamma = \delta/5$.

α	$t\backslash M$	40	80	160	320	Rate(δ)
	0.1	7.91e-3	4.34e-3	2.30e-3	1.20e-3	0.91(1.00)
0.5	0.5	3.51e-3	1.93e-3	1.02e-3	5.33e-4	0.91(1.00)
	0.9	2.41e-3	1.33e-3	7.13e-4	3.73e-4	0.90(1.00)

Table 3.3: Example (b): error of $\tilde{U}_0^\delta$, with $\delta = 1/M$, $h = \gamma = \delta^{\frac{4}{5}}$, $\tau = \delta^{\frac{8}{5}}$.

$\alpha\backslash M$	40	80	160	320	Rate(δ)
0.25	4.70e-1	4.07e-1	3.48e-1	2.96e-1	0.22(0.20)
0.5	5.08e-1	4.47e-1	3.85e-1	3.28e-1	0.21(0.20)
0.75	5.70e-1	5.17e-1	4.59e-1	3.98e-1	0.17(0.20)

Table 3.4: Example(b): error of $\tilde{U}_n^\delta$, with $\delta = 1/M$, $h = \delta^{\frac{7}{8}}$, $\tau = \delta^{\frac{7}{4}}$, and $\gamma = \delta/5$.

α	$t_n \backslash M$	40	80	160	320	Rate(δ)
	0.1	6.76e-3	3.82e-3	2.06e-3	1.08e-3	0.88(1.00)
0.5	0.5	3.46e-3	1.90e-3	1.01e-3	5.24e-4	0.91(1.00)
	0.9	2.55e-3	1.40e-3	7.47e-4	3.89e-4	0.90(1.00)

Example (c): 2D problem. Now we consider a two-dimensional problem in a unit square domain $\Omega = (0, 1)^2$. We choose the smooth initial condition

$$u_0(x, y) = x(1 - x)y(1 - y) \in \dot{H}^2(\Omega),$$

and zero source term $f \equiv 0$. In the computation, we divided Ω into regular right triangles with K equal subintervals of length $h = 1/K$ on each side of the domain. Here, we apply the conjugate gradient method to numerically solve the discrete system, instead of the direct approach by the spectral decomposition in Example (a) and (b).

For $t = 0$, we let $h = \gamma = \sqrt{\delta} = \sqrt{\tau}$, and we observe that the convergence rate is $O(\sqrt{\delta})$, see Table 3.5. Moreover, In Table 3.6, we test the convergence rate for $t = T/2$. By letting $h = \sqrt{\gamma} = \sqrt{\delta} = \sqrt{\tau}$, the experiments show that the convergence rate is $O(\delta)$. All empirical results agree well with our theoretical finding in Theorem 3.3. [1]

Table 3.5: Example(c): error of $\tilde{U}_0^\delta$, with $\delta = 1/M$, $h = \sqrt{\delta}$, $\tau = \delta$, and $\gamma = \sqrt{\delta}$.

$\alpha \backslash M$	800	1600	3200	6400	Rate(δ)
0.25	1.27e-2	9.57e-3	6.61e-3	3.96e-3	0.56(0.50)
0.5	1.57e-2	1.27e-2	9.53e-3	6.57e-3	0.42(0.50)
0.75	2.28e-3	1.96e-3	1.57e-3	1.11e-3	0.34(0.50)

Table 3.6: Example(c): error of $\tilde{U}_n^\delta$, with $t_n = T/2$, $\delta = 1/M$, $h = \sqrt{\delta}$, $\tau = \delta$, and $\gamma = \delta$.

$\alpha \backslash M$	800	1600	3200	6400	Rate(δ)
0.25	5.09e-5	2.59e-5	1.31e-5	6.59e-6	0.98(1.00)
0.5	6.00e-5	3.08e-5	1.56e-5	7.90e-6	0.98(1.00)
0.75	7.06e-5	3.71e-5	1.89e-5	9.55e-6	0.96(1.00)

[1]Chapter 3 is reprinted with permission from "Numerical analysis of backward subdiffusion problems", Zhengqi Zhang and Zhi Zhou, 2020, Inverse Problems 36 105006. The contribution of candidate mainly focus on the proof and coding.

CHAPTER 4.

STABILITY AND NUMERICAL ANALYSIS OF BACKWARD SUBDIFFUSION WITH TIME-DEPENDENT COEFFICIENTS

In this chapter, let $\Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$ be a convex polyhedral domain with boundary $\partial\Omega$, we are interested in the fractional evolution model with time-dependent coefficient:

$$\begin{aligned} \partial_t^\alpha u(x,t) + \nabla \cdot (a(x,t)\nabla u) &= f(x,t), && \text{in } \Omega \times (0,T], \\ u(x,t) &= 0, && \text{on } \partial\Omega, \\ u(x,0) &= u_0(x), && \text{in } \Omega, \end{aligned} \tag{4.1}$$

where $T > 0$ is a fixed final time, $f \in L^\infty(0,T; L^2(\Omega))$ and $u_0 \in L^2(\Omega)$ are given source term and initial data, respectively. $a(x,t) \in \mathbb{R}^{d\times d}$ is a symmetric matrix-valued diffusion coefficient such that for constants $c_0 \ge 1$ and $c_1 > 0$

$$c_0^{-1}|\xi|^2 \le a(x,t)\xi \cdot \xi \le c_0|\xi|^2, \qquad \forall\, \xi \in \mathbb{R}^d,\ \forall\, (x,t) \in \Omega \times \mathbb{R}^+, \tag{4.2}$$

$$|\partial_t a(x,t)| + |\nabla_x a(x,t)| + |\nabla_x \partial_t a(x,t)| \le c_1, \qquad \forall\, (x,t) \in \Omega \times \mathbb{R}^+. \tag{4.3}$$

Here $\cdot$ and $|\cdot|$ denote the standard Euclidean inner product and norm, respectively, and $\mathbb{R}^+ = [0,\infty)$. In this Chapter We focus on backward problem for the subdiffusion model (4.1): to recover the initial data $u_0(x)$ with $x \in \Omega$ from terminal observation

$$u(x,T) = g(x), \quad \text{for all } x \in \Omega.$$

In practice, the observational data often involves random noise. Here we denote the empirical observation by g_δ and assume it is noisy with a level $\delta > 0$ in the sense that

$$\|g_\delta - g\|_{L^2(\Omega)} = \delta. \tag{4.4}$$

The rest of this Chapter is organized as follows. In section 4.1 we provide some preliminary results about solution regularity, smoothing properties of solution operators and derive conditional stability of the inverse problem. In section 4.2 we discuss the regularization scheme by quasi-boundary value method. In section 4.3 we propose and analyze a fully discrete scheme for solving the backward problem. Finally, in section 4.4 we present some numerical examples to illustrate and complete the theoretical analysis.

Here we introduce some notations used throughout the paper. Under conditions (4.2)–(4.3), the abstract time-dependent elliptic operator $A(t) : H_0^1(\Omega) \cap H^2(\Omega) \to L^2(\Omega)$ is defined by

$$A(t)\phi = -\nabla \cdot (a(x,t)\nabla\phi)$$

with the domain $\mathrm{Dom}(A(t)) = H_0^1(\Omega) \cap H^2(\Omega)$ for all $t \in [0, T]$. By the complex interpolation method [96], this implies

$$\mathrm{Dom}(A(t)^\gamma) = \dot{H}^{2\gamma}(\Omega) = (L^2(\Omega), H_0^1(\Omega) \cap H^2(\Omega))_{[\gamma]}, \quad \forall\, t \in [0, T], \ \forall\, \gamma \in [0, 1],$$

Equivalently, it relates to the definition via spectral introduced in Section 2.3. Let $\{(\lambda_j, \varphi_j)\}_{j=1}^n$ be the eigenpairs of $A(t_*)$ for a fixed $t_* \in [0, T]$ with multiplicity counted and $\{\varphi_j\}_{j=1}^\infty$ be an orthonormal basis in $L^2(\Omega)$. Then the Hilbert space $\dot{H}^\gamma(\Omega)$ can be equivalently defined as

$$\dot{H}^\gamma(\Omega) = \Big\{ v \in L^2(\Omega) : \sum_{j=1}^\infty \lambda_j^\gamma (v, \varphi_j)^2 < \infty \Big\}.$$

For $\gamma \in [0, 2]$ we also denote by $\dot{H}^{-\gamma}(\Omega)$ the dual space of $\dot{H}^\gamma(\Omega)$. Then the norm of $\dot{H}^{-\gamma}(\Omega)$ satisfies

$$\|v\|_{\dot{H}^{-\gamma}(\Omega)} \sim \|A(t)^{-\frac{\gamma}{2}} v\|_{L^2(\Omega)} \quad \forall\, v \in \dot{H}^{-\gamma}(\Omega), \ \forall\, t \in [0, T].$$

4.1 Stability of the backward subdiffusion in Sobolev spaces

First we recall basic properties of the subdiffusion model with a time-independent diffusion coefficient, i.e., $a(x, t_*)$ for some $t_* \geq 0$. Accordingly, consider the problem

$$\partial_t^\alpha u(t) + A(t_*) u(t) = f(t) \quad \forall t \in (0, T], \quad \text{with } u(0) = u_0. \tag{4.5}$$

By means of Laplace transform, the solution $u(t)$ can be represented by [44, Section 4]

$$u(t) = F(t; t_*) u_0 + \int_0^t E(t - s; t_*) f(s) \mathrm{d}s, \tag{4.6}$$

where the solution operators $F(t; t_*)$ and $E(t; t_*)$ are defined by

$$F(t; t_*) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}} e^{zt} z^{\alpha-1} (z^\alpha + A(t_*))^{-1} \, \mathrm{d}z, \quad \text{and} \quad E(t; t_*) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}} e^{zt} (z^\alpha + A(t_*))^{-1} \, \mathrm{d}z \tag{4.7}$$

with integration over a contour $\Gamma_{\theta,\kappa} \subset \mathbb{C}$ (oriented with an increasing imaginary part):

$$\Gamma_{\theta,\kappa} = \{ z \in \mathbb{C} : |z| = \kappa, |\arg z| \leq \theta \} \cup \{ z \in \mathbb{C} : z = \rho e^{\pm \mathrm{i}\theta}, \rho \geq \kappa \}.$$

Throughout, we fix $\theta \in (\frac{\pi}{2}, \pi)$ so that $z^\alpha \in \Sigma_{\alpha\theta} \subset \Sigma_\theta := \{0 \neq z \in \mathbb{C} : \arg(z) \leq \theta\}$, for all $z \in \Sigma_\theta$.

The next lemma gives smoothing properties and asymptotics of $F(t; t_*)$ and $E(t; t_*)$. The proof follows from the resolvent estimate[4, Example 3.7.5 and Theorem 3.7.11]:

$$\|(z + A)^{-1}\| \leq c_\phi (|z|^{-1}, \lambda^{-1}) \quad \forall z \in \Sigma_\phi, \ \forall\, \phi \in (0, \pi), \tag{4.8}$$

where $\| \cdot \|$ denotes the operator norm from $L^2(\Omega)$ to $L^2(\Omega)$, and λ denotes the smallest eigenvalue of $-\Delta$ with homogeneous Dirichlet boundary condition. The proof of (i) and (ii) were given in [38, Theorems 6.4 and 3.2], and (iii) were proved by Sakamoto and Yamamoto in [89, Theorem 4.1].

Lemma 4.1. *Let $F(t;t_*)$ and $E(t;t_*)$ be the solution operators defined in* (4.7) *for any $t_* \geq 0$ Then they satisfy the following properties for all $t > 0$*

(i) $\|A(t_*)F(t;t_*)v\|_{L^2(\Omega)} + t^{1-(2-k)\alpha}\|A(t_*)^k E(t;t_*)v\|_{L^2(\Omega)} \leq ct^{-\alpha}\|v\|_{L^2(\Omega)}$ *with $k = 1, 2$;*

(ii) $\|F(t;t_*)v\|_{L^2(\Omega)} + t^{1-\alpha}\|E(t;t_*)v\|_{L^2(\Omega)} \leq c\min(1, t^{-\alpha})\|v\|_{L^2(\Omega)}$*;*

(iii) $\|F(t;t_*)^{-1}v\|_{L^2(\Omega)} \leq c(1 + t^\alpha)\|v\|_{\dot{H}^2(\Omega)}$ *for all $v \in \dot{H}^2(\Omega)$.*

The constants in all above estimates are uniform in t, but they are only dependent of t_* and T.

Next, we turn to the subdiffusion with a time-dependent coefficient. The overall proof strategy is to employ a perturbation argument [45], and then to properly resolve the singularity. Specifically, for any fixed $t_* \in (0, T]$, we rewrite problem (4.1) into

$$\begin{cases} \partial_t^\alpha u(t) + A(t_*)u(t) = (A(t_*) - A(t))u(t) + f(t), \quad \forall t \in (0, T], \\ u(0) = u_0. \end{cases} \tag{4.9}$$

By (4.6), the solution $u(t)$ of (4.9) is given by

$$u(t) = F(t;t_*)u_0 + \int_0^t E(t-s;t_*)(f(s) + (A(t_*) - A(s))u(s))\mathrm{d}s. \tag{4.10}$$

The following perturbation estimate will be used extensively. See similar results in [45, Corollary 3.1].

Lemma 4.2. *Under conditions* (4.2)–(4.3)*, there holds that*

$$\|(A(t) - A(s))v\|_{\dot{H}^p(\Omega)} \leq c\min(1, |t-s|)\|v\|_{\dot{H}^{p+2}(\Omega)}, \quad p \in [-2, 0].$$

Proof. The condition (4.3) implies the case that $p = 0$. The case $p = -2$ has been proved in [45, Corollary 3.1]. Then the intermediate case follows from the interpolation [37, Section 2.5]. $\square$

Next, we state a few regularity results. The proof of these results can be found in, e.g., [5, 89, 45].

Theorem 4.1. *Let $u(t)$ be the solution to* (4.1)*. Then the following statements hold.*

(i) *If $u_0 \in \dot{H}^q(\Omega)$ with $s \in [0, 2]$ and $f = 0$, then there holds*

$$\|\partial_t^{(m)}u(t)\|_{\dot{H}^p(\Omega)} \leq ct^{\frac{(s-p)\alpha}{2}-m}\|u_0\|_{\dot{H}^q(\Omega)}$$

with $0 \leq p - q \leq 2$ and $m = 0, 1$. The constant c in the estimate depends on T and α.

(ii) *If $u_0 = 0$ and $f \in L^p(0, T; L^2(\Omega))$ with $1 < p < \infty$, then there holds*

$$\|u\|_{L^p(0,T;\dot{H}^2(\Omega))} + \|\partial_t^\alpha u\|_{L^p(0,T;L^2(\Omega))} \leq c\|f\|_{L^p(0,T;L^2(\Omega))}.$$

Moreover, if $f \in L^p(0, T; L^2(\Omega))$ with $1/\alpha < p < \infty$, then $u(t)$ is the solution to problem (4.1) *such that $u \in C([0, T]; L^2(\Omega))$. The constant c in the estimate depends on T and α.*

The next lemma provides an a priori estimate similar to Theorem 4.1 (i). Note that the generic constant in the new estimate is independent of T.

Lemma 4.3. *Suppose that $u_0 \in L^2(\Omega)$ and $f = 0$. Let $u(t)$ be the solution to the subdiffusion problem* (4.1)*. Under conditions* (4.2)–(4.3)*, there holds*

$$\|u(t)\|_{L^2(\Omega)} \le c\min(1, t^{-\alpha})\|u_0\|_{L^2(\Omega)} \quad \text{and} \quad \|u(t)\|_{\dot H^2(\Omega)} \le c\, e^{ct} t^{-\alpha}\|u_0\|_{L^2(\Omega)} \quad \text{for all} \;\; t > 0 \tag{4.11}$$

Meanwhile, for any $\epsilon \in (0, 1/\alpha - 1)$ and $t > 0$, there holds that

$$\|u(t)\|_{\dot H^2(\Omega)} \le ct^{-(1-\epsilon)\alpha}\|u_0\|_{L^2(\Omega)}. \tag{4.12}$$

All the positive constants c in above estimates are independent of t and T.

Proof. We define an operator $\underline{A} = -c_0\Delta$. Then by condition 4.2, the operator $A(t) - \underline{A}$ is self-adjoint and positive semidefinite for all $t \ge 0$. Then we rewrite the equation (4.1) as

$$\partial_t^\alpha u(t) + \underline{A}u(t) = (\underline{A} - A(t))u(t) \quad \text{for all} \;\; t \in (0, \infty).$$

Taking inner product with $u(t)$ on the above equation and integrating by parts, we obtain

$$(\partial_t^\alpha u(t), u(t)) + c_0\|\nabla u(t)\|^2_{L^2(\Omega)} = \big((c_0 - a(\cdot, t))\nabla u(t), \nabla u(t)\big) \le 0 \quad \text{for all} \;\; t \in (0, \infty).$$

Using the facts that $(\partial_t^\alpha u(t), u(t)) \ge \|u(t)\|_{L^2(\Omega)}\partial_t^\alpha \|u(t)\|_{L^2(\Omega)}$ [38, Lemma 6.1(iii)] and Poincaré inequality we arrive at

$$\partial_t^\alpha \|u(t)\|_{L^2(\Omega)} + c\|u(t)\|_{L^2(\Omega)} \le 0 \quad \text{for all} \;\; t \in (0, \infty),$$

for some constant c uniform in t. Then the comparison principle for fractional ODEs [61, Theorem 2.3] leads to

$$\|u(t)\|_{L^2(\Omega)} \le E_{\alpha,1}(-ct^\alpha)\|u_0\| \le \frac{c}{1 + ct^\alpha}\|u_0\|_{L^2(\Omega)}.$$

This immediately leads to the desired claim (4.11).

Next, we apply the relation (4.10), Lemmas 4.1 and 4.2 (with $p = 2$) to obtain for any $t_* \in (0, T]$

$$\begin{aligned}\|u(t_*)\|_{\dot H^2(\Omega)} &\le \|F(t_*; t_*)u_0\|_{\dot H^2(\Omega)} + c\int_0^{t_*} \|A(t_*)E(t_* - s; t_*)\| \, \|(A(t_*) - A(s))u(s)\|_{L^2(\Omega)} \,\mathrm{d}s \\ &\le ct_*^{-\alpha}\|u_0\|_{L^2(\Omega)} + c\int_0^{t_*} \|u(s)\|_{\dot H^2(\Omega)} \,\mathrm{d}s.\end{aligned}$$

Then the Gronwall's inequality implies for any $t > 0$

$$\|u(t)\|_{\dot H^2(\Omega)} \le c\, e^{ct} t^{-\alpha}\|u_0\|_{L^2(\Omega)}.$$

Meanwhile, Lemma 4.2 leads to the estimate for $\beta = (1+\epsilon)\alpha$ with $\epsilon \in (0, 1/\alpha - 1)$

$$\begin{aligned}\|u(t_*)\|_{\dot H^2(\Omega)} &\le \|F(t_*;t_*)u_0\|_{\dot H^2(\Omega)} + \int_0^{t_*} \|A(t_*)^2 E(t_*-s;t_*)\| \, \|I - A(t_*)^{-1}A(s)\| \, \|u(s)\|_{L^2(\Omega)} \,\mathrm{d}s \\ &\le c t_*^{-\alpha}\|u_0\|_{L^2(\Omega)} + \int_0^{t_*} (t_*-s)^{-1+\epsilon\alpha} s^{-\alpha} \,\mathrm{d}s \le c_\epsilon t_*^{-(1-\epsilon)\alpha}\end{aligned}$$

for any $t_* > 0$. This completes the proof of (4.12). □

Using the superposition principle, we consider the homogeneous source condition, i.e., $f \equiv 0$, without loss of generality. Then the corresponding backward subdiffusion problem reads: find $u(0)$ such that

$$\partial_t^\alpha u + A(t)u = 0 \ \ \forall t \in (0,T] \quad \text{with} \quad u(T) = g \qquad \text{in } \Omega. \tag{4.13}$$

The next theorem provides a stability estimate for the backward problem of (4.13) when T is sufficiently small.

Theorem 4.2. *Suppose that $u_0 \in L^2(\Omega)$ and $f = 0$. Let $u(t)$ be the solution to* (4.1). *Under conditions* (4.2)–(4.3), *there exists a positive constant T_0 such that for any $T \le T_0$ there holds*

$$\|u_0\|_{L^2(\Omega)} \le c(1+T^\alpha)\|u(T)\|_{H^2(\Omega)},$$

where the constant c depends on T_0 and T.

Proof. We rearrange the terms in relation (4.10) with $t_* = T$ to obtain

$$u_0 = F(T;T)^{-1}\Big[u(T) - \int_0^T E(T-s;T)(A(T)-A(s))u(s)\mathrm{d}s\Big]. \tag{4.14}$$

Taking $L^2(\Omega)$ norm on both sides of the above relation, we apply Lemma 4.1 (iii) to obtain

$$\|u_0\|_{L^2(\Omega)} \le C(1+T^\alpha)\Big(\|u(T)\|_{\dot H^2(\Omega)} + \int_0^T \|A(T)E(T-s;T)\| \, \|(A(T)-A(s)))u(s)\|_{L^2(\Omega)} \,\mathrm{d}s\Big).$$

According to Lemmas 4.2 with $p = 0$ and 4.1 (i) we arrive at

$$\|u_0\|_{L^2(\Omega)} \le c(1+T^\alpha)\Big(\|u(T)\|_{\dot H^2(\Omega)} + \int_0^T \|u(s)\|_{\dot H^2(\Omega)} \,\mathrm{d}s\Big).$$

Then this together with the estimate (4.11) implies

$$\begin{aligned}\|u_0\|_{L^2(\Omega)} &\le c(1+T^\alpha)\Big(\|u(T)\|_{\dot H^2(\Omega)} + \int_0^T e^{cs}s^{-\alpha} \,\mathrm{d}s \|u_0\|_{L^2(\Omega)}\Big) \\ &\le c(1+T^\alpha)\Big(\|u(T)\|_{\dot H^2(\Omega)} + ce^{cT}T^{1-\alpha}\|u_0\|_{L^2(\Omega)}\Big)\end{aligned}$$

Let be the constant that

$$c(1+T_0^\alpha)e^{cT_0}T_0^{1-\alpha} < \frac{1}{2}, \quad T_0 < 1. \tag{4.15}$$

Then for any $T \le T_0$

$$\|u_0\|_{L^2(\Omega)} \le c(1+T^\alpha)\|u(T)\|_{\dot H^2(\Omega)}.$$

This completes the proof of the lemma. □

Next, we derive a stability estimate for a large T. To this end, we need the following assumption.

Assumption 4.3. *There exists constants $c_2 > 0$ and $\kappa > 0$ such that*

$$|\partial_t \nabla_x a(x,t)| + |\partial_t a(x,t)| \le c_2 t^{-\kappa} \quad \forall\, (x,t) \in \Omega \times (0,\infty).$$

Under the condition, we have the following perturbation estimate. The proof is similar to that of Lemma 4.2. The proof is provided in Appendix A for completeness.

Lemma 4.4. *Under Conditions* (4.2)-(4.3) *and Assumption 4.3, there holds for all $t, s \ge 1$*

$$\|(A(t) - A(s))v\|_{\dot H^p(\Omega)} \le c \min\big(1, \min(t,s)^{-\kappa}|t-s|\big)\|v\|_{\dot H^{p+2}(\Omega)}, \qquad \forall\;\; p \in [-2,0]$$

The next theorem provides a stability result in case of sufficiently large T.

Theorem 4.4. *Suppose that $u_0 \in L^2(\Omega)$ and $f = 0$. Let conditions* (4.2)-(4.3) *and Assumption 4.3 be valid. Let $u(t)$ be the solution to the subdiffusion problem* (4.1)*. Then there exists positive $T_1 > 1$ such that for any $T \ge T_1$ there holds*

$$\|u_0\|_{L^2(\Omega)} \le c(1 + T^\alpha)\|u(T)\|_{H^2(\Omega)},$$

where the constant c depends on T_1 and T.

Proof. Using (4.14) and taking L^2 norm on both sides, we apply again Lemma 4.1 (iii) to obtain

$$\|u_0\|_{L^2(\Omega)} \le c(1+T^\alpha)\Big(\|u(T)\|_{\dot H^2(\Omega)} + \Big\|\int_0^T A(T)E(T-s;T)\big(A(T) - A(s)\big)u(s)\,\mathrm{d}s\Big\|_{L^2(\Omega)}\Big).$$

Applying Lemma 4.4 with $p = -2$, we have for sufficiently small $\epsilon > 0$

$$\|(I - A(t)^{-1}A(s))v\|_{L^2(\Omega)} \le c \min(t,s)^{-\kappa\alpha(1+\epsilon)}|t-s|^{\alpha(1+\epsilon)}\|v\|_{L^2(\Omega)}$$

This together with Lemma 4.1 (i) and the a priori estimate (4.12), imply

$$\begin{aligned}
&\|A(T)E(T-s;T)\big(A(T) - A(s)\big)u(s)\|_{L^2(\Omega)}\\
&\le \|A(T)^2E(T-s;T)\|\,\|(I - A(T)^{-1}A(s))u(s)\|_{L^2(\Omega)}\\
&\le cT^{-\kappa\alpha(1+\epsilon)}(T-s)^{-1+\epsilon\alpha}\,\|u(s)\|_{L^2(\Omega)}\\
&\le cT^{-\kappa\alpha(1+\epsilon)}(T-s)^{-1+\epsilon\alpha}\,s^{-(1-\epsilon)\alpha}\|u(0)\|_{L^2(\Omega)}
\end{aligned}$$

for all $s \in [T/2, T]$. Then we arrive at

$$\Big\|\int_{T/2}^T A(T)E(T-s;T)\big(A(T) - A(s)\big)u(s)\,\mathrm{d}s\Big\|_{L^2(\Omega)} \le cT^{-\alpha-\kappa\alpha(1+\epsilon)+2\epsilon\alpha}\|u_0\|_{L^2(\Omega)}.$$

Meanwhile, we apply Lemmas 4.2 and 4.1 again to derive

$$\|A(T)^2E(T-s;T)\|\,\|I - A(T)^{-1}A(s)\| \le c(T-s)^{-1-\alpha} \quad \text{for all} \;\; s \in (0, T/2].$$

This together with the estimate (4.11) leads to

$$
\begin{aligned}
&\int_0^{T/2} \|A(T)^2 E(T-s;T)\| \, \|I - A(T)^{-1}A(s)\| \, \|u(s)\|_{L^2(\Omega)} \, \mathrm{d}s \\
&\leq c \int_0^{T/2} (T-s)^{-1-\alpha} s^{-(1-\epsilon)\alpha} \, \mathrm{d}s \|u(0)\|_{L^2(\Omega)} \leq c T^{-(2-\epsilon)\alpha} \|u(0)\|_{\dot H^2(\Omega)}.
\end{aligned}
$$

To sum up, we arrive at the estimate

$$
\|u_0\|_{L^2(\Omega)} \leq c(1+T^\alpha)\|u(T)\|_{\dot H^2(\Omega)} + c(1+T^\alpha)(T^{-\kappa\alpha(1+\epsilon)-\alpha+2\epsilon\alpha} + T^{-(2-\epsilon)\alpha})\|u_0\|_{L^2(\Omega)}
$$

Then choosing a sufficiently small ϵ, there exists $T_1 > 1$ sufficiently large such that

$$
c(1+T_1^\alpha)(T_1^{-\kappa\alpha(1+\epsilon)-\alpha+2\epsilon\alpha} + T_1^{-(2-\epsilon)\alpha}) = \frac{1}{2} \tag{4.16}
$$

and hence for any $T \geq T_1$, there holds the desired stability estimate. □

In Sections 4.2 and 4.3, we shall discuss respectively the regularization and a fully discrete scheme with rigorous numerical analysis. The stability estimate in Theorems 4.2 and 4.4 provides a key tool in the coming numerical analysis. Therefore, from now on, we suppose the following assumption are valid.

Assumption 4.5. *Suppose Conditions* (4.2)–(4.3) *and one of the following conditions are valid.*

(i) $T \leq T_0$*, where* T_0 *be a sufficiently small constant;*

(ii) Assumption 4.3 holds and $T \geq T_1$ *where* T_1 *be a sufficiently large constant.*

4.2 Regularization and convergence analysis

In practice, the observational data often suffers from noise, i.e., (4.4). In this section, we study a simple regularization scheme by using the quasi boundary value method. Let $u_\gamma^\delta(t) \in \dot H^1(\Omega)$ be the regularizing solution such that

$$
\partial_t^\alpha u_\gamma^\delta(t) + A(t)u_\gamma^\delta(t) = 0 \quad \forall\, t \in (0,T] \quad \text{with} \quad \gamma u_\gamma^\delta(0) + u_\gamma^\delta(T) \quad = g^\delta \tag{4.17}
$$

where γ denotes a positive regularization parameter. To derive an error estimate for $u_\gamma^\delta(0) - u(0)$, we introduce an auxiliary function $u_\gamma(t) \in \dot H^1(\Omega)$ satisfying

$$
\partial_t^\alpha u_\gamma(t) + A(t)u_\gamma(t) = 0 \ \ \forall\, t \in (0,T] \quad \text{with} \quad \gamma u_\gamma(0) + u_\gamma(T) = g. \tag{4.18}
$$

Then using the solution representation

$$
u_\gamma(T) = F(T;T)u_\gamma(0) + \int_0^T E(T-s;T)(A(T)-A(s))u_\gamma(s)\,\mathrm{d}s
$$

we have the relation

$$\gamma u_\gamma(0) + F(T;T)u_\gamma(0) + \int_0^T E(T-s;T)(A(T)-A(s))u_\gamma(s)\,\mathrm{d}s = g.$$

Therefore, we derive

$$u_\gamma(0) = (\gamma I + F(T;T))^{-1}\Big[g - \int_0^T E(T-s;T)(A(T)-A(s))u_\gamma(s)\,\mathrm{d}s\Big]. \tag{4.19}$$

Similarly, we have

$$u_\gamma^\delta(0) = (\gamma I + F(T;T))^{-1}\Big[g^\delta - \int_0^T E(T-s;T)(A(T)-A(s))u_\gamma^\delta(s)\,\mathrm{d}s\Big]. \tag{4.20}$$

We begin with the following lemma on solution operator with fixed-time operator $A(T)$. These estimates have been proved in [112, Lemma 3.3] by means of spectral decomposition.

Lemma 4.5. *Let $0 \le p \le q \le 2+p$. Then there holds the estimates for any $\gamma \in (0,1]$*

$$\begin{aligned}
&\|(\gamma I + F(T;T))^{-1}\|_{\dot H^p(\Omega)} \le c(1+T^\alpha)^{\frac{q-p}{2}}\gamma^{-(1+\frac{p-q}{2})}\|v\|_{\dot H^q(\Omega)}, \ \textit{and}\\
&\|F(T;T)(\gamma I + F(T;T))^{-1}\| \le c.
\end{aligned}$$

All the constants are independent of p, q, T and γ.

Also, we need the following regularity of the regularized solution.

Lemma 4.6. *Let $u_\gamma(t)$ be the solution to (4.18). Suppose Conditions (4.2)–(4.3) and one of the following conditions are valid.*

(i) $T \le T_0$, where T_0 be a sufficiently small constant;

(ii) Assumption 4.3 holds and $T \ge T_1$ where T_1 be a sufficiently large constant.

Then there holds for any $p \in [0,2]$,

$$\|u_\gamma(0)\|_{\dot H^p(\Omega)} \le c\gamma^{-\frac{p}{2}}\|u_0\|_{L^2(\Omega)}$$

where the constant c depends on T_0 and T_1.

Proof. By means of the representation (4.19), Theorem 4.1 and Lemma 4.5,

$$\begin{aligned}
\|u_\gamma(0)\|_{L^2(\Omega)} &= \Big\|(\gamma I + F(T;T))^{-1}\Big(g - \int_0^T E(T-s;T)(A(T)-A(s))u_\gamma(s)\mathrm{d}s\Big)\Big\|_{L^2(\Omega)}\\
&\le c(1+T^\alpha)\|g\|_{\dot H^2(\Omega)} + \|F(T;T)^{-1}\int_0^T E(T-s;T)(A(T)-A(s))u_\gamma(s)\mathrm{d}s\|_{L^2(\Omega)}\\
&\le c_T\|u_0\|_{L^2(\Omega)} + \|F(T;T)^{-1}\int_0^T E(T-s;T)(A(T)-A(s))u_\gamma(s)\mathrm{d}s\|_{L^2(\Omega)}.
\end{aligned}$$

Then the desired result with $p=0$ follows immediately from the proof of Theorems 4.2 and 4.4.

Next, we turn to the case that $p=2$. Similarly, we apply the representation (4.19) and Lemma 4.5 again to obtain

$$
\begin{aligned}
&\|u_\gamma(0)\|_{\dot H^2(\Omega)}\\
&\leq c\Big\|A(T)(\gamma I+F(T;T))^{-1}\Big(g-\int_0^T E(T-s;T)(A(T)-A(s))u_\gamma(s)\mathrm{d}s\Big)\Big\|_{L^2(\Omega)}\\
&\leq c\gamma^{-1}\|g\|_{\dot H^2(\Omega)}+\int_0^T \|F(T;T)^{-1}A(T)E(T-s;T)(A(T)-A(s))u_\gamma(s)\|_{L^2(\Omega)}\mathrm{d}s\\
&\leq c_T\gamma^{-1}\|u_0\|_{L^2(\Omega)}+c(1+T^\alpha)\int_0^T \|A(T)^2E(T-s;T)(A(T)-A(s))u_\gamma(s)\|_{L^2(\Omega)}\mathrm{d}s.
\end{aligned}
$$

Using Lemma 4.3 and Poincare inequality, we have

$$\|u_\gamma(t)\|_{\dot H^2(\Omega)}\leq ce^{ct}t^{-\alpha}\|u_\gamma(0)\|_{\dot H^2(\Omega)}\quad\text{and}\quad \|u_\gamma(t)\|_{\dot H^2(\Omega)}\leq ct^{-(1-\epsilon)\alpha}\|u_\gamma(0)\|_{\dot H^2(\Omega)}, \tag{4.21}$$

with any small parameter $\epsilon>0$ and $t>0$, and all the positive constants c in above estimates are independent of t and T. Next, we repeat the argument in Theorems 4.2 and 4.4. Now Lemmas 4.1 and 4.2 (with $p=0$) imply that

$$
\begin{aligned}
&\|u_\gamma(0)\|_{\dot H^2(\Omega)}\\
&\leq c\gamma^{-1}T^{-\alpha}\|u_0\|_{L^2(\Omega)}+c(1+T^\alpha)\int_0^T \|A(T)^2E(T-s;T)(A(T)-A(s))u_\gamma(s)\|_{L^2(\Omega)}\mathrm{d}s\\
&\leq c\gamma^{-1}T^{-\alpha}\|u_0\|_{L^2(\Omega)}+c(1+T^\alpha)\int_0^T (T-s)^{-\alpha}\|u_\gamma(s)\|_{\dot H^2(\Omega)}\mathrm{d}s\\
&\leq c\gamma^{-1}T^{-\alpha}\|u_0\|_{L^2(\Omega)}+c(1+T^\alpha)\int_0^T (T-s)^{-\alpha}e^{cs}s^{-\alpha}\|u_\gamma(0)\|_{\dot H^2(\Omega)}\mathrm{d}s.
\end{aligned}
$$

We combine this and (4.21) to arrive at

$$\|u_\gamma(0)\|_{\dot H^2(\Omega)}\leq c\gamma^{-1}T^{-\alpha}\|u_0\|_{L^2(\Omega)}+c(1+T^\alpha)T^{1-2\alpha}e^{cT}\|u_\gamma(0)\|_{\dot H^2(\Omega)}.$$

Then by choosing small T_0 such that $c(1+T_0^\alpha)T_0^{1-2\alpha}e^{cT_0}<\frac12$, we arrive at

$$\|u_\gamma(0)\|_{\dot H^2(\Omega)}\leq c\gamma^{-1}T^{-\alpha}\|u_0\|_{L^2(\Omega)}\qquad\text{for all }\ T\in(0,T_0).$$

Next we consider the case that T is sufficiently large, and we let Assumption 4.3 be valid. Then we apply Lemma 4.4 with $p=0$ to arrive at

$$\|(A(t)-A(s))v\|_{L^2(\Omega)}\leq c\min(t,s)^{-\kappa\alpha(1+\epsilon)}|t-s|^{\alpha(1+\epsilon)})\|v\|_{\dot H^2(\Omega)}$$

for sufficiently small ϵ. This together with Lemma 4.1 and the estimate (4.21) lead to

$$
\begin{aligned}
&\|A(T)^2E(T-s;T)\big(A(T)-A(s)\big)u_\gamma(s)\|_{L^2(\Omega)}\\
&\leq \|A(T)^2E(T-s;T)\|\,\|\big(A(T)-A(s)\big)u_\gamma(s)\|_{L^2(\Omega)}\\
&\leq cT^{-\kappa\alpha(1+\epsilon)}(T-s)^{-1+\epsilon\alpha}\,\|u_\gamma(s)\|_{\dot H^2(\Omega)}\\
&\leq cT^{-\kappa\alpha(1+\epsilon)}(T-s)^{-1+\epsilon\alpha}\,s^{-(1-\epsilon)\alpha}\|u_\gamma(0)\|_{\dot H^2(\Omega)}
\end{aligned}
$$

for all $s \in [T/2, T]$. Then we arrive at

$$\int_{T/2}^{T} \big\|A(T)^2 E(T-s;T)\big(A(T)-A(s)\big)u_\gamma(s)\big\|_{L^2(\Omega)}\,\mathrm{d}s \le cT^{-\alpha-\kappa\alpha(1+\epsilon)+2\epsilon\alpha}\|u_\gamma(0)\|_{\dot H^2(\Omega)}.$$

Meanwhile, we apply Lemmas 4.2 and 4.1 again to derive

$$\|A(T)^2 E(T-s;T)(A(t)-A(s))v\| \le c(T-s)^{-1-\alpha}\|v\|_{\dot H^2(\Omega)} \quad \text{for all} \quad s \in (0, T/2].$$

This together with the estimate (4.21) leads to

$$\begin{aligned}&\int_0^{T/2} \big\|A(T)^2 E(T-s;T)\big(A(T)-A(s)\big)u_\gamma(s)\big\|_{L^2(\Omega)}\,\mathrm{d}s\\ &\le c\int_0^{T/2}(T-s)^{-1-\alpha}s^{-(1-\epsilon)\alpha}\,\mathrm{d}s\|u_\gamma(0)\|_{\dot H^2(\Omega)} \le cT^{-(2-\epsilon)\alpha}\|u_\gamma(0)\|_{\dot H^2(\Omega)}.\end{aligned}$$

To sum up, we arrive at the estimate

$$\|u_\gamma(0)\|_{L^2(\Omega)} \le c\gamma^{-1}T^{-\alpha}\|u_0\|_{L^2(\Omega)} + c(1+T^\alpha)(T^{-\kappa\alpha(1+\epsilon)-\alpha+2\epsilon\alpha} + T^{-(2-\epsilon)\alpha})\|u_0\|_{L^2(\Omega)}$$

Then choosing a sufficiently small ϵ, there exists $T_1 > 1$ sufficiently large such that

$$c(1+T_1^\alpha)(T_1^{-\kappa\alpha(1+\epsilon)-\alpha+2\epsilon\alpha} + T_1^{-(2-\epsilon)\alpha}) = \frac{1}{2} \tag{4.22}$$

and hence for any $T \ge T_1$, there holds the desired stability estimate for $p = 2$. □

The following lemma is about the estimate of the regularization with the backward solution.

Lemma 4.7. *Let u and u_γ be the solutions to the backward problem* (4.13) *and regularized problem* (4.18)*, respectively. Suppose Assumption 4.5 is valid. Then if $u_0 \in \dot H^q(\Omega)$ with $q \in (0, 2]$ there holds*

$$\|u_\gamma(0) - u(0)\|_{L^2(\Omega)} \le c\gamma^{\frac{q}{2}}\|u_0\|_{\dot H^q(\Omega)}$$

where the constant c depends on T_0 and T_1. Moreover, for $u_0 \in L^2(\Omega)$, there holds

$$\lim_{\gamma\to 0^+}\|u_\gamma(0) - u(0)\|_{L^2(\Omega)} = 0.$$

Proof. We let $e := u_\gamma - u$, it would satisfy

$$\partial_t^\alpha e + A(t)e = 0, \quad \gamma e(0) + e(T) = -\gamma u_0,$$

which further implies

$$e(0) = (\gamma I + F(T;T))^{-1}\Big[-\gamma u(0) - \int_0^T E(T-s;T)(A(T)-A(s))e(s)\,\mathrm{d}s\Big], \tag{4.23}$$

Lemma 4.5 implies its estimate that

$$\begin{aligned}\|e(0)\|_{L^2(\Omega)} &\le c\gamma^{\frac{q}{2}}\|u_0\|_{\dot H^q(\Omega)} + \|(\gamma I + F(T;T))^{-1}\int_0^T E(T-s;T)(A(T)-A(s))e(s)\mathrm{d}s\|_{L^2(\Omega)}\\ &\le c\gamma^{\frac{q}{2}}\|u_0\|_{\dot H^q(\Omega)} + \|F(T;T)^{-1}\int_0^T E(T-s;T)(A(T)-A(s))e(s)\mathrm{d}s\|_{L^2(\Omega)}.\end{aligned}$$

Then the desired result follows immediately from the proof of theorems 4.2 and 4.4.

Next, we consider the case that $u_0 \in L^2(\Omega)$. For an arbitrary $\tilde{u}_0 \in \dot{H}^2(\Omega)$, let $\tilde{u}(t)$ and $\tilde{u}_\gamma(t)$ be the functions respectively satisfying

$$\partial_t^\alpha \tilde{u}(t) + A(t)\tilde{u}(t) = 0 \ \forall t \in (0,T] \quad \text{with} \quad \tilde{u}(0) = \tilde{u}_0,$$

and

$$\partial_t^\alpha \tilde{u}_\gamma(t) + A(t)\tilde{u}_\gamma(t) = 0 \ \forall t \in (0,T] \quad \text{with} \quad \gamma\tilde{u}_\gamma(0) + \tilde{u}_\gamma(T) = \tilde{u}(T).$$

We have proved that

$$\|\tilde{u}_\gamma(0) - \tilde{u}(0)\|_{L^2(\Omega)} \le c\gamma\|\tilde{u}_0\|_{\dot{H}^2(\Omega)}.$$

Meanwhile, using the argument in theorems 4.2 and 4.4, we have

$$\|\tilde{u}_\gamma(0) - u_\gamma(0)\|_{L^2(\Omega)} \le c\|u_0 - \tilde{u}_0\|_{L^2(\Omega)} \le c\epsilon.$$

As a result, we apply triangle inequality to obtain

$$\begin{aligned}\|u_\gamma(0) - u_0\|_{L^2(\Omega)} &\le \|u_0 - \tilde{u}_0\|_{L^2(\Omega)} + \|u_\gamma(0) - \tilde{u}_\gamma(0)\|_{L^2(\Omega)} + \|\tilde{u}_\gamma(0) - \tilde{u}_0\|_{L^2(\Omega)} \\ &\le c\|u_0 - \tilde{u}_0\|_{L^2(\Omega)} + c\gamma\|\tilde{u}_0\|_{\dot{H}^2(\Omega)}.\end{aligned}$$

Let ϵ be an arbitrarily small number. Using the density of $\dot{H}^2(\Omega)$ in $L^2(\Omega)$, we choose $\tilde{u}_0$ such that $c\|u_0 - \tilde{u}_0\|_{L^2(\Omega)} \le \frac{\epsilon}{2}$. Moreover, let γ_0 be the constant that $c\gamma_0\|\tilde{u}_0\|_{\dot{H}^2(\Omega)} < \frac{\epsilon}{2}$. Therefore, for all $\gamma \le \gamma_0$, we have $\|u_\gamma(0) - u(0)\|_{L^2(\Omega)} \le \epsilon$. Then the proof is complete. □

Then we are ready to state our main theorem to show the error for the regularizing solution $u_\gamma^\delta(0)$.

Theorem 4.6. *Let u and u_γ^δ be the solutions to the backward problem* (4.13) *and regularized problem* (4.17)*, respectively. Suppose Assumption 4.5 is valid. Then if $\|u_0\|_{\dot{H}^q(\Omega)} \le c$ with $q \in (0,2]$ there holds*

$$\|u_\gamma^\delta(0) - u(0)\|_{L^2(\Omega)} \le c\left(\delta\gamma^{-1} + \gamma^{\frac{q}{2}}\right).$$

Moreover, for $u_0 \in L^2(\Omega)$, there holds

$$\|u_\gamma^\delta(0) - u(0)\|_{L^2(\Omega)} \to 0 \quad \text{as} \ \ \delta,\ \gamma \to 0 \ \ \text{and} \ \ \frac{\delta}{\gamma} \to 0.$$

Proof. To show the error estimate, we consider the splitting

$$u_\gamma^\delta(t) - u(t) = (u_\gamma^\delta(t) - u_\gamma(t)) + (u_\gamma(t) - u(t)) = \vartheta(t) + \varrho(t).$$

Using the solution representation (4.19) and (4.20), we have

$$\begin{aligned}\|\vartheta(0)\|_{L^2(\Omega)} \le\ &\|(\gamma I + F(T;T))^{-1}(g - g^\delta)\|_{L^2(\Omega)} \\ &+ \|(\gamma I + F(T;T))^{-1}\int_0^T E(T-s;T)(A(T) - A(s))\theta(s)\,\mathrm{d}s\|_{L^2(\Omega)}.\end{aligned}$$

Using Lemma (4.5), we derive

$$\begin{aligned}\|\vartheta(0)\|_{L^2(\Omega)} &\le c\gamma^{-1}\|g-g^\delta\|_{L^2(\Omega)} + \|F(T;T)^{-1}\int_0^T E(T-s;T)(A(T)-A(s))\theta(s)\,\mathrm{d}s\|_{L^2(\Omega)}\\ &\le c\gamma^{-1}\delta + \|F(T;T)^{-1}\int_0^T E(T-s;T)(A(T)-A(s))\theta(s)\,\mathrm{d}s\|_{L^2(\Omega)}.\end{aligned}$$

Applying the argument in theorems 4.2 and 4.4, we conclude that $\|\vartheta(0)\|_{L^2(\Omega)} \le c\gamma^{-1}\delta$. This estimate and Lemma 4.7 lead to the desired result. □

4.3 Fully discretization scheme and error analysis

In this section, we shall propose and analyze a completely discrete scheme for solving the backward problem. To begin with, we study the semidiscrete scheme using the finite element methods. The semidiscrete solution plays an important role in the analysis of completely discrete scheme.

4.3.1 Semidiscrete scheme for solving the problem

To begin with, we study the semidiscrete scheme using the finite element methods studied in Section 2.5, where we define the piece-linear finite element space X_h, the $L^2(\Omega)$ projection P_h.

The semidiscrete standard Galerkin FEM of problem (4.1) reads: find $u_h \in X_h$ such that

$$(\partial_t^\alpha u_h(t),\chi) + (a(\cdot,t)\nabla u_h(t),\nabla\chi) = (f(\cdot,t),\chi), \quad \forall \chi \in X_h, \quad t\in(0,T], \text{ with } u_h(0) = P_h u_0. \tag{4.24}$$

We also need a time-dependent discrete elliptic operator $A_h(t) : X_h \to X_h$ by

$$(A_h(t)v_h,\chi) = (a(\cdot,t)\nabla v_h,\nabla\chi), \quad \forall v_h,\chi \in X_h.$$

With conditions (4.2)-(4.3), $A_h(t)$ is bounded and invertible on X_h, and problem (4.24) can be written as

$$\partial_t^\alpha u_h + A_h u_h = P_h f, \quad \forall t\in(0,T], \quad u_h(0) = P_h u_0. \tag{4.25}$$

Besides, we have the following perturbation result, which has been proved in [45, Remark 3.1].

Lemma 4.8. *Under condition* (4.2)-(4.3)*, there holds*

$$\|(I - A_h(t)^{-1}A_h(s))v_h\|_{L^2(\Omega)} \le c\min(1,|t-s|)\|v_h\|_{L^2(\Omega)}$$

Next, we introduce a time-dependent Ritz projection operator $R_h(t) : H_0^1(\Omega) \to X_h$:

$$(a(\cdot,t)\nabla R_h(t)\varphi,\nabla\chi) = (a(\cdot,t)\nabla\varphi,\nabla\chi), \quad \forall\varphi\in H_0^1(\Omega), \quad \chi\in X_h. \tag{4.26}$$

It is well-known that the Ritz projection satisfies the following approximation property [73, p.99]:

$$\|R_h(t)v - v\|_{L^2(\Omega)} + h\|\nabla(R_h(t)v - v)\|_{L^2(\Omega)} \le ch^q\|v\|_{H^q(\Omega)}, \quad \forall v\in\dot{H}^q(\Omega), \quad q=1,2. \tag{4.27}$$

Next, with Assumption 4.3, we have an updated version of the discrete perturbation estimate.

Lemma 4.9. *With conditions* (4.2)-(4.3) *and Assumption 4.3, we have for all* $v_h \in X_h$

$$\|(I - A_h(t)^{-1}A_h(s))v_h\|_{L^2(\Omega)} \le c\min(1, \min(t,s)^{-\kappa}|t-s|)\|v_h\|_{L^2(\Omega)}, \quad \forall t, s > 1.$$

Proof. Let $w_h = A_h(t)^{-1}A_h(s)v_h$. Then we have $A_h(t)w_h = A_h(s)v_h$ and hence

$$(a(\cdot,t)\nabla w_h, \nabla\chi_h) = (a(\cdot,s)\nabla v_h, \nabla\chi_h), \quad \forall \chi_h \in X_h.$$

This further implies the relation

$$(a(\cdot,t)\nabla(v_h - w_h), \nabla\chi_h) = ((a(\cdot,t) - a(\cdot,s))\nabla v_h, \nabla\chi_h), \quad \forall \chi \in X_h.$$

Let ϕ be the weak solution to the following elliptic problem:

$$(a(\cdot,t)\nabla\phi, \nabla\chi) = ((a(\cdot,t) - a(\cdot,s))\nabla v_h, \nabla\chi), \quad \forall \chi \in \dot H^1(\Omega).$$

Then Lax-Milgram lemma and Assumption 4.3 implies the following *a priori* estimate

$$\|\phi\|_{\dot H^1(\Omega)} \le c\|(a(\cdot,t) - a(\cdot,s))\nabla v_h\|_{L^2(\Omega)} \le c\min(1, \min(t,s)^{-\kappa}|t-s|)\|v_h\|_{\dot H^1(\Omega)},$$

Using the fact that $w_h - v_h = R_h(t)\phi$, the approximation property (4.27), and the inverse inequality, we derive

$$\begin{aligned}\|w_h - v_h - \phi\|_{L^2(\Omega)} &\le ch\|\varphi\|_{\dot H^1(\Omega)} \le ch\min(1, \min(t,s)^{-\kappa}|t-s|)\|v_h\|_{\dot H^1(\Omega)}\\ &\le c\min(1, \min(t,s)^{-\kappa}|t-s|)\|v_h\|_{L^2(\Omega)}.\end{aligned}$$

According triangle inequality we have

$$\|w_h - v_h\|_{L^2(\Omega)} \le c\min(1, \min(t,s)^{-\kappa}|t-s|)\|v_h\|_{L^2(\Omega)} + \|\phi\|_{L^2(\Omega)}.$$

Next, we apply the duality argument to derive a bound for $\|\phi\|_{L^2(\Omega)}$. Let $\xi \in \dot H^2(\Omega)$ be the function such that $A(t)\xi = \phi$. Then

$$\begin{aligned}\|\phi\|^2_{L^2(\Omega)} &= |(a(\cdot,t)\nabla\phi, \nabla\xi)| = |((a(\cdot,t) - a(\cdot,s))\nabla v_h, \nabla\xi)|\\ &\le |(v_h, (a(\cdot,t) - a(\cdot,s))\Delta\xi)| + |(v_h, \nabla(a(\cdot,t) - a(\cdot,s)) \cdot \nabla\xi)|\\ &\le c\min(1, \min(t,s)^{-\kappa}|t-s|)\|v_h\|_{L^2(\Omega)}\|\xi\|_{\dot H^2(\Omega)}\\ &\le c\min(1, \min(t,s)^{-\kappa}|t-s|)\|v_h\|_{L^2(\Omega)}\|\phi\|_{L^2(\Omega)}.\end{aligned}$$

This completes the proof of the lemma. □

Next we derive some semidiscrete solution representation analogue to (4.10), that is given any $t_* \in (0, T]$,

$$u_h(t) = F_h(t;t_*)u_h(0) + \int_0^t E_h(t-s;t_*)(P_hf(s) + (A_h(t_*) - A_h(s))u_h(s))ds \tag{4.28}$$

where the solution operators $F_h(t;t_*)$ and $E_h(t;t_*)$ can be written as

$$F_h(t;t_*) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}} e^{zt} z^{\alpha-1} (z^\alpha + A_h(t_*))^{-1} \, \mathrm{d}z, \quad \text{and} \quad E_h(t;t_*) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}} e^{zt} (z^\alpha + A_h(t_*))^{-1} \, \mathrm{d}z. \tag{4.29}$$

For any fixed t_*, the discrete operators $F_h(t;t_*)$ and $E_h(t;t_*)$ satisfy the following smoothing property, whose proof is identical to that of Lemma 4.1.

Lemma 4.10. *Let $F_h(t;t_*)$ and $E_h(t;t_*)$ be the discrete solution operators defined in* (4.29) *for any $t_* \in [0,T]$. Then they satisfy the following properties for all $t > 0$ and $v_h \in X_h$*

(i) $\|A_h(t_*)F_h(t;t_*)v_h\|_{L^2(\Omega)} + t^{1-(2-k)\alpha}\|A_h(t_*)^k E_h(t;t_*)v_h\|_{L^2(\Omega)} \le ct^{-\alpha}\|v_h\|_{L^2(\Omega)}$, *with $k = 1, 2$;*

(ii) $\|F_h(t;t_*)v_h\|_{L^2(\Omega)} + t^{1-\alpha}\|E_h(t;t_*)v_h\|_{L^2(\Omega)} \le c\min(1, t^{-\alpha})\|v_h\|_{L^2(\Omega)}$*;*

(iii) $\|F_h(t;t_*)^{-1}v_h\|_{L^2(\Omega)} \le c(1 + t^\alpha)\|A_h(t_*)v_h\|_{L^2(\Omega)}$.

The constants in all above estimates are uniform in t, but they are only dependent of t_* and T.

Analogue to Lemma 4.5, we have the following result.

Lemma 4.11. *Let $F_h(t;t_*)$ be the discrete solution operator defined in* (4.29). *For all $0 < t \le T$, $t_* \in (0,T]$ and $v_h \in X_h$, we have*

$$\|(\gamma I + F_h(T;T))^{-1}v_h\| \le c\gamma^{-1}\|v_h\|_{L^2(\Omega)} \text{ and } \|F_h(T;T)(\gamma I + F_h(T;T))^{-1}v_h\|_{L^2(\Omega)} \le c\|v_h\|_{L^2(\Omega)},$$

where the constant c is independent of t, γ and h.

The following Lemma provides an error estimate for the semidiscrete error of the direct problem, see [45, Theorem 3.2] for a detailed proof.

Lemma 4.12. *Let u and u_h be the solutions to* (4.1) *and* (4.24) *respectively. If $u_0 \in L^2$ and $f \equiv 0$, then there holds that*

$$\|(u_h - u)(t)\|_{L^2(\Omega)} \le ch^2 t^{-\alpha}\|u_0\|_{L^2(\Omega)} \quad \text{for all} \quad t \in (0,T],$$

where the constant c is independent of t and h.

After proposing many results about solving direct problem, we shall propose a semidiscrete scheme for solving the backward problem.

We apply the regularized semidiscrete scheme: find $u_{\gamma,h}(t) \in X_h$ such that

$$\partial_t^\alpha u_{\gamma,h}(t) + A_h(t)u_{\gamma,h}(t) = 0, \quad 0 < t \le T, \qquad \gamma u_{\gamma,h}(t) + u_{\gamma,h}(T) = P_h g. \tag{4.30}$$

Then analogue to (4.19) we have

$$u_{\gamma,h}(0) = (\gamma I + F_h(T;T))^{-1}\left[P_h g - \int_0^T E_h(T-s;T)(A_h(T) - A_h(s))u_{\gamma,h}(s)ds\right]. \tag{4.31}$$

Next we shall derive a preliminary estimate for the proof of the semidiscrete error $u_{\gamma,h} - u_\gamma$.

Lemma 4.13. *Let $u_\gamma(t)$ be the solution to the backward regularized problem* (4.30)*. Then fix any $t_* \in (0,T]$ there holds that*

$$\|\int_0^{t_*} E_h(t_*-s;t_*)A_h(s)(R_h(s)-P_h)u_\gamma(s)ds\|_{L^2(\Omega)} \le ch^2 \max\{t_*^{-\alpha}, t_*^{1-\alpha}\}\|u_\gamma(0)\|_{L^2}.$$

The constant c is independent of t and t_*.

Proof. Let φ_h be the solution to the following semidiscrete problem

$$\partial_t^\alpha \varphi_h(t) + A_h(t)\varphi_h(t) = 0, \qquad \varphi_h(0) = P_h u_\gamma(0).$$

Lemma 4.12 implies that

$$\|(\varphi_h - u_\gamma)(t)\|_{L^2(\Omega)} \le ch^2 t^{-\alpha}\|u_\gamma(0)\|_{L^2(\Omega)}.$$

Then we consider the splitting

$$(\varphi_h - u_\gamma)(t) = (\varphi_h - P_h u_\gamma)(t) + (P_h u_\gamma - u_\gamma)(t) := \zeta_h(t) + \rho(t).$$

The approximation property (2.17) and the regularity estimate in Theorem 4.1 give that

$$\|\rho(t)\|_{L^2(\Omega)} \le ch^2\|u_\gamma(t)\|_{\dot H^2(\Omega)} \le ch^2 t^{-\alpha}\|u_\gamma(0)\|_{L^2(\Omega)}.$$

Then by triangle's inequality, we obtain

$$\|\zeta_h(t)\|_{L^2(\Omega)} \le \|\rho(t)\|_{L^2(\Omega)} + \|(\varphi_h - u_\gamma)(t)\|_{L^2(\Omega)} \le ch^2 t^{-\alpha}\|u_\gamma(0)\|_{L^2(\Omega)}. \tag{4.32}$$

Meanwhile, notice that

$$\partial_t^\alpha \zeta_h(t) + A_h(t)\zeta_h(t) = A_h(t)(R_h(t)-P_h)u_\gamma(t), \quad T \ge t > 0, \qquad \zeta(0) = 0.$$

Then for any $t_* \in (0,T]$, $\zeta_h(t_*)$ could be written as

$$\zeta_h(t_*) = \int_0^{t_*} E_h(t_*-s;t_*)A_h(s)(R_h(s)-P_h)u_\gamma(s)ds + \int_0^{t_*} E_h(t_*-s;t_*)(A_h(t_*)-A_h(s))\zeta_h(s)ds.$$

We apply Lemmas 4.9 and 4.10, and the estimate (4.32) to derive

$$\begin{aligned}
&\|\int_0^{t} E_h(t-s;t_*)A_h(s)(R_h(s)-P_h)u_\gamma(s)ds\|_{L^2(\Omega)} \\
&\le \|\zeta_h(t)\|_{L^2(\Omega)} + c\int_0^{t_*}\|\zeta_h(s)\|_{L^2(\Omega)}\,\mathrm{d}s \le c(t_*^{-\alpha} + t_*^{1-\alpha})h^2\|u_\gamma(0)\|_{L^2(\Omega)} \\
&\le ch^2\max\{t_*^{-\alpha}, t_*^{1-\alpha}\}\|u_\gamma(0)\|_{L^2(\Omega)}.
\end{aligned}$$

□

Next, we state a key lemma providing an estimate for the discretization error $u_{\gamma,h} - u_\gamma$.

Lemma 4.14. *Let $u_\gamma(t)$, $u_{\gamma,h}(t)$ be the solutions to problem* (4.18) *and* (4.30) *respectively. Suppose Assumption 4.5 is valid. Then there holds*

$$\|u_{\gamma,h}(0) - u_\gamma(0)\| \le ch^2\gamma^{-1}\|u_0\|_{L^2(\Omega)},$$

where the constant c is independent on γ, h and t.

Proof. We use the splitting

$$(u_{\gamma,h} - u_\gamma)(0) = (u_{\gamma,h} - P_h u_\gamma)(0) + (P_h u_\gamma - u_\gamma)(0) := \zeta_h(0) + \rho(0).$$

From the approximation property (2.17) and Lemma 4.6, we obtain

$$\|\rho(0)\|_{L^2(\Omega)} \le ch^2\|u_\gamma(0)\|_{\dot H^2(\Omega)} \le ch^2\gamma^{-1}\|u_0\|_{L^2(\Omega)}.$$

Now we turn to the bound of $\zeta_h(t)$. Using the fact $A_h(t)R_h(t)v = P_h A(t)v$, we observe that

$$\partial_t^\alpha \zeta_h(t) + A_h(t)\zeta_h(t) = A_h(t)(R_h(t) - P_h)u_\gamma(t) \quad \text{for} \quad t \in (0,T], \quad \text{with} \quad \gamma\zeta_h(0) + \zeta_h(T) = 0. \tag{4.33}$$

For any $t_* \in (0,T]$, we have the solution representation from (4.28) that

$$\begin{aligned}\zeta_h(t) = F_h(t;t_*)\zeta_h(0) &+ \int_0^t E_h(t-s;t_*)A_h(s)(R_h(s) - P_h)u_\gamma(s)\,\mathrm{d}s\\ &+ \int_0^t E_h(t-s;t_*)(A_h(t_*) - A_h(s))\zeta_h(s)\,\mathrm{d}s.\end{aligned}$$

Then with $t = t_* = T$ we apply $\gamma\zeta_h(0) + \zeta_h(T) = 0$ to derive

$$\begin{aligned}\zeta_h(0) = (\gamma I + F_h(T;T))^{-1}&\int_0^T E_h(T-s;T)(A_h(s)(P_h - R_h(s))u_\gamma(s)\,\mathrm{d}s\\ &- (\gamma I + F_h(T;T))^{-1}\int_0^T E_h(T-s;T)(A_h(T) - A_h(s))\zeta(s)\,\mathrm{d}s.\end{aligned}$$

Now we apply Lemmas 4.11 and 4.13 to obtain

$$\begin{aligned}&\|\zeta_h(0)\|_{L^2(\Omega)}\\ &\le c\gamma^{-1}\int_0^T \|E_h(T-s;T)A_h(s)(P_h - R_h(s))u_\gamma(s)\|_{L^2(\Omega)}\mathrm{d}s\\ &+ \|F_h(T;T)^{-1}\int_0^T E_h(T-s;T)(A_h(T) - A_h(s))\zeta(s)\mathrm{d}s\|_{L^2(\Omega)}\\ &\le c_T h^2\gamma^{-1}\|u_\gamma(0)\|_{L^2(\Omega)} + c(1+T^\alpha)\int_0^T \|A_h(T;T)E_h(T-s;T)(A_h(T) - A_h(s))\zeta_h(s)\|_{L^2(\Omega)}\mathrm{d}s.\end{aligned}$$

Next, we split $\zeta_h(s)$ into homogeneous part and inhomogeneous part. Let $\zeta_h(t) := \zeta_1(t) + \zeta_2(t)$ where

$$\begin{aligned}&\partial_t^\alpha \zeta_1(t) + A_h(t)\zeta_1(t) = 0 \quad \text{for} \quad t \in (0,T], \quad \text{with} \quad \zeta_1(0) = \zeta_h(0),\\ &\partial_t^\alpha \zeta_2(t) + A_h(t)\zeta_2(t) = A_h(t)(R_h(t) - P_h)u_\gamma(t) \quad \text{for} \quad t \in (0,T], \quad \text{with} \quad \zeta_2(0) = 0.\end{aligned}$$

First of all, we fixed $t_* \in (0,T]$ and apply the solution representation in (4.28) and Lemmas 4.10, 4.13 and 4.8, and hence derive

$$\begin{aligned}\|\zeta_2(t_*)\|_{L^2(\Omega)} &\le \int_0^{t_*} \|E_h(t_*-s;t_*)A_h(s)(R_h(s)-P_h)u_\gamma(s)\|_{L^2(\Omega)}\mathrm{d}s \\ &\quad + \int_0^{t_*} \|E_h(t_*-s;t_*)(A_h(t_*)-A_h(s))\zeta_2(s)\|_{L^2(\Omega)}\mathrm{d}s \\ &\le ct_*^{-\alpha}h^2\|u_\gamma(0)\|_{L^2(\Omega)} + \int_0^{t_*} \|\zeta_2(s)\|_{L^2(\Omega)}\mathrm{d}s.\end{aligned}$$

Then Gronwall's inequality leads to

$$\|\zeta_2(t)\|_{L^2(\Omega)} \le ch^2e^{ct}t^{-\alpha}\|u_\gamma(0)\|_{L^2(\Omega)}. \tag{4.34}$$

For $\zeta_1(t)$, we apply the similar argument in Lemma 4.3 to obtain

$$\begin{aligned}&\|\zeta_1(t)\|_{L^2(\Omega)} \\ &\le c\min(1,t^{-\alpha})\|\zeta_h(0)\|_{L^2(\Omega)}, \text{ and} \\ &\|A_h(T)\zeta_1(t)\|_{L^2(\Omega)} \le c\,e^{ct}t^{-\alpha}\|\zeta_h(0)\|_{L^2(\Omega)} \quad \text{for all} \ \ t>0.\end{aligned}$$

All the positive constants c in above estimates are independent of t and T. As a result, we have

$$\begin{aligned}\|\zeta_h(0)\|_{L^2(\Omega)} &\le ch^2\gamma^{-1}\|u_\gamma(0)\|_{L^2(\Omega)} \\ &\qquad + \sum_{i=1}^{2} c(1+T^\alpha)\int_0^T \|A_h(T;T)E_h(T-s;T)(A_h(T)-A_h(s))\zeta_i(s)\mathrm{d}s\|_{L^2(\Omega)} \\ &\le ch^2\gamma^{-1}\|u_\gamma(0)\|_{L^2(\Omega)} \\ &\qquad + c(1+T^\alpha)\int_0^T \|A_h(T)E_h(T-s;T)(A_h(T)-A_h(s))\zeta_1(s)\|_{L^2(\Omega)}\mathrm{d}s.\end{aligned}$$

Applying the argument in theorems 4.2 and 4.4, we conclude that

$$\|\zeta_h(0)\|_{L^2(\Omega)} \le ch^2\gamma^{-1}\|u_\gamma(0)\|_{L^2(\Omega)}.$$

This completes the proof of the lemma. □

4.3.2 Fully discrete scheme and error analysis

To begin with, we apply the backward Euler convolution quadrature in Section 2.5. With $\varphi_j = \varphi(t_j)$ we have

$$\partial_t^\alpha \varphi(t_n) \approx \bar\partial_\tau^\alpha(\varphi(t_n)-\varphi(0)) = \frac{1}{\tau^\alpha}\sum_{j=0}^{n} b_j\varphi_{n-j}.$$

The fully discrete scheme for problem (4.25) reads: find $U_h^n \in X_h$ such that

$$\bar\partial_\tau^\alpha U_h^n + A_h(t_n)U_h^n = P_hf(t_n), \quad n=1,2,\dots,N, \quad \text{with} \ \ U_h^0 = P_hu_0, \tag{4.35}$$

By means of Laplace transform and perturbation argument, with $1 \leq n_* \leq N$, the fully discrete solution U^n can be written as [45, 111]

$$U_h^n = F_{h,\tau}^n(n_*)U_h^0 + \tau \sum_{k=1}^{n} E_{h,\tau}^{n-k}(n_*)P_h f(t_k) + \tau \sum_{k=1}^{n} E_{h,\tau}^{n-k}(n_*)(A_h(t_{n_*}) - A_h(t_k))U_h^k \tag{4.36}$$

with $n = 1, 2, \cdots, N$. Here the fully discrete operators $F_{h,\tau}^n(n_*)$ and $E_{h,\tau}^n(n_*)$ are defined by

$$\begin{aligned} F_{h,\tau}^n(n_*) &= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} e^{-z\tau} \delta_\tau(e^{-z\tau})^{\alpha-1} (\delta_\tau(e^{-z\tau})^\alpha + A_h(t_{n_*}))^{-1} \, \mathrm{d}z, \\ E_{h,\tau}^n(n_*) &= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} (\delta_\tau(e^{-z\tau})^\alpha + A_h(t_{n_*}))^{-1} \, \mathrm{d}z, \end{aligned} \tag{4.37}$$

with $\delta_\tau(\xi) = (1 - \xi)/\tau$ and the contour $\Gamma_{\theta,\sigma}^\tau := \{z \in \Gamma_{\theta,\sigma} : |\Im(z)| \leq \pi/\tau\}$ where $\theta \in (\pi/2, \pi)$ is close to $\pi/2$. (oriented with an increasing imaginary part).

The next lemma provides some approximation properties of solution operators $F_{h,\tau}^n(n_*)$ and $E_{h,\tau}^n(n_*)$. See [110, Lemma 4.2] and [41, Theorem 3.5] for the proof of the first estimate, and [45, Lemma 4.5] for the second estimate.

Lemma 4.15. *For the operator F_h^τ and E_h^τ defined in* (4.37)*, we have*

$$\|A_h(t_{n_*})^\beta (F_{h,\tau}^n(n_*) - F_h(t_n; t_{n_*}))\|_{L^2(\Omega)} \leq c\tau t_n^{-1-\beta\alpha},$$
$$\left\| \tau A_h^\beta E_{h,\tau}^{n_*-k}(n_*) - \int_{t_{k-1}}^{t_k} A_h^\beta(t_{n_*}) E_h(t_{n_*} - s; t_{n_*})) ds \right\| \leq c\tau^2 (t_{n_*} - t_k + \tau)^{-(2-(1-\beta)\alpha)}$$

for any $\beta \in [0, 1]$.

Note that the solution operators $F_{h,\tau}^n(n_*)$ and $E_{h,\tau}^n(n_*)$ satisfy the following smoothing properties, whose proof is identical to that of Lemma 4.1.

Lemma 4.16. *Let $F_h^\tau(n; n)$ and $E_h^\tau(n; n)$ be the operators defined in* (4.37)*. Then they satisfy the following properties for any $n \geq 1$ and $v_h \in X_h$,*

(i) $\|A_h(t_*)F_{h,\tau}^n(n_*)v_h\|_{L^2(\Omega)} + t_n^{1-(2-k)\alpha} \|A_h(t_*)^k E_{h,\tau}^n(n_*)v_h\|_{L^2(\Omega)} \leq ct_{n+1}^{-\alpha} \|v_h\|_{L^2(\Omega)}, \quad k = 1, 2;$

(ii) $\|F_{h,\tau}^n(n_*)v_h\|_{L^2(\Omega)} + t_n^{1-\alpha} \|E_{h,\tau}^n(n_*)v_h\|_{L^2(\Omega)} \leq c \min(1, t_n^{-\alpha}) \|v_h\|_{L^2(\Omega)};$

(iii) $\|F_{h,\tau}^n(n_*)^{-1}v_h\|_{L^2(\Omega)} \leq c(1 + t_n^\alpha) \|A_h(t_*)v_h\|_{L^2(\Omega)}.$

Next we introduce some *a priori* estimate for the discrete solution U_h^n in (4.36), analogue to Lemma 4.3 for the continuous problem. We provide the proof in Appendix B for completeness.

Lemma 4.17. *Let U_h^n be the solution to* (4.35)*, then we have the following a priori estimate ($f \equiv 0$)*

$$\|U_h^n\|_{L^2(\Omega)} \leq c \min(1, t_n^{-\alpha}) \|U_h^0\|_{L^2(\Omega)} \quad \textit{and} \quad \|A_h(T)U_h^n\|_{L^2(\Omega)} \leq ce^{ct_n} t_n^{-\alpha} \|U_h^0\|_{L^2(\Omega)} \quad \textit{for} \quad n \geq 1.$$

Moreover, for any $\epsilon \in (0, 1/\alpha - 1)$, there holds

$$\|A_h(T)U_h^n\|_{L^2(\Omega)} \leq c t_n^{-(1-\epsilon)\alpha} \|U_h^0\|_{L^2(\Omega)} \quad \text{for all} \quad n \geq 1.$$

All the constants in above estimates are independent of h, n, N, τ and T.

Now we introduce the fully discrete scheme for solving the backward problem: find $U_{h,\gamma}^{n,\delta} \in X_h$ for $n = 1, \ldots, N$ such that

$$\bar{\partial}_\tau U_{h,\gamma}^{n,\delta} + A_h(t_n)U_{h,\gamma}^{n,\delta} = 0 \quad \text{for all} \quad 1 \leq n \leq N, \quad \text{with} \quad \gamma U_{h,\gamma}^{0,\delta} + U_{h,\gamma}^{N,\delta} = P_h g_\delta. \tag{4.38}$$

Then $U_{h,\gamma}^{n,\delta}$ can be written as

$$U_{h,\gamma}^{0,\delta} = (\gamma I + F_{h,\tau}^N(N))^{-1} \Big[P_h g_\delta - \tau \sum_{k=1}^{N} E_{h,\tau}^{N-k}(N)(A_h(T) - A_h(t_k))U_{h,\gamma}^{k,\delta} \Big]. \tag{4.39}$$

The following lemma provides a useful estimate of the discrete operator $(\gamma I + F_{h,\tau}^N(N))^{-1}$; see a detailed proof in [112, Lemma 4.4].

Lemma 4.18. *Let $F_h^\tau(n; n_*)$ and $E_h^\tau(n; n_*)$ be the operators defined in (4.37). Then there holds*

$$\|(\gamma I + F_h^\tau(N;N))^{-1} v_h\|_{L^2(\Omega)} \leq c\gamma^{-1}\|v_h\|_{L^2(\Omega)} \quad \text{and} \quad \|F_h^\tau(N;N)(\gamma I + F_h^\tau(N;N))^{-1} v_h\|_{L^2(\Omega)} \leq c$$

where c is uniform in T, h, τ and γ.

To show the error between $U_{h,\gamma}^{N,\delta}$ and u_0, we introduce an auxiliary function $\bar{U}_{h,\gamma}^n \in X_h$ such that

$$\bar{\partial}_\tau \bar{U}_{h,\gamma}^n + A_h(t_n)\bar{U}_{h,\gamma}^n = P_h f(t_n) \quad \text{for all} \quad 1 \leq n \leq N, \quad \text{with} \quad \bar{U}_{h,\gamma}^n = u_{\gamma,h}(0), \tag{4.40}$$

Then we have the following error estimate for the direct problem, according to [45, Theorem 4.1].

Lemma 4.19. *Let $u_{\gamma,h}(t)$ and $\bar{U}_{h,\gamma}^n$ be the solution to (4.25) and (4.40) with $f \equiv 0$, then we have*

$$\|A_h(0)(\bar{U}_{h,\gamma}^n - u_{\gamma,h}(t_n))\|_{L^2(\Omega)} \leq c\tau \log(n+1) \max(t_n^{-\alpha-1}, t_n^{-\alpha}) \|u_{\gamma,h}(0)\|_{L^2(\Omega)}.$$

Proof. Let $e_n = \bar{U}_{h,\gamma}^n - u_{\gamma,h}(t_n)$. First of all, we recall [45, Theorem 4.1] that

$$\|e_n\|_{L^2(\Omega)} \leq c\tau t_n^{-1} \log(n+1) \|u_{\gamma,h}(0)\|_{L^2(\Omega)}. \tag{4.41}$$

We then use the solution representation (4.36) to obtain

$$\bar{U}_{h,\gamma}^n = F_{h,\tau}^n(n_*)u_{\gamma,h}(0) + \tau \sum_{k=1}^{n} E_{h,\tau}^{n-k}(n_*)(A_h(t_{n_*}) - A_h(t_k))\bar{U}_{h,\gamma}^k.$$

Then by means of (4.28), we have for fixed t_{n_*}

$$
\begin{aligned}
A_h(t_{n_*})e_{n_*} &= A_h(t_{n_*})(F^n_{h,\tau}(n_*) - F_h(t_n;t_{n_*}))u_{\gamma,h}(0)\\
+\tau\sum_{k=1}^{n_*} &A_h(t_{n_*})E^{n_*-k}_{h,\tau}(n_*)(A_h(t_{n_*}) - A_h(t_k))\bar U^k_{h,\gamma} -\\
&\int_0^{t_{n_*}} A_h(t_{n_*})E_h(t_{n_*}-s;t_{n_*})(A_h(t_{n_*}) - A_h(s))u_{\gamma,h}(s)\,\mathrm{d}s\\
+\tau\sum_{k=1}^{n_*} &A_h(t_{n_*})E^{n_*-k}_{h,\tau}(n_*)(A_h(t_{n_*}) - A_h(t_k))(\bar U^k_{h,\gamma} - u_{\gamma,h}(t_k)) = I_1 + I_2 + I_3.
\end{aligned}
$$

Lemma 4.15 immediately implies the bound for I_1:

$$\|I_1\|_{L^2(\Omega)} \le c\tau t_{n_*}^{-1-\alpha}\|u_{\gamma,h}(0)\|_{L^2(\Omega)}.$$

A slight modification of [45, Lemma 4.4] leads to a bound for I_2. In particular, we observe

$$
\begin{aligned}
I_2 = \sum_{k=1}^{n_*} \Big[&\tau A_h(t_{n_*})E^{n_*-k}_{h,\tau}(n_*)(A_h(t_{n_*}) - A_h(t_k))\\
&\qquad - \int_{t_{k-1}}^{t_k} A_h(t_{n_*})E_h(t_{n_*}-s;t_{n_*})(A_h(t_{n_*}) - A_h(s))\mathrm{d}s\Big]\bar U^k_{h,\gamma}\\
+\sum_{k=1}^{n_*}&\int_{t_{k-1}}^{t_k} A_h(t_{n_*})E_h(t_{n_*}-s;t_{n_*})(A_h(t_{n_*}) - A_h(s))\,\mathrm{d}s\, e_k\\
+\sum_{k=1}^{n_*}&\int_{t_{k-1}}^{t_k} A_h(t_{n_*})E_h(t_{n_*}-s;t_{n_*})(A_h(t_{n_*}) - A_h(s))(u_{\gamma,h}(t_k) - u_{\gamma,h}(s))\,\mathrm{d}s\\
:= I_{2,1} &+ I_{2,2} + I_{2,3},
\end{aligned}
$$

For $I_{2,1}$, by means of Lemma 4.15 with $\beta = 1$, 4.8 and 4.16 (i) with the solution representation (4.36), we arrive at

$$
\begin{aligned}
\|I_{2,1}\|_{L^2(\Omega)} &\le \sum_{k=1}^{n_*} \|\Big[\tau A_h(t_{n_*})E^{n_*-k}_{h,\tau}(n_*)(I - A_h(t_k)A_h(t_{n_*})^{-1})\\
&\qquad - \int_{t_{k-1}}^{t_k} A_h(t_{n_*})E_h(t_{n_*}-s;t_{n_*})(I - A_h(s)A_h(t_{n_*})^{-1})\mathrm{d}s\Big]\|\,\|A_h(t_{n_*})\bar U^k_{h,\gamma}\|_{L^2(\Omega)}\\
&\le c\sum_{k=1}^{n_*}\tau^2(t_{n_*} - t_k + \tau)^{-1}t_k^{-\alpha}\|u_{\gamma,h}(0)\|_{L^2(\Omega)}\\
&\le c\tau\log(n_*+1)t_n^{-\alpha}\|u_{\gamma,h}(0)\|_{L^2(\Omega)}.
\end{aligned}
$$

For $I_{2,2}$ we apply Lemmas 4.10 (i) with $k = 2$, Lemma 4.8 and *a priori* estimate (4.41) to derive

$$\|I_{2,2}\|_{L^2(\Omega)} \le c\tau t_{n_*}^{-\alpha-1}\log(n_*+1)\|u_{\gamma,h}(0)\|_{L^2(\Omega)}.$$

Last, for the error term $I_{2,3}$, we denote

$$Q_k = \int_{t_{k-1}}^{t_k} A_h(t_{n_*})E_h(t_{n_*}-s;t_{n_*})(A_h(t_{n_*}) - A_h(s))(u_{\gamma,h}(t_k) - u_{\gamma,h}(s)).$$

For $k=1$, we apply Lemmas 4.10 and 4.8 to derive the bound

$$\begin{aligned}\|Q_1\|_{L^2(\Omega)} &\leq \|\int_0^\tau A_h(t_{n_*})E_h(t_{n_*}-s;t_{n_*})(A_h(t_{n_*})-A_h(s))u_{\gamma,h}(\tau)\,\mathrm{d}s\|_{L^2(\Omega)}\\ &\quad+\|\int_0^\tau A_h(t_{n_*})E_h(t_{n_*}-s;t_{n_*})(A_h(t_{n_*})-A_h(s))u_{\gamma,h}(s)\,\mathrm{d}s\|_{L^2(\Omega)}\\ &\leq c\int_0^\tau (t_{n_*}-s)^{-\alpha}\mathrm{d}s\|u_{\gamma,h}(0)\|_{L^2(\Omega)} \leq c\tau t_{n_*}^{-\alpha}\|u_{\gamma,h}(0)\|_{L^2(\Omega)}.\end{aligned}$$

Meanwhile, for $k\geq 2$, there holds that

$$Q_k=\int_{t_{k-1}}^{t_k} A_h(t_{n_*})E_h(t_{n_*}-s;t_{n_*})(A_h(t_{n_*})-A_h(s))\int_s^{t_k} u'_{\gamma,h}(\xi)\mathrm{d}\xi\,\mathrm{d}s.$$

The discrete analogue to Theorem 4.1(i) (see detail proof in [45, Theorem 2.3(i)]), $u'_{\gamma,h}(t)$ can be bounded by

$$\|u'_{\gamma,h}(t)\|_{L^2(\Omega)} \leq ct^{-1}\|u_{\gamma,h}(0)\|_{L^2(\Omega)}. \tag{4.42}$$

Then by Lemmas 4.10, 4.8 and regularity estimate (4.42) there holds

$$\begin{aligned}\|Q_k\|_{L^2(\Omega)} &\leq c\int_{t_{k-1}}^{t_k} \|A_h(t_{n_*})E_h(t_{n_*}-s;t_{n_*})(A_h(t_{n_*})-A_h(s))\|\int_s^{t_k}\xi^{-1}\mathrm{d}\xi\,\mathrm{d}s\|u_{\gamma,h}(0)\|_{L^2(\Omega)}\\ &\leq c\int_{t_{k-1}}^{t_k}(t_{n_*}-s)^{-\alpha}\int_s^{t_k}\xi^{-1}\mathrm{d}\xi\,\mathrm{d}s\|u_{\gamma,h}(0)\|_{L^2(\Omega)}\\ &\leq c\tau\int_{t_{k-1}}^{t_k}(t_{n_*}-s)^{-\alpha}s^{-1}\mathrm{d}s\|u_{\gamma,h}(0)\|_{L^2(\Omega)}.\end{aligned}$$

Summing those terms from $k=2$ to $k=n_*$, we obtain

$$\begin{aligned}\sum_{k=2}^{n_*}\|Q_k\|_{L^2(\Omega)} &\leq c\tau\|u_{\gamma,h}(0)\|_{L^2(\Omega)}\int_\tau^{t_{n_*}}(t_{n_*}-s)^{-\alpha}s^{-1}\mathrm{d}s\\ &\leq c\tau t_{n_*}^{-\alpha-1}\log(n_*+1)\|u_{\gamma,h}(0)\|_{L^2(\Omega)}.\end{aligned}$$

As a result, we arrive at

$$\|I_2\|_{L^2(\Omega)} \leq c\tau t_{n_*}^{-\alpha-1}\log(n_*+1)\|u_{\gamma,h}(0)\|_{L^2(\Omega)}.$$

Finally, Lemmas 4.16, 4.8 and the estimate (4.41) imply that

$$\begin{aligned}\|I_3\|_{L^2(\Omega)} &\leq c\tau\sum_{k=1}^{n_*}\|A_h(t_{n_*})^2E_{h,\tau}^{n_*-k}(n_*)\|\,\|I-A_h(t_k)A_h(t_{n_*})^{-1}\|\,\|e_k\|_{L^2(\Omega)}\\ &\leq c\tau\sum_{k=1}^{n_*}(t_{n_*}-t_k)^{-\alpha}\|e_k\|_{L^2(\Omega)}\\ &\leq c\tau^2\sum_{k=1}^{n_*}(t_{n_*}-t_k)^{-\alpha}t_k^{-1}\log(k+1)\|u_{\gamma,h}(0)\|_{L^2(\Omega)}\\ &\leq c\tau\log(n_*+1)t_n^{-\alpha}\|u_{\gamma,h}(0)\|_{L^2(\Omega)}.\end{aligned}$$

This completes the proof of the lemma. □

Next, we introduce an auxiliary function

$$\bar{\partial}_\tau U_{h,\gamma}^n + A_h(t_n)U_{h,\gamma}^n = 0 \text{ for all } 1 \le n \le N, \quad \text{with } \gamma U_{h,\gamma}^0 + U_{h,\gamma}^N = P_h g. \tag{4.43}$$

Then $U_{h,\gamma}^0$ can be written as

$$U_{h,\gamma}^0 = (\gamma I + F_{h,\tau}^N(N))^{-1}\Big[P_h g - \tau\sum_{k=1}^N F_{h,\tau}^{N-k}(N)(A_h(T) - A_h(t_k))U_{h,\gamma}^k\Big]. \tag{4.44}$$

Then the next lemma provides an estimate for $U_{h,\gamma}^{0,\delta} - U_{h,\gamma}^0$.

Lemma 4.20. *Let $U_{h,\gamma}^{n,\delta}$ and $U_{h,\gamma}^n$ be the solution to problems (4.38) and (4.43) respectively. Suppose Assumption 4.5 is valid. Then there holds*

$$\|U_{h,\gamma}^{0,\delta} - U_{h,\gamma}^0\|_{L^2(\Omega)} \le c\delta\gamma^{-1},$$

where the constant c is independent on γ, h, τ and t.

Proof. Let $e_n = U_{h,\gamma}^{n,\delta} - U_{h,\gamma}^n$. Then e_n satisfies the relation that

$$\bar{\partial}_\tau e_n + A_h(t_n)e_n = 0 \text{ for all } 1 \le n \le N, \quad \text{with } \gamma e_0 + e_N = P_h(g_\delta - g) \tag{4.45}$$

Using representations (4.39) and (4.44) we obtain

$$e_0 = (\gamma I + F_{h,\tau}^N(N))^{-1}\Big[P_h(g_\delta - g) - \tau\sum_{k=1}^N E_{h,\tau}^{N-k}(N)(A_h(T) - A_h(t_k))e_k\Big].$$

Now we apply Lemmas 4.16 and 4.17 to obtain

$$\begin{aligned}\|e_0\|_{L^2(\Omega)} &\le c\delta\gamma^{-1} + \|F_h^\tau(N;N)^{-1}\tau\sum_{k=1}^N E_h^\tau(N-k;N)(A_h(T) - A_h(t_k))e_k\|_{L^2(\Omega)}\\ &\le c\delta\gamma^{-1} + c(1+T^\alpha)\sum_{k=1}^N \|\tau A_h(T)E_h^\tau(N-t_k;N)(A_h(T) - A_h(t_k))e_k\|_{L^2(\Omega)}.\end{aligned}$$

Then the desired results follows immediately from the a priori estimate in Lemma 4.17 and the same argument in theorems 4.2 and 4.4. □

Time discretization would give the following fully error estimate.

Lemma 4.21. *Let $u_{\gamma,h}(t)$ and $U_{h,\gamma}^n$ be the solutions to (4.30) and (4.43) respectively. Suppose Assumption 4.5 is valid. Then there holds*

$$\|u_{\gamma,h}(0) - U_{h,\gamma}^0\| \le c\tau|\log\tau|(h^2\gamma^{-1} + 1)\|u_0\|_{L^2(\Omega)},$$

where the constant c is independent on γ, h and t.

Proof. Let $\bar{U}^n_{h,\gamma}$ be the solution to (4.40) and $e_n = \bar{U}^n_{h,\gamma} - U^n_{h,\gamma}$, which satisfies the following equation

$$\bar\partial_\tau e_n + A_h(t_n)e_n = 0 \quad \text{for all} \quad 1 \le n \le N, \quad \text{with} \quad \gamma e_0 + e_N = \bar{U}^N_{h,\gamma} - u_{\gamma,h}(T) =: Q. \tag{4.46}$$

Then we apply the representation of fully discrete scheme to derive

$$e_0 = (\gamma I + F^N_{h,\tau}(N)))^{-1}\Big[Q - \sum_{k=1}^{N} \tau E^{N-k}_{h,\tau}(N)(A_h(T) - A_h(t_k))e_k\Big]. \tag{4.47}$$

Lemmas 4.16 and 4.18 give that

$$\begin{aligned}\|e_0\|_{L^2(\Omega)} &\le \Big\|F^N_{h,\tau}(N)^{-1}\Big[Q - \sum_{k=1}^{N} \tau \mathbb{E}^\tau_h(N-k;N)(A_h(T) - A_h(t_k))e_k\Big]\Big\|_{L^2(\Omega)} \\ &\le c_T\|A_h(T)Q\|_{L^2(\Omega)} + c(1+T^\alpha)\|\sum_{k=1}^{N} \tau A_h(T)E^{N-k}_{h,\tau}(N)(A_h(T) - A_h(t_k))e_k\|_{L^2(\Omega)}.\end{aligned}$$

This combined with Lemma 4.19 leads to

$$\|e_0\|_{L^2(\Omega)} \le c_T\tau|\log\tau|\|u_{\gamma,h}(0)\|_{L^2(\Omega)} + c(1+T^\alpha)\|\sum_{k=1}^{N} \tau A_h(T)E^{N-k}_{h,\tau}(N)(A_h(T) - A_h(t_k))e_k\|_{L^2(\Omega)}.$$

Then by applying the *a priori* estimate in Lemma 4.17 and the same argument in Theorems 4.2 and 4.4, we derive

$$\|e_0\|_{L^2(\Omega)} \le c_T\tau|\log\tau|\|u_{\gamma,h}(0)\|_{L^2(\Omega)}.$$

Finally, the Lemmas 4.6 and 4.14 leads to the desired result. □

Now we are ready to state the main theorem showing the error of the numerical reconstruction from noisy data. The proof is a direct result of Lemma 4.7, 4.14, 4.20 and 4.21.

Theorem 4.7. *Let $U^{0,\delta}_{h,\gamma}$ be the numerical reconstructed initial data using the fully discrete scheme* (4.38)*, and u_0 be the exact initial data. Suppose Assumption 4.5 is valid. Then if $\|u_0\|_{\dot H^q(\Omega)} \le c$ with $q \in (0,2]$ there holds*

$$\|U^{0,\delta}_{h,\gamma} - u_0\|_{L^2(\Omega)} \le c\Big(\gamma^{\frac{q}{2}} + \delta\gamma^{-1} + h^2\gamma^{-1} + \tau|\log\tau|(h^2\gamma^{-1}+1)\Big)$$

Moreover, for $u_0 \in L^2(\Omega)$, there holds

$$\|U^{0,\delta}_{h,\gamma} - u(0)\|_{L^2(\Omega)} \to 0 \quad \text{as} \quad \delta,\gamma,h,\tau \to 0, \quad \frac{\delta}{\gamma} \to 0 \quad \text{and} \quad \frac{h^2}{\gamma} \to 0.$$

The *a priori* error estimate in Theorem 4.7 gives a useful guideline to choose the regularization parameter γ and the discretization parameters h and τ according to the noise level δ. In particular, if $u_0 \in \dot H^q(\Omega)$, by choosing

$$\gamma \sim \delta^{\frac{2}{q+2}}, \quad h \sim \delta^{\frac12} \quad \text{and} \quad \tau|\log\tau| \sim \delta^{\frac{q}{q+2}},$$

we obtain the optimal approximation error

$$\|U^{0,\delta}_{h,\gamma} - u(0)\|_{L^2(\Omega)} \le c\delta^{\frac{q}{q+2}}.$$

4.4 Numerical Experiments

Now we test several two dimensional examples with $\Omega = (0,1)^2$ in order to illustrate our theoretical results. Throughout the section, we apply the standard Galerkin piecewise linear FEM with uniform mesh size $h = 1/(M+1)$ for the space discretization, and the backward Euler convolution quadrature method with uniform mesh size $\tau = T/N$ for time discretization. We solve the direct problem to obtain the exact observation data by using fine meshes, i.e. $h = 1/100$, $\tau = T/500$. Then we compute the noisy observational data by

$$g_\delta = u(T) + \varepsilon\delta \sup_{x\in\Omega} u(x,T)$$

where ε is generated from standard Gaussian distribution and δ denotes the related noisy level.

We begin with the following time-dependent diffusion coefficient:

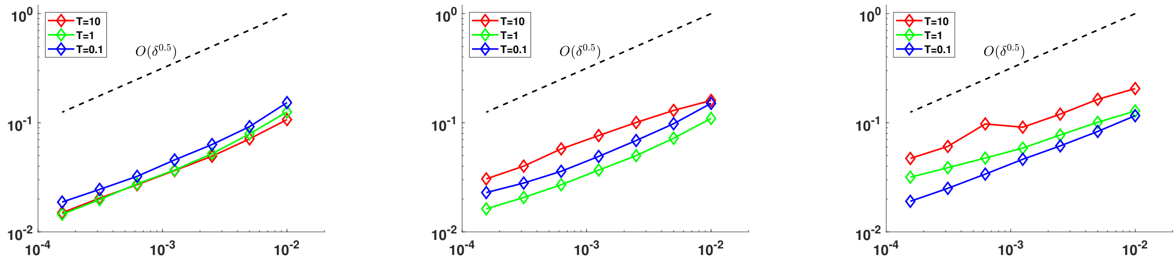
$$a_1(x,y,t) = \begin{pmatrix} y\sin((1+t)^{0.5}) + 2 & -0.1 \\ -0.1 & \sin(\pi x)(t+1.2)^{-0.8} + 2 \end{pmatrix},$$

satisfying conditions (4.2)-(4.3) and Assumption 4.3. We solve the linear system (4.38) by using the conjugate gradient method.

Example 5.1. Smooth initial data We begin with a smooth initial data:

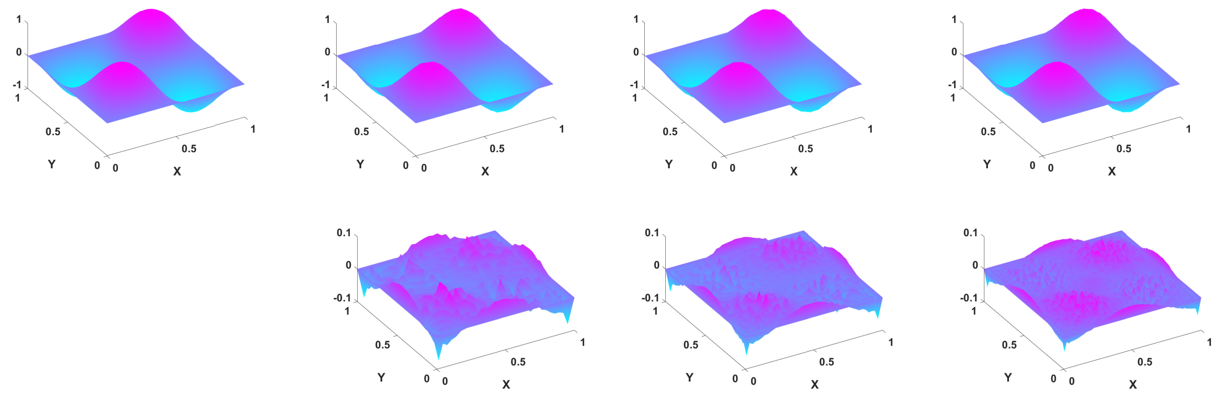
$$u_0 = \sin(2\pi x)\sin(2\pi y) \in \dot{H}^2(\Omega).$$

According to Theorem 4.7, we compute $U_{h,\gamma}^{0,\delta}$ with $\gamma \sim \sqrt{\delta}$ and $h, \tau \sim \sqrt{\delta}$, and expect a convergence of order $O(\sqrt{\delta})$. Numerical results presented in Figure 4.1 fully support the theoretical result. On the other hand, our numerical results indicate that the recovery is stable for all T, might be neither very large nor very small. This interesting phenomenon warrants further investigation in the future. In Figure 4.2, we present profiles of solutions and errors with different noise level.



(a) $\alpha = 0.25$. (b) $\alpha = 0.5$. (c) $\alpha = 0.75$.

Figure 4.1: Plot of error: $a_1(x,t)$ and smooth initial data; $h = \sqrt{\delta}$, $\tau\log(N+1) = \sqrt{\delta}/7$, $\gamma = \sqrt{\delta}/350$.



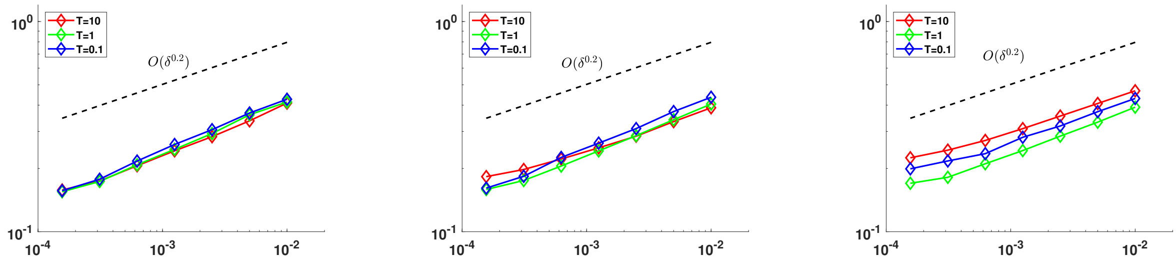
(a) $\delta = 1e-2$. (b) $\delta = 5e-3$. (c) $\delta = 2.5e-3$.

Figure 4.2: Profiles of Top left: Exact initial data u_0. Recover with $a_1(x,t)$, $\alpha = 0.5$, $T = 1$. The remaining three columns are profiles of numerical reconstructions $U_{h,\gamma}^{0,\delta}$ and theirs errors, with $h = \sqrt{\delta}$, $\tau = \sqrt{\delta}/5$, $\gamma = \sqrt{\delta}/350$.

Example 5.2. Nonsmooth initial data. In this example we consider the following nonsmooth initial condition

$$u_0 = \begin{cases} 1, & \text{if } 0.5 \le x \le 1, \\ 0, & \text{otherwise} \end{cases}$$

Note that $u_0 \in \dot{H}^{\frac{1}{2}-\varepsilon}(\Omega)$ for any $\varepsilon \in (0, \frac{1}{2})$. Then Theorem 4.7 indicate that the optimal convergence rate is almost $O(\delta^{0.2})$ provided that $\gamma = O(\delta^{0.8})$, $h = O(\sqrt{\delta})$ and $\tau = O(\delta^{0.2})$. This is fully supported by the numerical results presented in Figure 4.3. In Figure 4.4 we plot the profiles of solutions and errors, which also confirm that the numerical recovery is reliable.



(a) $\alpha = 0.25$. (b) $\alpha = 0.5$. (c) $\alpha = 0.75$.

Figure 4.3: Plot of error: $a_1(x,t)$ and smooth initial data; $h = \sqrt{\delta}$, $\tau = \delta^{0.2}/20$, $\gamma = \delta^{0.8}/200$.

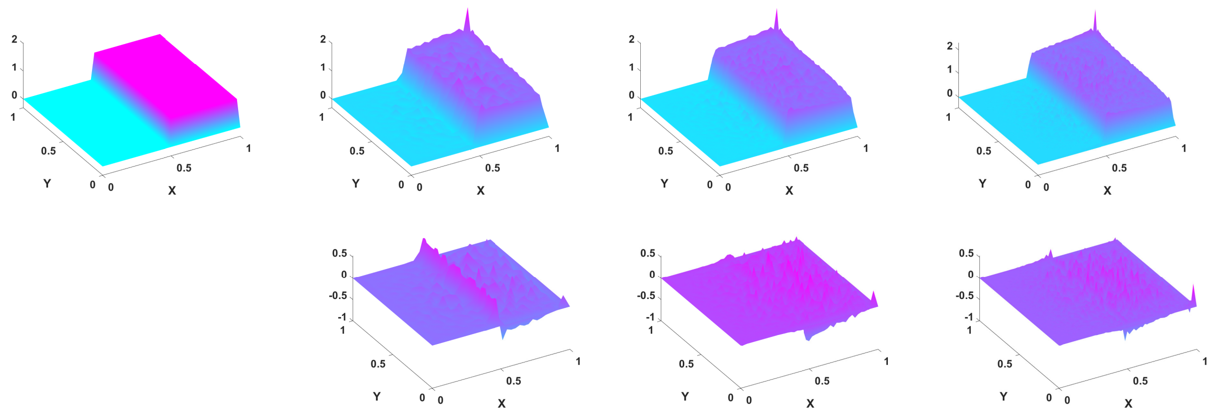


Figure 4.4: Top left: Exact initial data u_0. Recover with $a_1(x,t)$, $\alpha = 0.5$, $T = 1$. The remaining three columns are profiles of numerical reconstructions $U_{h,\gamma}^{0,\delta}$ and theirs errors, with $h = \sqrt{\delta}$, $\tau = \delta^{0.2}/20$, $\gamma = \delta^{0.8}/200$.

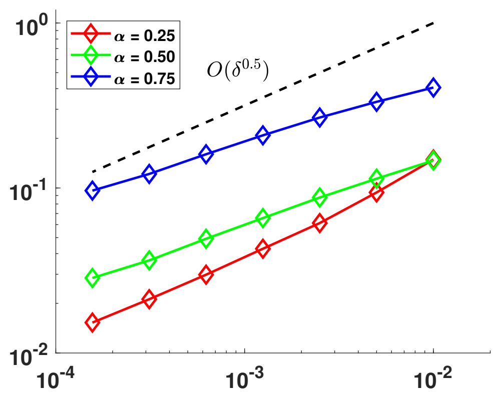


Figure 4.5: Plot of error: $a_2(x,t)$ and smooth initial data; $T = 10$, with $h = \sqrt{\delta}$, $\tau = \delta^{0.5}/5$, $\gamma = \delta^{0.5}/350$ for $\alpha = 0.25, 0.5$ and $\gamma = \delta^{0.5}/150$ for $\alpha = 0.75$.

Example 5.3. Diffusion coefficient violating Assumption 4.3. We also test the following diffusion coefficient

$$a_2(x,y,t) = \begin{pmatrix} e^{-x}\cos(t) + 2 & (1.5 - (t+1)^{-0.2})/10 \\ (1.5 - (t+1)^{-0.2})/10 & \cos(\pi y)\sin(t) + 2 \end{pmatrix}.$$

Note that a_2 satisfies conditions (4.2) and (4.3), but Assumption 4.3 is not fulfilled.

Numerical experiments show that the numerical reconstruction via the fully discrete scheme (4.38) still converges under proper parameter choices. For example, we test the smooth initial data $u_0 = \sin(2\pi x)\sin(2\pi y)$ and large terminal time $T = 10$. We choose $\gamma, h, \tau \sim \sqrt{\delta}$, and observe a convergence rate around $O(\sqrt{\delta})$, see cf. Figure 4.5. We will continue to consider the general case in our future studies.

Appendix

Appendix A. Proof of Lemma 4.4

For $p=0$, Conditions (4.2) and (4.3) and Assumption 4.3 imply

$$\begin{aligned}\|(A(t)-A(s))v\|_{L^2(\Omega)} &\le c\big(\|\nabla(a(t)-a(s))\|_{L^\infty(\Omega)}+\|a(t)-a(s)\|_{L^\infty(\Omega)}\big)\|v\|_{\dot H^2(\Omega)}\\ &\le c\min(1,\min(t,s)^{-\kappa}|t-s|)\|v\|_{\dot H^2(\Omega)}.\end{aligned}$$

For $p=-2$, from using the duality argument, we have

$$\begin{aligned}\|(A(t)-A(s))v\|_{\dot H^{-2}(\Omega)} &= \sup_{\varphi\in\dot H^2(\Omega)}\frac{\langle (A(t)-A(s))v,\varphi\rangle}{\|\varphi\|_{\dot H^2(\Omega)}}=\sup_{\varphi\in\dot H^2(\Omega)}\frac{(v,(A(t)-A(s))\varphi)}{\|\varphi\|_{\dot H^2(\Omega)}}\\ &\le \sup_{\varphi\in\dot H^2(\Omega)}\frac{\|v\|_{L^2(\Omega)}\|(A(t)-A(s))\varphi\|_{L^2(\Omega)}}{\|\varphi\|_{\dot H^2(\Omega)}}\\ &\le c\min(1,\min(t,s)^{-\kappa}|t-s|)\sup_{\varphi\in\dot H^2(\Omega)}\|v\|_{L^2(\Omega)}\end{aligned}$$

This completes the proof of the lemma.

Appendix B. Proof of Lemma 4.17

Recalling the fact that [51, Lemma 3.3]

$$U_h^n\bar\partial_\tau U_h^n \ge \frac{1}{2}\bar\partial_\tau|U_h^n|^2.$$

Therefore, like Lemma 4.3 we define an operator $\underline{A_h}=-c_0\Delta_h$. Condition 4.2 gives that the operator $A_h(t)-\underline{A_h}$ is self-adjoint and positive semidefinite for all $n\ge 1$. Rewrite the equation (4.35) as

$$\bar\partial_\tau(U_h^n-U_h^0)+\underline{A_h}U_n=(\underline{A_h}-A_h(t))U_h^n \quad \text{for all} \ \ 1\le n\le N.$$

Taking inner product with U_h^n on the above equation and by definition of $-\Delta_h$ and $A_h(t)$, we obtain

$$(\bar\partial_\tau(U_h^n-U_h^0),U_h^n)+c_0\|\nabla U_h^n\|^2_{L^2(\Omega)}=\big((c_0-a(\cdot,t))\nabla U_h^n,\nabla U_h^n\big)\le 0 \quad \text{for all} \ \ 1\le n\le N.$$

Using the above inequality and Poincaré inequality we arrive at

$$\begin{aligned}&\bar\partial_\tau(\|U_h^n\|_{L^2(\Omega)}-\|U_h^0\|_{L^2(\Omega)})+c\|U_h^n\|_{L^2(\Omega)}\\ &\le \bar\partial_\tau\Big[(\|U_h^n\|_{L(\Omega)}-\|U_h^0\|_{L^2(\Omega)})(1+\|U_h^0\|_{L^2(\Omega)}/\|U_h^n\|_{L^2(\Omega)})\Big]+c\|U_h^n\|_{L^2(\Omega)}\\ &\le 0 \quad \text{for all} \ \ n\ge 1,\end{aligned}$$

for a constant c uniform in t_n. Then the comparison principle for discrete fractional ODEs [65] leads to

$$\|U_h^n\|_{L^2(\Omega)}\le F_\tau^n(c)\|U_h^0\|_{L^2(\Omega)}\le\frac{c}{1+ct_n^\alpha}\|U_h^0\|_{L^2(\Omega)}$$

where the definition of $F_\tau^n(c)$ can be found in [111, 112]. This immediately leads to the desired result.

Next by solution representation (4.36) we have

$$
\begin{aligned}
&\|A_h(t_{n_*})U_h^n\|_{L^2(\Omega)}\\
&\le \|A_h(t_{n_*})F_{h,\tau}^n(n_*)U_h^0\|_{L^2(\Omega)} + \tau\|\sum_{k=1}^n A_h(t_{n_*})E_{h,\tau}^{n-k}(n_*)(I-A_h(t_k)A_h(t_{n_*})^{-1})A_h(t_{n_*})U_h^k\|_{L^2(\Omega)}\\
&\le ct_n^{-\alpha}\|U_h^0\|_{L^2(\Omega)} + \sum_{k=1}^n \|\tau A_h(t_{n_*})E_{h,\tau}^{n-k}(n_*)(I-A_h(t_k)A_h(t_{n_*})^{-1})\|\,\|A_h(t_{n_*})U_h^k\|_{L^2(\Omega)},
\end{aligned}
$$

lemma 4.16 and 4.8 show that

$$
\|A_h(t_{n_*})U_h^n\|_{L^2(\Omega)} \le ct_n^{-\alpha}\|U_h^0\|_{L^2(\Omega)} + \sum_{k=1}^n c\tau\|A_h(t_{n_*})U_h^k\|_{L^2(\Omega)},
$$

the discrete version of Gronwall's inequality [93, Lemma 10.5] gives that

$$
\|A_h(t_{n_*})U_h^n\|_{L^2(\Omega)} \le c\exp(ct_n)t_n^{-\alpha}\|U_h^0\|_{L^2(\Omega)}
$$

here c is uniform in n, τ and t_n.

Meanwhile, in the other hand $\|I-A(t_*)^{-1}A(s)\| \le c|t_*-s|^\beta$ for any $\beta\in[0,1]$. Then if $\beta=(1+\epsilon)\alpha$ with $\epsilon\in(0,1/\alpha-1)$ we can derive that[1]

$$
\begin{aligned}
&\|A_h(t_{n_*})U_h^n\|_{L^2(\Omega)}\\
&\le \|A_h(t_{n_*})F_{h,\tau}^n(n_*)U_h^0\|_{L^2(\Omega)} + \tau\|\sum_{k=1}^n A_h(t_{n_*})E_{h,\tau}^{n-k}(n_*)(I-A_h(t_k)A_h(t_{n_*})^{-1})A_h(t_{n_*})U_h^k\|_{L^2(\Omega)}\\
&\le ct_n^{-\alpha}\|U_h^0\|_{L^2(\Omega)} + \sum_{k=1}^n \|\tau A_h^2(t_{n_*})E_{h,\tau}^{n-k}(n_*)(I-A_h(t_{n_*})^{-1}A_h(t_k))\|\,\|U_h^k\|_{L^2(\Omega)}\\
&\le ct_n^{-\alpha}\|U_h^0\|_{L^2(\Omega)} + c\tau\sum_{k=1}^n (t_{n_*}-t_k)^{-1+\varepsilon\alpha}t_k^{-\alpha}\|U_h^0\|_{L^2(\Omega)}\\
&\le ct_n^{-\alpha}\|U_h^0\|_{L^2(\Omega)} + c\int_0^{t_n}(t_{n_*}-s)^{-1+\epsilon\alpha}s^{-\alpha}\mathrm{d}s\|U_h^0\|_{L^2(\Omega)} \le ct_n^{-(1-\epsilon)\alpha}\|U_h^0\|_{L^2(\Omega)}.
\end{aligned}
$$

[1] Chapter 4 is reprinted with permission from "Stability and numerical analysis of backward problem for subdiffusion with time-dependent coefficients", Zhengqi Zhang and Zhi Zhou, 2023, Inverse Problems 39 034001. The candidate mainly works on the research methodology discussion, the proof details and the coding and data collection in numerical experiments.

CHAPTER 5.

Backward Diffusion-Wave Problem: Stability and Numerical Analysis

In this Chapter Let $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$) be a convex polygonal domain with boundary $\partial\Omega$. We consider the following initial-boundary value problem of diffusion-wave equation with $\alpha \in (1, 2)$

$$\begin{aligned} \partial_t^\alpha u - \Delta u &= f, \quad && \text{in } \Omega \times (0, T], \\ u &= 0, && \text{on } \partial\Omega, \\ u(0) = a,\ \partial_t u(0) &= b, && \text{in } \Omega, \end{aligned} \tag{5.1}$$

where $T > 0$ is a fixed final time, $f \in L^\infty(0, T; L^2(\Omega))$ and $a, b \in L^2(\Omega)$ are given source term and initial data, respectively.

As Section 1.2, for the backward diffusion-wave problem, we want to simultaneously determine the initial data $u(x, 0)$ and $u_t(x, 0)$ with $x \in \Omega$ (and hence the function $u(x, t)$ for all $(x, t) \in \Omega \times (0, T)$) from two terminal observations

$$u(x, T_1) = g_1(x), \quad u(x, T_2) = g_2(x) \quad \text{for all } \ x \in \Omega, \tag{5.2}$$

where $T_1, T_2 \in (0, T]$ and $T_1 < T_2$.

The rest of this chapter is organized as follows. In section 5.1, we provide some preliminary results about solution representation, asymptotic behaviors of Mittag-Leffler functions, and regularization for the continuous problem. Then in sections 5.2 and 5.3, we propose and analyze spatially semi-discrete scheme and space-time fully discrete scheme, respectively. Finally, in section 5.4, we present some numerical examples to illustrate and complete the theoretical analysis.

The notation c denotes a generic constant, which may change at each occurrence, but it is always independent of the noise level δ, the regularization parameter γ, the mesh size h and time step τ etc.

By using Lemma 2.3, if $u(t)$ is the solution to the diffusion-wave equation, the function $w(t) = u(t) - \int_0^t E(t-s)f(s)\,\mathrm{d}s$ satisfies the diffusion-wave equation (2.12) with the trivial source term. Therefore, without loss of generality, throughout the paper we consider the homogeneous problem

$$\begin{aligned} \partial_t^\alpha u - \Delta u &= 0, \quad && \text{in } \Omega \times (0, T], \\ u &= 0, && \text{on } \partial\Omega, \\ u(0) = a,\ \partial_t u(0) &= b, && \text{in } \Omega. \end{aligned} \tag{5.3}$$

5.1 Stability and regularization for the backward diffuion-wave problems

5.1.1 Stability of the backward diffusion-wave problems

In this part, we intend to examine the well-posedness of the backward problem diffusion-wave problem for $0 < T_1 < T_2 \le T$

$$\begin{aligned} \partial_t^\alpha u - \Delta u = 0, &\quad \text{in } \Omega \times (0,T], \\ u = 0, &\quad \text{on } \partial\Omega, \\ u(T_1) = g_1,\ u(T_2) = g_2, &\quad \text{in } \Omega. \end{aligned} \tag{5.4}$$

Using the solution representation (2.13), we have the following relation

$$\begin{aligned} \begin{bmatrix} g_1 \\ g_2 \end{bmatrix} &= \mathcal{G}(T_1,T_2) \begin{bmatrix} a \\ b \end{bmatrix} := \begin{bmatrix} F(T_1) & \bar{F}(T_1) \\ F(T_2) & \bar{F}(T_2) \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} \\ &= \sum_{j=1}^\infty \begin{bmatrix} E_{\alpha,1}(-\lambda_j T_1^\alpha) & T_1 E_{\alpha,2}(-\lambda_j T_1^\alpha) \\ E_{\alpha,1}(-\lambda_j T_2^\alpha) & T_2 E_{\alpha,2}(-\lambda_j T_2^\alpha) \end{bmatrix} \begin{bmatrix} (a,\varphi_j)\varphi_j \\ (b,\varphi_j)\varphi_j \end{bmatrix}. \end{aligned} \tag{5.5}$$

In order to represent the inverse of the operator $\mathcal{G}(T_1,T_2)$, we define the function

$$\psi(T_1,T_2;\lambda_j) = T_2 E_{\alpha,1}(-\lambda_j T_1^\alpha) E_{\alpha,2}(-\lambda_j T_2^\alpha) - T_1 E_{\alpha,1}(-\lambda_j T_2^\alpha) E_{\alpha,2}(-\lambda_j T_1^\alpha). \tag{5.6}$$

Then $\mathcal{G}(T_1,T_2)^{-1}$ is well-defined, provided that $\psi(T_1,T_2;\lambda_j) \neq 0$ for all $j = 1, 2, \ldots$, and a direct computation leads to the relation

$$\begin{aligned} \begin{bmatrix} a \\ b \end{bmatrix} &= \mathcal{G}(T_1,T_2)^{-1} \begin{bmatrix} g_1 \\ g_2 \end{bmatrix} \\ &= \sum_{j=1}^\infty \psi(T_1,T_2;\lambda_j)^{-1} \begin{bmatrix} T_2 E_{\alpha,2}(-\lambda_j T_2^\alpha) & -T_1 E_{\alpha,2}(-\lambda_j T_1^\alpha) \\ -E_{\alpha,1}(-\lambda_j T_2^\alpha) & E_{\alpha,1}(-\lambda_j T_1^\alpha) \end{bmatrix} \begin{bmatrix} (g_1,\varphi_j)\varphi_j \\ (g_2,\varphi_j)\varphi_j \end{bmatrix}. \end{aligned} \tag{5.7}$$

The next lemma clarifies the conditions for $\psi(T_1,T_2;\lambda_j) \neq 0$ for all $j = 1, 2, \ldots$.

Lemma 5.1. *Let $\lambda > 0$ and $\psi(T_1,T_2;\lambda)$ be the function defined in (5.6). Then there exists a constant $M(\lambda)$ such that for all $T_2 > T_1 \ge M(\lambda)$, then*

$$\psi(T_1,T_2;\lambda) \le \frac{c(T_2-T_1)}{\Gamma(1-\alpha)\Gamma(2-\alpha)} \frac{1}{\lambda^2 T_1^\alpha T_2^\alpha} < 0,$$

where the constant c is independent of λ, T_1 and T_2.

Proof. By means of the asymptotic property of Mittag-Leffler functions in (2.6), we have

$$\psi(T_1,T_2;\lambda) = (T_2-T_1)\left(\frac{1}{\Gamma(1-\alpha)\Gamma(2-\alpha)} \frac{1}{\lambda^2 T_1^\alpha T_2^\alpha} + O\Big(\frac{1}{\lambda^4 T_1^{2\alpha} T_2^{2\alpha}}\Big)\right), \qquad \text{for } T_1, T_2 \to \infty. \tag{5.8}$$

For $\lambda > 0$ and $T_2 > T_1 > 0$, we know the leading term $\frac{1}{\Gamma(1-\alpha)\Gamma(2-\alpha)}\frac{1}{\lambda^2 T_1^\alpha T_2^\alpha} < 0$, and hence the asymptotic behavior (5.8) implies the existence of $M(\lambda)$ such that for all $T_2 > T_1 \geq M(\lambda)$

$$\psi(T_1, T_2; \lambda) \leq \frac{T_2 - T_1}{2\Gamma(1-\alpha)\Gamma(2-\alpha)}\frac{1}{\lambda^2 T_1^\alpha T_2^\alpha} < 0.$$

This completes the proof of the lemma. □

Combining Lemmas 2.1 and 5.1, we have the following stability estimate.

Theorem 5.1. *Let λ_1 be the smallest eigenvalue of $-\Delta$ with homogeneous Dirichlet boundary condition, and $M(\lambda_1)$ be the constant defined in Lemma 5.1. Suppose that $T_2 > T_1 \geq M(\lambda_1)$. Then for any $g_1, g_2 \in \dot{H}^2(\Omega)$, there exists $a, b \in L^2(\Omega)$ such that the solution u to (5.3) satisfies*

$$u(T_1) = g_1 \quad \text{and} \quad u(T_2) = g_2.$$

Meanwhile, there holds the following two-sided Lipschitz stability

$$c_1\Big(\|g_1\|_{\dot{H}^2(\Omega)} + \|g_2\|_{\dot{H}^2(\Omega)}\Big) \leq \|a\|_{L^2(\Omega)} + \|b\|_{L^2(\Omega)} \leq c_2\Big(\|g_1\|_{\dot{H}^2(\Omega)} + \|g_2\|_{\dot{H}^2(\Omega)}\Big). \tag{5.9}$$

Proof. By Lemma 5.1 and the asymptotic estimate (5.8), we have for all $T_2 > T_1 > M(\lambda_1)$ and $\lambda \geq \lambda_1$

$$|\psi(T_1, T_2; \lambda)| \geq \left|\frac{c(T_2 - T_1)}{\Gamma(1-\alpha)\Gamma(2-\alpha)}\frac{1}{\lambda^2 T_1^\alpha T_2^\alpha}\right| > 0, \tag{5.10}$$

where the constant c is independent of λ_j, T_1 and T_2. This together with (5.7) indicates the existence and uniqueness of initial data a and b.

Next we turn to the stability estimate. Noting that the first inequality has been confirmed by Lemma 2.3, so it suffices to verify the second one. The estimate (5.10) and the relation (5.7) imply

$$\begin{aligned}
\|a\|_{L^2(\Omega)}^2 + \|b\|_{L^2(\Omega)}^2 &\leq \frac{c}{(T_2 - T_1)^2}\sum_{j=1}^{\infty}\lambda_j^4\Big(\frac{(g_1, \varphi_j)^2}{(1 + \lambda_j T_2^\alpha)^2} + \frac{(g_2, \varphi_j)^2}{(1 + \lambda_j T_2^\alpha)^2}\Big) \\
&\leq \frac{c}{(T_2 - T_1)^2}\Big(\|g_1\|_{\dot{H}^2(\Omega)}^2 + \|g_2\|_{\dot{H}^2(\Omega)}^2\Big).
\end{aligned}$$

□

Remark 5.1. *Note that in the stability estimate* (5.9) *the constant c_2 is proportional to $(T_2 - T_1)^{-1}$. This is reasonable since one cannot recover two initial data $u(0)$ and $\partial_t u(0)$ from a single observation $u(T)$. Throughout our numerical analysis, we shall assume that $T_2 > T_1 \geq M(\lambda_1)$ and $T_2 - T_1 \geq c_0 > 0$.*

5.1.2 Regularization and convergence analysis

From now on, we shall assume that our observation is noisy with noise level δ, i.e.,

$$\|g_1 - g_1^\delta\|_{L^2(\Omega)} = \|g_2 - g_2^\delta\|_{L^2(\Omega)} = \delta. \tag{5.11}$$

Note that both g_1^δ and g_2^δ are nonsmooth. In order to regularize the mildly ill-posed problem, we apply the quasi-boundary value method [27, 108]: find $\tilde{u}^\delta(t)$ satisfies

$$\begin{aligned} \partial_t^\alpha \tilde{u}^\delta - \Delta \tilde{u}^\delta &= 0, && \text{in } \Omega \times (0,T], \\ \tilde{u}^\delta &= 0, && \text{on } \partial\Omega, \\ -\gamma \tilde{u}^\delta(0) + \tilde{u}^\delta(T_1) &= g_1^\delta, && \text{in } \Omega, \\ \gamma \partial_t \tilde{u}^\delta(0) + \tilde{u}^\delta(T_2) &= g_2^\delta, && \text{in } \Omega, \end{aligned} \tag{5.12}$$

where the constant $\gamma > 0$ denotes the regularization parameter. Recalling the definition of the operator $\mathcal{G}(T_1, T_2)$ in (5.5), the solution to the regularized problem (5.12) could be written as

$$\begin{aligned} \begin{bmatrix} g_1^\delta \\ g_2^\delta \end{bmatrix} &= (\gamma \mathcal{I} + \mathcal{G}(T_1,T_2)) \begin{bmatrix} \tilde{u}(0) \\ \partial_t \tilde{u}(0) \end{bmatrix} \\ &:= \sum_{j=1}^{\infty} \begin{bmatrix} -\gamma + E_{\alpha,1}(-\lambda_j T_1^\alpha) & T_1 E_{\alpha,2}(-\lambda_j T_1^\alpha) \\ E_{\alpha,1}(-\lambda_j T_2^\alpha) & \gamma + T_2 E_{\alpha,2}(-\lambda_j T_2^\alpha) \end{bmatrix} \begin{bmatrix} (\tilde{u}^\delta(0), \varphi_j)\varphi_j \\ (\partial_t \tilde{u}^\delta(0), \varphi_j)\varphi_j \end{bmatrix} \end{aligned}$$

where $\mathcal{I}$ denotes the matrix of operators

$$\mathcal{I} = \begin{bmatrix} -I & 0 \\ 0 & I \end{bmatrix} \tag{5.13}$$

where I is the identity operator.

Now we define an auxiliary function

$$\tilde{\psi}(T_1, T_2; \lambda_j) := \psi(T_1, T_2; \lambda_j) - \gamma^2 + \gamma[E_{\alpha,1}(-\lambda_j T_1^\alpha) - T_2 E_{\alpha,2}(-\lambda_j T_2^\alpha)]. \tag{5.14}$$

Lemma 2.1 implies that there exists a constant $z_0 > 0$ such that for $z \geq z_0$,

$$E_{\alpha,1}(-z) \leq \frac{1}{\Gamma(1-\alpha)} \frac{1}{z} < 0 \quad \text{and} \quad E_{\alpha,2}(-z) \geq \frac{1}{\Gamma(2-\alpha)} \frac{1}{z} > 0.$$

Without loss of generality, we assume that

$$M(\lambda_1)^\alpha > z_0/\lambda_1. \tag{5.15}$$

Then with $T_2 > T_1 \geq M(\lambda_1)$,

$$\tilde{\psi}(T_1, T_2; \lambda_j) \leq -c\Big(\lambda_j^{-2} + \gamma \lambda_j^{-1} + \gamma^2\Big) < 0, \tag{5.16}$$

where c is only dependent on T_1, T_2 and α.

Then based the discussion in Theorem 5.1 we would have uniqueness for the regularized backward problem (5.12).

Lemma 5.2. *Let λ_1 be the smallest eigenvalue of $-\Delta$ with homogeneous Dirichlet boundary condition, and $M(\lambda_1)$ be the constant satisfying* (5.15). *Suppose that $T_2 > T_1 \geq M(\lambda_1)$. Then for any $g_1^\delta, g_2^\delta \in L^2(\Omega)$, there exists $\tilde{u}^\delta(0) \in L^2(\Omega)$ and $\partial_t \tilde{u}^\delta(0) \in L^2(\Omega)$ such that the solution $\tilde{u}^\delta$ to* (5.12) *satisfies*

$$-\gamma \tilde{u}^\delta(0) + \tilde{u}^\delta(T_1) = g_1^\delta,$$
$$\gamma \partial_t \tilde{u}^\delta(0) + \tilde{u}^\delta(T_2) = g_2^\delta.$$

Proof. From solution representation (5.7) there holds the relation

$$\begin{aligned}\begin{bmatrix} \tilde{u}^\delta(0) \\ \partial_t \tilde{u}^\delta(0) \end{bmatrix} &= (\gamma \mathcal{I} + \mathcal{G}(T_1, T_2))^{-1} \begin{bmatrix} g_1^\delta \\ g_2^\delta \end{bmatrix} \\ &= \sum_{j=1}^\infty \widetilde{\psi}(T_1, T_2; \lambda_j)^{-1} \begin{bmatrix} \gamma + T_2 E_{\alpha,}(-\lambda_j T_2^\alpha) & -T_1 E_{\alpha,2}(-\lambda_j T_1^\alpha) \\ -E_{\alpha,1}(-\lambda_j T_2^\alpha) & -\gamma + E_{\alpha,1}(-\lambda_j T_1^\alpha) \end{bmatrix} \begin{bmatrix} (g_1^\delta, \varphi_j)\varphi_j \\ (g_2^\delta, \varphi_j)\varphi_j \end{bmatrix}.\end{aligned} \tag{5.17}$$

And from (5.15) if $T_2 > T_1 \geq M(\lambda_1)$, (5.16) shows that $(\gamma \mathcal{I} + \mathcal{G}(T1, T_1))$ is invertible therefore the uniqueness is followed. ∎

Meanwhile, with $\mathcal{F}(t) = [F(t)\ \bar{F}(t)]$, we know

$$\tilde{u}^\delta(t) = \mathcal{F}(t)(\gamma \mathcal{I} + \mathcal{G}(T_1, T_2))^{-1} \begin{bmatrix} g_1^\delta \\ g_2^\delta \end{bmatrix}. \tag{5.18}$$

Now we intend to establish estimates for $u(0) - \tilde{u}^\delta(0)$, $\partial_t u(0) - \partial_t \tilde{u}^\delta(0)$ and $u(t) - \tilde{u}^\delta(t)$. To this end, we need the following auxiliary function

$$\tilde{u}(t) = \mathcal{F}(t)(\gamma I + \mathcal{G}(T_1, T_2))^{-1} \begin{bmatrix} g_1 \\ g_2 \end{bmatrix} = \mathcal{F}(t)(\gamma I + \mathcal{G}(T_1, T_2))^{-1} \mathcal{G}(T_1, T_2) \begin{bmatrix} a \\ b \end{bmatrix}, \tag{5.19}$$

which is the solution to the following quasi boundary value problem:

$$\begin{aligned} \partial_t^\alpha \tilde{u} - \Delta \tilde{u} &= 0, && \text{in } \Omega \times (0, T], \\ \tilde{u} &= 0, && \text{on } \partial\Omega, \\ -\gamma \tilde{u}(0) + \tilde{u}(T_1) &= g_1, && \text{in } \Omega, \\ \gamma \partial_t \tilde{u}(0) + \tilde{u}(T_2) &= g_2, && \text{in } \Omega. \end{aligned} \tag{5.20}$$

The next lemma provides an estimate for the operator $\mathcal{F}(t)(\gamma \mathcal{I} + \mathcal{G}(T_1, T_2))^{-1}$.

Lemma 5.3. *Let $M(\lambda_1)$ be the constant defined in Lemma 5.1, and suppose that $T_2 > T_1 \geq M(\lambda_1)$. Let $\mathcal{F}(t)$ and $(\gamma \mathcal{I} + \mathcal{G}(T_1, T_2))^{-1}$ be defined in* (2.13) *and* (5.17)*, then for all $0 < t \leq T$, $v, w \in \dot{H}^q(\Omega)$, for any $0 \leq p \leq q \leq 2 + p$, we have*

$$\left\| \left(\frac{d}{dt}\right)^\ell \mathcal{F}(t)(\gamma \mathcal{I} + \mathcal{G}(T_1, T_2))^{-1} \begin{bmatrix} v \\ w \end{bmatrix} \right\|_{\dot{H}^p(\Omega)} \leq c t^{-\ell} \min(\gamma^{-(1+\frac{p-q}{2})}, t^{-\alpha(1+\frac{p-q}{2})})(\|v\|_{\dot{H}^q(\Omega)} + \|w\|_{\dot{H}^q(\Omega)}).$$

Meanwhile, we have

$$\left\| (\gamma \mathcal{I} + \mathcal{G}(T_1,T_2))^{-1} \begin{bmatrix} v \\ w \end{bmatrix} \right\|_{\dot H^p(\Omega)} \le c\gamma^{-(1+\frac{p-q}{2})}(\|v\|_{\dot H^q(\Omega)} + \|w\|_{\dot H^q(\Omega)}).$$

Proof. Firstly, for $0 < t \le T$, we let

$$\begin{aligned}\zeta(t) &= \mathcal{F}(t)(\gamma I + \mathcal{G}(T_1,T_2))^{-1} \begin{bmatrix} v \\ w \end{bmatrix} \\ &= \sum_{j=1}^{\infty} \tilde\psi(T_1,T_2;\lambda_j)^{-1} \begin{bmatrix} E_{\alpha,1}(-\lambda_j t^\alpha) & tE_{\alpha,2}(-\lambda_j t^\alpha) \end{bmatrix} \\ &\qquad \begin{bmatrix} \gamma + T_2 E_{\alpha,2}(-\lambda_j T_2^\alpha) & -T_1 E_{\alpha,2}(-\lambda_j T_1^\alpha) \\ -E_{\alpha,1}(-\lambda_j T_2^\alpha) & -\gamma + E_{\alpha,1}(-\lambda_j T_1^\alpha) \end{bmatrix} \begin{bmatrix} (v,\varphi_j)\varphi_j \\ (w,\varphi_j)\varphi_j \end{bmatrix}.\end{aligned}$$

By means of Lemmas 2.1, we arrive at

$$\begin{bmatrix} |E_{\alpha,1}(-\lambda_j t^\alpha)| & |tE_{\alpha,2}(-\lambda_j t^\alpha)| \end{bmatrix} \le \frac{c}{1+\lambda_j t^\alpha} \begin{bmatrix} 1 & t \end{bmatrix}. \tag{5.21}$$

Similarly, by Lemma 2.1 and the estimate (5.16)

$$|\partial_t \psi(T_1,T_2;\lambda_j)|^{-1} \begin{bmatrix} |\gamma + T_2 E_{\alpha,2}(-\lambda_j T_2^\alpha)| & |-T_1 E_{\alpha,2}(-\lambda_j T_1^\alpha)| \\ |-E_{\alpha,1}(-\lambda_j T_2^\alpha)| & |-\gamma + E_{\alpha,1}(-\lambda_j T_1^\alpha)| \end{bmatrix} \le \frac{c\lambda_j}{1+\gamma\lambda_j} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \tag{5.22}$$

Combining (5.21) and (5.22) we obtain

$$\begin{aligned}\lambda_j^p(\zeta(t),\varphi_j)^2 &\le c\left(\frac{\lambda_j^{1+\frac{p-q}{2}}}{(1+\gamma\lambda_j)(1+\lambda_j t^\alpha)}\right)^2 \lambda_j^q((v,\varphi_j)^2 + (w,\varphi_j)^2) \\ &\le c\Big(\min(\gamma^{-(1+\frac{p-q}{2})}, t^{-\alpha(1+\frac{p-q}{2})})\Big)^2 \lambda_j^q((v,\varphi_j)^2 + (w,\varphi_j)^2).\end{aligned}$$

As a result, we conclude that

$$\begin{aligned}\|\zeta(t)\|^2_{\dot H^p(\Omega)} &\le c\Big(\min(\gamma^{-(1+\frac{p-q}{2})}, t^{-\alpha(1+\frac{p-q}{2})})\Big)^2 \sum_{j=1}^{\infty} \lambda_j^q((v,\varphi_j)^2 + (w,\varphi_j)^2) \\ &= c\Big(\min(\gamma^{-(1+\frac{p-q}{2})}, t^{-\alpha(1+\frac{p-q}{2})})\Big)^2 \Big(\|v\|^2_{\dot H^q(\Omega)} + \|w\|^2_{\dot H^q(\Omega)}\Big).\end{aligned}$$

Now we turn to the second estimate. Noting that

$$\begin{aligned}\begin{bmatrix} \zeta \\ \xi \end{bmatrix} &= (\gamma I + \mathcal{G}(T_1,T_2))^{-1} \begin{bmatrix} v \\ w \end{bmatrix} \\ &= \sum_{j=1}^{\infty} \tilde\psi(T_1,T_2;\lambda_j)^{-1} \begin{bmatrix} \gamma + T_2 E_{\alpha,}(-\lambda_j T_2^\alpha) & -T_1 E_{\alpha,2}(-\lambda_j T_1^\alpha) \\ -E_{\alpha,1}(-\lambda_j T_2^\alpha) & -\gamma + E_{\alpha,1}(-\lambda_j T_1^\alpha) \end{bmatrix} \begin{bmatrix} (v,\varphi_j)\varphi_j \\ (w,\varphi_j)\varphi_j \end{bmatrix},\end{aligned}$$

the estimate (5.22) leads to

$$\begin{aligned}\|\zeta\|_{\dot H^p(\Omega)}^2+\|\xi\|_{\dot H^p(\Omega)}^2 &\le c\sum_{j=1}^{\infty}\Big(\frac{\lambda_j^{1+\frac{p-q}{2}}}{1+\gamma\lambda_j}\Big)^2\lambda_j^q\Big((v,\varphi_j)^2+(w,\varphi_j)^2\Big)\\ &\le c\gamma^{-(2+(p-q))}\Big(\|v\|_{\dot H^q(\Omega)}^2+\|w\|_{\dot H^q(\Omega)}^2\Big).\end{aligned}$$

This completes the proof of the lemma. □

Using the similar argument, we have the following estimates for higher regularity estimate for $\tilde u(0)$ and $\partial_t\tilde u(0)$, which will be intensively used in the next section.

Corollary 5.1. *Let $M(\lambda_1)$ be the constant defined in Lemma 5.1, and suppose that $T_2 > T_1 \ge M(\lambda_1)$. Let $\tilde u$ be the solution to*(5.20)*. Then there holds*

$$\|\tilde u(0)\|_{\dot H^q(\Omega)}+\|\partial_t\tilde u(0)\|_{\dot H^q(\Omega)}\le c\gamma^{-q/2}\Big(\|a\|_{L^2(\Omega)}+\|b\|_{L^2(\Omega)}\Big).$$

Proof. Recalling the representation (5.19), we apply the similar argument in the proof of Lemma 5.3 to derive

$$\begin{aligned}\begin{bmatrix}\lambda_j^q(\tilde u(0),\varphi_j)^2\\ \lambda_j^q(\partial_t\tilde u(0),\varphi_j)^2\end{bmatrix} &\le c\left(\frac{\lambda_j^{1+q/2}}{(1+\gamma\lambda_j)(1+\lambda_jT_1^\alpha)}\right)^2\Big((a,\varphi_j)^2+(b,\varphi_j)^2\Big)\begin{bmatrix}1\\1\end{bmatrix}\\ &\le c\left(\frac{\lambda_j^{q/2}}{1+\gamma\lambda_j}\right)^2\Big((a,\varphi_j)^2+(b,\varphi_j)^2\Big)\begin{bmatrix}1\\1\end{bmatrix}\\ &\le c\gamma^{-q}\Big((a,\varphi_j)^2+(b,\varphi_j)^2\Big)\begin{bmatrix}1\\1\end{bmatrix}.\end{aligned}$$

Then the desired result follows immediately. □

Lemma 5.3 with $p=q=0$ immediately leads to the estimate for $\tilde u^\delta-\tilde u$.

Corollary 5.2. *Let $M(\lambda_1)$ be the constant defined in Lemma 5.1, and suppose that $T_2 > T_1 \ge M(\lambda_1)$. Let $\tilde u^\delta$ and $\tilde u$ be solutions to* (5.12) *and* (5.20)*, respectively. Then for any $a,b\in L^2(\Omega)$ we have*

$$\|(\tilde u^\delta-\tilde u)(t)\|_{L^2(\Omega)}\le c\,\delta\min(\gamma^{-1},t^{-\alpha})\qquad\textit{for all}\ \ t\in(0,T]$$

and

$$\|(\tilde u^\delta-\tilde u)(0)\|_{L^2(\Omega)}+\|\partial_t(\tilde u^\delta-\tilde u)(0)\|_{L^2(\Omega)}\le c\,\delta\gamma^{-1}.$$

According to Lemma 5.3 we can derive the following estimate of $\tilde u(t)-u(t)$ with $t\in[0,T]$.

Lemma 5.4. *Let $M(\lambda_1)$ be the constant defined in Lemma 5.1, and suppose that $T_2 > T_1 \ge M(\lambda_1)$. Let $u(t)$ and $\tilde u(t)$ be the solutions of problems* (5.3) *and* (5.20)*, respectively.*

(i) For $a, b \in \dot{H}^q(\Omega)$ with $q \in [0,2]$, we have

$$\|(\tilde{u}-u)(0)\|_{L^2(\Omega)} + \|\partial_t(\tilde{u}-u)(0)\|_{L^2(\Omega)} \leq c\gamma^{\frac{q}{2}}$$

and for all $t \in (0,T]$

$$\|(\tilde{u}-u)(t)\|_{L^2(\Omega)} \leq c\gamma \min(\gamma^{-(1-\frac{q}{2})}, t^{-(1-\frac{q}{2})\alpha}).$$

(ii) In case that $a, b \in L^2(\Omega)$, we have for any small $s \in (0,1]$

$$\lim_{\gamma\to 0}\Big(\|(\tilde{u}-u)(0)\|_{L^2(\Omega)} + \|\partial_t(\tilde{u}-u)(0)\|_{\dot{H}^{-s}(\Omega)}\Big) = 0.$$

Proof. Recalling the definition of the operator $\mathcal{G}(T_1,T_2)$ in (5.5), we have the representation

$$\begin{aligned}
\begin{bmatrix} (\tilde{u}-u)(0) \\ \partial_t(\tilde{u}-u)(0) \end{bmatrix} &= (\gamma\mathcal{I}+\mathcal{G}(T_1,T_2))^{-1}\mathcal{G}(T_1,T_2)\begin{bmatrix} a \\ b \end{bmatrix} - \begin{bmatrix} a \\ b \end{bmatrix} \\
&= (\gamma\mathcal{I}+\mathcal{G}(T_1,T_2))^{-1}(\mathcal{G}(T_1,T_2) - (\gamma\mathcal{I}+\mathcal{G}(T_1,T_2)))\begin{bmatrix} a \\ b \end{bmatrix} \\
&= -\gamma(\gamma\mathcal{I}+\mathcal{G}(T_1,T_2))^{-1}\mathcal{I}\begin{bmatrix} a \\ b \end{bmatrix}.
\end{aligned}$$

From lemma 5.3 for $p=0$, we have

$$\|(\tilde{u}-u)(0)\|_{L^2(\Omega)} + \|\partial_t(\tilde{u}-u)(0)\|_{L^2(\Omega)} \leq c\gamma^{\frac{q}{2}}(\|a\|_{\dot{H}^q(\Omega)} + \|b\|_{\dot{H}^q(\Omega)}).$$

Similarly, we have the following representation to $(\tilde{u}-u)(t)$:

$$\begin{aligned}
(\tilde{u}-u)(t) &= \mathcal{F}(t)(\gamma\mathcal{I}+\mathcal{G}(T_1,T_2))^{-1}\mathcal{G}(T_1,T_2)\begin{bmatrix} a \\ b \end{bmatrix} - \mathcal{F}(t)\begin{bmatrix} a \\ b \end{bmatrix} \\
&= -\gamma\mathcal{F}(t)(\gamma\mathcal{I}+\mathcal{G}(T_1,T_2))^{-1}\mathcal{I}\begin{bmatrix} a \\ b \end{bmatrix}.
\end{aligned}$$

We apply Lemma 5.3 with $p=0$ again to obtain

$$\|(\tilde{u}-u)(t)\|_{L^2(\Omega)} \leq c\gamma \min(\gamma^{-(1-\frac{q}{2})}, t^{-(1-\frac{q}{2})\alpha}).$$

Now we show the estimate (ii) for $q=0$. In case that $a, b \in L^2(\Omega)$, we know that $\tilde{u}, u \in C([0,T]; L^2(\Omega))$. Then for any small ϵ, we choose t_0 small enough such that

$$\|\tilde{u}(t_0) - \tilde{u}(0)\|_{L^2(\Omega)} + \|u(t_0) - u(0)\|_{L^2(\Omega)} < \epsilon/2.$$

Then by the estimate in (i), we may find γ_0 small enough such that

$$\|\tilde{u}(t_0) - u(t_0)\|_{L^2(\Omega)} < \epsilon/2 \quad \text{for all } \gamma < \gamma_0.$$

By triangle inequality, we obtain that for any $\gamma < \gamma_0$

$$\|\tilde{u}(0) - u(0)\|_{L^2(\Omega)} < \epsilon.$$

Therefore, $\tilde{u}(0)$ converges to $u(0)$ in L^2-sense, as $\gamma \to 0$. Finally, the convergence of $\partial_t \tilde{u}(0)$ in H^{-s} follows from (i) and a shift argument. □

Combining Corollary 5.2 and Lemma 5.4, we obtain the following convergence result.

Theorem 5.2. *Let $M(\lambda_1)$ be the constant defined in Lemma 5.1, and suppose that $T_2 > T_1 \geq M(\lambda_1)$. Let $u(t)$ and $\tilde{u}^\delta(t)$ be the solutions of problems* (5.3) *and* (5.12)*, respectively.*

(i) For $a, b \in \dot{H}^q(\Omega)$ with $q \in [0, 2]$, we have

$$\|(\tilde{u}^\delta - u)(0)\|_{L^2(\Omega)} + \|\partial_t(\tilde{u}^\delta - u)(0)\|_{L^2(\Omega)} \leq c\Big(\gamma^{\frac{q}{2}} + \delta\gamma^{-1}\Big)$$

and for all $t \in (0, T]$

$$\|(\tilde{u}^\delta - u)(t)\|_{L^2(\Omega)} \leq c\big(\gamma \min(\gamma^{-(1-\frac{q}{2})}, t^{-\alpha(1-\frac{q}{2})}) + \delta \min(\gamma^{-1}, t^{-\alpha})\big).$$

(ii) In case that $a, b \in L^2(\Omega)$, we have for any small $s \in (0, 1]$

$$\|(\tilde{u}^\delta - u)(0)\|_{L^2(\Omega)} + \|\partial_t(\tilde{u}^\delta - u)(0)\|_{\dot{H}^{-s}(\Omega)} \to 0 \quad \text{for} \quad \delta, \gamma \to 0, \frac{\delta}{\gamma} \to 0.$$

Remark 5.2. *To approximate $u(t)$ with $t > 0$, Theorem 5.2 indicates an optimal regularized parameter $\gamma \sim \delta$, and the error is of the order $O(\delta)$ which is independent of the smoothness of initial data. Meanwhile, for $t = 0$, the choice $\gamma \sim \delta^{\frac{2}{q+2}}$ leads to the optimal approximation $O(\delta^{\frac{q}{q+2}})$ if $a, b \in \dot{H}^q(\Omega)$ with $q \in (0, 2]$.*

5.2 Spatially semidiscrete scheme and error analysis

In this section, we shall propose and analyze a spatially semidiscrete scheme for solving the backward diffusion wave problem. The semidiscrete scheme would give an insight view to understand the role of the regularity of problem data and plays an important role in the analysis of fully discrete scheme.

5.2.1 Semidiscrete scheme for solving direct problem

We would also use the piecewise linear finite element methods for space discretization. And we introduce the space discretization parameter h, the finite element space X_h, the L^2 projection P_h and the Ritz projection R_h in Section 2.5.

Then the semidiscrete standard Galerkin FEM for problem (5.3) reads: find $u_h(t) \in X_h$ such that

$$\begin{aligned} &(\partial_t^\alpha u_h, \chi) + (\nabla u_h, \nabla \chi) = (f, \chi),\ \forall \chi \in X_h,\ T \geq t > 0, \\ &u_h(0) = P_h a, \quad \partial_t u_h(0) = P_h b. \end{aligned} \tag{5.23}$$

By introducing the discrete Laplacian $-\Delta_h : X_h \to X_h$ such that

$$(-\Delta_h \xi, \chi) = (\nabla \xi, \nabla \chi),\ \forall \xi, \chi \in X_h,$$

spatially semidiscrete problem (5.23) could be written as

$$\begin{aligned} \partial_t^\alpha u_h - \Delta_h u_h &= f_h,\ T \geq t > 0, \\ u_h(0) = P_h a, \quad \partial_t u_h(0) &= P_h b. \end{aligned} \tag{5.24}$$

Let $\{\lambda_j^h, \varphi_j^h\}_{j=1}^J$ be eigenpairs of $-\Delta_h$ with $\lambda_1^h \leq \lambda_2^h \leq \dots \lambda_J^h$. By the Courant minimax principle and the fact that $X_h \subset H_0^1(\Omega)$, we know

$$\lambda_1^h = \min_{\phi_h \in X_h} \frac{(-\Delta_h \phi_h, \phi_h)}{\|\phi_h\|_{L^2(\Omega)}^2} = \min_{\phi_h \in X_h} \frac{(\nabla \phi_h, \nabla \phi_h)}{\|\phi_h\|_{L^2(\Omega)}^2} \geq \min_{\phi \in H_0^1} \frac{(\nabla \phi, \nabla \phi)}{\|\phi\|_{L^2(\Omega)}^2} = \lambda_1. \tag{5.25}$$

Analogue to (2.13), the solution to the semidiscrete problem (5.24) could be written as

$$\begin{aligned} u_h(t) &:= \mathcal{F}_h(t) \begin{bmatrix} P_h a \\ P_h b \end{bmatrix} + \int_0^t E_h(t-s) P_h f_h(s)\, \mathrm{d}s \\ &:= \begin{bmatrix} F_h & \bar{F}_h \end{bmatrix} \begin{bmatrix} P_h a \\ P_h b \end{bmatrix} + \int_0^t E_h(t-s) P_h f_h(s)\, \mathrm{d}s \end{aligned} \tag{5.26}$$

where the solution operators $F(t)$, $\bar{F}(t)$ and $E(t)$ are respectively defined by

$$\begin{aligned} F_h(t) v_h &= \sum_{j=1}^J E_{\alpha,1}(-\lambda_j^h t^\alpha)(v_h, \varphi_j^h)\varphi_j^h, \quad \bar{F}_h(t) v_h = \sum_{j=1}^J t E_{\alpha,2}(-\lambda_j^h t^\alpha)(v_h, \varphi_j^h)\varphi_j^h, \\ E_h(t) v_h &= \sum_{j=1}^J t^{\alpha-1} E_{\alpha,\alpha}(-\lambda_j^h t^\alpha)(v_h, \varphi_j^h)\varphi_j^h \end{aligned} \tag{5.27}$$

for any $v_h \in X_h$. By Laplace Transform, we have the following integral representations of the solution operators:

$$\begin{aligned} F_h(t) &= \frac{1}{2\pi i} \int_{\Gamma_{\theta,\sigma}} e^{zt} z^{\alpha-1} (z^\alpha - \Delta_h)^{-1} dz, \quad \bar{F}_h(t) = \frac{1}{2\pi i} \int_{\Gamma_{\theta,\sigma}} e^{zt} z^{\alpha-2} (z^\alpha - \Delta_h)^{-1} dz, \\ E_h(t) &= \frac{1}{2\pi i} \int_{\Gamma_{\theta,\sigma}} e^{zt} (z^\alpha - \Delta_h)^{-1} dz. \end{aligned} \tag{5.28}$$

The discrete solution operator $E_h(t)$ satisfies the following smoothing property. See the proof for the case $\alpha \in (0,1)$ in [40, Lemma 3.2] and the proof for the diffusion wave-model is the same exactly.

Lemma 5.5. *Let $E_h(t)$ be the operator defined in* (5.27). *Then we have for all $t > 0$ and $q \in [0,1]$*

$$\|(-\Delta_h)^q E_h(t) v_h\|_{L^2(\Omega)} \leq c t^{(1-q)\alpha - 1} \|v_h\|_{L^2(\Omega)} \quad \textit{for all} \ \ v_h \in X_h.$$

The following Lemma provides an error estimate of the semidiscrete approximation (5.24) with trivial source $f \equiv 0$. See [41, Theorem 3.2] for detailed proof.

Lemma 5.6. *Let u and u_h are the solutions to* (5.3) *and* (5.24)*, respectively, with $a, b \in \dot H^q(\Omega)$ and $f \equiv 0$. Then there holds that*

$$\|(u - u_h)(t)\|_{L^2(\Omega)} \le ch^2 t^{-\alpha(2-q)/2} \left(\|a\|_{\dot H^q(\Omega)} + t\|b\|_{\dot H^q(\Omega)}\right).$$

5.2.2 Semidiscrete scheme for solving backward problem

In order to solve the inverse problem, we apply the following regularized semidiscrete scheme: find $\tilde u_h^\delta(t) \in X_h$ such that

$$\begin{aligned} \partial_t^\alpha \tilde u_h^\delta - \Delta_h \tilde u_h^\delta &= 0,\ T \ge t > 0, \\ -\gamma \tilde u_h^\delta(0) + \tilde u_h^\delta(T_1) &= P_h g_1^\delta, \\ \gamma \partial_t \tilde u_h^\delta(0) + \tilde u_h^\delta(T_2) &= P_h g_2^\delta. \end{aligned} \tag{5.29}$$

We define the operator $\mathcal{G}_h(T_1, T_2)$ as

$$\mathcal{G}_h(T_1,T_2) = \begin{bmatrix} F_h(T_1) & \bar F_h(T_1) \\ F_h(T_2) & \bar F_h(T_2) \end{bmatrix}. \tag{5.30}$$

Then from (5.26) the solutions can be represented as

$$\begin{bmatrix} \tilde u_h^\delta(0) \\ \partial_t \tilde u_h^\delta(0) \end{bmatrix} = (\gamma \mathcal{I} + \mathcal{G}_h(T_1,T_2))^{-1} \begin{bmatrix} P_h g_1^\delta \\ P_h g_2^\delta \end{bmatrix} \quad \text{and} \quad \tilde u_h^\delta(t) = \mathcal{F}_h(t)(\gamma \mathcal{I} + \mathcal{G}_h(T_1,T_2))^{-1} \begin{bmatrix} P_h g_1^\delta \\ P_h g_2^\delta \end{bmatrix}, \tag{5.31}$$

where the operator $\mathcal{I}$ is given by (5.13). Meanwhile, we shall introduce an auxiliary function $\tilde u_h(t)$, a semidiscrete solution satisfying

$$\begin{aligned} \partial_t^\alpha \tilde u_h - \Delta_h \tilde u_h &= 0,\ T \ge t > 0, \\ -\gamma \tilde u_h(0) + \tilde u_h(T_1) &= P_h g_1, \\ \gamma \partial_t \tilde u_h(0) + \tilde u_h(T_2) &= P_h g_2. \end{aligned} \tag{5.32}$$

Then we would write the solutions as

$$\begin{bmatrix} \tilde u_h(0) \\ \partial_t \tilde u_h(0) \end{bmatrix} = (\gamma \mathcal{I} + \mathcal{G}_h(T_1,T_2))^{-1} \begin{bmatrix} P_h g_1 \\ P_h g_2 \end{bmatrix} \quad \text{and} \quad \tilde u_h(t) = \mathcal{F}_h(t)(\gamma \mathcal{I} + \mathcal{G}_h(T_1,T_2))^{-1} \begin{bmatrix} P_h g_1 \\ P_h g_2 \end{bmatrix}. \tag{5.33}$$

The next lemma confirms the invertibility of the operator $\gamma \mathcal{I} + \mathcal{G}_h(T_1,T_2)$.

Lemma 5.7. *Let $M(\lambda_1)$ be the constant defined in Lemma 5.1, and suppose that $T_2 > T_1 \ge M(\lambda_1)$. Then the operator $\gamma \mathcal{I} + \mathcal{G}_h(T_1,T_2)$ is invertible. Meanwhile, there holds for all $v_h, w_h \in X_h$*

$$\left\| \mathcal{F}_h(t)(\gamma \mathcal{I} + \mathcal{G}_h(T_1,T_2))^{-1} \begin{bmatrix} v_h \\ w_h \end{bmatrix} \right\|_{L^2(\Omega)} \le c \min(\gamma^{-1}, t^{-\alpha}) \Big(\|v_h\|_{L^2(\Omega)} + \|w_h\|_{L^2(\Omega)} \Big)$$

Meanwhile, we have

$$\left\|(\gamma\mathcal{I}+\mathcal{G}_h(T_1,T_2))^{-1}\begin{bmatrix}v_h\\ w_h\end{bmatrix}\right\|_{L^2(\Omega)} \le c\gamma^{-1}\Big(\|v_h\|_{L^2(\Omega)}+\|w_h\|_{L^2(\Omega)}\Big)\begin{bmatrix}1\\1\end{bmatrix}.$$

Proof. By (5.10) and the fact (5.25), we obtain for any $1\le j\le J$

$$|\psi(T_1,T_2;\lambda_j^h)| \ge \left|\frac{c(T_2-T_1)}{\Gamma(1-\alpha)\Gamma(2-\alpha)}\frac{1}{(\lambda_j^h)^2T_1^\alpha T_2^\alpha}\right| > 0, \tag{5.34}$$

where the constant c is independent of λ_j^h, T_1 and T_2. Then by the assumption (5.15) we have

$$\begin{aligned}\tilde\psi(T_1,T_2;\lambda_j^h) &= \psi(T_1,T_2;\lambda_j^h)-\gamma^2+\gamma[E_{\alpha,1}(-\lambda_j^hT_1^\alpha)-T_2E_{\alpha,2}(-\lambda_j^hT_2^\alpha)]\\ &\le -c\Big((\lambda_j^h)^{-2}+\gamma(\lambda_j^h)^{-1}+\gamma^2\Big)<0\end{aligned} \tag{5.35}$$

and hence the operator $\gamma\mathcal{I}+\mathcal{G}_h(T_1,T_2)$ is invertible. Finally, the desired two stability estimates follow by the same argument in the proof of Lemma 5.3 with $p=q=0$. □

This lemma together with the representations (5.31) and (5.33) implies the following estimate

Corollary 5.3. *Suppose that $M(\lambda_1)$ is the constant defined in Lemma 5.1, and $T_2>T_1\ge M(\lambda_1)$. Let $\tilde u_h^\delta(t)$ and $\tilde u_h(t)$ be the solutions of problems* (5.29) *and* (5.32). *Then there holds for all* $0<t\le T$

$$\|(\tilde u_h^\delta-\tilde u_h)(t)\|_{L^2(\Omega)}\le c\delta\min(\gamma^{-1},t^{-\alpha})\quad\text{and}\quad\begin{bmatrix}\|(\tilde u_h^\delta-\tilde u_h)(0)\|_{L^2(\Omega)}\\ \|\partial_t(\tilde u_h^\delta-\tilde u_h)(0)\|_{L^2(\Omega)}\end{bmatrix}\le c\delta\gamma^{-1}\begin{bmatrix}1\\1\end{bmatrix},$$

where c is independent on δ, γ, h and t.

Next, we aim to derive a bound for the discretization error $\tilde u_h-\tilde u$. To this end, we need the following preliminary estimate.

Lemma 5.8. *Suppose that $M(\lambda_1)$ is the constant defined in Lemma 5.1, and $T_2>T_1\ge M(\lambda_1)$. Let $\tilde u$ be the solution to the backward regularization problem* (5.20). *Then there holds for* $0\le q\le 2$

$$\|(\mathbb{E}_h*\Delta_h(P_h-R_h)\tilde u)(t)\|_{L^2(\Omega)}\le ch^2t^{-\alpha(2-q)/2}\Big(\|\tilde u(0)\|_{\dot H^q(\Omega)}+t\|\partial_t\tilde u(0)\|_{\dot H^q(\Omega)}\Big).$$

Proof. Let w_h be the solution to the semidiscrete problem

$$\begin{aligned}\partial_t^\alpha w_h-\Delta_hw_h=0,\ T\ge t>0,\\ w_h(0)=P_h\tilde u(0),\ \partial_tw_h(0)=P_h\partial_t\tilde u(0).\end{aligned} \tag{5.36}$$

Then Lemma 5.6 implies the estimate

$$\|(w_h-\tilde u)(t)\|\le ch^2t^{-\alpha(2-q)/2}\Big(\|\tilde u(0)\|_{\dot H^q(\Omega)}+t\|\partial_t\tilde u(0)\|_{\dot H^q(\Omega)}\Big). \tag{5.37}$$

Meanwhile, we apply the following splitting

$$(w_h - \tilde{u})(t) = (w_h - P_h\tilde{u})(t) + (P_h\tilde{u} - \tilde{u})(t) =: \zeta(t) + \rho(t).$$

From the approximation of L^2 projection (2.17) and the regularity estimate in Lemma 2.3, we arrive at

$$\|\rho(t)\|_{L^2(\Omega)} \le ch^2\|\tilde{u}(t)\|_{\dot{H}^2(\Omega)} \le ch^2 t^{-\alpha(2-q)/2}\Big(\|\tilde{u}(0)\|_{\dot{H}^q(\Omega)} + t\|\partial_t\tilde{u}(0)\|_{\dot{H}^q(\Omega)}\Big). \tag{5.38}$$

Moreover, we observe that the function $\zeta(t)$ satisfies

$$\begin{aligned}
&\partial_t^\alpha\zeta(t) - \Delta_h\zeta(t) = \Delta_h(P_h - R_h)\tilde{u}(t),\ T \ge t > 0,\\
&\zeta(0) = 0,\ \partial_t\zeta(0) = 0.
\end{aligned}$$

Then (5.26) indicates the representation $\zeta(t) = (\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u})(t)$. Then the desired result follows immediately from (5.37), (5.38) and the triangle inequality. □

Then we are ready to state a key lemma providing an estimate for the discretization error $\tilde{u}_h - \tilde{u}$.

Lemma 5.9. *Assume that $a, b \in L^2(\Omega)$. Let $\tilde{u}$ be the solution to the regularized problem* (5.20) *and $\tilde{u}_h$ be the solution to the corresponding semidiscrete problem* (5.32)*, then there holds for all* $0 < t \le T$

$$\|(\tilde{u}_h - \tilde{u})(t)\|_{L^2(\Omega)} \le ch^2\min(\gamma^{-1}, t^{-\alpha})\Big(\|a\|_{L^2} + \|b\|_{L^2(\Omega)}\Big)$$

and

$$\|(\tilde{u}_h - \tilde{u})(0)\|_{L^2(\Omega)} + \|\partial_t(\tilde{u}_h - \tilde{u})(0)\|_{L^2(\Omega)} \le ch^2\gamma^{-1}\Big(\|a\|_{L^2} + \|b\|_{L^2(\Omega)}\Big)$$

where both c are independent on γ, h and t.

Proof. First of all, for $t \in (0, T]$, we use the splitting

$$(\tilde{u}_h - \tilde{u})(t) = (\tilde{u}_h - P_h\tilde{u})(t) + (P_h\tilde{u} - \tilde{u})(t) =: \zeta(t) + \rho(t).$$

From the approximation property of the L^2-projection in (2.17), we arrive at

$$\begin{aligned}
\|\rho(t)\|_{L^2(\Omega)} \le ch^2\|\tilde{u}(t)\|_{\dot{H}^2(\Omega)} &\le ch^2\min\left(\gamma^{-1}, t^{-\alpha}\right)\left(\|g_1\|_{\dot{H}^2(\Omega)} + \|g_2\|_{\dot{H}^2(\Omega)}\right)\\
&\le ch^2\min\left(\gamma^{-1}, t^{-\alpha}\right)\left(\|a\|_{L^2(\Omega)} + \|b\|_{L^2(\Omega)}\right)
\end{aligned}$$

where the second inequality follows from (5.19) and Lemma 5.3 (with $p = q = 2$), and the last inequality follows from the regularity estimate in Lemma 2.3.

Now we turn to the term $\zeta = \tilde{u}_h - P_h\tilde{u}$ which satisfies the error equation

$$\begin{cases}
\partial_t^\alpha\zeta - \Delta_h\zeta = \Delta_h(P_h - R_h)\tilde{u}(t), \quad T \ge t > 0,\\
-\gamma\zeta(0) + \zeta(T_1) = 0,\\
\gamma\partial_t\zeta(0) + \zeta(T_2) = 0.
\end{cases} \tag{5.39}$$

From solution representation we have

$$\begin{bmatrix} \zeta(T_1) \\ \zeta(T_2) \end{bmatrix} = \mathcal{G}_h(T_1,T_2) \begin{bmatrix} \zeta(0) \\ \partial_t\zeta(0) \end{bmatrix} + \begin{bmatrix} (\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u})(T_1) \\ (\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u})(T_2) \end{bmatrix}.$$

Then we add $(-\gamma\zeta(0), \gamma\partial_t\zeta(0))^T$ at both sides and derive

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} = (\gamma\mathcal{I} + \mathcal{G}_h(T_1,T_2)) \begin{bmatrix} \zeta(0) \\ \partial_t\zeta(0) \end{bmatrix} + \begin{bmatrix} (\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u})(T_1) \\ (\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u})(T_2) \end{bmatrix}. \tag{5.40}$$

This immediately implies a representation to $\zeta(t)$:

$$\begin{aligned} \zeta(t) &= \mathcal{F}_h(t) \begin{bmatrix} \zeta(0) \\ \partial_t\zeta(0) \end{bmatrix} + (\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u})(t) \\ &= -\mathcal{F}_h(t)(\gamma\mathcal{I} + \mathcal{G}_h(T_1,T_2))^{-1} \begin{bmatrix} (\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u})(T_1) \\ (\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u})(T_2) \end{bmatrix} + (\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u})(t) \\ &=: I_1(t) + I_2(t). \end{aligned}$$

Then Lemmas 5.7 and 5.8 lead to the estimate for all $t \in (0,T]$

$$\begin{aligned} \|I_1(t)\|_{L^2(\Omega)} &\le c\min(\gamma^{-1}, t^{-\alpha})\Big(\|(\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u})(T_1)\|_{L^2(\Omega)} + \|(\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u})(T_2)\|_{L^2(\Omega)}\Big) \\ &\le ch^2 \min(\gamma^{-1}, t^{-\alpha})(\|\tilde{u}(0)\|_{L^2(\Omega)} + \|\partial_t\tilde{u}(0)\|_{L^2(\Omega)}). \end{aligned}$$

Recalling Corollary 5.1 with $q = 0$, we derive for all $t \in (0,T]$

$$\|I_1(t)\|_{L^2(\Omega)} \le ch^2 \min(\gamma^{-1}, t^{-\alpha})(\|a\|_{L^2(\Omega)} + \|b\|_{L^2(\Omega)}).$$

Similarly, using Lemma 5.8 with $q = 2$ and Corollary 5.1 with $q = 2$, we bound the term I_2 by

$$\|I_2(t)\|_{L^2(\Omega)} \le ch^2(\|\tilde{u}(0)\|_{\dot{H}^2(\Omega)} + \|\partial_t\tilde{u}(0)\|_{\dot{H}^2(\Omega)}) \le ch^2\gamma^{-1}(\|a\|_{L^2(\Omega)} + \|b\|_{L^2(\Omega)})$$

for all $t \in (0,T]$. Meanwhile, using Lemma 5.8 with $q = 0$ and Corollary 5.1 with $q = 0$, we have

$$\|I_2(t)\|_{L^2(\Omega)} \le ch^2 t^{-\alpha}(\|\tilde{u}(0)\|_{L^2} + \|\partial_t\tilde{u}(0)\|_{L^2}) \le ch^2 t^{-\alpha}(\|a\|_{L^2(\Omega)} + \|b\|_{L^2(\Omega)}).$$

Therefore, we conclude that

$$\|(\tilde{u} - \tilde{u}_h)(t)\|_{L^2(\Omega)} \le ch^2 \min(\gamma^{-1}, t^{-\alpha})\Big(\|a\|_{L^2} + \|b\|_{L^2(\Omega)}\Big).$$

Similarly, for $t = 0$, the relation (5.40) implies

$$\begin{bmatrix} \zeta(0) \\ \partial_t\zeta(0) \end{bmatrix} = -\,(\gamma\mathcal{I} + \mathcal{G}_h(T_1,T_2))^{-1} \begin{bmatrix} (\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u})(T_1) \\ (\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u})(T_2) \end{bmatrix}.$$

Then we apply Lemmas 5.3 (with $p = 0$ and $q = 0$), 5.7 (with $q = 0$) and Corollary 5.8 (with $q = 0$) to derive

$$
\begin{aligned}
&\|\zeta(0)\|_{L^2(\Omega)} + \|\partial_t\zeta(0)\|_{L^2(\Omega)} \\
&\le c\gamma^{-1}\Big(\|\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u}(T_1)\|_{L^2(\Omega)} + \|\mathbb{E}_h * \Delta_h(P_h - R_h)\tilde{u}(T_2)\|_{L^2(\Omega)}\Big) \\
&\le ch^2\gamma^{-1}\Big(\|\tilde{u}(0)\|_{L^2(\Omega)} + \|\partial_t\tilde{u}(0)\|_{L^2(\Omega)}\Big) \\
&\le ch^2\gamma^{-1}\Big(\|a\|_{L^2(\Omega)} + \|b\|_{L^2(\Omega)}\Big).
\end{aligned}
$$

This completes the proof of the lemma. □

Then Lemma 5.4, Corollary 5.3 and Lemma 5.9 would lead to the following error estimate.

Theorem 5.3. *Assume that $a, b \in \dot{H}^q(\Omega)$, $q \in [0, 2]$. Let u be the solution to the problem (5.3) and $\tilde{u}_h^\delta$ be the solution to the regularized semidiscrete problem (5.29), then there holds*

$$
\|(\tilde{u}_h^\delta - u)(t)\|_{L^2(\Omega)} \le c\Big[\gamma \min(\gamma^{-(1-\frac{q}{2})}, t^{-(1-\frac{q}{2})\alpha}) + (h^2 + \delta)\min(\gamma^{-1}, t^{-\alpha})\Big], \quad \forall t \in (0, T],
$$

and

$$
\|(\tilde{u}_h^\delta - u)(0)\|_{L^2(\Omega)} + \|\partial_t(\tilde{u}_h^\delta - u)(0)\|_{L^2(\Omega)} \le c\Big[\gamma^{\frac{q}{2}} + \gamma^{-1}(h^2 + \delta)\Big]
$$

where c depends on T_1, T_2, a and b, but is always independent of h, γ, δ and t.

Remark 5.3. *For $a, b \in \dot{H}^q(\Omega)$ and $t \ge t_0$, then Theorem 5.3 provides an estimate*

$$
\|(\tilde{u}_h^\delta - u)(t)\|_{L^2(\Omega)} \le c(\gamma + (h^2 + \delta)).
$$

With a priori *choice of parameter $\gamma \sim \delta$ and $h \sim \sqrt{\delta}$, we obtain the optimal convergence rate $\|(\tilde{u}_h^\delta - u)(t)\|_{L^2(\Omega)} \le c\delta$. For $t = 0$, according to Theorem 5.3, we choose $\gamma \sim \delta^{\frac{2}{2+q}}$ and $h \sim \sqrt{\delta}$ to obtain the best convergence rate*

$$
\|(\tilde{u}_h^\delta - u)(0)\|_{L^2(\Omega)} + \|\partial_t(\tilde{u}_h^\delta - u)(0)\|_{L^2(\Omega)} \le c\delta^{\frac{q}{2+q}}.
$$

In case that $q = 0$, we can also show the convergence, provided a suitable choice of parameters. According to Lemma 5.4, Corollary 5.3 and Theorem 5.3, there holds for any $s \in (0, 1]$

$$
\|(\tilde{u}_h^\delta - u)(0)\|_{L^2(\Omega)} + \|\partial_t(\tilde{u}_h^\delta - u)(0)\|_{\dot{H}^{-s}(\Omega)} \to 0, \qquad \text{as } \delta, \gamma, h \to 0,\ \frac{\delta}{\gamma} \to 0 \text{ and } \frac{h^2}{\gamma} \to 0.
$$

5.3 Fully discrete scheme and error analysis

Now we intend to propose a fully discrete scheme for approximately solving the backward diffusion-wave problem, and derive *a priori* error estimate in terms of data regularity.

5.3.1 Fully discrete scheme for the direct problem

To begin with, we introduce the fully discrete scheme for the direct problem. We divide the time interval $[0, T]$ into a uniform grid, with $t_n = n\tau$, $n = 0, \ldots, N$, and $\tau = T/N$ being the time step size. In case that $\varphi(0) = 0$ and $\varphi'(0) = 0$, we approximate the Riemann-Liouville fractional derivative

$$^{RL}\partial_t^\alpha \varphi(t) = \frac{1}{\Gamma(2-\alpha)} \frac{\mathrm{d}^2}{\mathrm{d}t^2} \int_0^t (t-s)^{1-\alpha} \varphi(s) \mathrm{d}s$$

by the backward Euler convolution quadrature (with $\varphi_j = \varphi(t_j)$) [71, 43]:

$$^{RL}\partial_t^\alpha \varphi(t_n) \approx \tau^{-\alpha} \sum_{j=0}^{n} b_j \varphi_{n-j} := \bar{\partial}_\tau^\alpha \varphi_n, \quad \text{ with } \sum_{j=0}^{\infty} b_j \xi^j = (1-\xi)^\alpha.$$

The fully discrete scheme for problem (2.12) reads: find $U_n \in X_h$ such that

$$\bar{\partial}_\tau (U_n - P_h a - t_n P_h b) - \Delta_h U_n = P_h f(t_n), \quad n = 1, 2, \ldots, N, \tag{5.41}$$

with the initial condition $U_0 = P_h a \in X_h$. Here we use the relation between Riemann-Liouville and Caputo fractional derivatives with $\alpha \in (1, 2)$ [57, p. 91]:

$$\partial_t^\alpha u(t_n) = \partial_t^\alpha (u(t_n) - a - tb) = {}^{RL}\partial_t^\alpha (u(t_n) - a - tb) \approx \bar{\partial}_\tau^\alpha (u(t_n) - a - tb).$$

By means of discrete Laplace transform, the fully discrete solution U_n is given by

$$\begin{aligned} U_n &= \mathcal{F}_{h,\tau}^n \begin{bmatrix} P_h a \\ P_h b \end{bmatrix} + \tau \sum_{k=1}^{n} E_{h,\tau}^{n-k} P_h f(t_k) \\ &:= \begin{bmatrix} F_{h,\tau}^n & \bar{F}_{h,\tau}^n \end{bmatrix} \begin{bmatrix} P_h a \\ P_h b \end{bmatrix} + \tau \sum_{k=1}^{n} E_{h,\tau}^{n-k} P_h f(t_k), \end{aligned} \tag{5.42}$$

with $n = 1, 2, \ldots, N$, where the fully discrete operators $F_{h,\tau}^n$, $\bar{F}_{h,\tau}^n$ and $E_{h,\tau}^n$ are respectively defined by (see e.g., [43])

$$\begin{aligned} F_{h,\tau}^n &= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} e^{-z\tau} \delta_\tau(e^{-z\tau})^{\alpha-1} (\delta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1} \, \mathrm{d}z, \\ F_{h,\tau}^n &= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} e^{-z\tau} \delta_\tau(e^{-z\tau})^{\alpha-2} (\delta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1} \, \mathrm{d}z, \\ E_{h,\tau}^n &= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} (\delta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1} \, \mathrm{d}z, \end{aligned} \tag{5.43}$$

with $\delta_\tau(\xi) = (1-\xi)/\tau$ and the contour $\Gamma_{\theta,\sigma}^\tau := \{z \in \Gamma_{\theta,\sigma} : |\Im(z)| \leq \pi/\tau\}$ where $\theta \in (\pi/2, \pi)$ is close to $\pi/2$. (oriented with an increasing imaginary part). The next lemma gives elementary properties of the kernel $\delta_\tau(e^{-z\tau})$. The detailed proof has been given in [43, Lemma B.1].

Lemma 5.10. *For a fixed $\theta' \in (\pi/2, \pi/\alpha)$, there exists $\theta \in (\pi/2, \pi)$ and positive constants c, c_1, c_2 (independent of τ) such that for all $z \in \Gamma_{\theta,\sigma}^{\tau}$*

$$c_1|z| \le |\delta_\tau(e^{-z\tau})| \le c_2|z|, \qquad \delta_\tau(e^{-z\tau}) \in \Sigma_{\theta'}.$$
$$|\delta_\tau(e^{-z\tau}) - z| \le c\tau|z|^2, \qquad |\delta_\tau(e^{-z\tau})^\alpha - z^\alpha| \le c\tau|z|^{1+\alpha}.$$

In case that $f \equiv 0$, with the spectral decomposition, we can write

$$U_n = F_{h,\tau}^n P_h a + \bar{F}_{h,\tau}^n P_h b = \sum_{j=1}^{J} \left[F_\tau^n(\lambda_j^h)(a, \varphi_j^h)\varphi_j^h + \bar{F}_\tau^n(\lambda_j^h)(b, \varphi_j^h)\varphi_j^h \right] \tag{5.44}$$

where $F_\tau^n(\lambda_j^h)$ and $\bar{F}_\tau^n(\lambda_j^h)$ are the solutions to the discrete initial value problems

$$\bar{\partial}_\tau[F_\tau^n(\lambda_j^h) - 1] + \lambda_j^h F_\tau^n(\lambda_j^h) = 0, \quad \text{with} \quad F_\tau^0(\lambda_j^h) = 1$$

and

$$\bar{\partial}_\tau[\bar{F}_\tau^n(\lambda_j^h) - t_n] + \lambda_j^h \bar{F}_\tau^n(\lambda_j^h) = 0, \quad \text{with} \quad \bar{F}_\tau^0(\lambda_j^h) = 0$$

respectively. From (5.43), we write $F_\tau^n(\lambda_j^h)$ and $\bar{F}_\tau^n(\lambda_j^h)$ as

$$\begin{aligned} F_\tau^n(\lambda_j^h) &= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} e^{-z\tau} \delta_\tau(e^{-z\tau})^{\alpha-1} (\delta_\tau(e^{-z\tau})^\alpha + \lambda_j^h)^{-1} \, \mathrm{d}z \\ \bar{F}_\tau^n(\lambda_j^h) &= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} e^{-z\tau} \delta_\tau(e^{-z\tau})^{\alpha-2} (\delta_\tau(e^{-z\tau})^\alpha + \lambda_j^h)^{-1} \, \mathrm{d}z. \end{aligned} \tag{5.45}$$

Next we derive some useful properties of $F_\tau^n(\lambda_j^h)$ and $\bar{F}_\tau^n(\lambda_j^h)$,

Lemma 5.11. *Let $F_\tau^n(\lambda)$ and $\bar{F}_\tau^n(\lambda)$ be defined as in* (5.45)*. Then for $\lambda > 0$, there holds for $1 \le n \le N$,*

$$\left|E_{\alpha,1}(-\lambda t_n^\alpha) - F_\tau^n(\lambda)\right| + t_n^{-1}\left|t_n E_{\alpha,2}(-\lambda t^\alpha) - \bar{F}_\tau^n(\lambda)\right| \le \frac{cn^{-1}}{1 + \lambda t_n^\alpha}. \tag{5.46}$$

Meanwhile, there holds

$$\lambda^{-1}\Big(\left|E_{\alpha,1}(-\lambda t_n^\alpha) - F_\tau^n(\lambda)\right| + t_n^{-1}\left|t_n E_{\alpha,2}(-\lambda t_n^\alpha) - \bar{F}_\tau^n(\lambda)\right|\Big) \le c\tau t_n^{\alpha-1}. \tag{5.47}$$

Here c is the generic positive constant independent of λ, t and τ.

Proof. The estimate for $E_{\alpha,1}(-\lambda t_n^\alpha) - F_\tau^n(\lambda)$ follows from the same argument in the proof of [111, Lemma 4.2]. Then it suffices to establish a bound for $t_n E_{\alpha,2}(-\lambda t^\alpha) - \bar{F}_\tau^n(\lambda)$, we recall representations (2.15) and (5.45) and derive

$$\begin{aligned} |t_n E_{\alpha,2}(-\lambda t_n^\alpha) - \bar{F}_\tau^n(\lambda)| &\le \left| \frac{1}{2\pi i} \int_{\Gamma_{\theta,\sigma} \backslash \Gamma_{\theta,\sigma}^\tau} e^{zt_n} z^{\alpha-2} (z^\alpha + \lambda)^{-1} dz \right| \\ &\quad + \left| \frac{1}{2\pi i} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} (z^{\alpha-2}(z^\alpha + \lambda)^{-1} - e^{-z\tau}\delta_\tau(e^{-z\tau})^{\alpha-2}(\delta_\tau(e^{-z\tau})^\alpha + \lambda)^{-1}) dz \right| \\ &:= I_1 + I_2. \end{aligned}$$

With $\sigma = t_n^{-1}$, the bound for I_1 follows from the direct computation

$$\begin{aligned}
I_1 &\le c\int_{\Gamma_{\theta,\sigma}\backslash\Gamma_{\theta,\sigma}^\tau} |e^{zt_n}||z^{\alpha-2}||(z^\alpha+\lambda)^{-1}||\mathrm{d}z| \le c\int_{\pi/(\tau\sin\theta)}^\infty \frac{e^{\rho(\cos\theta)t_n}\rho^{\alpha-2}}{\rho^\alpha}\mathrm{d}\rho\\
&\le ct_n\int_{cn}^\infty e^{-c\rho}\rho^{-2}\mathrm{d}\rho \le ct_n n^{-1}
\end{aligned}$$

and

$$\begin{aligned}
I_1 &\le c\int_{\pi/(\tau\sin\theta)}^\infty \frac{e^{\rho(\cos\theta)t_n}\rho^{\alpha-2}}{\lambda}\mathrm{d}\rho \le ct_n(\lambda t_n^\alpha)^{-1}\int_{cn}^\infty e^{-c\rho}\rho^{\alpha-2}d\rho\\
&\le ct_n(\lambda t_n^\alpha)^{-1}n^{-1}\int_{cn}^\infty e^{-c\rho}\rho^{\alpha-1}d\rho \le ct_n(\lambda t_n^\alpha)^{-1}n^{-1}.
\end{aligned}$$

As a result, we obtain $I_1 \le \frac{cn^{-1}}{(1+\lambda t_n^\alpha)}t_n$.

Next we turn to the term I_2. According to Lemma 5.10, we have for all $z\in\Gamma_{\theta,\sigma}^\tau$,

$$\begin{aligned}
\left|\frac{z^{\alpha-2}}{z^\alpha+\lambda} - \frac{e^{-z\tau}\delta_\tau(e^{-z\tau})^{\alpha-2}}{\delta_\tau(e^{-z\tau})^\alpha+\lambda}\right| &\le \left|\frac{z^{\alpha-2}}{z^\alpha+\lambda} - \frac{\delta_\tau(e^{-z\tau})^{\alpha-2}}{\delta_\tau(e^{-z\tau})^\alpha+\lambda}\right| + \left|\frac{(1-e^{-z\tau})\delta_\tau(e^{-z\tau})^{\alpha-2}}{\delta_\tau(e^{-z\tau})^\alpha+\lambda}\right|\\
&\le \left|\frac{z^{\alpha-2}\delta_\tau(e^{-z\tau})^{\alpha-2}(\delta_\tau(e^{-z\tau})^2-z^2)}{(z^\alpha+\lambda)(\delta_\tau(e^{-z\tau})^\alpha+\lambda)}\right| + \left|\frac{(z^{\alpha-2}-\delta_\tau(e^{-z\tau})^{\alpha-2})\lambda}{(z^\alpha+\lambda)(\delta_\tau(e^{-z\tau})^\alpha+\lambda)}\right|\\
&\quad + |(1-e^{-z\tau})|\left|\frac{\delta_\tau(e^{-z\tau})^{\alpha-2}}{\delta_\tau(e^{-z\tau})^\alpha+\lambda}\right|\\
&\le c\tau\frac{|z|^{\alpha-1}}{|z^\alpha+\lambda|}.
\end{aligned}$$

Therefore, with $\sigma = t_n^{-1}$, the term I_2 can be bounded as

$$I_2 \le c\tau\int_{\Gamma_{\theta,\sigma}^\tau}|e^{zt_n}|\frac{|z|^{\alpha-1}}{|z^\alpha+\lambda|}|dz| \le c\tau\lambda^{-1}\Big(\int_\sigma^\infty e^{\rho\cos\theta t_n}\rho^{\alpha-1}d\rho + \sigma^\alpha\int_{-\theta}^\theta d\psi\Big) \le c\tau(\lambda t_n^\alpha)^{-1}$$

and

$$I_2 \le c\tau\int_{\Gamma_{\theta,\sigma}^\tau}|e^{zt_n}||z|^{-1}|dz| \le c\tau\Big(\int_1^\infty e^{\rho\cos\theta}\rho^{-1}d\rho + \int_{-\theta}^\theta d\psi\Big) \le c\tau.$$

Then (5.46) follows immediately.

For the second estimate, we note that

$$\begin{aligned}
t_nE_{\alpha,2}(-\lambda t_n^\alpha) &= t_n - \frac{\lambda}{2\pi i}\int_{\Gamma_{\theta,\sigma}} e^{zt_n}z^{-2}(z^\alpha+\lambda)^{-1}dz,\\
\bar F_\tau^n(\lambda) &= t_n - \frac{\lambda}{2\pi i}\int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n}e^{-z\tau}\delta_\tau(e^{-z\tau})^{-2}(\delta_\tau(e^{-z\tau})^\alpha+\lambda)^{-1}dz,
\end{aligned}$$

with $n\ge1$. Then we use the spliiting

$$\begin{aligned}
\lambda^{-1}|t_nE_{\alpha,2}(-\lambda t_n^\alpha) - \bar F_\tau^n(\lambda)| &\le \left|\frac{1}{2\pi i}\int_{\Gamma_{\theta,\sigma}\backslash\Gamma_{\theta,\sigma}^\tau} e^{zt_n}z^{-2}(z^\alpha+\lambda)^{-1}dz\right|\\
&\quad+\left|\frac{1}{2\pi i}\int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n}[z^{-2}(z^\alpha+\lambda)^{-1} - e^{-z\tau}\delta_\tau(e^{-z\tau})^{-2}(\delta_\tau(e^{-z\tau})^\alpha+\lambda)^{-1}]dz\right|\\
&:= I_1 + I_2.
\end{aligned}$$

According to Lemma 5.10 we have for all $z \in \Gamma_{\theta,\sigma}^{\tau}$,

$$\begin{aligned}I_1 &\le c\int_{\Gamma_{\theta,\sigma}\setminus\Gamma_{\theta,\sigma}^{\tau}} |e^{zt_n}||z|^{-\alpha-2}|dz| \le c\int_{\pi/(\tau\sin\theta)} e^{\rho\cos\theta t_n}\rho^{-\alpha-2}d\rho\\ &\le ct_n^{\alpha+1}\int_{cn}^{\infty} e^{-c\rho}\rho^{-\alpha-2}d\rho \le ct_n^{\alpha+1}n^{-3}\int_0^{\infty} e^{-c\rho}\rho^{-\alpha+1}d\rho \le ct_n^{\alpha-2}\tau^3.\end{aligned}$$

And also we have

$$|z^{-2}(z^\alpha+\lambda)^{-1} - e^{-z\tau}\delta_\tau(e^{-z\tau})^{-2}(\delta_\tau(e^{-z\tau})^\alpha+\lambda)^{-1}| \le c\tau|z|^{-\alpha-1},$$

and therefore with $\sigma = t_n^{-1}$, we have the bound for $n \ge 1$

$$I_2 \le c\tau\int_{\Gamma_{\theta,\sigma}^{\tau}} |e^{zt_n}||z|^{-\alpha-1}|dz| \le c\tau\left(\int_\sigma^\infty e^{-c\rho t_n}\rho^{-\alpha-1}d\rho + \sigma^{-\alpha}\int_{-\theta}^{\theta} d\psi\right) \le c\tau t_n^\alpha.$$

This completes the proof of (5.47). □

Then Lemmas 2.1 and 5.11 lead to the following asymptotic behaviors of $F_\tau^n(\lambda)$ and $\bar{F}_\tau^n(\lambda)$.

Corollary 5.4. *Let $F_\tau^n(\lambda)$ and $\bar{F}_\tau^n(\lambda)$ be defined as in* (5.45)*. Then there exists $\tau_0 > 0$ such that for all $\tau \in (0,\tau_0)$, $\lambda > \lambda_1$ and $t_n \ge M(\lambda_1)$*

$$-c_0\lambda^{-1}t_n^{-\alpha} \le F_\tau^n(\lambda) \le -c_1\lambda^{-1}t_n^{-\alpha} \quad \textit{and} \quad \tilde{c}_0\lambda^{-1}t_n^{1-\alpha} \le \bar{F}_\tau^n(\lambda) \le \tilde{c}_1\lambda^{-1}t_n^{1-\alpha},$$

with positive constants c_0, c_1, $\tilde{c}_0$, $\tilde{c}_1$ independent of λ, t and τ.

Now we define two integers N_1 and N_2 such that $N_1\tau = T_1$ and $N_2\tau = T_2$, and define

$$\mathcal{G}_{h,\tau}(T_1,T_2) = \begin{bmatrix} F_{h,\tau}^{N_1} & \bar{F}_{h,\tau}^{N_1}\\ F_{h,\tau}^{N_2} & \bar{F}_{h,\tau}^{N_2}\end{bmatrix}, \quad G_\tau(T_1,T_2;\lambda_j^h) = \begin{bmatrix} F_\tau^{N_1}(\lambda_j^h) & \bar{F}_\tau^{N_1}(\lambda_j^h)\\ F_\tau^{N_2}(\lambda_j^h) & \bar{F}_\tau^{N_2}(\lambda_j^h)\end{bmatrix}. \tag{5.48}$$

Then according to (5.44), we have the representation

$$\begin{aligned}\begin{bmatrix} U_{N_1}\\ U_{N_2}\end{bmatrix} &= \mathcal{G}_{h,\tau}(T_1,T_2)\begin{bmatrix} P_h a\\ P_h b\end{bmatrix} = \sum_{j=1}^{J} G_\tau(T_1,T_2;\lambda_j^h)\begin{bmatrix}(a,\varphi_j^h)\varphi_j^h\\ (b,\varphi_j^h)\varphi_j^h\end{bmatrix}\\ &= \sum_{j=1}^{J}\begin{bmatrix} F_\tau^{N_1}(\lambda_j^h) & \bar{F}_\tau^{N_1}(\lambda_j^h)\\ F_\tau^{N_2}(\lambda_j^h) & \bar{F}_\tau^{N_2}(\lambda_j^h)\end{bmatrix}\begin{bmatrix}(a,\varphi_j^h)\varphi_j^h\\ (b,\varphi_j^h)\varphi_j^h\end{bmatrix}.\end{aligned}$$

The next lemma provides the invertibility of $\gamma\mathcal{I} + \mathcal{G}_{h,\tau}(T_1,T_2)$.

Lemma 5.12. *Let $M(\lambda_1)$ be the constant defined in Lemma 5.1, and suppose that $T_2 > T_1 \ge M(\lambda_1)$. Then the operator $\gamma\mathcal{I} + \mathcal{G}_{h,\tau}(T_1,T_2)$ is invertible, and there holds for $v_h, w_h \in X_h$*

$$\Big\|\mathcal{F}_{h,\tau}^n(\gamma\mathcal{I} + \mathcal{G}_{h,\tau}(T_1,T_2))^{-1}\begin{bmatrix} v_h\\ w_h\end{bmatrix}\Big\|_{L^2(\Omega)} \le c\min(\gamma^{-1}, t_n^{-\alpha})\Big(\|v_h\|_{L^2(\Omega)} + \|w_h\|_{L^2(\Omega)}\Big)$$

and

$$\Big\|(\gamma\mathcal{I} + \mathcal{G}_{h,\tau}(T_1,T_2))^{-1}\begin{bmatrix} v_h\\ w_h\end{bmatrix}\Big\|_{L^2(\Omega)} \le c\gamma^{-1}\Big(\|v_h\|_{L^2(\Omega)} + \|w_h\|_{L^2(\Omega)}\Big)\begin{bmatrix}1\\ 1\end{bmatrix}.$$

Proof. Let $\psi_\tau(T_1, T_2; \lambda_j^h)$ be the determinant of $G_\tau(T_1, T_2; \lambda_j^h)$. We define

$$\partial_t \psi_\tau(T_1, T_2; \lambda_j^h) = \psi_\tau(T_1, T_2; \lambda_j^h) - \gamma^2 + \gamma[F_{h,\tau}^{N_1} - \bar{F}_{h,\tau}^{N_2}],$$

Then from Lemma 5.11 and Corollary 5.4 we have for $\lambda > \lambda_1$

$$\begin{aligned}
&|\psi_\tau(T_1, T_2; \lambda) - \psi(T_1, T_2; \lambda)| \\
&\leq |(F_\tau^{N_1}(\lambda) - E_{\alpha,1}(-\lambda T_1^\alpha)\bar{F}_\tau^{N_2}(\lambda)| + |E_{\alpha,1}(-\lambda T_1^\alpha)(\bar{F}_\tau^{N_2}(\lambda) - T_2 E_{\alpha,2}(-\lambda T_2^\alpha))| \\
&+ |(T_1 E_{\alpha,2}(-\lambda T_1^\alpha) - \bar{F}_\tau^{N_1}(\lambda))F_\tau^{N_2}(\lambda)| + |T_1 E_{\alpha,2}(-\lambda T_1^\alpha)(E_{\alpha,1}(-\lambda T_2^\alpha) - F_\tau^{N_2}(\lambda))| \leq c\frac{\tau}{\lambda^2 T_1^\alpha T_2^\alpha}.
\end{aligned}$$

Combining (5.10) with the fact $\lambda_j^h \geq \lambda_1^h > \lambda_1$ by (5.25) we have

$$\psi_\tau(T_1, T_2; \lambda_j^h) \leq \frac{c}{(\lambda_j^h)^2 T_1^\alpha T_2^\alpha} < 0.$$

This together with the Corollary 5.4 leads to

$$|\partial_t \psi_\tau(T_1, T_2; \lambda_j^h)| \geq c\Big((\lambda_j^h)^{-2} + \gamma(\lambda_j^h)^{-1} + \gamma^2\Big) > 0, \tag{5.49}$$

where c is only dependent on T_1, T_2 and α. Therefore, the operator $\gamma\mathcal{I} + \mathcal{G}_{h,\tau}(T_1, T_2)$ is invertible. Finally, the desired stability estimates follows by an argument similar to the proof of Lemma 5.3 with $p = q = 0$ and Corollary 5.4. $\square$

5.3.2 Fully discrete scheme for the inverse problem

Now, we propose a fully discrete scheme for solving the backward diffusion-wave problem. Given g_1^δ and g_2^δ, we look for $\tilde{a}_{h,\tau}^\delta$, $\tilde{b}_{h,\tau}^\delta$ and $\tilde{U}_n^\delta \in X_h$ with $n = 1, 2, \ldots, N$ such that

$$\begin{aligned}
\bar{\partial}_\tau(\tilde{U}_n^\delta - \tilde{a}_{h,\tau}^\delta - t_n \tilde{b}_{h,\tau}^\delta) - \Delta_h \tilde{U}_n^\delta = 0, \quad \forall\, n = 1, 2, \ldots, N, \\
-\gamma \tilde{a}_{h,\tau}^\delta + \tilde{U}_{N_1}^\delta = P_h g_1^\delta, \\
\gamma \tilde{b}_{h,\tau}^\delta + \tilde{U}_{N_2}^\delta = P_h g_2^\delta
\end{aligned} \tag{5.50}$$

with $\tilde{U}_0^\delta = \tilde{a}_{h,\tau}^\delta$. Then by Lemma 5.12, the problem (5.50) is uniquely solvable, and $\tilde{U}_n^\delta$ could be represented as

$$\tilde{U}_n^\delta = \mathcal{F}_{h,\tau}^n \begin{bmatrix} \tilde{a}_{h,\tau}^\delta \\ \tilde{b}_{h,\tau}^\delta \end{bmatrix} = \mathcal{F}_{h,\tau}^n (\gamma\mathcal{I} + \mathcal{G}_{h,\tau}(T_1, T_2))^{-1} \begin{bmatrix} P_h g_1^\delta \\ P_h g_2^\delta \end{bmatrix} \tag{5.51}$$

while $\tilde{a}_{h,\tau}^\delta$ and $\tilde{b}_{h,\tau}^\delta$ could be written as

$$\begin{bmatrix} \tilde{a}_{h,\tau}^\delta \\ \tilde{b}_{h,\tau}^\delta \end{bmatrix} = (\gamma\mathcal{I} + \mathcal{G}_{h,\tau}(T_1, T_2))^{-1} \begin{bmatrix} P_h g_1^\delta \\ P_h g_2^\delta \end{bmatrix}. \tag{5.52}$$

Similarly, we could define auxiliary functions $\tilde{a}_{h,\tau}$, $\tilde{b}_{h,\tau}$ and $\tilde{U}_n \in X_h$ with $n = 1, 2, \ldots, N$ such that

$$\begin{aligned} \bar{\partial}_\tau(\tilde{U}_n - \tilde{a}_{h,\tau} - t_n\tilde{b}_{h,\tau}) - \Delta_h\tilde{U}_n = 0, \quad \forall\, n = 1, 2, \ldots, N, \\ -\gamma\tilde{a}_{h,\tau} + \tilde{U}_{N_1} = P_h g_1, \\ \gamma\tilde{b}_{h,\tau} + \tilde{U}_{N_2} = P_h g_2 \end{aligned} \tag{5.53}$$

with $\tilde{U}_0 = \tilde{a}_{h,\tau}$. Then the function $\tilde{U}_n^\delta$ could be represented as

$$\tilde{U}_n = \mathcal{F}_{h,\tau}^n \begin{bmatrix} \tilde{a}_{h,\tau} \\ \tilde{b}_{h,\tau} \end{bmatrix} = \mathcal{F}_{h,\tau}^n(\gamma\mathcal{I} + \mathcal{G}_{h,\tau}(T_1, T_2))^{-1} \begin{bmatrix} P_h g_1 \\ P_h g_2 \end{bmatrix} \tag{5.54}$$

while $\tilde{a}_{h,\tau}$ and $\tilde{b}_{h,\tau}$ could be written as

$$\begin{bmatrix} \tilde{a}_{h,\tau} \\ \tilde{b}_{h,\tau} \end{bmatrix} = (\gamma\mathcal{I} + \mathcal{G}_{h,\tau}(T_1, T_2))^{-1} \begin{bmatrix} P_h g_1 \\ P_h g_2 \end{bmatrix}. \tag{5.55}$$

Then Lemma 5.12 immediately implies following estimates for $\tilde{a}_{h,\tau} - \tilde{a}_{h,\tau}^\delta$, $\tilde{b}_{h,\tau} - \tilde{b}_{h,\tau}^\delta$ and $\tilde{U}_n - \tilde{U}_n^\delta$.

Lemma 5.13. *Let $M(\lambda_1)$ be the constant defined in Lemma 5.1, and suppose that $T_2 > T_1 \geq M(\lambda_1)$. Let $\tilde{a}_{h,\tau}^\delta$, $\tilde{b}_{h,\tau}^\delta$ and $\tilde{U}_n^\delta$ be solutions to* (5.50)*, and $\tilde{a}_{h,\tau}$, $\tilde{b}_{h,\tau}$ and $\tilde{U}_n$ be solutions to* (5.53)*. Then there holds*

$$\|\tilde{U}_n - \tilde{U}_n^\delta\|_{L^2(\Omega)} \leq c\delta \min(\gamma^{-1}, t_n^{-\alpha})\big(\|a\|_{L^2(\Omega)} + \|b\|_{L^2(\Omega)}\big)$$

and

$$\|\tilde{a}_{h,\tau} - \tilde{a}_{h,\tau}^\delta\|_{L^2(\Omega)} + \|\tilde{b}_{h,\tau} - \tilde{b}_{h,\tau}^\delta\|_{L^2(\Omega)} \leq c\delta\gamma^{-1}\big(\|a\|_{L^2(\Omega)} + \|b\|_{L^2(\Omega)}\big).$$

Next, we aim to compare two auxiliary problems, i.e. (5.53) and (5.32).

Lemma 5.14. *Let $M(\lambda_1)$ be the constant defined in Lemma 5.1, and suppose $T_2 > T_1 \geq M(\lambda_1)$. Let $\tilde{a}_{h,\tau}$, $\tilde{b}_{h,\tau}$ and $\tilde{U}_n$ be the solutions to* (5.53)*, and $\tilde{u}_h(t)$ be the solution to the semidiscrete problem* (5.32)*. Then there holds*

$$\|\tilde{a}_{h,\tau} - \tilde{u}_h(0)\|_{L^2(\Omega)} + \|\tilde{b}_{h,\tau} - \partial_t\tilde{u}_h(0)\|_{L^2(\Omega)} \leq c\big(\tau + h^2\gamma^{-1}\big)\big(\|a\|_{L^2(\Omega)} + \|b\|_{L^2(\Omega)}\big)$$

and

$$\|\tilde{U}_n - \tilde{u}_h(t_n)\|_{L^2(\Omega)} \leq c\big(\tau t_n^{\alpha-1} + h^2\big) \min(\gamma^{-1}, t_n^{-\alpha})\big(\|a\|_{L^2(\Omega)} + \|b\|_{L^2(\Omega)}\big).$$

Proof. Using representations (5.55) and (5.33), we derive

$$
\begin{aligned}
&\begin{bmatrix} \tilde a_{h,\tau} - \tilde u_h(0) \\ \tilde b_{h,\tau} - \partial_t \tilde u(0) \end{bmatrix} \\
&= \Big(\gamma\mathcal{I} + \mathcal{G}_{h,\tau}(T_1,T_2)\Big)^{-1} \begin{bmatrix} P_h g_1 \\ P_h g_2 \end{bmatrix} - \Big(\gamma\mathcal{I} + \mathcal{G}_{h}(T_1,T_2)\Big)^{-1} \begin{bmatrix} P_h g_1 \\ P_h g_2 \end{bmatrix} \\
&= \Big(\gamma\mathcal{I} + \mathcal{G}_{h,\tau}(T_1,T_2)\Big)^{-1} \begin{bmatrix} (P_h - R_h) g_1 \\ (P_h - R_h) g_2 \end{bmatrix} + \Big(\gamma\mathcal{I} + \mathcal{G}_{h}(T_1,T_2)\Big)^{-1} \begin{bmatrix} (R_h - P_h) g_1 \\ (R_h - P_h) g_2 \end{bmatrix} \\
&+ \Big(\mathcal{G}_h(T_1,T_2) - \mathcal{G}_{h,\tau}(T_1,T_2)\Big)\Big(\gamma\mathcal{I} + \mathcal{G}_{h,\tau}(T_1,T_2)\Big)^{-1}\Big(\gamma\mathcal{I} + \mathcal{G}_{h}(T_1,T_2)\Big)^{-1} \begin{bmatrix} R_h g_1 \\ R_h g_2 \end{bmatrix} \\
&= I_1 + I_2 + I_3.
\end{aligned}
$$

Using Lemmas 5.7 and 5.12 we can obtain an estimate for I_1 and I_2:

$$
\begin{aligned}
\|I_1\|_{L^2(\Omega)} + \|I_2\|_{L^2(\Omega)} &\le ch^2\gamma^{-1}(\|g_1\|_{\dot H^2(\Omega)} + \|g_2\|_{\dot H^2(\Omega)}) \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\
&\le ch^2\gamma^{-1}(\|a\|_{L^2(\Omega)} + \|b\|_{L^2(\Omega)}) \begin{bmatrix} 1 \\ 1 \end{bmatrix},
\end{aligned}
$$

where in the last inequality we use the regularity estimate in Lemma 2.3. Then for the term I_3, we apply Lemma 5.11 and Corollary 5.4 again to derive

$$
\begin{aligned}
\|I_3\|^2_{L^2(\Omega)} &\le c \sum_{j=1}^J \frac{(R_h g_1, \varphi_j^h)^2 + (R_h g_2, \varphi_j^h)^2}{\partial_t \psi_\tau(T_1,T_2;\lambda_j^h)^2 \partial_t \psi(T_1,T_2;\lambda_j^h)^2 (\lambda_j^h T_1^\alpha)^6 N_1^2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\
&\le c\tau^2 \sum_{j=1}^J (\lambda_j^h)^2 \Big((R_h g_1, \varphi_j^h)^2 + (R_h g_2, \varphi_j^h)^2 \Big) \begin{bmatrix} 1 \\ 1 \end{bmatrix}.
\end{aligned}
$$

Noting that $\Delta_h R_h = P_h \Delta$, then we apply Lemma 2.3 to obtain

$$
\begin{aligned}
\|\Delta_h R_h g_1\|_{L^2(\Omega)} + \|\Delta_h R_h g_2\|_{L^2(\Omega)} &= \|P_h \Delta g_1\|_{L^2(\Omega)} + \|P_h \Delta g_2\|_{L^2(\Omega)} \\
&\le (\|\Delta g_1\|_{L^2(\Omega)} + \|\Delta g_2\|_{L^2(\Omega)}) \\
&\le c(\|a\|_{L^2(\Omega)} + \|b\|_{L^2(\Omega)}).
\end{aligned} \tag{5.56}
$$

In conclusion, we obtain

$$
\|\partial_t a_{h,\tau} - \tilde u_h(0)\|_{L^2(\Omega)} + \|\partial_t b_{h,\tau} - \partial_t \tilde u_h(0)\|_{L^2(\Omega)} \le c(\tau + h^2\gamma^{-1})(\|a\|_{L^2(\Omega)} + \|b\|_{L^2(\Omega)}).
$$

Next, from (5.31) and (5.54) we derive the splitting that

$$
\begin{aligned}
&\partial_t U_n - \tilde{u}_h(t_n) \\
&= \mathcal{F}_{h,\tau}^n \Big(\gamma \mathcal{I} + \mathcal{G}_{h,\tau}(T_1,T_2)\Big)^{-1} \begin{bmatrix} P_h g_1 \\ P_h g_2 \end{bmatrix} - \mathcal{F}_h(t_n)\Big(\gamma \mathcal{I} + \mathcal{G}_h(T_1,T_2)\Big)^{-1} \begin{bmatrix} P_h g_1 \\ P_h g_2 \end{bmatrix} \\
&= \left(\mathcal{F}_{h,\tau}^n \Big(\gamma \mathcal{I} + \mathcal{G}_{h,\tau}(T_1,T_2)\Big)^{-1} \begin{bmatrix} (P_h - R_h) g_1 \\ (P_h - R_h) g_2 \end{bmatrix} + \mathcal{F}_h(t_n)\Big(\gamma \mathcal{I} + \mathcal{G}_h(T_1,T_2)\Big)^{-1} \begin{bmatrix} (R_h - P_h) g_1 \\ (R_h - P_h) g_2 \end{bmatrix} \right) \\
&\quad + \left(\mathcal{F}_{h,\tau}^n \Big(\gamma \mathcal{I} + \mathcal{G}_{h,\tau}(T_1,T_2)\Big)^{-1} \begin{bmatrix} R_h g_1 \\ R_h g_2 \end{bmatrix} - \mathcal{F}_h(t_n)\Big(\gamma \mathcal{I} + \mathcal{G}_h(T_1,T_2)\Big)^{-1} \begin{bmatrix} R_h g_1 \\ R_h g_2 \end{bmatrix} \right) \\
&=: I_1 + I_2.
\end{aligned}
$$

To bound the first term I_1, we apply approximation properties of P_h and R_h, Lemmas 5.7 and 5.12, and the argument (5.56) to obtain

$$
\begin{aligned}
\|I_1\|_{L^2(\Omega)} &\le ch^2 \min(\gamma^{-1}, t_n^{-\alpha})(\|\Delta_h R_h g_1\|_{L^2(\Omega)} + \|\Delta_h R_h g_2\|_{L^2(\Omega)}) \\
&\le ch^2 \min(\gamma^{-1}, t_n^{-\alpha})(\|g_1\|_{\dot{H}^2(\Omega)} + \|g_2\|_{\dot{H}^2(\Omega)}) \\
&\le ch^2 \min(\gamma^{-1}, t_n^{-\alpha})(\|a\|_{L^2(\Omega)} + \|b\|_{L^2(\Omega)}),
\end{aligned}
$$

where in the last inequality we use the regularity estimate in Lemma 2.3. For the other term I_2, we split it into three parts

$$
\begin{aligned}
I_2 &= \gamma(\mathcal{F}_{h,\tau}^n - \mathcal{F}_h(t_n))\mathcal{I}\Big(\gamma \mathcal{I} + \mathcal{G}_{h,\tau}(T_1,T_2)\Big)^{-1}\Big(\gamma \mathcal{I} + \mathcal{G}_h(T_1,T_2)\Big)^{-1} \begin{bmatrix} R_h g_1 \\ R_h g_2 \end{bmatrix} \\
&\quad + \mathcal{F}_{h,\tau}^n(\mathcal{G}_h(T_1,T_2) - \mathcal{G}_{h,\tau}(T_1,T_2))\Big(\gamma \mathcal{I} + \mathcal{G}_{h,\tau}(T_1,T_2)\Big)^{-1}\Big(\gamma \mathcal{I} + \mathcal{G}_h(T_1,T_2)\Big)^{-1} \begin{bmatrix} R_h g_1 \\ R_h g_2 \end{bmatrix} \\
&\quad + \mathcal{G}_{h,\tau}(T_1,T_2)(\mathcal{F}_{h,\tau}^n - \mathcal{F}_h(t_n))\Big(\gamma \mathcal{I} + \mathcal{G}_{h,\tau}(T_1,T_2)\Big)^{-1}\Big(\gamma \mathcal{I} + \mathcal{G}_h(T_1,T_2)\Big)^{-1} \begin{bmatrix} R_h g_1 \\ R_h g_2 \end{bmatrix} \\
&=: \sum_{i=1}^{3} I_{2,i}.
\end{aligned}
$$

Then we intend to establish bounds for those terms one by one. For the term $I_{2,1}$, we apply the spectral decomposition to obtain

$$
\begin{aligned}
I_{2,1} = \sum_{j=1}^{J} \gamma &\Big[-(F_\tau^n(\lambda_j^h) - E_{\alpha,1}(-\lambda_j^h t_n^\alpha)) \quad \bar{F}_\tau^n(\lambda_j^h) - t_n E_{\alpha,2}(-\lambda_j^h t_n^\alpha) \Big] \\
&\partial_t \psi_\tau(T_1,T_2;\lambda_j^h)^{-1} \begin{bmatrix} \gamma + \bar{F}_\tau^{N_2}(\lambda_j^h) & -\bar{F}_\tau^{N_1}(\lambda_j^h) \\ -F_\tau^{N_2}(\lambda_j^h) & -\gamma + F_\tau^{N_1}(\lambda_j^h) \end{bmatrix} \\
&\partial_t \psi(T_1,T_2;\lambda_j^h)^{-1} \begin{bmatrix} \gamma + T_2 E_{\alpha,2}(-\lambda_j^h T_2^\alpha) & -T_1 E_{\alpha,2}(-\lambda_j^h T_1^\alpha) \\ -E_{\alpha,1}(-\lambda_j^h T_2^\alpha) & -\gamma + E_{\alpha,1}(-\lambda_j^h T_1^\alpha) \end{bmatrix} \begin{bmatrix} (R_h g_1, \varphi_j^h)\varphi_j^h \\ (R_h g_2, \varphi_j^h)\varphi_j^h \end{bmatrix}.
\end{aligned}
$$

Using Corollary 5.4 and the estimate (5.49), we obtain

$$|\partial_t\psi_\tau(T_1,T_2;\varphi_j^h)|^{-1}\begin{bmatrix}|\gamma+\bar F_\tau^{N_2}(\lambda_j^h)| & |-\bar F_\tau^{N_1}(\lambda_j^h)|\\ |-F_\tau^{N_2}(\lambda_j^h)| & |-\gamma+F_\tau^{N_1}(\lambda_j^h)|\end{bmatrix}\le\frac{c\lambda_j}{1+\gamma\lambda_j}\begin{bmatrix}1&1\\1&1\end{bmatrix}\le c\min(\gamma^{-1},\lambda_j^h)\begin{bmatrix}1&1\\1&1\end{bmatrix}.$$

The first estimate in Lemma 5.11 and the estimates (5.22) and (5.56) imply

$$\begin{aligned}\|I_{2,1}\|_{L^2(\Omega)}^2&\le c\tau^2t_n^{-2}\sum_{j=1}^J\left(\frac{\lambda_j^h}{1+\lambda_j^ht_n^\alpha}\right)^2\big((R_hg_1,\varphi_j^h)^2+(R_hg_2,\varphi_j^h)^2\big)\\&\le c\tau^2t_n^{-2}\sum_{j=1}^J(\lambda_j^h)^2\big((R_hg_1,\varphi_j^h)^2+(R_hg_2,\varphi_j^h)^2\big),\\&=c\tau^2t_n^{-2}\big(\|\Delta_hR_hg_1\|_{L^2(\Omega)}^2+\|\Delta_hR_hg_2\|_{L^2(\Omega)}^2\big)\\&\le c\tau^2t_n^{-2}\big(\|a\|_{L^2(\Omega)}+\|b\|_{L^2(\Omega)}\big)\end{aligned}$$

while the second estimate in Lemma 5.11 indicates

$$\begin{aligned}\|I_{2,1}\|_{L^2(\Omega)}^2&\le c\tau^2t_n^{2\alpha-2}\gamma^{-2}\sum_{j=1}^J(\lambda_j^h)^2\big((R_hg_1,\varphi_j^h)^2+(R_hg_2,\varphi_j^h)^2\big)\\&\le c\tau^2t_n^{2\alpha-2}\gamma^{-2}\big(\|a\|_{L^2(\Omega)}+\|b\|_{L^2(\Omega)}\big).\end{aligned}$$

Combining these two estimates we arrive at

$$\|I_{2,1}\|_{L^2(\Omega)}\le c\tau t_n^{\alpha-1}\min(\gamma^{-1},t_n^{-\alpha})\big(\|a\|_{L^2(\Omega)}+\|b\|_{L^2(\Omega)}\big).$$

The estimates for $I_{2,2}$ and $I_{2,3}$ follows analogously. □

Then we combine Lemmas 5.4, 5.9, 5.13 and 5.14 to obtain the following error estimate for the fully discrete scheme (5.50).

Theorem 5.4. *Let $M(\lambda_1)$ be the constant defined in Lemma 5.1, and suppose that $T_2>T_1\ge M(\lambda_1)$. Let $\tilde a_{h,\tau}^\delta$, $\tilde b_{h,\tau}^\delta$ and $\tilde U_n^\delta$ be the solutions to* (5.50)*, and u be the exact solution to the problem* (5.3)*. If $a,b\in\dot H^q(\Omega)$ with $q\in[0,2]$, then there holds*

$$\|\tilde a_{h,\tau}^\delta-a\|_{L^2(\Omega)}+\|\tilde b_{h,\tau}^\delta-b\|_{L^2(\Omega)}\le c\big(\gamma^{\frac q2}+\tau+(h^2+\delta)\gamma^{-1}\big)$$

and

$$\|\tilde U_n^\delta-u(t_n)\|_{L^2(\Omega)}\le c\Big[\gamma\min(\gamma^{-(1-\frac q2)},t_n^{-(1-\frac q2)\alpha})+\big(\tau t_n^{\alpha-1}+h^2+\delta\big)\min(\gamma^{-1},t_n^{-\alpha})\Big].$$

Moreover, if $a,b\in L^2(\Omega)$, then for any $s\in(0,1]$

$$\|\tilde a_{h,\tau}^\delta-a\|_{L^2(\Omega)}+\|\tilde b_{h,\tau}^\delta-b\|_{H^{-s}(\Omega)}\to0,\qquad as\ \ \gamma,\tau\to0,\ \frac\delta\gamma\to0,\ \frac h\gamma\to0.$$

In the estimate, the constant c may depend on T_1, T_2, T, a and b, but is always independent of τ, h, γ, δ and t.

5.4 Numerical results

In this section, we illustrate our theoretical results by presenting some one- and two-dimensional examples. Throughout, we consider the observation data

$$g_\delta = u(T) + \varepsilon\delta \sup_{x\in\Omega} u(x,T) \quad \text{and} \quad g_\delta = u(T) + \varepsilon\delta \sup_{x\in\Omega} u(x,T),$$

ε is generated following the standard Gaussian distribution and δ denotes the (relative) noise level. Throughout this section, we fix $T_1 = 1$ and $T_2 = 1.2$.

To examine *a priori* estimates in Sections 5.2 and 6.3, we begin with a one-dimensional diffusion-wave model (5.3) in the unit interval $\Omega = (0,1)$. We use the standard piecewise linear FEM with uniform mesh size $h = 1/(J+1)$ for the space discretization, and the backward Euler convolution quadrature method with uniform step size $\tau = T/N$ for the time discretization.

To solve the discrete system (5.50), we apply the following direct method by spectral decomposition. For the uniform mesh size $h = 1/(J+1)$, we let $x_i = ih$ for all $i = 0, 1, \ldots, J+1$. Then the eigenvalues and eigenfunctions of $-\Delta_h$ have the closed form:

$$\lambda_j^h = \frac{6}{h^2}\frac{1-\cos(j\pi h)}{2+\cos(j\pi h)}, \quad \varphi_j^h(x_i) = \sqrt{2}\sin(j\pi x_i), \quad i,j = 1,2,\cdots,J. \tag{5.57}$$

We compute the observation data $u(T_1)$, $u(T_2)$ and reference solution $u(t)$ by using the semidiscrete scheme with a very fine mesh size, i.e., $h = 1/2000$.

For each example, we measure the errors of semidiscrete scheme

$$e_{\mathrm{ini},s} = \frac{\|\tilde{u}_h^\delta(0) - a\|_{L^2(\Omega)}}{\|a\|_{L^2(\Omega)}} + \frac{\|\partial_t \tilde{u}_h^\delta(0) - b\|_{L^2(\Omega)}}{\|b\|_{L^2(\Omega)}},$$
$$e_s(t) = \|\tilde{u}_h^\delta(t) - u(t)\|_{L^2(\Omega)}/\|u(t)\|_{L^2(\Omega)} \quad \text{for some} \quad t > 0,$$

and the errors of fully discrete scheme

$$e_{\mathrm{ini},f} = \frac{\|\tilde{a}_{h,\tau}^\delta - a\|_{L^2(\Omega)}}{\|a\|_{L^2(\Omega)}} + \frac{\|\tilde{b}_{h,\tau}^\delta - b\|_{L^2(\Omega)}}{\|b\|_{L^2(\Omega)}},$$
$$e_f^n = \|\tilde{U}_n^\delta - u(t_n)\|_{L^2(\Omega)}/\|u(t_n)\|_{L^2(\Omega)} \quad \text{for some} \quad n \geq 1.$$

The normalization enables us to observe the behavior of the error with respect to α and t.

Example (a): smooth initial data. We start with the smooth initial condition

$$a(x) = -\sin(\pi x), \quad b(x) = x(1-x) \in \dot{H}^2(\Omega) = H^2(\Omega) \cap H_0^1(\Omega),$$

and source term $f \equiv 0$. We compute the solution of the regularized semidiscrete scheme (5.31),

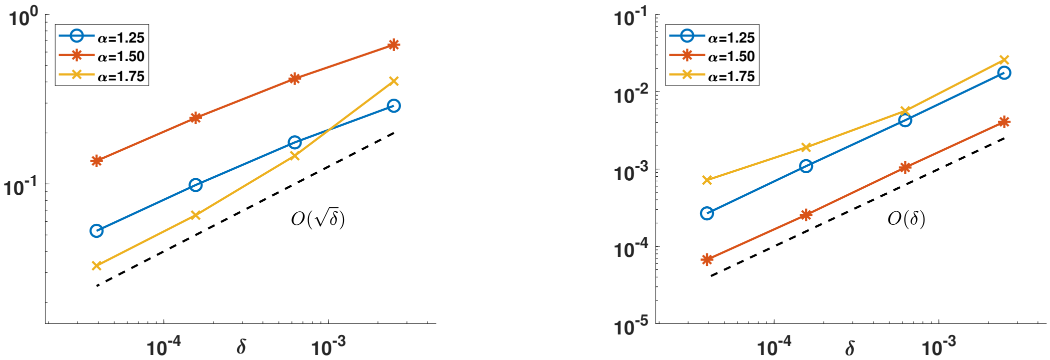
$$\begin{bmatrix} \tilde{u}_h^\delta(0) \\ \partial_t \tilde{u}_h^\delta(0) \end{bmatrix} = (\gamma\mathcal{I} + \mathcal{G}_h(T_1,T_2))^{-1} \begin{bmatrix} P_h g_1^\delta \\ P_h g_2^\delta \end{bmatrix} \quad \text{and} \quad \tilde{u}_h^\delta(t) = \mathcal{F}_h(t)(\gamma\mathcal{I} + \mathcal{G}_h(T_1,T_2))^{-1} \begin{bmatrix} P_h g_1^\delta \\ P_h g_2^\delta \end{bmatrix} \tag{5.58}$$

by using the formulae

$$\begin{bmatrix} \tilde{u}_h^\delta(0) \\ \partial_t \tilde{u}_h^\delta(0) \end{bmatrix} = \sum_{j=1}^J \partial_t \psi(T_1, T_2; \lambda_j^h)^{-1} \begin{bmatrix} \gamma + T_2 E_{\alpha,2}(-\lambda_j^h T_2^\alpha) & -T_1 E_{\alpha,2}(-\lambda_j^h T_1^\alpha) \\ -E_{\alpha,1}(-\lambda_j^h T_2^\alpha) & -\gamma + E_{\alpha,1}(-\lambda_j^h T_1^\alpha) \end{bmatrix} \begin{bmatrix} (P_h g_1^\delta, \varphi_j^h)\varphi_j^h \\ (P_h g_2^\delta, \varphi_j^h)\varphi_j^h \end{bmatrix},$$

$$\tilde{u}_h^\delta(t) = \sum_{j=1}^J \tilde{\psi}(T_1, T_2; \lambda_j^h)^{-1} \begin{bmatrix} E_{\alpha,1}(-\lambda_j^h t^\alpha) & t E_{\alpha,2}(-\lambda_j^h t^\alpha) \end{bmatrix}$$
$$\begin{bmatrix} \gamma + T_2 E_{\alpha,2}(-\lambda_j^h T_2^\alpha) & -T_1 E_{\alpha,2}(-\lambda_j^h T_1^\alpha) \\ -E_{\alpha,1}(-\lambda_j^h T_2^\alpha) & -\gamma + E_{\alpha,1}(-\lambda_j^h T_1^\alpha) \end{bmatrix} \begin{bmatrix} (P_h g_1^\delta, \varphi_j^h)\varphi_j^h \\ (P_h g_2^\delta, \varphi_j^h)\varphi_j^h \end{bmatrix}$$

where $(\lambda_j^h, \varphi_j^h)$, for $j = 1, \cdots, J$ are given by (5.57). To accurately evaluate the Mittag-Leffler functions, we employ the numerical algorithm developed in [91].



(a) $e_{\text{ini},s}$.

(b) $e_s(t)$ with $t = 0.5$.

Figure 5.1: Example (a): plot of semidiscrete errors. Left: error for approximating initial data, where $h = \sqrt{\delta}$, and $\gamma = \sqrt{\delta}/12, \sqrt{\delta}, \sqrt{\delta}/2$ for $\alpha = 1.25, 1.5, 1.75$ respectively. Right: error for approximating solution $u(t)$ at $t = 0.5$, where $h = \sqrt{\delta}$ and $\gamma = \sqrt{\delta}/5, \sqrt{\delta}/5, \sqrt{\delta}/2$ for $\alpha = 1.25, 1.5, 1.75$ respectively.

By Theorem 5.3, we compute $\tilde{u}_h^\delta(0)$ and $\partial_t \tilde{u}_h^\delta(0)$ by choosing the parameters $\gamma \sim \sqrt{\delta}$ and $h \sim \sqrt{\delta}$ for a given δ, and expect a convergence of order $O(\sqrt{\delta})$. For $t > 0$, we compute $\tilde{u}_h^\delta(t)$ by choosing the parameters $h \sim \sqrt{\delta}$, $\gamma \sim \delta$ for a given δ, and expect a convergence of order $O(\delta)$. In Figure 5.1, we plot the errors of semidiscrete solutions (5.58) with different fractional order α. Our numerical experiments fully support our theoretical results in Theorem 5.3. It is interesting to observe that the error in case of $\alpha = 1.5$ is bigger when reconstructing the initial condition, while the error for $\alpha = 1.5$ becomes smaller when we compute the solution at time level $t > 0$.

Similarly, we compute the numerical solutions to the fully discrete scheme (5.50)

$$\begin{bmatrix} \tilde{a}_{h,\tau}^\delta \\ \tilde{b}_{h,\tau}^\delta \end{bmatrix} = (\gamma \mathcal{I} + \mathcal{G}_{h,\tau}(T_1, T_2))^{-1} \begin{bmatrix} P_h g_1^\delta \\ P_h g_2^\delta \end{bmatrix} \quad \text{and} \quad \tilde{U}_n^\delta = \mathcal{F}_{h,\tau}^n (\gamma \mathcal{I} + \mathcal{G}_{h,\tau}(T_1, T_2))^{-1} \begin{bmatrix} P_h g_1^\delta \\ P_h g_2^\delta \end{bmatrix}, \text{for all } \forall n \geq 1.$$

We compute them by using the formulae

$$\begin{bmatrix} \partial_t a^\delta_{h,\tau} \\ \partial_t b^\delta_{h,\tau} \end{bmatrix} = \sum_{j=1}^{J} \partial_t \psi_\tau(T_1, T_2; \lambda^h_j)^{-1} \begin{bmatrix} \gamma + \bar{F}^{N_2}_{h,\tau} & -\bar{F}^{N_1}_{h,\tau} \\ -F^{N_2}_{h,\tau} & -\gamma + F^{N_1}_{h,\tau} \end{bmatrix} \begin{bmatrix} (P_h g^\delta_1, \varphi^h_j)\varphi^h_j \\ (P_h g^\delta_2, \varphi^h_j)\varphi^h_j \end{bmatrix},$$

$$\partial_t U^\delta_n = \sum_{j=1}^{J} \tilde{\psi}_\tau(T_1, T_2; \lambda^h_j)^{-1} \begin{bmatrix} F^n_{h,\tau} & \bar{F}^n_{h,\tau} \end{bmatrix} \begin{bmatrix} \gamma + \bar{F}^{N_2}_{h,\tau} & -\bar{F}^{N_1}_{h,\tau} \\ F^{N_2}_{h,\tau} & -\gamma + F^{N_1}_{h,\tau} \end{bmatrix} \begin{bmatrix} (P_h g^\delta_1, \varphi^h_j)\varphi^h_j \\ (P_h g^\delta_2, \varphi^h_j)\varphi^h_j \end{bmatrix}.$$

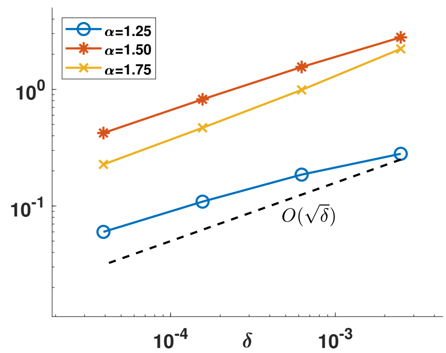
Then Theorem 5.4 implies that for $a, b \in \dot{H}^2(\Omega)$

$$\|a^\delta_{h,\tau} - a\|_{L^2(\Omega)} + \|b^\delta_{h,\tau} - b\|_{L^2(\Omega)} \le c(\gamma + \tau + (h^2 + \delta)\gamma^{-1}),$$

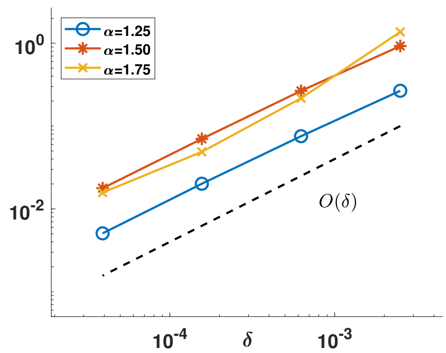
and

$$\|\partial_t U^\delta_n - u(t_n)\|_{L^2(\Omega)} \le c(\gamma + \tau + h^2 + \delta), \quad \text{for a fixed } \; t_n > 0.$$

Therefore, with a given noise level δ, to recover the initial data a and b, we choose parameters $h \sim \sqrt{\delta}$, $\tau \sim \sqrt{\delta}$ and $\gamma \sim \sqrt{\delta}$, while to approximate solution $u(t_n)$ with some $t_n > 0$, we let $h \sim \sqrt{\delta}$, $\tau \sim \delta$, $\gamma \sim \delta$. According to Theorem 5.4, we expect that the convergence rate for the error $e_{\mathrm{ini},f}$ is $O(\sqrt{\delta})$ while the error e^n_f converges to zero as $O(\delta)$ for any fixed $t_n > 0$. They are fully supported by numerical results plotted in Figure 5.2.



(a) $e_{ini,f}$.

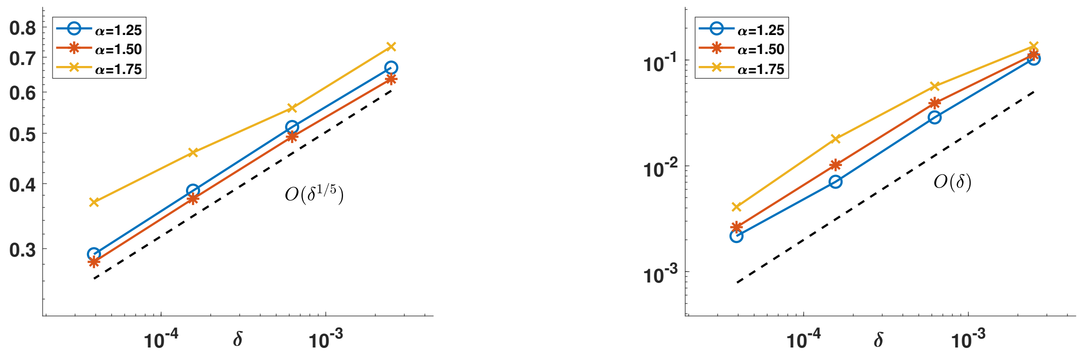


(b) e^n_f with $t_n = 0.5$.

Figure 5.2: Example (a): fully discrete errors. Left: error for approximating initial data, where $h = \sqrt{\delta}$, $\tau = \sqrt{\delta}/2$ and $\gamma = \sqrt{\delta}/10$, $\sqrt{\delta}/10$, $\sqrt{\delta}/15$ for $\alpha = 1.25, 1.5, 1.75$ respectively, Right: error for approximating solution $u(t_n)$ at $t_n = 0.5$, where $h = \sqrt{\delta}$, $\tau = 10\delta$ and $\gamma = \delta$, $\delta/2$, $\delta/2$ for $\alpha = 1.25, 1.5, 1.75$ respectively.

Example (b): non-smooth initial data. Next, we turn to the case of nonsmooth data and expect to examine the influence of weak regularity of problem data. Consider

$$a(x) = \begin{cases} 0, & 0 \le x \le 0.5; \\ 1, & 0.5 \le x \le 1. \end{cases}, \quad b(x) = \begin{cases} 1, & 0 \le x \le 0.5; \\ 0, & 0.5 \le x \le 1 \end{cases}$$

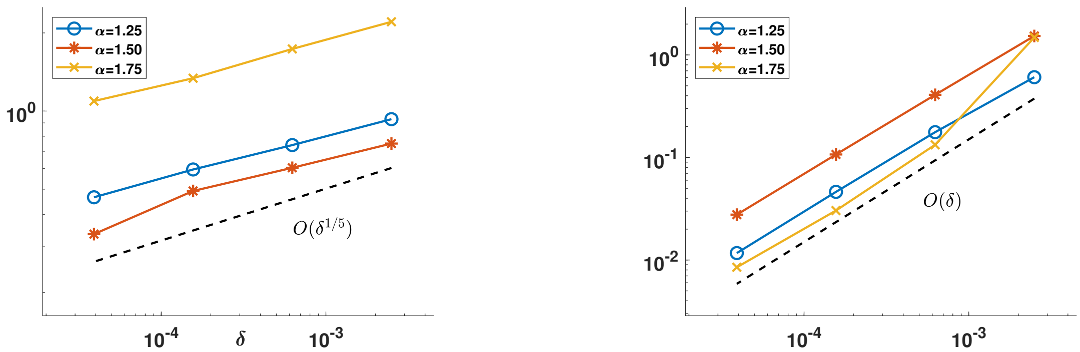


(a) $e_{ini,s}$.

(b) $e_s(t)$ with $t = 0.5$.

Figure 5.3: Example (b): semidiscrete errors. Left: error for reconstructing initial data, where $h = \sqrt{\delta}$ and $\gamma = \delta^{4/5}/15, \delta^{4/5}/15, \delta^{4/5}/8$ for $\alpha = 1.25, 1.5, 1.75$ respectively. Right: error for approximately solving $u(t)$ at $t = 0.5$, where $h = \sqrt{\delta}$ and $\gamma = \delta/10, \delta/5, \delta/5$ for $\alpha = 1.25, 1.5, 1.75$ respectively

.



(a) $e_{ini,f}$.

(b) e_f^n with $t_n = 0.5$.

Figure 5.4: Example (b): fully discrete errors. Left: error for reconstructing initial data, where $h = \sqrt{\delta}$, $\tau = \delta^{1/5}/20$ and $\gamma = \delta^{4/5}/2, \delta^{4/5}/15, \delta^{4/5}/2$ for $\alpha = 1.25, 1.5, 1.75$ respectively. Right: error for approximately solving $u(t_n)$ at $t_n = 0.5$, where $h = \sqrt{\delta}$, $\tau = 10\delta$, $\gamma = \delta/10, \delta, \delta/2$ for $\alpha = 1.25, 1.5, 1.75$ respectively.

and source term $f \equiv 0$. It is well-known that $a, b \in \dot{H}^{\frac{1}{2}-\varepsilon}(\Omega)$ for any $\varepsilon \in (0, \frac{1}{2}]$. According to Theorem 5.3, the error of the semidiscrete discrete solution satisfies

$$\|\tilde{u}_h^\delta - a\|_{L^2(\Omega)} + \|\partial_t \tilde{u}_h^\delta - b\|_{L^2(\Omega)} \leq c(\gamma^{\frac{q}{2}} + (h^2 + \delta)\gamma^{-1}),$$
$$\|(\tilde{u}_h^\delta - u)(t)\|_{L^2(\Omega)} \leq c(\gamma + h^2 + \delta), \quad \text{for a given } \ t > 0.$$

Therefore, for given δ, to numerically reconstruct the initial data a and b, we let $h = \sqrt{\delta}$, and $\gamma \sim \delta^{4/5}$ and expect that the error converges to zero as $O(\delta^{\frac{1}{5}})$, while to approximate $u(t)$ for some $t > 0$, we let $h \sim \sqrt{\delta}$ and $\gamma \sim \delta$ and expect a convergence of order $O(\delta)$. The theoretical results agree well with the numerical results in Figure 5.3.

In Figure 5.4 we plot errors of the numerical reconstruction by fully discrete scheme (5.50). According to Theorem 5.4 we have the error estimate that (with $q = \frac{1}{2} - \varepsilon$)

$$\|a_{h,\tau}^\delta - a\|_{L^2(\Omega)} + \|b_{h,\tau}^\delta - b\|_{L^2(\Omega)} \leq c(\gamma^{\frac{q}{2}} + \tau + (h^2 + \delta)\gamma^{-1}),$$
$$\|\partial_t U_n^\delta - u(t_n)\|_{L^2(\Omega)} \leq c(\gamma + \tau + h^2 + \delta), \quad \text{for any fixed } \ t_n > 0.$$

Therefore, we choose parameters $h \sim \sqrt{\delta}$, $\tau \sim \delta^{1/5}$ and $\gamma \sim \delta^{4/5}$ for the numerical reconstruction of initial data, while we let $h \sim \sqrt{\delta}$, $\tau \sim \delta$ and $\gamma \sim \delta$ for approximately solving the solution $u(t_n)$ for some $t_n > 0$. The empirical convergence results show that $e_{\mathrm{ini},f} \sim \delta^{\frac{1}{5}}$ and $e_f^n \sim \delta$, which are consistent with our theoretical findings. Finally, in figure 5.5, we provide the profiles of solutions to semidiscrete and fully discrete schemes with different noise levels, which show clearly the convergence of the discrete approximation as the noise level δ decreases.

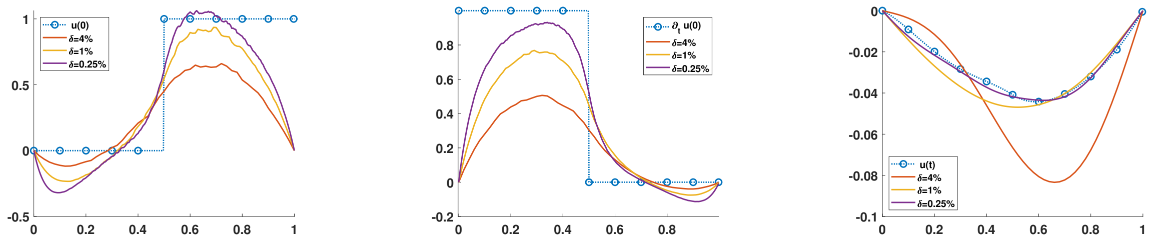
Example (c): 2D examples. Finally, we test a two dimensional diffusion-wave model in $\Omega = (0, 1)^2$ with smooth initial conditions:

$$a(x, y) = \sin(2\pi x)\sin(2\pi y), \quad b(x, y) = 4x(1 - x)y(1 - y) \in \dot{H}^2(\Omega) = H^2(\Omega) \cap H_0^1(\Omega),$$

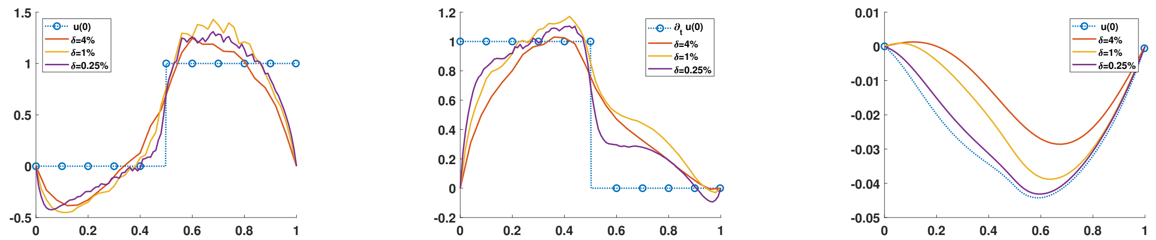
and source term $f \equiv 0$. The reference solution is computed with $h = 1/150$, $\tau = 1/1000$. Noting that the fully discrete system is not symmetric, we apply the biconjugate gradient stabilized method [98].

In Figure 5.6 and 5.7, we plot profiles of (numerical) reconstruction of initial data a, b and approximation errors, with different noise level δ as well as different parameters γ, h, τ chosen according to δ. The empirical observations are in excellent agreement with theoretical results, e.g., convergence as the noise level δ decreases to zero.[1]

[1] Chapter 5 is reprinted with permission from "Backward Diffusion-Wave Problem: Stability, Regularization, and Approximation", Zhengqi Zhang and Zhi Zhou, 2022, SIAM Journal on Scientific Computing Vol. 44 Iss. 5. The candidate mainly works on the research idea and Methodology, the proof details, the coding and data collection in numerical experiments.

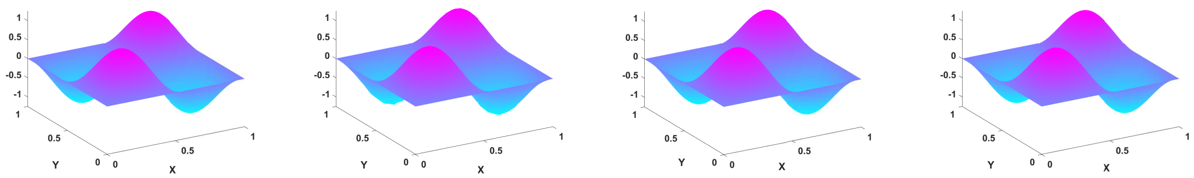


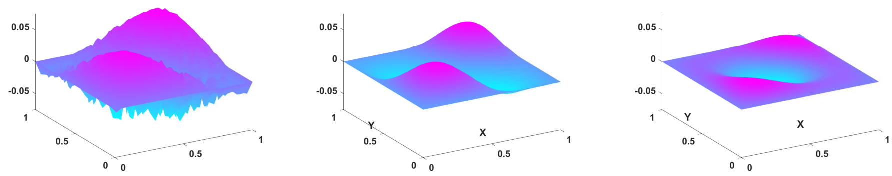
(a) $\tilde{u}_h^\delta(0)$ (b) $\partial_t \tilde{u}_h^\delta(0)$ (c) $\tilde{u}_h^\delta(t)$ with $t = 0.5$



(d) $\tilde{a}_{h,\tau}^\delta$ (e) $\tilde{b}_{h,\tau}^\delta$ (f) $\tilde{U}_n^\delta$, with $t_n = 0.5$

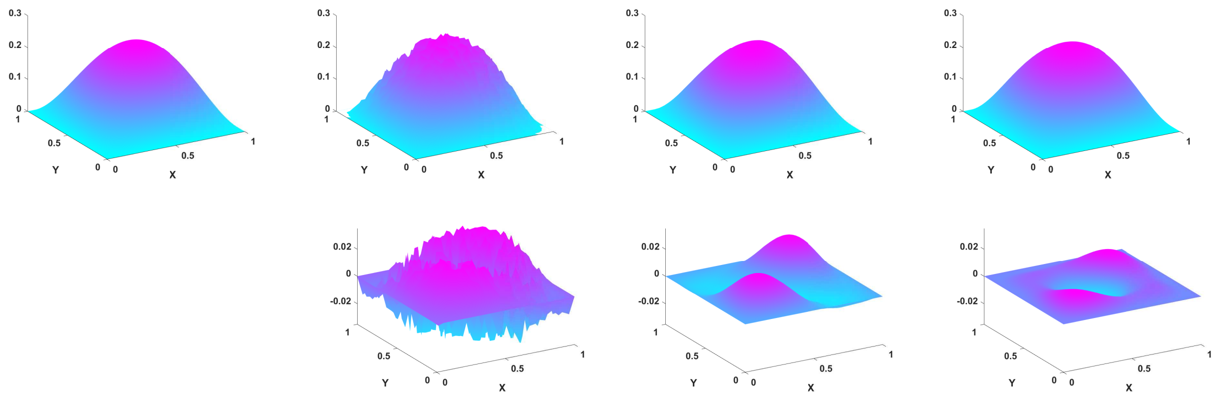
Figure 5.5: Example(b): profiles of semidiscrete and fully discrete solutions with $\alpha = 1.5$ for $\delta = 4\%, 1\%, 0.25\%$. Up row: $h = \sqrt{\delta}/10$, $\gamma = \delta^{4/5}/5$ for both (a) and (b); $h = \sqrt{\delta}/10$, $\gamma = \delta/5$ for (c). Down row : $h = \sqrt{\delta}/10$, $\tau = \delta^{1/5}/10$, $\gamma = \delta^{4/5}/15$ for both (d) and (e); $h = \sqrt{\delta}/10$, $\tau = \delta$, $\gamma = \delta/10$ for (f).





(a) $\delta = 1e-2$. (b) $\delta = 5e-3$. (c) $\delta = 2.5e-3$.

Figure 5.6: Example(c): Top left: Exact initial data a. The remaining three columns are profiles of numerical reconstructions $a_{h,\tau}^\delta$ and theirs errors, with $h = \sqrt{\delta}/4$, $\tau = \sqrt{\delta}/20$, $\gamma = \sqrt{\delta}/4000$.



(a) $\delta = 1e-2$. (b) $\delta = 5e-3$. (c) $\delta = 2.5e-3$.

Figure 5.7: Example(c): Top left: Exact initial data b. The remaining three columns are profiles of numerical reconstructions $b^{\delta}_{h,\tau}$ and their errors, with $h = \sqrt{\delta}/4$, $\tau = \sqrt{\delta}/20$, $\gamma = \sqrt{\delta}/4000$.

CHAPTER 6.

Inverse Potential In Diffusion Equations from terminal Observation

In this chapter we consider an inverse potential problem for the diffusion model with a space-dependent potential and its rigorous numerical analysis. Let $\Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$ be a convex polyhedral domain with a boundary $\partial\Omega$. Fixing $T > 0$ as the final time, we consider the following initial-boundary value problem for the diffusion model with $\alpha \in (0, 1]$:

$$\begin{cases} \partial_t^\alpha u(x,t) - \Delta u(x,t) + q(x)u(x,t) = f(x), & (x,t) \in \Omega \times (0,T], \\ u(x,t) = b(x), & (x,t) \in \partial\Omega \times (0,T], \\ u(x,0) = v(x), & x \in \Omega, \end{cases} \tag{6.1}$$

where v denotes the initial condition, b and f are space-dependent boundary data and source term, respectively. The function q refers to the radiativity or reaction coefficient or potential in the standard parabolic case ($\alpha = 1$), dependent of the specific applications. Throughout, we assume that the potential q is space-dependent.

The notation $\partial_t^\alpha u$ denotes the conventional first-order derivative when $\alpha = 1$, and the Djrbashian-Caputo fractional derivative in time t for $\alpha \in (0, 1)$ defined in (2.3).

We study the following **inverse potential problem** for the (sub)diffusion model (6.1): setting appropriate problem data v, f, b and measuring the final time data $g(x) := u(x, T; q^\dagger)$, then we aim to recover the unknown potential term $q^\dagger(x) \in L^\infty(\Omega)$ such that

$$u(x, T; q^\dagger) = g(x) \quad \text{in } \Omega.$$

Here we denote the solution corresponding to the potential q by $u(x, t; q)$. We also consider the numerical reconstruction from a noisy data

$$g_\delta(x) = u(x, T; q^\dagger) + \xi(x) \quad \text{in } \Omega,$$

and ξ denotes the measurement noise. The accuracy of the observational data g_δ is measured by the noise level $\|g_\delta - g\|_{C(\overline{\Omega})} = \delta$. This inverse potential problem arises in many practical applications, where $q^\dagger$ represents the radiativity coefficient in heat conduction [106] and perfusion coefficient in Pennes' bio-heat equation in human physiology [86].

In the following, we construct an operator K from the PDE (6.1) as follows:

$$K\psi(x) = \frac{f(x) - \partial_t^\alpha u(x, T; \psi) + \Delta g(x)}{g(x)}.$$

From the observational data $g(x) := u(x,T;q)$, we see that the exact potential $q^\dagger$ is one of the fixed points of K. We show the monotonicity of K and use it to construct a decreasing sequence converging to one fixed point. With this monotone sequence, we prove that there is at most one fixed point, which immediately leads to the uniqueness result of the inverse problem (Theorem 6.2). Besides, this argument also deduces a simple reconstruction algorithm. Noting that such the operator K has been considered in [34, 113], but the argument is substantially different. For instance, in [34], the proof of uniqueness relied on a unique continuation result of the solution u, while the proof in [113] used some inverse spectral estimates, which are only valid in the one-dimensional case (cf. [113, Lemma 2.2]). In this work, our analysis mainly relies on the monotonicity of the operator K, which works for convex polyhedral domains in higher dimensions. This novel argument also provides the feasibility of applying the approach in other PDE models. Moreover, under some conditions on problem data, we show a Lipschitz-type stability in Hilbert spaces (Theorem 6.3)

$$\|q_1 - q_2\|_{L^2(\Omega)} \le C\|u(T;q_1) - u(T;q_2)\|_{H^2(\Omega)}, \qquad \text{for all} \;\; q_1, q_2 \in \mathcal{Q}.$$

The proof relies heavily on the smoothing properties and asymptotics of solution operators. This conditional stability plays an essential role in the numerical analysis of our reconstruction algorithm with fully discretization in space and time.

The rest of the Chapter is organized as follows. In Section 6.1, we provide some preliminary results and show the uniqueness of the inverse potential problem by constructing a monotone fixed point iteration. Then in Section 6.2, we prove a conditional stability of the inverse problem in Hilbert spaces by using the smoothing properties and asymptotics of solution operators. The numerical reconstruction with fully discretization is developed and analyzed in Section 6.3, where we show the linear convergence of the iterative algorithm and establish *a priori* error estimates (in terms of discretization parameters and noise level) for the reconstructed potential. Finally, in Section 6.4, we present illustrative one- and two-dimensional numerical results to complement the analysis.

Now we conclude with some useful notations. For any $k \ge 0$ and $p \ge 1$, the space $W^{k,p}(\Omega)$ denotes the standard Sobolev spaces of the kth order, and we write $H^k(\Omega)$ when $p = 2$. The notation $(\cdot,\cdot)$ denotes the $L^2(\Omega)$ inner product. We use the Bochner spaces $W^{k,p}(0,T;B)$ etc., with B being a Banach space. Throughout, the notations c and C, with or without a subscript, denote generic constants which may change at each occurrence, but they are always independent of space mesh size h, time step size τ and noise level δ.

6.1 Unique identification by the monotone iteration

The aim of this section is to investigate the uniqueness of the inverse potential problem. Our approach is to propose a monotone operator which generates a pointwise decreasing sequence converging to the exact potential.

To begin with, we collect some preliminary setting for the controllable conditions v, b, f, and the (unknown) exact potential $q^\dagger$. Throughout, we assume that the exact potential

$$q^\dagger \in \mathcal{Q} \cap C(\overline{\Omega}) \quad \text{with the set} \quad \mathcal{Q} := \{\psi \in L^\infty(\Omega) : 0 \le \psi \le M_1\}. \tag{6.2}$$

Now we recall the maximum principle for the diffusion model (6.1). See [21] for the normal diffusion, [72] and [38, Section 6.5] for the subdiffusion.

Lemma 6.1. *Let $q \in \mathcal{Q} \cap C(\overline{\Omega})$, $f \in L^\infty(0,T;L^2(\Omega))$, $v \in L^2(\Omega)$ and $b = 0$. Assume that v and f are non-negative functions. Then the solution u to equation* (6.1) *satisfies $u \ge 0$ a.e. in $\Omega \times (0,T)$.*

Next, we present the solution representation of the initial-boundary value problem (6.1). For the simplicity of notations, we let I be the identity operator and $A(q)$ be the realization of $-\Delta + qI$ with the homogeneous Dirichlet boundary condition, where the domain is $\mathrm{Dom}(A(q)) = \{\psi \in H_0^1(\Omega) : A(q)\psi \in L^2(\Omega)\} = H_0^1(\Omega) \cap H^2(\Omega)$. If $q \in \mathcal{Q}$, for any $\psi \in H_0^1(\Omega) \cap H^2(\Omega)$, the full elliptic regularity implies (see e.g. [64, Lemma 2.1] and [23, Theorems 3.3 and 3.4])

$$c_1 \|\psi\|_{H^2(\Omega)} \le \|A(q)\psi\|_{L^2(\Omega)} + \|\psi\|_{L^2(\Omega)} \le c_2 \|\psi\|_{H^2(\Omega)} \tag{6.3}$$

with constants c_1 and c_2 independent of q.

Let $D(q)$ be the Dirichlet map by $\phi = D(q)\psi$ with ϕ satisfying

$$-\Delta\phi + q\phi = 0 \ \text{ in } \Omega \ \text{ and } \ \phi = \psi \ \text{ in } \partial\Omega.$$

In particular, for any $q \in \mathcal{Q}$, there exists a constant c independent of q such that

$$\|D(q)\psi\|_{H^2(\Omega)} \le C\|\psi\|_{H^{\frac{3}{2}}(\partial\Omega)} \qquad \text{for all } \ \psi \in H^{\frac{3}{2}}(\partial\Omega). \tag{6.4}$$

This is a direct result of the regularity of the Dirichlet operator $D(0)$ [62, (1.2.2)] and a simple shift argument.

Then the solution u of problem (6.1) could be represented by [62, eq. (2.2)]

$$\begin{aligned} u(t) &= F(t;q)v + A(q)\int_0^t E(s;q)D(q)b \,\mathrm{d}s + \int_0^t E(s;q) f \,\mathrm{d}s \\ &= F(t;q)v + (I - F(t;q))D(q)b + (I - F(t;q))A(q)^{-1} f, \end{aligned} \tag{6.5}$$

where the operators $F(t;q)$ and $E(t;q)$ are defined by [38, eq. (6.25) and (6.26)]

$$F(t;q) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}} e^{zt} z^{\alpha-1} (z^\alpha + A(q))^{-1} \, \mathrm{d}z \quad \text{and} \quad E(t;q) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}} e^{zt} (z^\alpha + A(q))^{-1} \, \mathrm{d}z, \tag{6.6}$$

respectively. Here $\Gamma_{\theta,\kappa}$ denotes the integral contour in the complex plane $\mathbb{C}$ oriented counterclockwise, defined by $\Gamma_{\theta,\kappa} = \{z \in \mathbb{C} : |z| = \kappa, |\arg z| \le \theta\} \cup \{z \in \mathbb{C} : z = \kappa e^{\pm i\theta}, \rho \ge \kappa\}$, with $\kappa \ge 0$ and $\theta \in (\frac{\pi}{2}, \pi)$. Throughout, we fix $\theta \in (\frac{\pi}{2}, \pi)$ so that $z^\alpha \in \Sigma_{\alpha\theta} \subset \Sigma_\theta := \{0 \ne z \in \mathbb{C} : \arg(z) \le \theta\}$, for all $z \in \Sigma_\theta$. Note that $E(t;q) = -A(q)\frac{d}{dt}F(t;q)$, and in case that $\alpha = 1$ there holds $F(t;q) = E(t;q)$.

The next lemma gives smoothing properties and asymptotics of $F(t;q)$ and $E(t;q)$. The proof follows from the resolvent estimate (for any $q \in \mathcal{Q}$) [4, Example 3.7.5 and Theorem 3.7.11]:

$$\|(z + A(q))^{-1}\| \le c_\theta(|z|^{-1}, \lambda^{-1}) \quad \forall z \in \Sigma_\theta, \ \forall \theta \in (0, \pi), \tag{6.7}$$

where $\|\cdot\|$ denotes the operator norm from $L^2(\Omega)$ to $L^2(\Omega)$, and λ denotes the smallest eigenvalue of $-\Delta$ with homogeneous Dirichlet boundary condition. In case that $q \in \mathcal{Q}$, the constant c_θ can be chosen independent of q. The full proof of the following lemma has been given in [38, Theorems 6.4 and 3.2].

Lemma 6.2. *Let λ be the smallest eigenvalue of $-\Delta$ with homogeneous boundary condition. Let $F(t;q)$ and $E(t;q)$ be the solution operators defined in* (6.6) *with potential coefficient $q \in \mathcal{Q}$. Then they satisfy the following properties:*

(i) $\|A(q)F(t;q)v\|_{L^2(\Omega)} + t^{1-\alpha}\|A(q)E(t;q)v\|_{L^2(\Omega)} \le ct^{-\alpha}\|v\|_{L^2(\Omega)}, \quad \forall t \in (0,T]$;

(ii) $\|F(t;q)v\|_{L^2(\Omega)} + t^{1-\alpha}\|E(t;q)v\|_{L^2(\Omega)} \le c\min(1, \lambda^{-1}t^{-\alpha})\|v\|_{L^2(\Omega)}, \quad \forall t \in (0,T]$,

where the constants are independent of q and t.

Throughout the paper, we also need the following assumption on the problem data.

Assumption 6.1. *Let the initial data v, the boundary data b and the source term f satisfy the following conditions:*

(i) $v \in H^2(\Omega)$, $v \ge M_2 > 0$ *in* Ω, $v(x) = b(x)$ *for all* $x \in \partial\Omega$;

(ii) $b \in H^2(\partial\Omega)$, $b \ge M_2 > 0$ *in* $\partial\Omega$;

(iii) $f \in W^{1,p}(\Omega) \subset C(\overline{\Omega})$ *(with* $p > \max(d,2)$*)*, $f \ge 0$ *and* $f + \Delta v - M_1 v \ge 0$ *in* Ω.

Under Assumption 6.1, we have the following results about the solution regularity and behaviors for the direct problem (6.1).

Lemma 6.3. *Let $q \in \mathcal{Q}$ and Assumption 6.1 be valid. Let $u(t)$ be the solution to problem* (6.1) *with potential q. Then The following statements are valid.*

(i) $u \in C([0,T]; H^2(\Omega))$, $\partial_t^\alpha u \in C((0,T]; H^2(\Omega))$, *and there exists a constant* C *independent of* q *such that* $\|u\|_{C(\overline{\Omega}\times[0,T])} \le C$.

Moreover, if $q \in C(\overline{\Omega}) \cap \mathcal{Q}$, *then*

(ii) $\partial_t^\alpha u(x,t) \ge 0$, $u(x,t) \ge M_2$ *for all* $(x,t) \in \overline{\Omega} \times (0,T]$;

(iii) $\Delta u(x,t) \in C(\overline{\Omega})$, $f(x) + \Delta u(x,t) \ge q(x) M_2$ *for all* $t > 0$ *and* $x \in \overline{\Omega}$.

Proof. By the smoothing property in Lemma 6.2, we observe that

$$A(q)[F(t;q)v - F(t;q)D(q)b - F(t;q)A(q)^{-1}f] \in L^2(\Omega).$$

Then the elliptic regularity (see [64, Lemma 2.1] and [23, Theorems 3.3 and 3.4]) implies that $F(t;q)v - F(t;q)D(q)b - F(t;q)A(q)^{-1}f \in H^2(\Omega)$. Besides, we observe that $D(q)b$ and $A(q)^{-1}f$ belong to $H^2(\Omega)$ (see e.g. [1, Proposition 2.12] and [17, Theorem B.54]). These together with (6.5) imply that $u \in C([0,T]; H^2(\Omega))$. Finally, we define an auxiliary function $\phi(x,t)$ satisfying

$$\begin{cases} \partial_t^\alpha \phi(x,t) - \Delta\phi(x,t) = f(x), & (x,t) \in \Omega \times (0,T], \\ \phi(x,t) = b(x), & (x,t) \in \partial\Omega \times (0,T], \\ \phi(x,0) = v(x), & x \in \Omega. \end{cases} \tag{6.8}$$

With Assumption 6.1 and the maximal L^p regularity (see e.g. [64, Lemma 2.1] for parabolic equation and [38, Theorem 6.11] for fractional evolution equations), we know that

$$\phi \in W^{\alpha,p}(0,T; L^2(\Omega)) \cap L^p(0,T; H^2(\Omega)) \quad \text{for any} \quad p \in (1,\infty).$$

Then by means of the Sobolev embedding and the interpolation between $W^{\alpha,p}(0,T;L^2(\Omega))$ and $L^p(0,T;H^2(\Omega))$ with $p > 4/\alpha$ (see e.g., [3, Theorem 5.2]), we have $\phi \in C([0,T]\times\overline{\Omega})$. As a result, the comparison principle, i.e. Lemma 6.1, implies $\|u\|_{C([0,T]\times\overline{\Omega})} \le \|\phi\|_{C([0,T]\times\overline{\Omega})} \le C$, where the constant C is independent of potential q.

Next, we let $w = \partial_t^\alpha u$, which is the solution to the following initial-boundary value problem

$$\begin{cases} \partial_t^\alpha w(x,t) - \Delta w(x,t) + q(x)w(x,t) = 0, & (x,t) \in \Omega \times (0,T], \\ w(x,t) = 0, & (x,t) \in \partial\Omega \times (0,T], \\ w(x,0) = f(x) + \Delta v(x) - q(x)v(x), & x \in \Omega. \end{cases} \tag{6.9}$$

Noting that $w(x,0) \in L^2(\Omega)$ by Assumption 6.1, then we apply Lemma 6.2 to arrive that

$$A(q)w(t) = A(q)F(t;q)[f + \Delta v - qv] \in L^2(\Omega).$$

Then the elliptic regularity implies $\partial_t^\alpha u(t) = w(t) \in H^2(\Omega) \cap H_0^1(\Omega)$ for $t > 0$. Then we complete the proof of (i).

Next, we let $q \in C(\overline{\Omega}) \cap \mathcal{Q}$. Recalling Assumption 6.1 (i) and (iii), we have $f(x)+\Delta v(x)-q(x)v(x) \geq 0$ a.e. in Ω. This and Lemma 6.1 indicate the $\partial_t^\alpha u(x,t) \geq 0$ for all $(x,t) \in \overline{\Omega} \times (0,T]$. This further implies for all $t > 0$ and $x \in \overline{\Omega}$

$$u(x,t) = u(x,0) + \int_0^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)} \partial_s^\alpha u(x,s)\,\mathrm{d}s \geq u(x,0) \geq M_2$$

Then we complete the proof of (ii).

Finally, the facts that $u(t), \partial_t^\alpha u(t), f \in C(\overline{\Omega})$ and $q \in C(\overline{\Omega})$ lead to $\Delta u(t) \in C(\overline{\Omega})$. By the non-negativity of $\partial_t^\alpha u(x,t)$ we conclude that for any $t > 0$,

$$f(x) + \Delta u(x,t) = \partial_t^\alpha u(x,t) + q(x)u(x,t) \geq q(x)u(x,t) \geq q(x)M_2 \quad \text{in } \Omega. \tag{6.10}$$

This completes the proof of (iii). □

From now on, we use the notation $u(q)$ to denote the solution to (6.1) with the potential q. Let $q^\dagger \in C(\overline{\Omega}) \cap \mathcal{Q}$ be the exact potential to be reconstructed. Under Assumption 6.1, according to Lemma 6.3, the (exact) observation $g(x) = u(x,T;q^\dagger)$ satisfies

$$g \in C(\overline{\Omega}), \quad \Delta g \in C(\overline{\Omega}), \quad f(x) + \Delta g(x) \geq 0, \quad \text{and} \quad g(x) \geq M_2 > 0 \text{ for all } x \in \overline{\Omega}. \tag{6.11}$$

To show the uniqueness of the potential, we define an operator

$$Kq(x) = \frac{f(x) - \partial_t^\alpha u(x,T;q) + \Delta g(x)}{g(x)} \quad \text{for} \quad q \in \mathcal{Q}. \tag{6.12}$$

Under Assumption 6.1, Lemma 6.3 implies that the exact potential $q^\dagger$ belongs to $C(\overline{\Omega}) \cap \mathcal{S}$, where

$$\mathcal{S} := \Big\{ \psi \in L^\infty(\Omega) : 0 \leq \psi \leq \frac{f(x) + \Delta g(x)}{g(x)} \Big\}.$$

Next, we intend to show that the inverse potential problem is equivalent to find a fixed point of the operator K in the set $\mathcal{D}(K)$. This is given by the following lemma.

Lemma 6.4. *Let Assumption 6.1 be valid and the data g satisfy the a priori estimate* (6.11). *The operator K is defined by* (6.12). *Then we have the following equivalence.*

(i) If $q^\dagger \in \mathcal{Q} \cap C(\overline{\Omega})$ satisfies $u(x,T;q^\dagger) = g(x)$, then $q^\dagger$ is a fixed point of K in $\mathcal{S}$.

(ii) If $q^* \in \mathcal{S}$ is a fixed point of K, then $q^* \in C(\overline{\Omega})$ and q^* satisfies $u(x,T;q^*) = g(x)$.

Proof. It is obvious that $u(x,T;q^\dagger) = g(x)$ implies that $q^\dagger$ is the fixed point of K. Then the relation (6.11) and the fact that $\partial_t^\alpha u(x,t;q^\dagger) \geq 0$ (by Lemma 6.3) yield that $q^\dagger \in \mathcal{S}$.

Then it suffices to show the reversed conclusion. We assume that $q^* \in \mathcal{S}$ is one fixed point of the operator K. According to the *a priori* estimate (6.11), we have $g, \Delta g, f \in C(\overline{\Omega})$ and $g \geq M_2$. This together with the fact that $\partial_t^\alpha u(T;q^*) \in C(\overline{\Omega})$ in Lemma 6.3 (i) indicates

$$q^* = \frac{f(x) - \partial_t^\alpha u(x,T;q^*) + \Delta g(x)}{g(x)} \in C(\overline{\Omega}) \cap \mathcal{S}.$$

Moreover, we note that

$$f(x) - \partial_t^\alpha u(x,T;q^*) = q^*(x)g(x) - \Delta g(x) = -\Delta u(x,T;q^*) + q^*(x)u(x,T;q^*).$$

Therefore, $w = u(x,T;q^*) - g(x)$ satisfies the elliptic system

$$\begin{cases} -\Delta w(x) + q^*(x)w(x) = 0, & x \in \Omega, \\ w(x) = 0, & x \in \partial\Omega. \end{cases}$$

Then the comparison principle of elliptic equation implies $w = 0$. Hence, $u(x,T;q^*) = g(x)$, which implies that q^* generates the terminal measurement $g(x)$. $\square$

Due to the equivalence given by Lemma 6.4 and the fact that $q^\dagger \in C(\overline{\Omega}) \cap \mathcal{Q}$, we aim to verify that the fixed point of K is unique in $\mathcal{S}$. To this end, we intend to show that K generates a decreasing sequence in $\mathcal{S}$ from an *a priori* chosen starting value. Then the uniqueness of the fixed point follows immediately.

Lemma 6.5 (Monotonicity)**.** *Let Assumption 6.1 be valid and the data g satisfy the* a priori *estimate* (6.11)*. The operator K is defined by* (6.12)*. Then K is a monotone operator, i.e., $Kq_1 \le Kq_2$ for any $q_1, q_2 \in C(\overline{\Omega}) \cap \mathcal{S}$ with $q_1 \le q_2$ in Ω.*

Proof. First of all, we recall Lemma 6.3 which implies that $\partial_t^\alpha u(x,t;q_2) \ge 0$ in $(0,T] \times \Omega$. Then for $w(t) = \partial_t^\alpha u(t;q_1) - \partial_t^\alpha u(t;q_2)$, and note that w satisfies

$$\begin{cases} (\partial_t^\alpha - \Delta + q_1(x))w(x,t) = (q_2 - q_1)\partial_t^\alpha u(x,t;q_2), & (x,t) \in \Omega \times (0,T], \\ w(x,t) = 0, & (x,t) \in \partial\Omega \times (0,T], \\ w(x,0) = (q_2 - q_1)v(x), & x \in \Omega. \end{cases}$$

Since $(q_2 - q_1)v(x)$ and $(q_2 - q_1)\partial_t^\alpha u(x,t;q_2) \ge 0$, using Lemma 6.1 to the above system yields that

$$w(x,t) = \partial_t^\alpha u(x,t;q_1) - \partial_t^\alpha u(x,t;q_2) \ge 0 \quad \text{a.e. in} \quad \Omega.$$

Note that $w(T) \in C(\overline{\Omega})$ according to Lemma 6.3 (i), and hence $w(T) \ge 0$ in $\overline{\Omega}$. From the definition of K in (6.12) and the fact that $g(x) \ge M_2 > 0$ in Ω by (6.11), we have

$$Kq_1 - Kq_2 = \frac{\partial_t^\alpha u(x,T;q_2) - \partial_t^\alpha u(x,T;q_1)}{g(x)} \le 0 \quad \text{in} \quad \Omega.$$

This completes the proof of the lemma. $\square$

Then the monotonicity of K immediately implies the following lemma.

Lemma 6.6. *Let Assumption 6.1 be valid and the data g satisfy the* a priori *estimate* (6.11)*. The operator K is defined by* (6.12)*. If $q_1, q_2 \in C(\overline{\Omega}) \cap \mathcal{S}$ are both fixed points of K and $q_1 \le q_2$, then $q_1 = q_2$.*

Proof. Let $w(x,t) = u(x,t;q_1) - u(x,t;q_2) \in H^2(\Omega)$, then w satisfies

$$\begin{cases} (\partial_t^\alpha - \Delta + q_1(x))w(x,t) = (q_2 - q_1)u(x,t;q_2), & (x,t) \in \Omega \times (0,T], \\ w(x,t) = 0, & (x,t) \in \partial\Omega \times (0,T], \\ w(x,0) = 0, & x \in \Omega. \end{cases} \tag{6.13}$$

From Lemma 6.3 (ii), we have $u(x,t;q_2) \geq M_2 > 0$ in $\overline{\Omega} \times [0,T]$, which leads to the non-negativity of the source $(q_2 - q_1)u(x,t;q_2)$. This yields that $w(x,t) \geq 0$ in $\overline{\Omega} \times [0,T]$. From the proof of Lemma 6.5, we have $\partial_t^\alpha(u(x,t;q_1) - u(x,t;q_2)) = \partial_t^\alpha w(x,t) \geq 0$. The relation

$$w(t) = w(0) + \int_0^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)} \partial_s^\alpha w(s)\ dt$$

together with the observations

$$w(T) = u(T;q_1) - u(T;q_2) = 0, \quad w(0) = 0 \ \text{ and } \ \partial_t^\alpha w(t) \geq 0$$

immediately yields that $\partial_t^\alpha w(t) = 0$ a.e. in $(0,T)$, and hence $w(t) = 0$ for all $t \in [0,T]$. This and the equation (6.13) imply that $(q_2 - q_1)u(x,t;q_2) = 0$ in $\overline{\Omega} \times [0,T]$. This together with the strict positivity of $u(x,t;q_2)$ in $\overline{\Omega} \times [0,T]$ leads to $q_1 = q_2$. $\square$

The above results motivate us to define the iteration:

$$q_0(x) = \frac{f(x) + \Delta g(x)}{g(x)} \in C(\overline{\Omega}) \cap \mathcal{S} \quad \text{and} \quad q_n = Kq_{n-1} \ \text{ for } \ n \in \mathbb{N}^+. \tag{6.14}$$

Note that the initial guess q_0 is set to be the upper bound of the set $\mathcal{S}$. Next, we shall state the main theorem in this section which shows that the fixed point of K must be the limit of the sequence $\{q_n\}_{n=0}^\infty$ generated by (6.14) and hence it is unique.

Theorem 6.2. *Suppose that v, f, b satisfy Assumption 6.1 and the exact potential $q^\dagger$ belongs to $C(\overline{\Omega}) \cap \mathcal{Q}$. Then the sequence $\{q_n\}_{n=0}^\infty$ generated by (6.14) is included in $C(\overline{\Omega}) \cap \mathcal{S}$ and converges decreasingly to $q^\dagger$. Moreover, the fixed point of the operator K in $\mathcal{S}$ is unique.*

Proof. Since $q^\dagger \in C(\overline{\Omega}) \cap \mathcal{Q}$, we conclude that the data g satisfy the *a priori* estimate (6.11). According to Lemma 6.3 (i), we know that $\partial_t^\alpha u(T;q_{n-1}) \in C(\overline{\Omega})$ and hence $q_n \in C(\overline{\Omega})$.

From the proof of Lemma 6.5, we obtain that $\partial_t^\alpha u(T;q_0) \geq 0$ in $\overline{\Omega}$. This further implies

$$q_1 = Kq_0 = \frac{f(x) - \partial_t^\alpha u(x,T;q_0) + \Delta g(x)}{g(x)} \leq \frac{f(x) + \Delta g(x)}{g(x)} = q_0(x) \quad \text{in } \overline{\Omega}.$$

Meanwhile, we know that $q^\dagger \in \mathcal{S}$ and so $q^\dagger \leq q_0$. This and Lemma 6.5 result in

$$0 \leq q^\dagger = Kq^\dagger \leq Kq_0 = q_1.$$

As a result, we obtain $0 \le q^\dagger \le q_1 \le q_0$. Using Lemma 6.5 again, we have $Kq^\dagger \le Kq_1 \le Kq_0$, namely $q^\dagger \le q_2 \le q_1$. Continuing this argument, we can conclude that

$$0 \le q^\dagger \le \cdots \le q_{n+1} \le q_n \le \cdots \le q_0.$$

Now we have proved that the sequence $\{q_n\}_{n=0}^\infty$ is decreasing. It is bounded by $q^\dagger$ from below and q_0 from above. Therefore, this sequence is included in $C(\overline{\Omega}) \cap \mathcal{S}$.

Next, we show that the sequence $\{q_n\}_{n=0}^\infty$ converges to $q^\dagger$. Note that the sequence $\{q_n\}_{n=0}^\infty$ is decreasing, and it has a lower bound, therefore this sequence converges pointwise, and we denote the limit by $q^* \in \mathcal{S}$. Moreover, there holds $q^\dagger \le q^*$ since $q^\dagger$ is a lower bound of $\{q_n\}_{n=0}^\infty$, and $q^\dagger \le q^* \le q_0$ indicates that $q^* \in \mathcal{S}$. Then q^* is one fixed point of the operator K in $\mathcal{S}$, and we apply Lemma 6.4 (ii) to conclude that $q^* \in C(\overline{\Omega}) \cap \mathcal{S}$. Meanwhile, Lemma 6.4 (i) implies that $q^\dagger \in C(\overline{\Omega})$ is also a fixed point of K in $\mathcal{S}$. Therefore, we apply Lemma 6.6 and hence conclude that $q^\dagger = q^*$. □

6.2 Conditional stability

The aim of this section is to establish a stability of the inverse potential problem. Note that [113] provides a conditional stability in a Hilbert space setting for one dimensional diffusion problem by applying a spectrum perturbation argument (cf. [113, Lemma 2.2] and [88]), which is not applicable in high dimensional cases. We refer interested readers to [9, 10, 50] for some conditional stability results for sufficiently small T.

Let us begin with the following *a priori* estimate for $\partial_t^\alpha u(t;q)$.

Lemma 6.7. *Let $q \in \mathcal{Q}$ and $u(q)$ be the solution to problem* (6.1)*. Then we have the estimate*

$$\|\partial_t^\alpha u(t;q)\|_{H^s(\Omega)} \le c \min(t^{-s\alpha/2}, t^{-\alpha}) \quad \textit{for all} \quad s \in [0,2],$$

where c is independent of q and t.

Proof. According to (6.9), we have the representation

$$\partial_t^\alpha u(t;q) = F(t;q)(\Delta v - qv + f) \in H^2(\Omega) \cap H_0^1(\Omega) \quad \text{for all} \quad t > 0. \tag{6.15}$$

Then applying Lemma 6.2, we obtain

$$\|\partial_t^\alpha u(t;q)\|_{L^2(\Omega)} \le \|F(t;q)(\Delta v - qv + f)\|_{L^2(\Omega)} \le c \min(1, t^{-\alpha}) \big(\|v\|_{H^2(\Omega)} + \|f\|_{L^2(\Omega)}\big).$$

Next, by applying the norm equivalence in (6.3) and the estimate in Lemma 6.2, we derive

$$\begin{aligned}
\|\partial_t^\alpha u(t;q)\|_{H^2(\Omega)} &\le c\Big(\|F(t;q)(\Delta v - qv + f)\|_{L^2(\Omega)} + \|A(q)F(t;q)(\Delta v - qv + f)\|_{L^2(\Omega)}\big) \\
&\le c\big(\min(1, t^{-\alpha})\|\Delta v - qv + f\|_{L^2(\Omega)} + ct^{-\alpha}\|\Delta v - qv + f\|_{L^2(\Omega)} \\
&\le ct^{-\alpha}\big(\|v\|_{H^2(\Omega)} + \|f\|_{L^2(\Omega)}\big).
\end{aligned}$$

These together with interpolation between $L^2(\Omega)$ and $H^2(\Omega)\cap H_0^1(\Omega)$ immediately lead to the desired result. $\square$

For different potentials $q_1, q_2 \in \mathcal{Q}$, we denote the solution to (6.1) with potential q_i by $u(q_i)$. Then the following lemma provides an important *a priori* estimate which (and whose discrete analogue) plays a crucial role in our error analysis.

Lemma 6.8. *Let Assumption 6.1 be valid and $q_1, q_2 \in \mathcal{Q}$. Then for any $t > t_0$ and any positive parameter $\epsilon < \min(1, 2-\frac{d}{2})$ there holds*

$$\|\partial_t^\alpha(u(q_1)-u(q_2))(t)\|_{L^2(\Omega)} \le c\max(t^{-\alpha}, t^{-(1-\epsilon)\alpha})\|q_1-q_2\|_{L^2(\Omega)},$$

where the constant c is independent of q_1, q_2 and t.

Proof. Let $\phi(x,t) = \partial_t^\alpha(u(q_1)-u(q_2))(t)$. Then we note that $\phi(x,t)\in H_0^1(\Omega)$ satisfies

$$(\partial_t^\alpha - \Delta + q_1(x))\phi(x,t) = (q_2-q_1)\partial_t^\alpha u(x,t;q_2) \quad \text{for} \quad (x,t)\in\Omega\times(0,T] \tag{6.16}$$

with the initial condition $\phi(0) = (q_2-q_1)v$. We apply the solution representation (6.5) to derive

$$\phi(t) = F(t;q_1)\phi(0) + \int_0^t E(s;q_1)(q_2-q_1)\partial_t^\alpha u(t-s;q_2)\,\mathrm{d}s.$$

Taking L^2 norm on the above relation, Lemma 6.2 and Assumption 6.1 lead to for any $\epsilon\in(0,1)$

$$\begin{aligned}\|\phi(t)\|_{L^2(\Omega)} &= \|F(t;q_1)\|\,\|(q_2-q_1)v\|_{L^2(\Omega)} + \int_0^t \|E(s;q_1)\|\,\|(q_2-q_1)\partial_t^\alpha u(t-s;q_2)\|_{L^2(\Omega)}\,\mathrm{d}s\\ &\le c\|q_2-q_1\|_{L^2(\Omega)}\Big(t^{-\alpha} + \int_0^t s^{-1+\epsilon\alpha/2}\|\partial_t^\alpha u(t-s;q_2)\|_{L^\infty(\Omega)}\,\mathrm{d}s\Big).\end{aligned}$$

Here we use the estimate that $\|E(s;q_1)\| \le cs^{-1+\epsilon\alpha/2}$ which is a direct result of the second assertion of Lemma 6.2 and the interpolation. Then according to Lemma 6.7 and the Sobolev embedding theorem, we obtain for $r > \frac{d}{2}$ and $d = 1,2,3$,

$$\begin{aligned}\|\phi(t)\|_{L^2(\Omega)} &\le c\|q_2-q_1\|_{L^2(\Omega)}\Big(t^{-\alpha} + \int_0^t s^{-1+\epsilon\alpha/2}\|\partial_t^\alpha u(t-s;q_2)\|_{L^\infty(\Omega)}\,\mathrm{d}s\Big)\\ &\le c\|q_2-q_1\|_{L^2(\Omega)}\Big(t^{-\alpha} + \int_0^t s^{-1+\epsilon\alpha/2}\|\partial_t^\alpha u(t-s;q_2)\|_{H^r(\Omega)}\,\mathrm{d}s\Big)\\ &\le c\|q_2-q_1\|_{L^2(\Omega)}\Big(t^{-\alpha} + \int_0^t s^{-1+\epsilon\alpha/2}(t-s)^{-r\alpha/2}\,\mathrm{d}s\Big)\\ &\le c\|q_2-q_1\|_{L^2(\Omega)}\big(t^{-\alpha} + t^{\epsilon\alpha/2-r\alpha/2}\big).\end{aligned}$$

Finally, the choice that $r = 2-\epsilon$ leads to the estimate that

$$\|\phi(t)\|_{L^2(\Omega)} \le c\|q_2-q_1\|_{L^2(\Omega)}\big(t^{-\alpha}+t^{-\alpha(1-\epsilon)}\big) \le c\max(t^{-\alpha}, t^{-(1-\epsilon)\alpha})\|q_1-q_2\|_{L^2(\Omega)}.$$

This completes the proof of the lemma. $\square$

Next, we state the main theorem of this section, which shows the conditional stability of the inverse potential problem.

Theorem 6.3. *Let Assumption 6.1 be valid, $q_1, q_2 \in \mathcal{Q}$, and $u(t; q_i)$ be the solution to* (6.1) *with the potential q_i. Then there exists $T_0 \geq 0$ such that for any $T \geq T_0$ there holds*

$$\|q_1 - q_2\|_{L^2(\Omega)} \leq C\|u(T; q_1) - u(T; q_2)\|_{H^2(\Omega)},$$

where the constant C is independent of q_1, q_2 and T.

Proof. Recalling that, for $i = 1, 2$, q_i could be written as

$$q_i = \frac{f - \partial_t^\alpha u(T; q_i) + \Delta u(T; q_i)}{u(T; q_i)}.$$

Then we split $q_1 - q_2$ into three parts:

$$\begin{aligned} q_1 - q_2 = f\frac{u(T; q_2) - u(T; q_1)}{u(T; q_1)u(T; q_2)} &+ \frac{u(T; q_1)\partial_t^\alpha u(T; q_2) - u(T; q_2)\partial_t^\alpha u(T; q_1)}{u(T; q_1)u(T; q_2)} \\ &+ \frac{u(T; q_2)\Delta u(T; q_1) - u(T; q_1)\Delta u(T; q_2)}{u(T; q_1)u(T; q_2)}. \end{aligned}$$

Using Assumption 6.1, we conclude that $u_i \geq M_2 > 0$ and hence

$$\Big\|f\frac{u(T; q_2) - u(T; q_1)}{u(T; q_1)u(T; q_2)}\Big\|_{L^2(\Omega)} \leq \frac{\|f\|_{L^\infty(\Omega)}}{M_2^2}\|u(T; q_2) - u(T; q_1)\|_{L^2(\Omega)}.$$

Besides, we use the fact that $\|u_i(T)\|_{L^\infty(\Omega)}$ and $\|\partial_t^\alpha u_i(T)\|_{L^\infty(\Omega)}$ are bounded uniformly in q (Lemma 6.3) and Lemma 6.8 to derive for any ϵ close to 0,

$$\begin{aligned} &\Big\|\frac{u(T; q_1)\partial_t^\alpha u(T; q_2) - u(T; q_2)\partial_t^\alpha u(T; q_1)}{u(T; q_1)u(T; q_2)}\Big\|_{L^2(\Omega)} \\ &\leq c\Big(\|u(T; q_1)\|_{L^\infty(\Omega)}\|\partial_t^\alpha(u(T; q_2) - u(T; q_1))\|_{L^2(\Omega)} + \|\partial_t^\alpha u(T; q_1)\|_{L^\infty(\Omega)}\|u(T; q_1) - u(T; q_2)\|_{L^2(\Omega)}\Big) \\ &\leq c\Big(\max(T^{-\alpha}, T^{-(1-\epsilon)\alpha})\|q_1 - q_2\|_{L^2(\Omega)} + \|u(T; q_1) - u(T; q_2)\|_{L^2(\Omega)}\Big). \end{aligned}$$

Similarly, we apply the fact that $\|u_i(T)\|_{L^\infty(\Omega)}$ and $\|\Delta u_i(T)\|_{L^\infty(\Omega)}$ are bounded uniformly in q_i (Lemma 6.3) to arrive at

$$\begin{aligned} &\Big\|\frac{u(T; q_2)\Delta u(T; q_1) - u(T; q_1)\Delta u(T; q_2)}{u(T; q_1)u(T; q_2)}\Big\|_{L^2(\Omega)} \\ &\leq c\Big(\|u(T; q_1)\|_{L^\infty(\Omega)}\|\Delta(u(T; q_2) - u(T; q_1))\|_{L^2(\Omega)} + \|\Delta u(T; q_1)\|_{L^\infty(\Omega)}\|u(T; q_1) - u(T; q_2)\|_{L^2(\Omega)}\Big) \\ &\leq c\Big(\|\Delta(u(T; q_1) - u(T; q_1))\|_{L^2(\Omega)} + \|u(T; q_1) - u(T; q_2)\|_{L^2(\Omega)}\Big). \end{aligned}$$

As a result, we arrive at

$$\|q_1 - q_2\|_{L^2(\Omega)} \leq c_1\|u(T; q_1) - u(T; q_2)\|_{H^2(\Omega)} + c_2\max(T^{-\alpha}, T^{-(1-\epsilon)\alpha})\|q_1 - q_2\|_{L^2(\Omega)}.$$

Then for T_0 such that $c_2\max(T_0^{-\alpha}, T_0^{-(1-\epsilon)\alpha}) \leq c_3$ for some constant $c_3 \in (0, 1)$, and $T \geq T_0$, we have

$$\|q_1 - q_2\|_{L^2(\Omega)} \leq \frac{c_1}{1 - c_3}\|u(T; q_1) - u(T; q_2)\|_{H^2(\Omega)}.$$

This completes the proof of the lemma. $\square$

6.3 Completely discrete scheme

In this section, we shall develop a fully discrete scheme for solving the inverse potential problem. To this end, we shall introduce the time stepping method using convolution quadrature in the first part, then discuss the spatial discretization using finite element method. A reconstruction algorithm will be presented to recover the potential from the noisy observational data. Finally, we establish an *a priori* error bound showing the way to choose the (space/time) mesh sizes according to the noise level.

6.3.1 Time stepping scheme for solving the direct problem

The literature on the numerical approximation for the nonlocal-in-time subdiffusion equation (6.1) is vast, see e.g., [42] for an overview of existing schemes. Here we apply the convolution quadrature to discretize the fractional derivative on uniform grids studied in Section 2.5. Let $\{t_n = n\tau\}_{n=0}^N$ be a uniform partition of the time interval $[0,T]$, with a time step size $\tau = T/N$. The convolution quadrature (CQ) was first proposed by Lubich [71] for discretizing Volterra integral equations. This approach provides a systematic framework to construct high-order numerical methods to discretize fractional derivatives, and has been the foundation of many early works. The time stepping scheme for problem (6.1) reads: given $u^0(q) = v$, find $u^n(q) \in H^1(\Omega)$ such that $\gamma_0(u^n(q)) = b$ and

$$\bar\partial_\tau^\alpha u^n(q) - \Delta u^n(q) + qu^n(q) = f \quad \text{with} \quad n = 1, 2, \dots, N, \tag{6.17}$$

In particular, when $\alpha = 1$, the operator $\bar\partial_\tau^\alpha$ reduces to the standard backward difference quotient: $\bar\partial_\tau^1 \varphi^n = \frac{\varphi^n - \varphi^{n-1}}{\tau}$, and the scheme (6.17) reduces to the standard backward Euler scheme.

Using the superposition principle, the time stepping solution in (6.17) could be written in the operational form as ([49, equation (2.5)] and [111, equations (4.3)-(4.4)])

$$\begin{aligned} u^n(q) &= F_\tau(n;q)(v - D(q)b) + D(q)b + \tau \sum_{j=1}^n E_\tau(j;q) f \\ &= F_\tau(n;q)(v - D(q)b) + D(q)b + (I - F_\tau(n;q))A(q)^{-1} f. \end{aligned} \tag{6.18}$$

Here the time discrete operators $F_\tau(n;q)$ and $E_\tau(n;q)$ are defined by the discrete inverse Laplace transform

$$\begin{aligned} F_\tau(n;q) &= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} e^{-z\tau} \delta_\tau(e^{-z\tau})^{\alpha-1} (\delta_\tau(e^{-z\tau})^\alpha + A(q))^{-1} \, \mathrm{d}z, \\ E_\tau(n;q) &= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} e^{-z\tau} (\delta_\tau(e^{-z\tau})^\alpha + A(q))^{-1} \, \mathrm{d}z, \end{aligned} \tag{6.19}$$

with $\delta_\tau(\xi) = (1-\xi)/\tau$ and the contour $\Gamma_{\theta,\sigma}^\tau := \{z \in \Gamma_{\theta,\sigma} : |\Im(z)| \le \pi/\tau\}$ where $\theta \in (\pi/2, \pi)$ is close to $\pi/2$ (oriented with an increasing imaginary part).

For any $q \in \mathcal{Q}$, Lemma 2.4 and resolvent estimate of elliptic operator (6.7) immediately lead to

$$\|(\delta_\tau(e^{-z\tau})^\alpha + A(q))^{-1}\| \le C \min(|z^{-\alpha}|, \lambda^{-1}), \quad \forall z \in \Sigma_\phi, \ \forall \phi \in (0, \pi), \tag{6.20}$$

for a constant C independent of q. Next we give some useful properties of $F_\tau(n;q)$ and $E_\tau(n;q)$.

The first lemma provides an estimate for $F_\tau(n;q)-F(t_n;q)$. It has been proved in the earlier work [111, Lemma 4.2, eq. (4.7)], so we omit its proof here.

Lemma 6.9. *Let $F_\tau(n;q)$ and $E_\tau(n;q)$ be defined as in* (6.19)*, and λ be the smallest eigenvalue of $-\Delta$ with homogeneous Dirichlet boundary condition. Then for $q\in\mathcal{Q}$, there holds*

$$\|(F_\tau(n;q)-F(t_n;q))v\|_{L^2(\Omega)} \le c\,n^{-1}\min(1,\lambda^{-1}t_n^{-\alpha})\|v\|_{L^2(\Omega)} \quad \textit{for all} \;\; n\ge 1,$$

and

$$\|A(q)(F_\tau(n;q)-F(t_n;q))v\|_{L^2(\Omega)} \le c\,n^{-1}t_n^{-\alpha}\|v\|_{L^2(\Omega)} \quad \textit{for all} \;\; n\ge 1,$$

where the constants are independent of q, τ and t_n.

The next lemma provides some smoothing and asymptotic properties of operators $F_\tau(t;q)$ and $E_\tau(t;q)$. This is a discrete analogue to Lemma 6.2. The proof follows from the solution representation (6.18)-(6.19), Lemma 2.4, the resolvent estimate (6.20), and the same argument of the proof of Lemma 6.2 in [38, Theorem 6.4 and 3.2].

Lemma 6.10. *Let $F_\tau(n;q)$ and $E_\tau(n;q)$ be defined as* (6.19)*, and λ be the smallest eigenvalue of $-\Delta$ with homogeneous boundary condition. Then for $q\in\mathcal{Q}$, there holds*

$$\|A(q)F_\tau(n;q)v\|_{L^2(\Omega)} + t_n^{1-\alpha}\|A(q)E_\tau(n;q)v\|_{L^2(\Omega)} \le ct_n^{-\alpha}\|v\|_{L^2(\Omega)}$$

and

$$\|F_\tau(n;q)v\|_{L^2(\Omega)} + t_n^{1-\alpha}\|E_\tau(n;q)v\|_{L^2(\Omega)} \le c\min(1,\lambda^{-1}t_n^{-\alpha})\|v\|_{L^2(\Omega)}, \quad n\ge 1.$$

Here c is the generic constant independent of τ, t_n and q.

Proof. The asymptotics of $A(q)F_\tau(n;q)$ could be derived directly from Lemmas 6.2 and 6.9:

$$\begin{aligned}\|A(q)F_\tau(n;q)v\|_{L^2(\Omega)} &\le \|A(q)(F_\tau(n;q)-F(t_n;q))v\|_{L^2(\Omega)} + \|A(q)F(t_n;q)v\|_{L^2(\Omega)}\\ &\le c(n^{-1}+1)t_n^{-\alpha}\|v\|_{L^2(\Omega)} \le ct_n^{-\alpha}\|v\|_{L^2(\Omega)}.\end{aligned}$$

Similarly, for $F_\tau(n;q)$, we apply Lemmas 6.2 and 6.9 again to derive

$$\begin{aligned}\|F_\tau(n;q)v\|_{L^2(\Omega)} &\le \|(F_\tau(n;q)-F(t_n;q))v\|_{L^2(\Omega)} + \|F(t_n;q)v\|_{L^2(\Omega)}\\ &\le c(n^{-1}+1)\min(1,\lambda^{-1}t_n^{-\alpha})\|v\|_{L^2(\Omega)} \le c\min(1,\lambda^{-1}t_n^{-\alpha})\|v\|_{L^2(\Omega)}.\end{aligned}$$

Next, we turn to the estimate of $A(q)E_\tau(n;q)$. Using the representation (6.19), resolvent estimate (6.20) and Lemma 2.4, we derive

$$\begin{aligned}\|A(q)E_\tau(n;q)v\|_{L^2(\Omega)} &\le c\int_{\Gamma_{\theta,\sigma}^\tau} |e^{zt_n}||e^{-z\tau}|\|A(q)(\delta_\tau(e^{-z\tau})^\alpha + A(q))^{-1}v\|_{L^2(\Omega)}|\mathrm{d}z|\\ &\le c\int_{\Gamma_{\theta,\sigma}^\tau} |e^{zt_n}|\Big(\|v\|_{L^2(\Omega)} + |\delta_\tau(e^{-z\tau})^\alpha|\|(\delta_\tau(e^{-z\tau})^\alpha + A(q))^{-1}v\|_{L^2(\Omega)}\Big)|\mathrm{d}z|\\ &\le c\|v\|_{L^2(\Omega)}\int_{\Gamma_{\theta,\sigma}^\tau}|e^{zt_n}||\mathrm{d}z| \le c\|v\|_{L^2(\Omega)}\left(\int_\sigma^\infty e^{-c\rho t_n}d\rho + c\sigma\int_{-\theta}^{\theta}\mathrm{d}\psi\right) \le c\sigma\|v\|_{L^2(\Omega)}.\end{aligned}$$

Then we let $\sigma = t_n^{-1}$ to derive the desired estimate for $A(q)E_\tau(n;q)$.

The estimate for $E_\tau(n;q)$ could be derived using similar argument. By letting $\sigma = t_n^{-1}$, we apply the resolvent estimate (6.20) and Lemma 2.4 to deduce

$$\begin{aligned}
\|E_\tau(n;q)v\|_{L^2(\Omega)} &\le c\int_{\Gamma^\tau_{\theta,\sigma}} |e^{zt_n}| \|(\delta_\tau(e^{-z\tau})^\alpha + A(q))^{-1}v\|_{L^2(\Omega)}|\mathrm{d}z| \\
&\le c\|v\|_{L^2(\Omega)} \int_{\Gamma^\tau_{\theta,\sigma}} |e^{zt_n}| \min(|z|^{-\alpha}, \lambda^{-1})|\mathrm{d}z| \\
&\le c\|v\|_{L^2(\Omega)} \min(t_n^{\alpha-1}, \lambda^{-1}t_n^{-1}).
\end{aligned}$$

Then we complete the proof of Lemma 6.10. □

Next, we are ready to show some *a priori* estimate of the time stepping solution.

Lemma 6.11. *Let Assumption 6.1 be valid and $q \in \mathcal{Q}$. Then the solution $u^n(q)$ to the time stepping scheme* (6.17) *satisfies*

$$\|u^n(q)\|_{L^\infty(\Omega)} \le c \quad \textit{for all} \quad n = 1, 2, \ldots, N.$$

Moreover, there holds for all $s \in [0, 2]$,

$$\|\bar\partial_\tau^\alpha u^n(q)\|_{H^s(\Omega)} \le c \min(t_n^{-s\alpha/2}, t_n^{-\alpha}) \quad \textit{for} \quad n = 1, 2, \ldots, N.$$

Here the generic constants are independent of τ, t_n and q.

Proof. Using the solution representation (6.18) and triangle inequality we arrive at

$$\begin{aligned}
\|u^n(q)\|_{H^2(\Omega)} &\le \|F_\tau(n;q)(v - D(q)b) + D(q)b + (I - F_\tau(n;q))A(q)^{-1}f\|_{H^2(\Omega)} \\
&\le \|F_\tau(n;q)(v - D(q)b)\|_{H^2(\Omega)} + \|D(q)b\|_{H^2(\Omega)} + \|(I - F_\tau(n;q))A(q)^{-1}f\|_{H^2(\Omega)}.
\end{aligned}$$

We use the norm equivalence (6.3) and Lemma 6.10 to obtain

$$\begin{aligned}
\|F_\tau(n;q)(v - D(q)b)\|_{H^2(\Omega)} &\le c\Big(\|F_\tau(n;q)A(q)(v - D(q)b)\|_{L^2(\Omega)} + \|F_\tau(n;q)(v - D(q)b)\|_{L^2(\Omega)}\Big) \\
&\le c\Big(\|A(q)(v - D(q)b)\|_{L^2(\Omega)} + \|v - D(q)b\|_{L^2(\Omega)}\Big) \\
&\le c\|v - D(q)b\|_{H^2(\Omega)} \le c\Big(\|v\|_{H^2(\Omega)} + \|D(q)b\|_{L^2(\Omega)}\Big).
\end{aligned}$$

Then the estimate (6.4) implies

$$\|F_\tau(n;q)(v - D(q)b)\|_{H^2(\Omega)} \le c(\|v\|_{H^2(\Omega)} + \|b\|_{H^{\frac{3}{2}}(\partial\Omega)}).$$

This combined with Sobolev embedding theorem yields $\|u^n(q)\|_{L^\infty(\Omega)} \le c$ where the constant c is independent of τ, t_n and q.

Next, we let $w^n(q) = \bar\partial_\tau^\alpha u^n(q)$. By a simple computation, we obtain that $w^n(q) \in H_0^1(\Omega)$ and

$$\bar\partial_\tau^\alpha w^n(q) + A(q)w^n(q) = 0 \quad \text{for all} \quad 1 \le n \le N \quad \text{and} \quad w^0(q) = f + \Delta v - qv. \tag{6.21}$$

Then the solution representation (6.18) leads to

$$w^n(q) = \bar{\partial}_\tau^\alpha u^n(q) = F_\tau(n;q)(f + \Delta v - qv). \tag{6.22}$$

Applying Lemma 6.10 and the condition $q \in \mathcal{Q}$, we obtain

$$\|\bar{\partial}_\tau^\alpha u^n(q)\|_{L^2(\Omega)} = \|F_\tau(n;q)(f + \Delta v - qv)\|_{L^2(\Omega)} \le c\min(1, t^{-\alpha})\big(\|v\|_{H^2(\Omega)} + \|f\|_{L^2(\Omega)}\big).$$

Next, the norm equivalence (6.3) and Lemma 6.10 yield

$$\|\bar{\partial}_\tau^\alpha u^n(q)\|_{H^2(\Omega)} \le c\big(\|\bar{\partial}_\tau^\alpha u^n(q)\|_{L^2(\Omega)} + \|A(q)\bar{\partial}_\tau^\alpha u^n(q)\|_{L^2(\Omega)}\big) \le ct_n^{-\alpha}(\|v\|_{H^2(\Omega)} + \|f\|_{L^2(\Omega)}).$$

Here c is independent of τ, t_n and q. The case that $s \in (0,1)$ follows immediately by interpolation. This completes the proof of the lemma. □

Finally, we shall provide a useful *a priori* error estimate for $\bar{\partial}_\tau^\alpha u^n(q) - \partial_t^\alpha u(t_n;q)$.

Lemma 6.12. *Let Assumption 6.1 be valid and $q \in \mathcal{Q}$. Let $u^n(q)$ and $u(t;q)$ be the solutions to* (6.17) *and* (6.1)*, respectively. Then there holds*

$$\|\bar{\partial}_\tau^\alpha u^n(q) - \partial_t^\alpha u(t_n;q)\|_{L^2(\Omega)} \le c\tau t_n^{-\alpha-1}$$

with the constant independent of q, τ and n.

Proof. Combining (6.15) with (6.21), we obtain

$$\bar{\partial}_\tau^\alpha u^n(q) - \partial_t^\alpha u(t_n;q) = (F_\tau(n;q) - F(t_n;q))(\Delta v - qv + f).$$

Then we apply Lemma 6.9 with $s = 0$ and note that $q \in \mathcal{Q}$ to derive

$$\|\bar{\partial}_\tau^\alpha u^n(q) - \partial_t^\alpha u(t_n;q)\|_{L^2(\Omega)} \le c\tau t_n^{-\alpha-1}\Big(\|v\|_{H^2(\Omega)} + \|f\|_{L^2(\Omega)}\Big).$$

This completes the proof of the lemma. □

6.3.2 Fully discrete scheme

In this section, we shall discuss the completely discrete scheme to solve the inverse potential problem. We use the convolution quadrature for the time discretization and use Galerkin finite element method for the space discretization. To begin with, we introduce some settings for the finite element methods.

To illustrate the main idea, we consider the square region $\Omega = (a,b)^d \subset \mathbb{R}^d$, with $1 \le d \le 3$ and the discussion could be extended to general convex polyhedral domain. For all $i = 1, \dots, d$, we denote by $a = x_0 < x_1 < \cdots < x_M = b$ a partition of the interval $[a,b]$ with a uniform mesh size $h = x_i - x_{i-1} = (b-a)/M$ for all $i = 1, \dots, M$. Then domain Ω is now separated into M^d subrectangles by all grid points $(x_{j_1}, \ldots, x_{j_d})$, with $0 \le j_i \le M$ and $i = 1, \ldots, d$. We denote this partition by $\mathcal{T}_h$, and note that h is the mesh size of the partition $\mathcal{T}_h$.

Then we apply the tensor-product Lagrange finite elements on the partition $\mathcal{T}_h$. Let Q_1 be the space of polynomials in the variables $x_1, \ldots, x_d$, with real coefficients and of degree at most one in each variable, i.e.,

$$Q_1 = \Big\{ \sum_{0 \le \beta_1, \beta_2, \ldots, \beta_d \le 1} c_{\beta_1 \beta_2 \ldots \beta_d} x_1^{\beta_1} \cdots x_d^{\beta_d}, \quad \text{with} \;\; c_{\beta_1 \beta_2 \ldots \beta_d} \in \mathbb{R} \Big\}.$$

The H^1-conforming tensor-product finite element space, denoted by X_h, is defined as

$$X_h = \{ v \in H^1(\Omega) : v|_K \in Q_1 \text{ for all } K \in \mathcal{T}_h \}. \tag{6.23}$$

Besides, we define

$$X_h^0 = X_h \cap H_0^1(\Omega) = \{ v \in H_0^1(\Omega) : v|_K \in Q_1 \text{ for all } K \in \mathcal{T}_h \}. \tag{6.24}$$

We let $\mathcal{I}_h$ denote the Lagrange interpolation operator associated with the finite element space X_h. It satisfies the following error estimates for $s = 1, 2$ and $1 \le p \le \infty$ with $sp > d$ [17, Theorem 1.103]:

$$\|v - \mathcal{I}_h v\|_{L^p(\Omega)} + h \|v - \mathcal{I}_h v\|_{W^{1,p}(\Omega)} \le c h^s \|v\|_{W^{s,p}(\Omega)}, \quad \forall v \in W^{s,p}(\Omega). \tag{6.25}$$

Similarly, we let $\mathcal{I}_h^\partial$ denote the Lagrange interpolation operator on the boundary.

We define the orthogonal L_2-projection $P_h : L^2(\Omega) \to X_h^0$ and the Ritz projection $R_h(q) : H_0^1(\Omega) \to X_h^0$ by

$$\begin{aligned} (P_h \psi, \chi_h) &= (\psi, \chi_h), & \forall \chi \in X_h^0, \\ (\nabla R_h(q) \psi, \nabla \chi_h) &= (\nabla \psi, \nabla \chi_h) + (q \psi, \chi_h), & \forall \chi \in X_h^0. \end{aligned}$$

It is well-known that the operators P_h and $R_h(q)$ (with $q \in \mathcal{Q}$) have the following approximation property, cf. [93, Lemma 1.1] or [17, Theorems 3.16 and 3.18], for $s \in [1, 2]$,

$$\|P_h \psi - \psi\|_{L^2(\Omega)} + \|R_h(q) \psi - \psi\|_{L^2(\Omega)} \le c h^s \|\psi\|_{H^s(\Omega)}, \quad \forall \psi \in H^s(\Omega) \cap H_0^1(\Omega). \tag{6.26}$$

Noting that $q \in \mathcal{Q}$, the constant c is independent of q.

Let γ_0 be the trace operator [17, Section B.3.5], and the set $X_h^\partial = \{\gamma_0(\chi_h) : \; \chi_h \in X_h\}$. Now we introduce a discrete operator $D_h(q) : X_h^\partial \to X_h$ such that $w_h = D_h(q) b_h$ for $b_h \in X_h^\partial$ satisfies

$$(\nabla w_h, \nabla \chi_h) + (q w_h, \chi_h) = 0 \quad \text{for all} \;\; \chi_h \in X_h^0, \qquad \text{and} \;\; \gamma_0(w_h) = b_h.$$

Then for any $q \in \mathcal{Q}$ and $b \in H^2(\partial\Omega)$, there holds the estimate [17, Lemma 3.28]

$$\|D(q) b - D_h(q) \mathcal{I}_h^\partial b\|_{L^2(\Omega)} \le c h^2 \|b\|_{H^2(\partial\Omega)}. \tag{6.27}$$

To discretize the problem (6.1), we consider the weak formulation to find $u(t) \in H^1(\Omega)$ such that for all $\varphi \in H_0^1(\Omega)$ and $t > 0$,

$$(\partial_t^\alpha u(t), \varphi) + (\nabla u(t), \nabla \varphi) + (qu(t), \varphi) = (f, \varphi), \quad \text{with} \quad u(\cdot, t) = b \quad \text{in } \partial\Omega \quad \text{and} \quad u(0) = v.$$

Then the fully discrete scheme for (6.1) reads: find $u_h^n(q) \in X_h$ for $t \geq 0$ such that $\gamma_0(u_h^n(q)) = \mathcal{I}_h^\partial b$ on $\partial\Omega$ and for all $\varphi_h \in X_h^0$ and $n = 1, 2, \ldots, N$,

$$(\bar{\partial}_\tau^\alpha u_h^n(q), \varphi_h) + (\nabla u_h^n(q), \nabla \varphi_h) + (q u_h^n(q), \varphi_h) = (f, \varphi_h) \quad \text{with} \quad u_h^0(q) = \mathcal{I}_h v. \tag{6.28}$$

For $q \in \mathcal{Q}$ we define the discrete operator $A_h(q) : X_h^0 \to X_h^0$ such that

$$(A_h(q)\xi_h, \chi_h) = (\nabla \xi_h, \nabla \chi_h) + (q\xi_h, \chi_h) \quad \text{for all} \quad \xi_h, \chi_h \in X_h^0.$$

Then by splitting the fully discrete solution to (6.28) as $u_h^n(q) = \varphi_h^n(q) + D_h(q)\mathcal{I}_h^\partial b$, we observe that $\varphi_h^n(q) \in X_h^0$ satisfies

$$\bar{\partial}_\tau^\alpha \varphi_h^n(q) + A_h(q)\varphi_h^n(q) = P_h f \qquad \text{for } t > 0,$$

with $\varphi_h^0(q) = \mathcal{I}_h v - D_h(q)\mathcal{I}_h^\partial b$. In particular, we define $\Delta_h = -A_h(0)$. Then analogue to (6.18), the fully discrete solution in (6.28) could be written in the operational form

$$\begin{aligned} u_h^n(q) &= F_\tau^h(n;q)\big(\mathcal{I}_h v - D_h(q)\mathcal{I}_h^\partial b\big) + D_h(q)\mathcal{I}_h^\partial b + \tau \sum_{j=1}^n E_\tau^h(j;q) P_h f \\ &= F_\tau^h(n;q)\big(\mathcal{I}_h v - D_h(q)\mathcal{I}_h^\partial b\big) + D_h(q)\mathcal{I}_h^\partial b + (I - F_\tau^h(n;q))A_h(q)^{-1} P_h f, \end{aligned} \tag{6.29}$$

where the fully discrete operators $F_\tau^h(n;q)$ and $E_\tau^h(n;q)$ are defined as

$$\begin{aligned} F_\tau^h(n;q) &= \frac{1}{2\pi\mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} e^{-z\tau} \delta_\tau(e^{-z\tau})^{\alpha-1} (\delta_\tau(e^{-z\tau})^\alpha + A_h(q))^{-1} \, \mathrm{d}z, \\ E_\tau^h(n;q) &= \frac{1}{2\pi\mathrm{i}} \int_{\Gamma_{\theta,\sigma}^\tau} e^{zt_n} e^{-z\tau} (\delta_\tau(e^{-z\tau})^\alpha + A_h(q))^{-1} \, \mathrm{d}z. \end{aligned} \tag{6.30}$$

Let λ be the smallest eigenvalue of $-\Delta$ with the homogeneous Dirichlet boundary condition, and $\lambda_h(q)$ be the smallest eigenvalue of discrete operator $A_h(q)$. Recalling that the finite element space X_h^0 is conforming in $H_0^1(\Omega)$ and $q \in \mathcal{Q}$, the Courant minimax principle implies the relation that $0 < \lambda \leq \lambda_h(0) \leq \lambda_h(q)$. Then we have the resolvent estimate for the (discrete) elliptic operator $A_h(q)$: with fixed $\phi \in (0, \pi)$

$$\|(\delta_\tau(e^{-z\tau})^\alpha + A_h(q))^{-1}\| \leq C \min(|z^{-\alpha}|, \lambda_h(q)^{-1}) \leq C \min(|z^{-\alpha}|, \lambda^{-1}), \quad \forall z \in \Sigma_\phi,$$

for a constant C independent of q and h. This immediately indicates the following result for the fully discrete scheme (6.28), similar to Lemmas 6.2 and 6.10.

Lemma 6.13. *Let $F_\tau^h(n;q)$ and $E_\tau^h(n;q)$ be the operators defined in* (6.30)*. Let λ be the smallest eigenvalue of $-\Delta$ with homogeneous boundary condition. Then for any $q \in \mathcal{Q}$ and $v_h \in X_h^0$, there holds for $n \geq 1$,*

$$\|A_h(q)F_\tau^h(n;q)v_h\|_{L^2(\Omega)} + t_n^{1-\alpha}\|A_h(q)E_\tau^h(n;q)v_h\|_{L^2(\Omega)} \leq ct_n^{-\alpha}\|v_h\|_{L^2(\Omega)},$$
$$\|F_\tau^h(n;q)v\|_{L^2(\Omega)} + t_n^{1-\alpha}\|E_\tau^h(n;q)v_h\|_{L^2(\Omega)} \leq c\min(1, \lambda^{-1}t_n^{-\alpha})\|v_h\|_{L^2(\Omega)}.$$

Here c is the generic constant independent of τ, t_n and q.

Next, we recall the following useful inverse inequality of finite element functions (see e.g., [17, Corollary 1.141]).

Lemma 6.14. *Let X_h and X_h^0 be the finite dimensional spaces defined in* (6.23) *and* (6.24) *respectively. Then we have the inverse estimates*

$$\|\phi_h\|_{L^p(\Omega)} \leq Ch^{d(\frac{1}{p}-\frac{1}{q})}\|\phi_h\|_{L^q(\Omega)} \quad \text{for all} \quad 1 \leq q \leq p \leq \infty \quad \text{and} \quad \phi_h \in X_h,$$
$$\|\Delta_h\phi_h\|_{L^2(\Omega)} + h^{-1}\|\nabla\phi_h\| \leq Ch^{-2}\|\phi_h\|_{L^2(\Omega)} \quad \text{for all} \quad \phi_h \in X_h^0.$$

Next, we intend to derive an a *priori* estimate for $\bar\partial_\tau^\alpha u_h^n(q) - \bar\partial_\tau^\alpha u^n(q)$.

Lemma 6.15. *Let Assumption 6.1 be valid and $q \in \mathcal{Q}$. Let $u^n(q)$ and $u_h^n(q)$ be the solutions to* (6.17) *and* (6.28)*, respectively. Then there holds for any $\epsilon \in (0,1)$,*

$$\|\bar\partial_\tau^\alpha(u_h^n(q) - u^n(q))\|_{L^2(\Omega)} \leq ch^{2-\epsilon}\max(t_n^{-\alpha}, t_n^{-(1-\epsilon)\alpha}).$$

Here the constants are independent of q, τ and n.

Proof. First of all, we recall that $w^n(q) = \bar\partial_\tau^\alpha u^n(q) \in H_0^1(\Omega)$, and it satisfies (6.21). Meanwhile, Assumption (6.4) implies that the fully discrete approximation $w_h^n(q) = \bar\partial_\tau^\alpha u_h^n(q) \in X_h^0$ satisfies

$$\bar\partial_\tau^\alpha w_h^n(q) + A_h(q)w_h^n(q) = 0, \quad n \geq 1, \quad \text{with} \quad w_h^0(q) = P_h f - A_h(q)(\mathcal{I}_h v - D_h(q)\mathcal{I}_h^\partial b). \tag{6.31}$$

To derive an estimate for $w_h^n(q) - w^n(q)$, we apply the splitting

$$w_h^n(q) - w^n(q) = \big(w_h^n(q) - P_h w^n(q)\big) + \big(P_h w^n(q) - w^n(q)\big) =: \theta_h^n + \rho^n.$$

Then the bound of ρ^n can be derived from (6.25) and Lemma 6.11 as

$$\|\rho^n\|_{L^2(\Omega)} \leq ch^2\|\bar\partial_\tau^\alpha u^n(q)\|_{H^2(\Omega)} \leq ch^2 t_n^{-\alpha}.$$

Next we turn to derive an estimate for $\theta_h^n \in X_h^0$, which satisfies

$$\bar\partial_\tau^\alpha\theta_h^n + A_h(q)\theta_h^n = A_h(q)(R_h(q) - P_h)w^n(q) \quad \text{for all} \quad n = 1, 2, \ldots, N,$$
$$\theta_h^0 = A_h(q)R_h(q)(v - D(q)b) - A_h(q)(\mathcal{I}_h v - D_h(q)\mathcal{I}_h^\partial b),$$

where we use the fact that $A_h(q)R_h(q)\psi = P_hA(q)\psi$ for $\psi \in H^2(\Omega)\cap H_0^1(\Omega)$. By the representation (6.29) we have

$$\theta_h^n = F_\tau^h(n;q)\theta_h(0) + \tau\sum_{j=1}^n E_\tau^h(j;q)A_h(q)(R_h(q)-P_h)w^{n+1-j}(q) =: I + II. \tag{6.32}$$

From Assumption 6.1, we have $v - D(q)b \in H^2(\Omega)\cap H_0^1(\Omega)$. Then (6.25), (6.26), (6.27) and Lemma 6.13 imply

$$\begin{aligned}
\|I\|_{L^2(\Omega)} &\le ct_n^{-\alpha}\|R_h(q)(v-D(q)b) - (\mathcal{I}_hv - D_h(q)\mathcal{I}_h^\partial b)\|_{L^2(\Omega)}\\
&\le ct_n^{-\alpha}\Big(\|(R_h(q)-I)(v-D(q)b)\|_{L^2(\Omega)} + \|v-\mathcal{I}_hv\|_{L^2(\Omega)} + \|D(q)b - D_h(q)\mathcal{I}_h^\partial b\|_{L^2(\Omega)}\Big)\\
&\le ch^2t_n^{-\alpha}\Big(\|v\|_{H^2(\Omega)} + \|b\|_{H^2(\partial\Omega)}\Big).
\end{aligned}$$

Now we turn to the estimate for the term II. By Lemma 6.13, we have

$$\|A_h(q)^sE_\tau^h(n;q)v_h\|_{L^2(\Omega)} \le ct_n^{(1-s)\alpha-1}\|v_h\|_{L^2(\Omega)}.$$

Meanwhile, the second inverse inequality in Lemma 6.14 implies

$$\|A_h(q)^sv_h\|_{L^2(\Omega)} \le ch^{-2s}\|v_h\|_{L^2(\Omega)}.$$

The fact $q\in\mathcal{Q}$ implies that the constant c is independent of q. Then we apply the above estimates combined with Lemma 6.11 for $s = 2-\epsilon$, and obtain

$$\begin{aligned}
\|II\|_{L^2(\Omega)} &\le \tau\sum_{j=1}^n \|E_\tau^h(j;q)A_h(q)^{1-\epsilon/2}\|\,\|A_h(q)^{\epsilon/2}(R_h(q)-P_h)w^{n+1-j}(q)\|_{L^2(\Omega)}\\
&\le c\tau\sum_{j=1}^n t_j^{-1+\epsilon\alpha/2}\,\|(R_h(q)-P_h)w^{n+1-j}(q)\|_{L^2(\Omega)}h^{-\epsilon}\\
&\le ch^{2-\epsilon}\tau\sum_{j=1}^n t_j^{-1+\epsilon\alpha/2}\,\|w^{n+1-j}(q)\|_{H^{2-\epsilon}(\Omega)}\\
&\le ch^{2-\epsilon}\tau\sum_{j=1}^n t_j^{-1+\epsilon\alpha/2}t_{n+1-j}^{-\alpha+\epsilon\alpha/2} \le ch^{2-\epsilon}t_n^{-\alpha+\epsilon\alpha}.
\end{aligned}$$

This completes the proof of the lemma. □

The next result provides an *a priori* estimate for $\bar\partial_\tau^\alpha u_h^n(q_1) - \bar\partial_\tau^\alpha u_h^n(q_2)$, which plays a key role in the stability analysis for the numerical solution of the inverse potential problem.

Lemma 6.16. *Suppose that Assumption 6.1 is valid and $q_1, q_2 \in \mathcal{Q}$. For $i = 1,2$, let $u_h^n(q_i)$ be the solution to the fully discrete scheme* (6.28)*, with potential q_i, respectively. Then there holds for any positive parameter $\epsilon < \min(1, 2-\frac{d}{2})$,*

$$\|\bar\partial_\tau^\alpha(u_h^n(q_1) - u_h^n(q_2))\|_{L^2(\Omega)} \le c\max(t_n^{-\alpha}, t_n^{-(1-\epsilon)\alpha})\|q_1-q_2\|_{L^2(\Omega)},$$

where the constant c is independent of h, τ, q_1, q_2 and t_n.

Proof. We let $\theta_h^n = \bar\partial_\tau^\alpha (u_h^n(q_1) - u_h^n(q_2))$. Note that $\theta_h^n \in X_h^0$ and it satisfies

$$\bar\partial_\tau^\alpha \theta_h^n + A_h(q_1)\theta_h^n = P_h[(q_2-q_1)\bar\partial_\tau^\alpha u_h^n(q_2)] \quad \text{with} \quad \theta_h^0 = P_h[(q_2-q_1)\mathcal{I}_h v].$$

Now we apply the stability of L^2-projection P_h to obtain

$$\begin{aligned}\|\theta_h(0)\|_{L^2(\Omega)} &\le \|(q_2-q_1)\mathcal{I}_h v\|_{L^2(\Omega)} \le \|q_2-q_1\|_{L^2(\Omega)}\|\mathcal{I}_h v\|_{L^\infty(\Omega)}\\ &\le \|q_2-q_1\|_{L^2(\Omega)}\|v\|_{L^\infty(\Omega)}.\end{aligned} \tag{6.33}$$

Meanwhile, using the stability of P_h and the inverse inequality in Lemma 6.14 we arrive at

$$\begin{aligned}&\|P_h[(q_2-q_1)\bar\partial_\tau^\alpha u^n(q_2)]\|_{L^2(\Omega)}\\ &\le c\|q_2-q_1\|_{L^2(\Omega)}\|\bar\partial_\tau^\alpha u^n(q_2)\|_{L^\infty(\Omega)}\\ &\le c\|q_2-q_1\|_{L^2(\Omega)}\left(\|\bar\partial_\tau^\alpha (u_h^n(q_2) - \mathcal{I}_h u^n(q_2)\|_{L^\infty(\Omega)} + \|\mathcal{I}_h\bar\partial_\tau^\alpha u^n(q_2)\|_{L^\infty(\Omega)}\right)\\ &\le c\|q_2-q_1\|_{L^2(\Omega)}\left(h^{-\frac{d}{2}}\|\bar\partial_\tau^\alpha (u_h^n(q_2) - \mathcal{I}_h u^n(q_2)\|_{L^2(\Omega)} + \|\bar\partial_\tau^\alpha u^n(q_2)\|_{L^\infty(\Omega)}\right).\end{aligned}$$

Then we apply the Sobolev embedding theorem to derive that for $\epsilon < \min(1, 2-\frac{d}{2})$,

$$\begin{aligned}&\|P_h[(q_2-q_1)\bar\partial_\tau^\alpha u^n(q_2)]\|_{L^2(\Omega)}\\ &\le c\|q_2-q_1\|_{L^2(\Omega)}\left(h^{-\frac{d}{2}}\|\bar\partial_\tau^\alpha (u_h^n(q_2) - \mathcal{I}_h u^n(q_2)\|_{L^2(\Omega)} + \|\bar\partial_\tau^\alpha u^n(q_2)\|_{H^{2-\epsilon}(\Omega)}\right).\end{aligned}$$

This together with Lemma 6.11 leads to

$$\|P_h[(q_2-q_1)\bar\partial_\tau^\alpha u^n(q_2)]\|_{L^2(\Omega)} \le c\|q_2-q_1\|_{L^2(\Omega)}\left(h^{-\frac{d}{2}}\|\bar\partial_\tau^\alpha (u_h^n(q_2) - \mathcal{I}_h u^n(q_2))\|_{L^2(\Omega)} + t_n^{-(1-\epsilon/2)\alpha}\right).$$

Then using Lemmas 6.11 and 6.15, we obtain for $\epsilon < \min(1, 2-\frac{d}{2})$,

$$\begin{aligned}&h^{-\frac{d}{2}}\|\bar\partial_\tau^\alpha (u_h^n(q_2) - \mathcal{I}_h u^n(q_2)\|_{L^2(\Omega)}\\ &\le h^{-\frac{d}{2}}\left(\|\bar\partial_\tau^\alpha (u_h^n(q_2) - u^n(q_2)\|_{L^2(\Omega)} + \|\bar\partial_\tau^\alpha (\mathcal{I}_h u^n(q_2) - u^n(q_2))\|_{L^2(\Omega)}\right)\\ &\le ch^{2-\frac{d}{2}-\epsilon}\left(t_n^{-(1-\epsilon/2)\alpha} + \|\bar\partial_\tau^\alpha u^n(q_2)\|_{H^{2-\epsilon}(\Omega)}\right) \le ch^{2-\frac{d}{2}-\epsilon}t_n^{-(1-\epsilon/2)\alpha}.\end{aligned}$$

As a result, we conclude that for $\epsilon < \min(1, 2-\frac{d}{2})$,

$$\|P_h[(q_2-q_1)\bar\partial_\tau^\alpha u^n(q_2)]\|_{L^2(\Omega)} \le ct_n^{-(1-\epsilon/2)\alpha}\|q_2-q_1\|_{L^2(\Omega)}. \tag{6.34}$$

Now, using the representation (6.29), we derive

$$\theta_h^n = F_\tau^h(n;q_1)\theta_h^0 + \tau\sum_{j=1}^n E_\tau^h(j;q_1)P_h[(q_2-q_1)\bar\partial_\tau^\alpha u_h^{n+1-j}(q_2)].$$

Then Lemma 6.13 indicates that for any $\epsilon < \min(1, 2-\frac{d}{2})$,

$$\begin{aligned}\|\theta_h^n\|_{L^2(\Omega)} &\le \|F_\tau^h(n;q_1)\theta_h(0)\|_{L^2(\Omega)} + \tau\sum_{j=1}^n \|E_\tau^h(j;q_1)P_h[(q_2-q_1)\bar\partial_\tau^\alpha u_h^{n+1-j}(q_2)]\|_{L^2(\Omega)}\\ &\le ct_n^{-\alpha}\|\theta_h^0\|_{L^2(\Omega)} + \tau\sum_{j=1}^n t_j^{-1+\epsilon\alpha/2}\|P_h[(q_2-q_1)\bar\partial_\tau^\alpha u_h^{n+1-j}(q_2)]\|_{L^2(\Omega)}.\end{aligned}$$

This combined with (6.33) and (6.34) leads to the desired result. □

6.3.3 The inverse potential problem: numerical reconstruction and error estimate

In this part, we shall design a robust completely discrete scheme for the recovery of the potential. Throughout this section, we need the following assumption.

Assumption 6.4. *We assume that the exact potential $q^\dagger$ and noisy observational data g_δ satisfy the following conditions:*

(i) $q^\dagger \in C(\bar{\Omega}) \cap \mathcal{Q} \cap W^{1,p}(\Omega)$ with some $p > \max(d,2)$ and $q^\dagger|_{\partial\Omega}$ is a priori known;

(ii) $g_\delta(x) \in C(\overline{\Omega})$ is noisy and it satisfies $g_\delta \geq M_2$, $\gamma_0(g_\delta) = \gamma_0(g) = b$ and $\|g_\delta - g\|_{C(\overline{\Omega})} = \delta$.

Remark 6.1. *According to the a priori estimate (6.11), the exact data $g \geq M_2$ with an a priori known positive constant M_2. Therefore, it is reasonable to assume that the noisy data $g_\delta \geq M_2$. Otherwise, we may revise the observational data by*

$$\widetilde{g}_\delta(x) = \max(g_\delta(x), M_2), \qquad \textit{for all} \;\; x \in \overline{\Omega}.$$

Here $g_\delta \in C(\overline{\Omega})$ implies $\widetilde{g}_\delta \in C(\overline{\Omega})$. Moreover, we have

$$\|\widetilde{g}_\delta - g\|_{C(\overline{\Omega})} \leq \|g_\delta - g\|_{C(\overline{\Omega})} = \delta.$$

Then we may use the function $\tilde{g}_\delta$ as the observational data in our computation, where $\widetilde{g}_\delta \geq M_2 > 0$.

Based on Assumption 6.1 and Assumption 6.4 (i), we have $f, q^\dagger \in W^{1,p}(\Omega)$ for some $p > \max(d,2)$. Moreover, Lemma 6.3 indicates that $\partial_t^\alpha u(T, q^\dagger), u(T; q^\dagger) \in H^2(\Omega) \subset W^{1,p}(\Omega) \subset L^\infty(\Omega)$ with $p \in (\max(d,2), 6)$. Therefore, we conclude that for some $p \in (\max(d,2), 6)$

$$\Delta g(x) = \Delta u(T; q^\dagger) = -f + \partial_t^\alpha u(T, q^\dagger) + q^\dagger u(T; q^\dagger) \in W^{1,p}(\Omega). \tag{6.35}$$

Besides, Assumption 6.4 (i) and (ii) imply

$$\gamma_0(\Delta g) = \gamma_0(qg - f) = \gamma_0(q)b - \gamma_0(f),$$

which is *a priori* known. Note that Δg_δ might not be well-defined in $L^2(\Omega)$. Therefore, we need a numerical approximation to the unknown function Δg. Now we define a function $\psi_h \in X_h$ such that

$$\gamma_0(\psi_h) = \mathcal{I}_h^\partial(\gamma_0(q)b - \gamma_0(f)) \quad \text{and} \quad (\psi_h, \phi_h) = -(\nabla \mathcal{I}_h g_\delta, \nabla \phi_h) \;\; \text{for all} \;\; \phi_h \in X_h^0. \tag{6.36}$$

Then we have $\psi_h \approx \Delta g$ provided that $h = O(\delta^{\frac{1}{3}})$. This is given by the following lemma.

Lemma 6.17. *Suppose that Assumptions 6.1 and 6.4 are valid. Let $\psi_h \in X_h$ be the function defined in (6.36). Then there holds*

$$\|\psi_h - \Delta g\|_{L^2(\Omega)} \leq c\Big(\frac{\delta}{h^2} + h\Big),$$

where the constant c is independent of h and δ.

Proof. To derive the estimate, we define the auxiliary function $\tilde{\psi}_h \in X_h$ such that

$$\gamma_0(\tilde{\psi}_h) = \mathcal{I}_h^{\partial}(\gamma_0(q)b - \gamma_0(f)) \quad \text{and} \quad (\tilde{\psi}_h, \phi_h) = -(\nabla \mathcal{I}_h g, \nabla \phi_h) \ \text{ for all } \ \phi_h \in X_h^0.$$

Then we consider the split

$$\psi_h - \Delta g = (\psi_h - \tilde{\psi}_h) + (\tilde{\psi}_h - \mathcal{I}_h \Delta g) + (\mathcal{I}_h \Delta g - \Delta g).$$

According to the definition of ψ_h and $\tilde{\psi}_h$, we know $\psi_h - \tilde{\psi}_h \in X_h^0$. Then the inverse inequality in Lemma 6.14 implies

$$\begin{aligned}
\|\psi_h - \tilde{\psi}_h\|_{L^2(\Omega)} &= \sup_{\phi_h \in X_h^0} \frac{(\psi_h - \tilde{\psi}_h, \phi_h)}{\|\phi_h\|_{L^2(\Omega)}} = \sup_{\phi_h \in X_h^0} \frac{(\nabla(\mathcal{I}_h g - \mathcal{I}_h g_\delta), \nabla \phi_h)}{\|\phi_h\|_{L^2(\Omega)}} \\
&\le ch^{-2} \|\mathcal{I}_h g - \mathcal{I}_h g_\delta\|_{L^2(\Omega)} \le c\delta h^{-2}.
\end{aligned}$$

Meanwhile, using the fact that $\Delta g \in W^{1,p}(\Omega)$ for some $p \in (\max(2, d), 6)$ by (6.35), the approximation property of $\mathcal{I}_h$ in (6.25) implies

$$\|\mathcal{I}_h \Delta g - \Delta g\|_{L^2(\Omega)} \le \|\mathcal{I}_h \Delta g - \Delta g\|_{L^p(\Omega)} \le ch \|\Delta g\|_{W^{1,p}(\Omega)}.$$

Finally, according to the definition of $\tilde{\psi}_h$, we know $\tilde{\psi}_h - \mathcal{I}_h \Delta g \in X_h^0$, and hence

$$\begin{aligned}
\|\tilde{\psi}_h - \mathcal{I}_h \Delta g\|_{L^2(\Omega)} &= \sup_{\phi_h \in X_h^0} \frac{(\tilde{\psi}_h - \mathcal{I}_h \Delta g, \phi_h)}{\|\phi_h\|_{L^2(\Omega)}} = \sup_{\phi_h \in X_h^0} \frac{(\tilde{\psi}_h - \Delta g, \phi_h) + (\Delta g - \mathcal{I}_h \Delta g, \phi_h)}{\|\phi_h\|_{L^2(\Omega)}} \\
&= \sup_{\phi_h \in X_h^0} \frac{(\nabla(g - \mathcal{I}_h g), \nabla \phi_h)}{\|\phi_h\|_{L^2(\Omega)}} + ch \|\Delta g\|_{W^{1,p}(\Omega)}.
\end{aligned}$$

Then the superconvergence [68, Theorem 4.1]

$$(\nabla(g - \mathcal{I}_h g), \nabla \phi_h) \le ch^2 \|g\|_{H^3(\Omega)} \|\phi_h\|_{H^1(\Omega)},$$

together with the inverse inequality in Lemma 6.14 leads to

$$\|\tilde{\psi}_h - \mathcal{I}_h \Delta g\|_{L^2(\Omega)} \le \sup_{\phi_h \in X_h^0} \frac{ch^2 \|\phi_h\|_{H^1(\Omega)}}{\|\phi_h\|_{L^2(\Omega)}} + ch \le \sup_{\phi_h \in X_h^0} \frac{ch \|\phi_h\|_{L^2(\Omega)}}{\|\phi_h\|_{L^2(\Omega)}} + ch \le ch.$$

This completes the proof of the lemma. □

Now we define the operator $K_{h,\tau} : \mathcal{Q} \to \mathcal{Q}$ such that

$$K_{h,\tau} q(x) := P_{[0,M_1]} \Big(\frac{f(x) - \bar{\partial}_\tau^\alpha u_h^N(x; q) + \psi_h(x)}{g_\delta(x)} \Big), \tag{6.37}$$

where the function $P_{[0,M_1]} : \mathbb{R} \to \mathbb{R}$ denotes a truncation function defined by

$$P_{[0,M_1]}(a) := \max(\min(M_1, a), 0). \tag{6.38}$$

The next lemma shows a contraction property of the operator $K_{h,\tau}$.

Lemma 6.18. *Let $q_1, q_2 \in \mathcal{Q}$. Then there holds for any positive $\epsilon < \min(1, 2-\frac{d}{2})$,*

$$\|K_{h,\tau}q_1 - K_{h,\tau}q_2\|_{L^2(\Omega)} \leq c\max(T^{-\alpha}, T^{-(1-\epsilon)\alpha})\|q_1 - q_2\|_{L^2(\Omega)}.$$

Proof. By the definition (6.37) and the property that $|P_{[0,M_1]}(a) - P_{[0,M_1]}(b)| \leq |a-b|$, there holds

$$|(K_{h,\tau}q_1 - K_{h,\tau}q_2)(x)| \leq \Big|\frac{\bar\partial_\tau^\alpha(u_h^N(x;q_2) - u_h^N(x;q_1))}{g_\delta(x)}\Big| \leq \frac{|\bar\partial_\tau^\alpha(u_h^N(x;q_2) - u_h^N(x;q_1))|}{M_2 - \delta},$$

where the second inequality follows from the facts that $g(x) = u(x,T) \geq M_2$ (Lemma 6.3) and $\|g - g_\delta\|_{C(\overline{\Omega})} = \delta$. Then Lemma 6.16 yields for any positive $\epsilon < \min(1, 2-\frac{d}{2})$,

$$\begin{aligned}\|K_{h,\tau}q_1 - K_{h,\tau}q_2\|_{L^2(\Omega)} &\leq c\|\bar\partial_\tau^\alpha(u_h^N(q_2) - u_h^N(q_1))\|_{L^2(\Omega)}\\ &\leq c\max(T^{-\alpha}, T^{-(1-\epsilon)\alpha})\|q_1 - q_2\|_{L^2(\Omega)}.\end{aligned}$$

This completes the proof of the lemma. □

Now we are ready to present the main theorem of this section.

Theorem 6.5. *Suppose that Assumptions 6.1 and 6.4 are valid. Let $K_{h,\tau}$ be the operator defined in* (6.37)*. Then with sufficiently large T, for any $q_0 \in \mathcal{Q}$, the iteration*

$$q_{n+1} = K_{h,\tau}q_n, \qquad \forall\ \ n = 0, 1, \ldots, \tag{6.39}$$

linearly converges to a unique fixed point $q^* \in L^\infty(\Omega)$ of $K_{h,\tau}$ with $0 \leq q^* \leq M_1$ s.t.

$$\|q^* - q_{n+1}\|_{L^2(\Omega)} \leq cT^{-(1-\epsilon)\alpha}\|q^* - q_n\|_{L^2(\Omega)} \qquad \textit{for}\ \ n \geq 0.$$

Moreover, there holds

$$\|q^* - q^\dagger\|_{L^2(\Omega)} \leq c\Big(\frac{\delta}{h^2} + h + \tau\Big),$$

where $q^\dagger$ is the exact potential and the constant c is independent of τ, h and δ.

Proof. Choosing an arbitrary initial guess $q_0 \in \mathcal{Q}$, the contraction mapping theorem and Lemma 6.18 (with sufficiently large terminal time T) imply that the iteration (6.39) generates a Cauchy sequence $\{q_n\}_{n=1}^\infty$ in $L^2(\Omega)$ sense. Therefore, the sequence $\{q_n\}$ converges to a fixed point of $K_{h,\tau}$ as $n \to \infty$, denoted by $q^* \in L^2(\Omega)$. Then the use of the box restriction $P_{[0,M_1]}$ indicates $0 \leq q^* \leq M_1$.

Next, we show the error estimate between q^* and $q^\dagger$. Since $q^\dagger \in \mathcal{Q}$, it holds that

$$\begin{aligned}\|q^\dagger - q^*\|_{L^2(\Omega)} &\leq \Big\|\frac{f - \partial_t^\alpha u(T;q^\dagger) + \Delta g}{g} - \frac{f - \bar\partial_\tau^\alpha u_h^N(q^*) + \psi_h}{g_\delta}\Big\|_{L^2(\Omega)}\\ &\leq \Big\|\frac{f - \partial_t^\alpha u(T;q^\dagger) + \Delta g}{g} - \frac{f - \partial_t^\alpha u(T;q^\dagger) + \Delta g}{g_\delta}\Big\|_{L^2(\Omega)}\\ &\quad + \Big\|\frac{f - \partial_t^\alpha u(T;q^\dagger) + \Delta g}{g_\delta} - \frac{f - \bar\partial_\tau^\alpha u_h^N(q^*) + \psi_h}{g_\delta}\Big\|_{L^2(\Omega)} =: I + II.\end{aligned}$$

Due to the fact that $f(x),\ \partial_t^\alpha u(x,t;q^\dagger),\ \Delta g \in L^2(\Omega)$, it is straightforward to see that the first term satisfies $I \le c\delta$. So it suffices to establish a bound for II. First, we observe that for any positive $\epsilon < \min(1, 2-\frac{d}{2})$,

$$
\begin{aligned}
&\|\partial_t^\alpha u(T;q^\dagger) - \bar\partial_\tau^\alpha u_h^N(q^*)\|_{L^2(\Omega)} \\
&\le \|\partial_t^\alpha u(T;q^\dagger) - \bar\partial_\tau^\alpha u^N(q^\dagger)\|_{L^2(\Omega)} + \|\bar\partial_\tau^\alpha u^N(q^\dagger) - \bar\partial_\tau^\alpha u_h^N(q^\dagger)\|_{L^2(\Omega)} + \|\bar\partial_\tau^\alpha u_h^N(q^\dagger) - \bar\partial_\tau^\alpha u_h^N(q^*)\|_{L^2(\Omega)} \\
&\le c(h^2 + \tau T^{-1})T^{-(1-\epsilon)\alpha} + cT^{-(1-\epsilon)\alpha}\|q^\dagger - q^*\|_{L^2(\Omega)},
\end{aligned}
$$

where for the last inequality we apply Lemmas 6.12, 6.15 and 6.16. This combined with Lemma 6.18 implies that with T away from 0 there holds

$$II \le c\Big(\frac{\delta}{h^2} + h + \tau\Big) + cT^{-(1-\epsilon)\alpha}\|q^\dagger - q^*\|_{L^2(\Omega)}.$$

Then we arrive at

$$\|q^\dagger - q^*\|_{L^2(\Omega)} \le c_1\Big(\frac{\delta}{h^2} + h + \tau\Big) + c_2 T^{-(1-\epsilon)\alpha}\|q^\dagger - q^*\|_{L^2(\Omega)}.$$

Therefore, there exists a constant T_0 sufficiently large such that $c_2 T_0^{-(1-\epsilon)\alpha} \le c_0$ with some constant $c_0 \in (0,1)$ and for any $T \ge T_0$ there holds

$$\|q^\dagger - q^*\|_{L^2(\Omega)} \le \frac{c_1}{1-c_0}\Big(\frac{\delta}{h^2} + h + \tau\Big) \le c\Big(\frac{\delta}{h^2} + h + \tau\Big).$$

This completes the proof of the theorem. □

Remark 6.2. *The error estimate in Theorem 6.5 provides useful guidelines to choose discretization parameters h and τ according to the* a priori *known noise level δ. For example, the choice $\tau, h = O(\delta^{\frac{1}{3}})$ leads to the best convergence rate $O(\delta^{\frac{1}{3}})$. This is fully supported by our numerical results in Section 6.4.*

6.4 Numerical experiments

In this section, we present some two-dimensional numerical results to illustrate the theoretical results. The noisy data g_δ is generated by

$$g_\delta(x_i) = u(x_i, T) + \delta\zeta(x_i),$$

where ζ follows the standard uniform distribution in $[-1,1]$, and x_i are grid points of a fine partition of Ω. Then to compute the numerical reconstruction q^*, we follow the idea in Section 6.3 and design the iterative algorithm 1. All the computations are carried out on a personal desktop with MATLAB 2021.

Algorithm 1: An iterative algorithm for finding fixed point q^* from g_δ

Data: Order α, terminal time T, source term f, initial condition v, boundary data b, noisy observation g_δ, upper bound constant M_1, discretization parameter h and τ;

Result: Approximate potential q^*.

Compute ψ_h by (6.36); set $q_0 = P_{[0,M_1]}\Big[\dfrac{f+\psi_h}{g_\delta}\Big]$, $k=0$ and $e^0 = 1$;

while $e^k > tol = 10^{-10}$ **do**

  Compute $u_h^n(q_k)$, the fully discrete solution to (6.28) with potential q_k;

  Update the potential by

$$q_{k+1} = K_{h,\tau} q_k = P_{[0,M_1]}\Big[\frac{f - \bar\partial_\tau^\alpha u_h^N(q_k) + \psi_h}{g_\delta}\Big];$$

  Compute error

$$e^{k+1} = \|q_{k+1} - q_k\|_{L^2(\Omega)};$$

  $k \leftarrow k+1$;

end

$q^* \leftarrow q_k$;

output: The approximated potential q^*.

We present numerical experiments for a two-dimensional problem with the domain $(x,y) \in \Omega = (0,3)^2$ and the problem data

$$f(x,y) = 10, \quad b(x,y) = \frac{x(3-x)}{4} + 1, \quad v(x,y) = x(3-x)\Big(\frac{1}{4} + \frac{y(3-y)}{10}\Big) + 1. \tag{6.40}$$

Note that those problem data satisfy Assumption 6.1. We test the following three (exact) potentials:

(1) Smooth potential:

$$q_1^\dagger = 3 - \cos(\pi x)\cos(\pi y).$$

(2) Piecewise smooth potential: $q_2^\dagger$ is a pyramid-shape function, i.e.

$$q_2^\dagger(x,y) = 3 + 1.5 \times (-1)^{j+k}\psi(x-j, y-k), \quad (x,y) \in [j,j+1]\times[k,k+1], \quad j,k = 0,1,2,$$

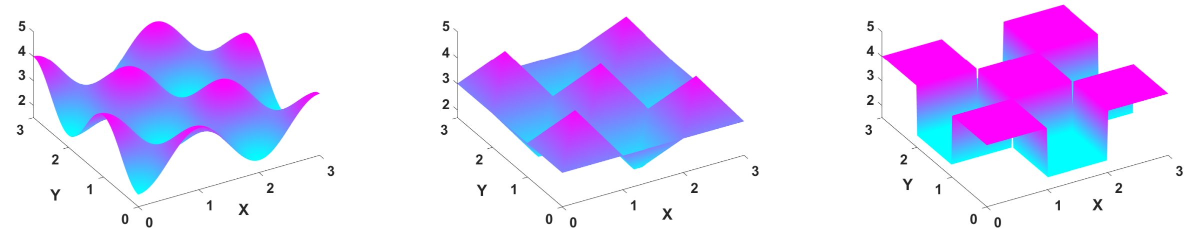
where for any $(x,y) \in [0,1]\times[0,1]$,

$$\psi(x,y) = \begin{cases} 2y, \quad x \ge y, \quad \text{and} \quad x+y>1, \quad \text{and} \quad y<0.5, \\ 2x, \quad x<y, \quad \text{and} \quad x+y \le 1, \quad \text{and} \quad x<0.5, \\ 2(1-y), \quad x<y, \quad \text{and} \quad x+y>1, \quad \text{and} \quad y>0.5, \\ 2(1-x), \quad x \ge y, \quad \text{and} \quad x+y \ge 1, \quad \text{and} \quad x \ge 0.5. \end{cases}$$

(3) Discontinuous potential: $q_3^\dagger$ is a step function where

$$q_3^\dagger(x, y) = 3 + (-1)^{j+k}, \quad (x, y) \in [j, j+1] \times [k, k+1], \quad j, k = 0, 1, 2.$$

We plot the profiles of these potential functions in Figure 6.1. Note that $q_1^\dagger$ and $q_2^\dagger$ satisfy Assumption (6.4) (i), while $q_3^\dagger \in H^{\frac{1}{2}-\epsilon}(\Omega)$ for any $\epsilon \in (0, 1/2)$.



(a) Smooth potential $q_1^\dagger$ (b) Piecewise smooth potential $q_2^\dagger$ (c) Discontinuous potential $q_3^\dagger$

Figure 6.1: Profiles of three exact potentials.

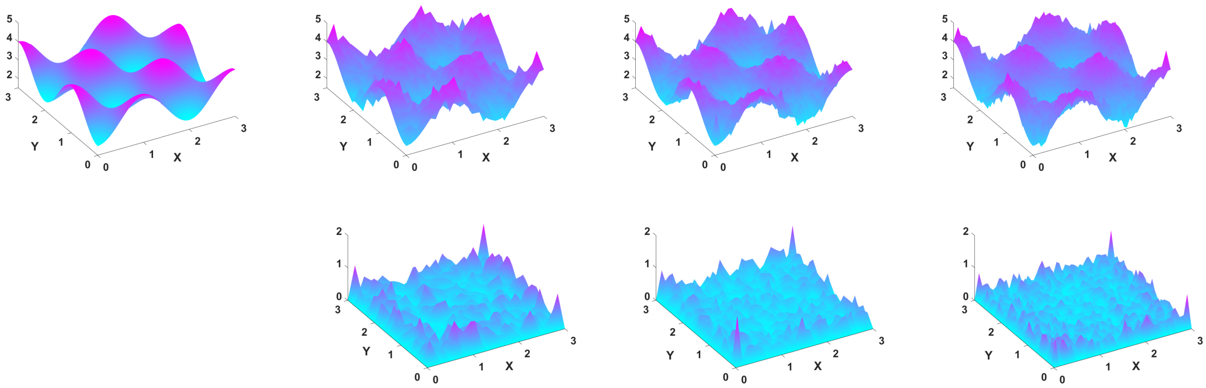
As we discussed in Section 6.3, we use the standard piecewise bilinear FEM with uniform mesh size h for the space discretization, and apply the backward Euler (convolution quadrature) method with uniform step size τ for the time discretization. Since the closed form of the exact solution is unavailable, we compute the exact observational data $g(x) = u(T; q^\dagger) \approx u_h^N(q^\dagger)$ by the fully discrete scheme (6.28) with fine meshes, i.e. $h = 10^{-2}$ and $\tau = 10^{-3}$.

For the *a priori* known noise level δ, we choose the discretization parameters $h, \tau \sim \delta^{1/3}$, and examine the relative error

$$e_q = \|q^\dagger - q^*\|_{L^2(\Omega)} / \|q^\dagger\|_{L^2(\Omega)}, \tag{6.41}$$

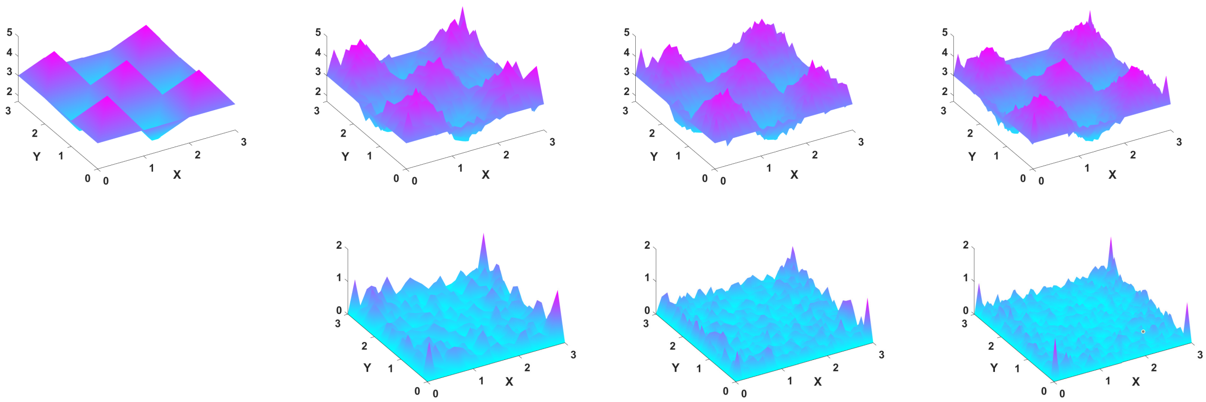
where $q^\dagger$ is the exact potential and q^* is the numerical reconstruction by Algorithm 1. Theorem 6.5 indicates that Algorithm 1 produces a sequence $\{q_k\}$ linearly converging to a fixed point q^*, and the error satisfies $e_q = O(\delta^{1/3})$. In Figure 6.2-6.4 we present the profiles of exact potentials and reconstructed potentials under different δ, with terminal time $T = 1$, $\alpha = 0.5$ and $h, \tau \sim \delta^{1/3}$. Meanwhile, we also plot profiles of absolute error in the second row of each figure. We observe that the numerical reconstructions are close to the exact potentials in all cases.

Next, we test the rate of convergence of numerical reconstruction. In Figure 6.5, we plot the relative error e_q defined by (6.41) versus δ, with different α. The numerical results show that for the $q_1^\dagger$ and $q_2^\dagger$, the convergence rate is $O(\delta^{1/3})$, which agrees well with our theory in Theorem 6.5. However, if the potential is discontinuous (and hence fails to satisfy Assumption (6.4) (i)), the convergence rate is clearly less than order 1/3 (cf. Figure 6.5 (c)). This illustrates the necessity of the Assumption on the smoothness of exact potential. Meanwhile, the experiments indicate that the error is robust with



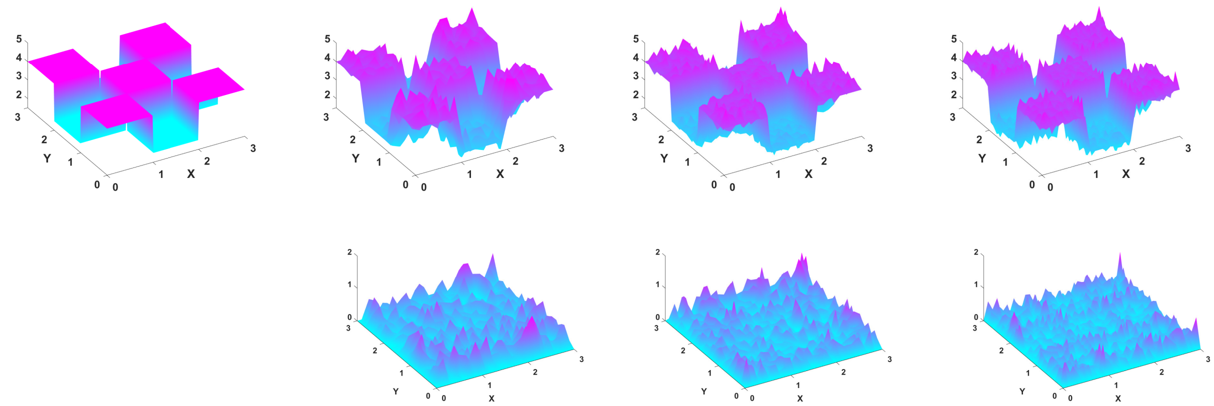
(a) $\delta = 10^{-2}$ (b) $\delta = 10^{-3}$ (c) $\delta = 10^{-4}$

Figure 6.2: Top left: Exact potential $q_1^\dagger$. The other three columns are profiles of numerical reconstructions q^* and corresponding pointwise error $e = |q^* - q_2^\dagger|$, with $T = 1$, $\alpha = 0.5$, $h = \delta^{\frac{1}{3}}$ and $\tau = \delta^{\frac{1}{3}}/15$.



(a) $\delta = 10^{-2}$ (b) $\delta = 10^{-3}$ (c) $\delta = 10^{-4}$

Figure 6.3: Top left: Exact potential $q_2^\dagger$. The other three columns are profiles of numerical reconstructions q^* and corresponding pointwise error $e = |q^* - q_2^\dagger|$, with $T = 1$, $\alpha = 0.5$, $h = \delta^{\frac{1}{3}}$ and $\tau = \delta^{\frac{1}{3}}/15$.



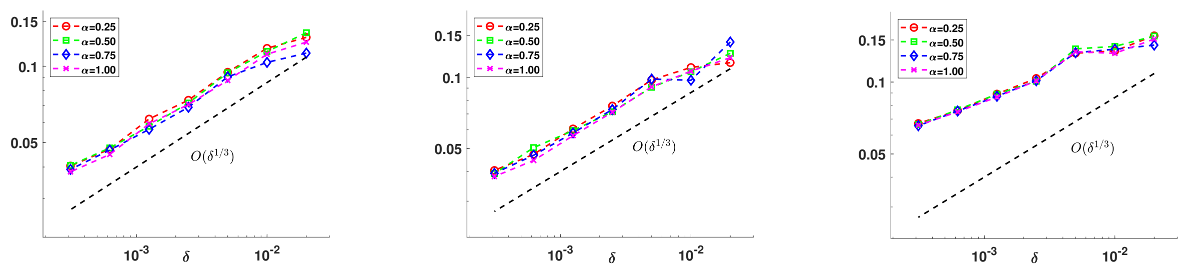
(a) $\delta = 10^{-2}$ (b) $\delta = 10^{-3}$ (c) $\delta = 10^{-4}$

Figure 6.4: Top left: Exact potential $q_3^\dagger$. The other three columns are profiles of numerical reconstructions q^* and corresponding pointwise error $e = |q^* - q_3^\dagger|$, with $T = 1$, $\alpha = 0.5$, $h = \delta^{\frac{1}{3}}$ and $\tau = \delta^{\frac{1}{3}}/15$.

respect to the order α. Moreover, we also test the sharpness of error estimate in Theorem 6.5, i.e.,

$$\|q^* - q^\dagger\|_{L^2(\Omega)} \le c\Big(\frac{\delta}{h^2} + h + \tau\Big).$$

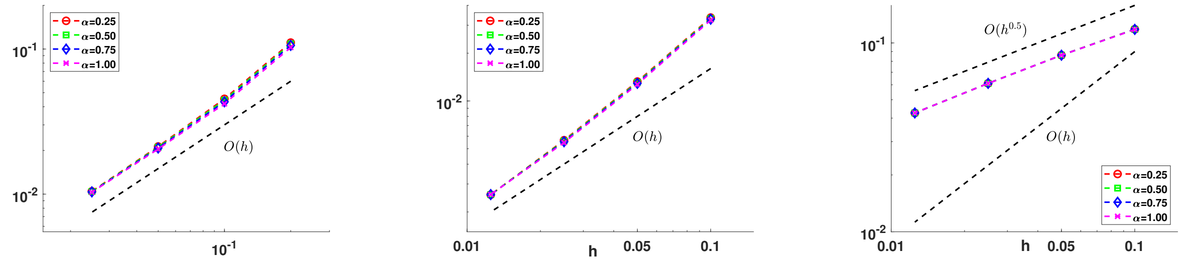
We let $\delta = 0$ and examine that the discretization error is $O(h+\tau)$. This is supported by the numerical results presented in Figure 6.6 and 6.7. In Figure 6.6, we fix $\tau = T/1000$ and test the convergence of space discretization. The empirical convergence rate is of order $O(h)$ for potentials $q_1^\dagger$ and $q_2^\dagger$. For $q_3^\dagger$ the empirical convergence rate is of order around $O(h^{\frac{1}{2}})$. This is due to the nonsmoothness of the discontinuous potential. In Figure 6.7, we present the convergence rate for time discretization with fixed $h = 3/200$. We observe that the empirical rate of convergence is of order $O(\tau)$ for all three cases. To test the term δ/h^2 in the error estimate, we let $\tau = \sqrt{\delta}/15$ and $h = \sqrt{\delta}$. Then Figure 6.8 shows that the error e_q hardly decays as $\delta \to 0$, it illustrates the sharpness of the term δ/h^2 in the error estimate.



(a) Smooth potential $q_1^\dagger$ (b) Piecewise smooth potential $q_2^\dagger$ (c) Discontinuous potential $q_3^\dagger$

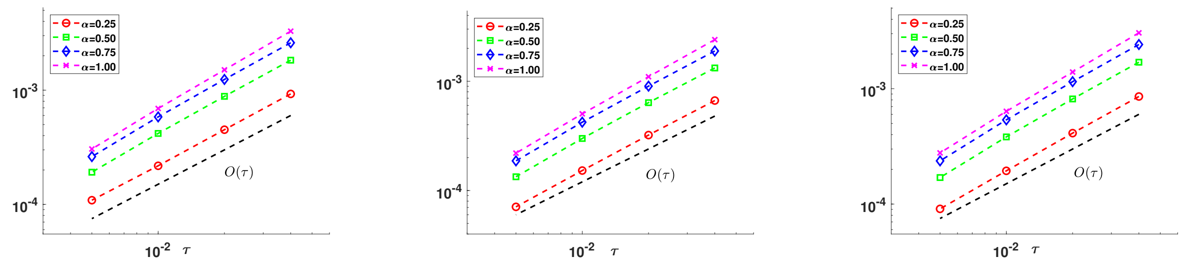
Figure 6.5: Relative error e_q versus noise level δ, where $T = 1$, $h = \delta^{\frac{1}{3}}$, $\tau = \delta^{\frac{1}{3}}/15$.

Next, we consider the continuous and piecewise smooth potential $q_2^\dagger$ and test the convergence of the numerical reconstruction with different terminal time T. We report the reconstruction error (6.41)



(a) Smooth potential: $q_1^\dagger$ (b) Piecewise smooth potential: $q_2^\dagger$ (c) Nonsmooth potential: $q_3^\dagger$

Figure 6.6: Relative error e_q versus h, where $\delta = 0$, $T = 1$, $\tau = T/1000$.



(a) Smooth potential: $q_1^\dagger$ (b) Piecewise smooth potential: $q_2^\dagger$ (c) Nonsmooth potential: $q_3^\dagger$

Figure 6.7: Relative error e_q versus τ, where $\delta = 0$, $T = 1$, $h = 3/200$.

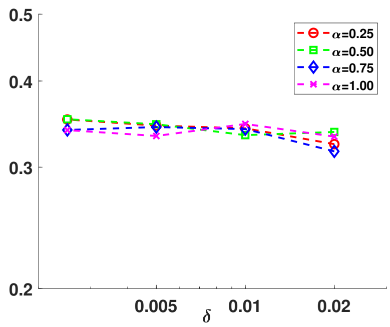
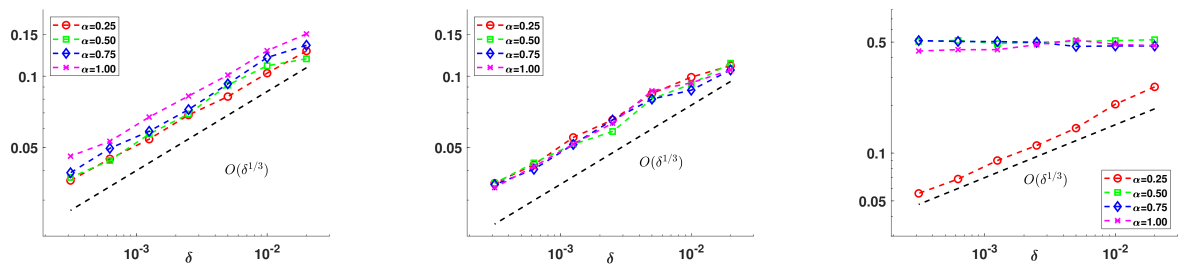


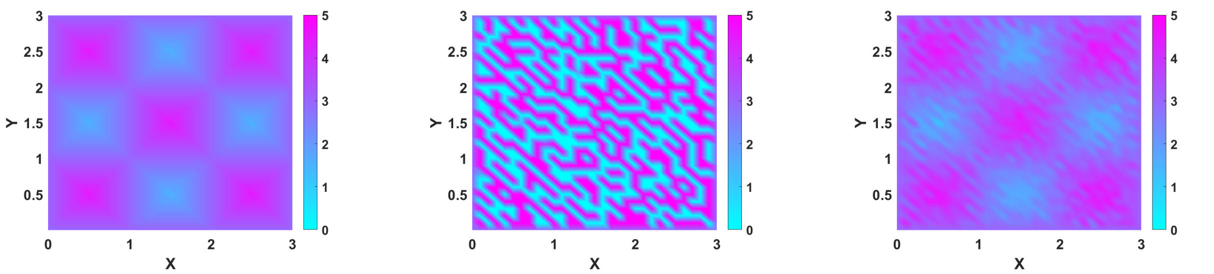
Figure 6.8: Relative error e_q with $T = 1$ and $q^\dagger = q_2^\dagger$, $h = \sqrt{\delta}$ and $\tau = \sqrt{\delta}/15$.

versus noise level δ, where we set $h = \delta^{\frac{1}{3}}$ and $\tau = \delta^{\frac{1}{3}} \times T/15$. For $T = 0.1$ and $T = 5$, we clearly observe the convergence rate $O(\delta^{\frac{1}{3}})$, cf. Figure 6.9 (a) and (b). However, in case that T is very small, i.e. $T = 10^{-7}$, our numerical results show that Algorithm 1 (with tolerance $\delta = 10^{-6}$) does not provide a good reconstruction q^* with $\alpha = 0.5$, 0.75 and 1, which might be due to the loss of the stability for small T, cf. Figure 6.9 (c). Interestingly, when $T = 10^{-7}$, we still observe the convergence of order $O(\delta^{\frac{1}{3}})$ for $\alpha = 0.25$. This might be due to the faster decay of $\partial_t^\alpha u(t)$ for small α when t is close to zero. The exact reason still awaits further theoretical investigation. Moreover, in Figure 6.10 (b) and (c) we plot the numerical reconstructions for $T = 10^{-7}$ and $T = 1$ respectively, where we set $\alpha = 0.75$, $\delta = 10^{-3}$, $h = 0.1$ and $\tau = T/150$, here we let $tol = 10^{-8}$. The numerical results show that Algorithm 1 produces an excellent reconstruction for $T = 1$, while the numerical reconstruction is inaccurate when T is small. This observation shows the necessity of the assumption in Theorems 6.3 and 6.5 that the terminal time T should be sufficiently large.



(a) $T = 0.1$ (b) $T = 5$ (c) $T = 10^{-7}$

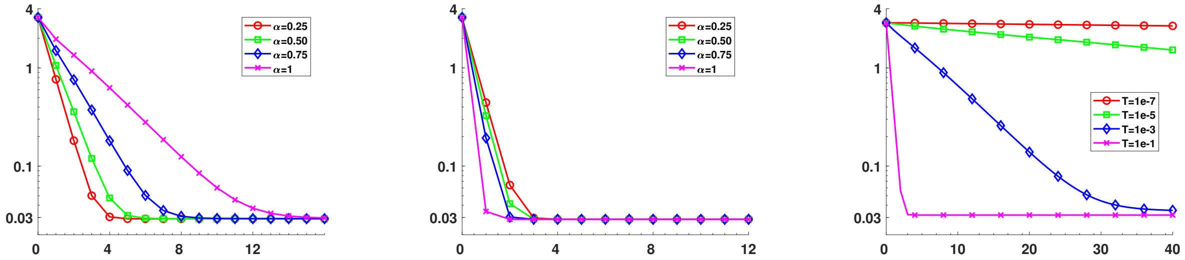
Figure 6.9: Relative error e_q versus noise level δ with $q_2^\dagger$, where $h = \delta^{\frac{1}{3}}$, $\tau = T \times \delta^{\frac{1}{3}}/15$ and $\alpha = 0.25, 0.5, 0.75, 1$.



(a) Exact potential $q_2^\dagger$ (b) Reconstruction with $T = 10^{-7}$ (c) Reconstruction with $T = 1$

Figure 6.10: Profiles of numerical reconstruction. (a): exact potential $q_2^\dagger$; (b): $T = 10^{-7}$, 2470 iterations and $\|q^{2470} - q^{2469}\|_{L^2(\Omega)} \leq 10^{-8}$; (c): $T = 1$, 9 iterations and $\|q^9 - q^{10}\|_{L^2(\Omega)} \leq 10^{-8}$.

Finally, we test the convergence of the iteration produced by Algorithm 1, with different α and T. In the experiments, we use the problem data (6.40) and the exact potential $q^\dagger = q_2^\dagger$. Meanwhile, we fix $\delta = 10^{-6}$, $h = 0.1$, $\tau = T/150$ and $q_0 = 3 - x(3-x)y(3-y)/3$. We let q_k be the numerical solution



(a) $T = 0.1$. (b) $T = 2$. (c) $\alpha = 0.5$.

Figure 6.11: Convergence histories of Algorithm 1 with different T and α, where $\delta = 10^{-6}$, $h = 0.03$, $\tau = T/500$.

obtained by k-th iteration in Algorithm 1, and compute the error at each iteration:

$$e_k = \|q_k - q^\dagger\|_{L^2(\Omega)} \qquad \text{for all} \quad k \geq 0.$$

In Figure 6.11 (a) and (b), we report the convergence histories for $T = 0.1$ and $T = 2$ with different α. We clearly observe that the iteration converges linearly, and the convergence factor decreases as T becomes larger. Besides, the convergence appears to be robust to the order of time derivative. Moreover, in Figure 6.11(c), we fix $\alpha = 0.5$ and test the convergence behavior for both large T and small T. Our experiments show that for small T, e.g. $T = 10^{-7}$, the iteration does not converge to a reasonable approximation to the exact potential.[1]

[1]Chapter 6 is reprinted with permission from "Identification of Potential in Diffusion Equations from Terminal Observation: Analysis and Discrete Approximation", Zhengqi Zhang Zhidong Zhang and Zhi Zhou, 2022, SIAM Journal on Numerical Analysis Vol. 60 Iss. 5. The candidate mainly works on the Methodology, the proof details, the coding and data collection in numerical experiments.

CHAPTER 7.

Conclusion and future works

This thesis has provided a complete and rigorous analysis of various inverse problems related to time-fractional differential equations, including backward diffusion of subdiffusion problem with time-dependent and time-independent coefficients, backward diffusion-wave problem and inverse potential problem.

Chapter 3–5 focus on the backward diffusion problems of time-fractional models. In Chapter 3, the classical finite element method and backward Euler convolution quadrature are applied to numerically approximate the time-fractional models. A quasi-boundary regularization method is used and, we give a thorough numerical analysis to the backward subdiffusion problem with time-independent coefficients. In Chapter 4, while the spatial diffusion coefficient is dependent on time, the spectral method may fail, then we provide a perturbation argument in the analysis of backward diffusion. Similarly, the discretization and regularization methods are applied. Then we extend our ideas to the backward diffusion-wave problem in Chapter 5, to simultaneously determine two initial conditions from two different observations. A novel quasi boundary value method is applied to this problem and, we provide a complete analysis.

Chapter 6 considers the inverse potential problem arising in diffusion models. To overcome the non-convergence approximation for Laplacian of observation, we apply a bilinear finite element method and obtain a numerical convergence.

In the following, we list several perspectives of our future research:

1. In Chapter 4, we show the backward subdiffusion problem with time dependent coefficients. However, we must assume the coefficient satisfies some assumption 4.3, 4.5. Our theoretical results are strongly dependent on the behavior of the coefficient, which decays to a constant at long time. However, for the high frequency coefficient, i.e., assumption 4.3 fail, the backward stability still holds from numerical experiments. We hope to derive theoretical backward stability for this case.

2. In Chapter 6, we give a fully numerical analysis for the inverse potential problem. However, the observation is assumed to be continuous in assumption 6.4 since we haven't applied regularization in this problem. Therefore, it is still our future work to find appropriate regularization methods for example smooth extension([113, 11]). Then we could assume the observation in L^2 sense, and we hope to derive some error estimates based on regularization.

3. Recently, there is a rapid arising interests in machine learning. Also, learning operator in inverse problems by Neural Networks is a popular topic these years, see [24, 19]. We hope to extend their ideas to the inverse potential problem of time(space)-fractional PDEs.

Bibliography

[1] P. Acquistapace, F. Flandoli, and B. Terreni. Initial-boundary value problems and optimal control for nonautonomous parabolic systems. *SIAM J. Control Optim.*, 29(1):89–118, 1991.

[2] E Eric Adams and Lynn W Gelhar. Field study of dispersion in a heterogeneous aquifer: 2. spatial moments analysis. *Water Res. Research*, 28(12):3293–3307, 1992.

[3] Herbert Amann. Compact embeddings of vector-valued Sobolev and Besov spaces. *Glas. Mat. Ser. III*, 35(55)(1):161–177, 2000.

[4] Wolfgang Arendt, Charles J.K. Batty, Matthias Hieber, and Frank Neubrander. *Vector-valued Laplace Transforms and Cauchy Problems.* Birkhäuser, Basel, 2nd edition, 2011.

[5] Emilia G Bajlekova. *Fractional Evolution Equations in Banach Spaces.* PhD thesis, Eindhoven University of Technology, 2001.

[6] Karel Van Bockstal. Uniqueness for inverse source problems of determining a space-dependent source in time-fractional equations with non-smooth solutions. *Fractal and Fractional*, 5(4):169, oct 2021.

[7] G. Chavent, G. Cohen, and M. Espy. Determination of relative permeabilities and capillary pressures by an automatic adjustment method. In *All Days.* SPE, sep 1980.

[8] De-Han Chen, Daijun Jiang, and Jun Zou. Convergence rates of Tikhonov regularizations for elliptic and parabolic inverse radiativity problems. *Inverse Problems*, page in press, 2020.

[9] Mourad Choulli and Masahiro Yamamoto. Generic well-posedness of an inverse parabolic problem—the Hölder-space approach. *Inverse Problems*, 12(3):195–205, 1996.

[10] Mourad Choulli and Masahiro Yamamoto. An inverse parabolic problem with non-zero initial condition. *Inverse Problems*, 13(1):19–27, 1997.

[11] Peter Craven and Grace Wahba. Smoothing noisy data with spline functions. *Numerische Mathematik*, 31(4):377–403, December 1978.

[12] Christopher B. Croke. *Geometric Methods in Inverse Problems and PDE Control.* Springer New York, 2004.

[13] Zui-Cha Deng, Jian-Ning Yu, and Liu Yang. Optimization method for an evolutional type inverse heat conduction problem. *J. Phys. A*, 41(3):035201, 20, 2008.

[14] Albert Einstein. Über die von der molekularkinetischen theorie der wärme geforderte bewegung von in ruhenden flüssigkeiten suspendierten teilchen. *Annalen der physik*, 4, 1905.

[15] Heinz W. Engl, Martin Hanke, and Andreas Neubauer. *Regularization of Inverse Problems.* Kluwer, Dordrecht, 1996.

[16] Heinz W. Engl, Karl Kunisch, and Andreas Neubauer. Convergence rates for Tikhonov regularisation of nonlinear ill-posed problems. *Inverse Problems*, 5(4):523–540, 1989.

[17] Alexandre Ern and Jean-Luc Guermond. *Theory and Practice of Finite Elements.* Springer-Verlag, New York, 2004.

[18] Richard E. Ewing. The approximation of certain parabolic equations backward in time by sobolev equations. *SIAM Journal on Mathematical Analysis*, 6(2):283–294, 1975.

[19] Yuwei Fan and Lexing Ying. Solving electrical impedance tomography with deep learning. *Journal of Computational Physics*, 404:109119, March 2020.

[20] G. Floridia and M. Yamamoto. Backward problems in time for fractional diffusion-wave equation. *Inverse Problems*, 36(12):125016, 14, 2020.

[21] Avner Friedman. Remarks on the maximum principle for parabolic equations and its applications. *Pacific J. Math.*, 8:201–211, 1958.

[22] Ido Golding and Edward C. Cox. Physical nature of bacterial cytoplasm. *Physical Review Letters*, 96(9):098102, mar 2006.

[23] Michael Grüter and Kjell-Ove Widman. The Green function for uniformly elliptic equations. *Manuscripta Math.*, 37(3):303–342, 1982.

[24] Ruchi Guo, Shuhao Cao, and Long Chen. Transformer meets boundary value inverse problems. *ICLR*, 2023.

[25] Jacques Salomon Hadamard. *Lectures on Cauchy's problem in linear partial differential equations*, volume 18. Yale University Press, 1923.

[26] E. Hairer and Gerhard Wanner. *Solving Ordinary Differential Equations II.* Springer, 2004.

[27] Dinh Nho Hào, Jijun Liu, Nguyen Van Duc, and Nguyen Van Thang. Stability results for backward time-fractional parabolic equations. *Inverse Problems*, 35(12):125006, 25, 2019.

[28] Alemdar Hasanov Hasanoglu and Vladimir G. Romanov. *Introduction to Inverse Problems for Differential Equations.* Springer, 2018.

[29] Yuko Hatano and Naomichi Hatano. Dispersive transport of ions in column experiments: An explanation of long-tailed profiles. *Water Res. Research*, 34(5):1027–1033, 1998.

[30] A. S. Hendy and K. Van Bockstal. On a reconstruction of a solely time-dependent source in a time-fractional diffusion equation with non-smooth solutions. *Journal of Scientific Computing*, 90(1), dec 2021.

[31] W. Höhn. Finite elements for parabolic equations backwards in time. *Numerische Mathematik*, 40(2):207–227, jun 1982.

[32] David S. Holder. *Electrical Impedance Tomography.* Taylor & Francis, 2004.

[33] Rui Huang, Xiaodong Wu, Ruihe Wang, and Hui Li. Inverse problem models of oil-water two-phase flow based on buckley-leverett theory. *Journal of Applied Mathematics*, 2013:1–6, 2013.

[34] Victor Isakov. Inverse parabolic problems with the final overdetermination. *Comm. Pure Appl. Math.*, 44(2):185–209, 1991.

[35] Hiroshi Isozaki. *Inverse Spectral and Scattering Theory.* Springer Singapore Pte. Limited, 2020.

[36] Kazufumi Ito and Bangti Jin. *Inverse Problems: Tikhonov Theory and Algorithms.* World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ, 2015.

[37] Enrico Magenes Jacques Louis Lions. *Non-Homogeneous Boundary Value Problems and Applications.* Springer Berlin Heidelberg, November 2011.

[38] Bangti Jin. *Fractional differential equations—an approach via fractional derivatives*, volume 206 of *Applied Mathematical Sciences*. Springer, Cham, [2021] ©2021.

[39] Bangti Jin, Raytcho Lazarov, Vidar Thomée, and Zhi Zhou. On nonnegativity preservation in finite element methods for subdiffusion equations. *Math. Comp.*, 86(307):2239–2260, 2017.

[40] Bangti Jin, Raytcho Lazarov, and Zhi Zhou. Error estimates for a semidiscrete finite element method for fractional order parabolic equations. *SIAM J. Numer. Anal.*, 51(1):445–466, jan 2013.

[41] Bangti Jin, Raytcho Lazarov, and Zhi Zhou. Two fully discrete schemes for fractional diffusion and diffusion-wave equations with nonsmooth data. *SIAM J. Sci. Comput.*, 38(1):A146–A170, 2016.

[42] Bangti Jin, Raytcho Lazarov, and Zhi Zhou. Numerical methods for time-fractional evolution equations with nonsmooth data: A concise overview. *Comput. Methods Appl. Mech. Engrg.*, 346:332–358, 2019.

[43] Bangti Jin, Buyang Li, and Zhi Zhou. Correction of high-order BDF convolution quadrature for fractional evolution equations. *SIAM J. Sci. Comput.*, 39(6):A3129–A3152, 2017.

[44] Bangti Jin, Buyang Li, and Zhi Zhou. Numerical analysis of nonlinear subdiffusion equations. *SIAM J. Numer. Anal.*, 56(1):1–23, 2018.

[45] Bangti Jin, Buyang Li, and Zhi Zhou. Subdiffusion with a time-dependent coefficient: analysis and numerical solution. *Math. Comp.*, 88(319):2157–2186, 2019.

[46] Bangti Jin, Buyang Li, and Zhi Zhou. Subdiffusion with time-dependent coefficients: improved regularity and second-order time stepping. *Numerische Mathematik*, 145(4):883–913, jun 2020.

[47] Bangti Jin, Xiliang Lv, Qimeng Quan, and Zhi Zhou. Convergence rate analysis of Galerkin approximation of inverse potential problem. Preprint, 2021.

[48] Bangti Jin and William Rundell. A tutorial on inverse problems for anomalous diffusion processes. *Inverse Problems*, 31(3):035003, 40, 2015.

[49] Bangti Jin and Zhi Zhou. Incomplete iterative solution of subdiffusion. *Numer. Math.*, 145(3):693–725, 2020.

[50] Bangti Jin and Zhi Zhou. An inverse potential problem for subdiffusion: stability and reconstruction. *Inverse Problems*, 37(1):Paper No. 015006, 26, 2021.

[51] Bangti Jin and Zhi Zhou. Numerical estimation of a diffusion coefficient in subdiffusion. *SIAM J. Control Optim.*, 59(2):1466–1496, 2021.

[52] Barbara Kaltenbacher. *Iterative regularization methods for nonlinear ill-posed problems.* Walter de Gruyter, 2008.

[53] Barbara Kaltenbacher and William Rundell. On an inverse potential problem for a fractional reaction-diffusion equation. *Inverse Problems*, 35(6):065004, 31, 2019.

[54] Barbara Kaltenbacher and William Rundell. The inverse problem of reconstructing reaction-diffusion systems. *Inverse Problems*, 36(6):065011, 34, 2020.

[55] Barbara Kaltenbacher and William Rundell. Recovery of multiple coefficients in a reaction-diffusion equation. *J. Math. Anal. Appl.*, 481(1):123475, 23, 2020.

[56] Yavar Kian and Masahiro Yamamoto. Reconstruction and stable recovery of source terms and coefficients appearing in diffusion equations. *Inverse Problems*, 35(11):115006, 24, 2019.

[57] Anatoly A. Kilbas, Hari M. Srivastava, and Juan J. Trujillo. *Theory and Applications of Fractional Differential Equations*, volume 204 of *North-Holland Mathematics Studies*. Elsevier Science B.V., 2006.

[58] Ildoo Kim, Kyeong-Hun Kim, and Sungbin Lim. An $l_q(l_p)$-theory for the time fractional evolution equations with variable coefficients. *Advances in Mathematics*, 306:123–176, jan 2017.

[59] Michael V. Klibanov, Jingzhi Li, and Wenlong Zhang. Convexification for an inverse parabolic problem. , arXiv:2001.01880, 2020.

[60] Adam Kubica, Katarzyna Ryszewska, and Masahiro Yamamoto. *Time-Fractional Differential Equations*. Springer Singapore Pte. Limited, 2020.

[61] V. Lakshmikantham and Aghalaya S. Vatsala. Theory of fractional differential inequalities and applications. *Communications in Applied Analysis*, 11, 2007.

[62] Irena Lasiecka. Unified theory for abstract parabolic boundary problems—a semigroup approach. *Appl. Math. Optim.*, 6(4):287–333, 1980.

[63] Robert Lattés. *The method of quasi-reversibility*. American Elsevier Pub. Co., 1969.

[64] Buyang Li and Weiwei Sun. Maximal L^p analysis of finite element solutions for parabolic equations with nonsmooth coefficients in convex polyhedra. *Math. Comp.*, 86(305):1071–1102, 2017.

[65] Lei Li and Dongling Wang. Complete monotonicity-preserving numerical methods for time fractional ODEs. *Communications in Mathematical Sciences*, 19(5):1301–1336, 2021.

[66] Zhiyuan Li, Yikan Liu, and Masahiro Yamamoto. Inverse problems of determining parameters of the fractional partial differential equations. In *Handbook of fractional calculus with applications. Vol. 2*, pages 431–442. De Gruyter, Berlin, 2019.

[67] Zhiyuan Li and Masahiro Yamamoto. Inverse problems of determining coefficients of the fractional partial differential equations. In *Handbook of fractional calculus with applications. Vol. 2*, pages 443–464. De Gruyter, Berlin, 2019.

[68] Qun Lin and Jiafu Lin. *Finite element methods: accuracy and improvement*, volume 1. Elsevier, 2006.

[69] J.J. Liu and M. Yamamoto. A backward problem for the time-fractional diffusion equation. *Applicable Analysis*, 89(11):1769–1788, nov 2010.

[70] Yikan Liu, Zhiyuan Li, and Masahiro Yamamoto. Inverse problems of determining sources of the fractional partial differential equations. *Handbook of fractional calculus with applications*, 2:411–430, 2019.

[71] Ch. Lubich. Discretized fractional calculus. *SIAM J. Math. Anal.*, 17(3):704–719, 1986.

[72] Yuri Luchko and Masahiro Yamamoto. On the maximum principle for a time-fractional diffusion equation. *Fract. Calc. Appl. Anal.*, 20(5):1131–1145, 2017.

[73] Mitchell Luskin and Rolf Rannacher. On the smoothing property of the Galerkin method for parabolic equations. *SIAM J. Numer. Anal.*, 19(1):93–113, 1982.

[74] Francesco Mainardi. Fractional relaxation-oscillation and fractional diffusion-wave phenomena. *Chaos Solitons Fractals*, 7(9):1461–1477, 1996.

[75] Francesco Mainardi. *Fractional calculus and waves in linear viscoelasticity.* Imperial College Press, London, 2010. An introduction to mathematical models.

[76] William McLean, Kassem Mustapha, Raed Ali, and Omar Knio. Well-posedness of time-fractional advection-diffusion-reaction equations. *Fractional Calculus and Applied Analysis*, 22(4):918–944, aug 2019.

[77] William McLean, Kassem Mustapha, Raed Ali, and Omar M. Knio. Regularity theory for time-fractional advection–diffusion–reaction equations. *Comput.Math.Appl.*, 79(4):947–961, feb 2020.

[78] William McLean, Kassem Mustapha, Raed Ali, and Omar M. Knio. Erratum to "regularity theory for time-fractional advection-diffusion-reaction equations" [comput. math. appl. 79 (2020) 947–961]. *Comput.Math.Appl.*, 85:82–83, mar 2021.

[79] Donald W. McRobbie, Elizabeth A. Moore, Martin J. Graves, and Martin R. Prince. *MRI from Picture to Proton.* Cambridge University Press, sep 2006.

[80] Ralf Metzler, Jae-Hyung Jeon, Andrey G. Cherstvy, and Eli Barkai. Anomalous diffusion models and their properties: non-stationarity, non-ergodicity, and ageing at the centenary of single particle tracking. *Phys. Chem. Chem. Phys.*, 16:24128, 37 pp., 2014.

[81] Ralf Metzler and Joseph Klafter. The random walk's guide to anomalous diffusion: a fractional dynamics approach. *Phys. Rep.*, 339(1):1–77, 2000.

[82] Luc Miller and Masahiro Yamamoto. Coefficient inverse problem for a fractional diffusion equation. *Inverse Problems*, 29(7):075013, 8, 2013.

[83] Kassem Mustapha. FEM for time-fractional diffusion equations, novel optimal error analyses. *Math. Comp.*, 87(313):2259–2272, 2018.

[84] Frank Natterer. *The Mathematics of Computerized Tomography (Classics in Applied Mathematics)*. SIAM: Society for Industrial and Applied Mathematics, 2001.

[85] RR Nigmatullin. The realization of the generalized transfer equation in a medium with fractal geometry. *Phys. Stat. Sol. B*, 133(1):425–430, 1986.

[86] H. H. Pennes. Analysis of tissue and arterial blood temperatures in the resting human forearm. *J. Appl. Physiol.*, 1(2):93–122, 1948.

[87] Igor Podlubny. *Fractional differential equations*, volume 198 of *Mathematics in Science and Engineering*. Academic Press, Inc., San Diego, CA, San Diego, 1999. An introduction to fractional derivatives, fractional differential equations, to methods of their solution and some of their applications.

[88] Jürgen Pöschel and Eugene Trubowitz. *Inverse spectral theory*, volume 130 of *Pure and Applied Mathematics*. Academic Press, Inc., Boston, MA, 1987.

[89] Kenichi Sakamoto and Masahiro Yamamoto. Initial value/boundary value problems for fractional diffusion-wave equations and applications to some inverse problems. *J. Math. Anal. Appl.*, 382(1):426–447, oct 2011.

[90] Thomas Schuster. *The method of approximate inverse*. Springer, 2007.

[91] Hansjörg Seybold and Rudolf Hilfer. Numerical algorithm for calculating the generalized Mittag-Leffler function. *SIAM J. Numer. Anal.*, 47(1):69–88, 2008/09.

[92] A. M. Stuart. Inverse problems: A bayesian perspective. *Acta Numerica*, 19:451–559, may 2010.

[93] Vidar Thomée. *Galerkin Finite Element Methods for Parabolic Problems*. Springer-Verlag, Berlin, 2nd edition, 2006.

[94] A. N. Tikhonov. *Solutions of ill-posed problems*. Winston, 1977.

[95] A. N. Tikhonov, A. Goncharsky, V. V. Stepanov, and Anatoly G. Yagola. *Numerical Methods for the Solution of Ill-Posed Problems*. Springer, 2013.

[96] Hans Triebel. *Interpolation Theory, Function Spaces, Differential Operators*. North-Holland Publishing Co., Amsterdam-New York, 1978.

[97] Gunther Uhlmann. Inverse problems: seeing the unseen. *Bulletin of Mathematical Sciences*, 4(2):209–279, jun 2014.

[98] H. A. van der Vorst. Bi-CGSTAB: A fast and smoothly converging variant of bi-CG for the solution of nonsymmetric linear systems. *SIAM Journal on Scientific and Statistical Computing*, 13(2):631–644, mar 1992.

[99] Vicente Vergara and Rico Zacher. Optimal decay estimates for time-fractional and other Non-Local subdiffusion equations via energy methods. *SIAM Journal on Mathematical Analysis*, 47(1):210–239, jan 2015.

[100] Jun-Gang Wang and Ting Wei. An iterative method for backward time-fractional diffusion problem. *Numer. Methods Partial Differential Equations*, 30(6):2029–2041, 2014.

[101] Lijuan Wang and Jun Zou. Error estimates of finite element methods for parameter identifications in elliptic and parabolic systems. *Discrete Contin. Dyn. Syst. Ser. B*, 14(4):1641–1670, 2010.

[102] Liyan Wang and Jijun Liu. Total variation regularization for a backward time-fractional diffusion problem. *Inverse Problems*, 29(11):115013, 22, 2013.

[103] Ting Wei and Jun-Gang Wang. A modified quasi-boundary value method for the backward time-fractional diffusion problem. *ESAIM Math. Model. Numer. Anal.*, 48(2):603–621, 2014.

[104] Ting Wei and Yun Zhang. The backward problem for a time-fractional diffusion-wave equation in a bounded domain. *Comput. Math. Appl.*, 75(10):3632–3648, 2018.

[105] Carl Wunsch. *The Ocean Circulation Inverse Problem.* Cambridge University Press, 1996.

[106] Masahiro Yamamoto and Jun Zou. Simultaneous reconstruction of the initial temperature and heat radiative coefficient. *Inverse Problems*, 17(4):1181–1202, 2001. Special issue to celebrate Pierre Sabatier's 65th birthday (Montpellier, 2000).

[107] Liu Yang, Jian-Ning Yu, and Zui-Cha Deng. An inverse problem of identifying the coefficient of parabolic equation. *Appl. Math. Model.*, 32(10):1984–1995, 2008.

[108] Ming Yang and Jijun Liu. Solving a final value fractional diffusion problem by boundary condition regularization. *Appl. Numer. Math.*, 66:45–58, 2013.

[109] V. Zaburdaev, S. Denisov, and J. Klafter. Lévy walks. *Reviews of Modern Physics*, 87(2):483–530, jun 2015.

[110] Zhengqi Zhang, Zhidong Zhang, and Zhi Zhou. Identification of potential in diffusion equations from terminal observation: Analysis and discrete approximation. *SIAM Journal on Numerical Analysis*, 60(5):2834–2865, oct 2022.

[111] Zhengqi Zhang and Zhi Zhou. Numerical analysis of backward subdiffusion problems. *Inverse Problems*, 36(10):105006, oct 2020.

[112] Zhengqi Zhang and Zhi Zhou. Backward diffusion-wave problem: stability, regularization and approximation. *SIAM J. Sci. Comput., in press. arXiv: 2109.07114*, 2021.

[113] Zhidong Zhang and Zhi Zhou. Recovering the potential term in a fractional diffusion equation. *IMA J. Appl. Math.*, 82(3):579–600, 2017.