# An Analysis of the Crank-Nicolson Method for Subdiffusion

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**Abstract**

In this work, we analyze a Crank-Nicolson type time stepping scheme for the subdiffusion equation, which involves a Caputo fractional derivative of order $\alpha \in (0, 1)$ in time. It hybridizes the backward Euler convolution quadrature with a $\theta$-type method, with the parameter $\theta$ dependent on the fractional order $\alpha$ by $\theta = \alpha/2$, and naturally generalizes the classical Crank-Nicolson method. We develop essential initial corrections at the starting two steps for the Crank-Nicolson scheme, and together with the Galerkin finite element method in space, obtain a fully discrete scheme. The overall scheme is easy to implement, and robust with respect to data regularity. A complete error analysis of the fully discrete scheme is provided, and a second-order accuracy in time is established for both smooth and nonsmooth problem data. Extensive numerical experiments are provided to illustrate its accuracy, efficiency and robustness, and a comparative study also indicates its competitive with existing schemes.

**Keywords**: Crank-Nicolson method, subdiffusion, initial correction, error estimates, nonsmooth data, convolution quadrature

## 1 Introduction

Let $\Omega$ be a bounded convex polygonal domain in $\mathbb{R}^d$ $(d = 1, 2, 3)$ with a boundary $\partial\Omega$, and $T > 0$ be a fixed value. We are interested in efficient numerical methods for the following fractional-order evolution equation of $u(t) : (0, T) \to H_0^1(\Omega) \cap H^2(\Omega)$:

$$\partial_t^\alpha u(t) - \Delta u(t) = f(t) \quad \text{for } t \in (0, T), \tag{1.1}$$

where $\Delta : H_0^1(\Omega) \cap H^2(\Omega) \to L^2(\Omega)$ denotes the Laplacian, $f : (0, T) \to L^2(\Omega)$ is a given function, and the notation $\partial_t^\alpha u$, $0 < \alpha < 1$, denotes the Caputo fractional derivative of order $\alpha$ with respect to $t$, defined by [15, pp. 91]

$$\partial_t^\alpha u(t) := \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \frac{d}{ds} u(s)\, ds, \tag{1.2}$$

with $\Gamma(\cdot)$ being the Gamma function defined by $\Gamma(s) := \int_0^\infty t^{s-1} e^{-t} dt$ for $\Re(s) > 0$. The model (1.1) is subject to a zero boundary condition $u = 0$ on $\partial\Omega \times (0, T]$, and the following initial condition

$$u(0) = v, \quad \text{in } \Omega,$$

where $v$ is a given function defined on the domain $\Omega$. The model (1.1) with $0 < \alpha < 1$ is popular for modeling subdiffusion processes, in which the mean-squared displacement of particle motion grows only

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sublinearly with the time $t$, instead of the linear growth for normal diffusion. It has been applied in several fields, e.g., solute transport in heterogeneous media and cytoplasmic crowding in living cells; see [23] for an extensive list.

Recently, there has been much interest in developing efficient numerical schemes for (1.1). A number of time stepping schemes have been proposed, which roughly can be divided into two groups, i.e., L1 type scheme and convolution quadrature (CQ). L1 type schemes are of finite difference nature, and can be derived by polynomial interpolation [6, 17, 8, 1, 3, 21]. These schemes were derived under the assumption that the solution $u$ is smooth, and require high solution regularity for error estimates. See also [22, 24] for discontinuous Galerkin methods. CQ due to [18, 19] presents a flexible framework for devising high-order time stepping schemes for (1.1), and merits excellent stability property. Thus it has been customarily applied [29, 5, 12, 7, 30]. For both L1 type and CQ schemes, proper corrections are necessary in order to obtain high-order convergence for general problem data, including very smooth data. However, to the best of our limited knowledge, for problem (1.1), so far this has been only done in [5] and [12] for CQ generated by the second-order BDF. Hence, it remains imperative to develop and analyze high-order schemes robust with respect to data regularity.

In this paper, we present an analysis of a robust $O(\tau^2)$ accurate fractional Crank-Nicolson scheme, with finite element space discretization. Let $\tau$ be the constant time step size and $h$ the mesh size. Using the time-stepping scheme developed in [7] and standard Galerkin finite element method in space, we propose a fully discrete scheme approximates the solution $u(t_n)$ by $U_h^n$, $n = 1, 2, \ldots, N$:

$$\bar\partial_\tau^\alpha(U_h^n - v_h) - \big(1 - \tfrac{\alpha}{2}\big)\Delta_h U_h^n - \tfrac{\alpha}{2}\Delta_h U_h^{n-1} = \big(1 - \tfrac{\alpha}{2}\big)F_h^n + \tfrac{\alpha}{2}F_h^{n-1}, \tag{1.3}$$

where $\Delta_h : X_h \to X_h$ denotes the Galerkin approximation of the Laplacian on a finite element subspace $X_h \subset H_0^1(\Omega)$, $F_h^n = P_h f(t_n)$ denotes the $L^2$-projection of $f(t_n)$ onto $X_h$, and $v_h \in X_h$ is an approximation to the initial data $v$. In (1.3), $\bar\partial_\tau^\alpha \varphi^n$ denotes the backward Euler CQ approximation to the Riemann-Liouville fractional derivative ${}^R\partial_t^\alpha \varphi(t_n)$ (cf. (2.3) below) defined by:

$$\bar\partial_\tau^\alpha \varphi^n := \tau^{-\alpha}\sum_{j=0}^{n} b_{n-j}\varphi^j, \quad \text{with} \quad \sum_{j=0}^{\infty} b_j \xi^j := (1-\xi)^\alpha, \tag{1.4}$$

where the weights $b_j$ are available in closed form: $b_j = (-1)^j \frac{\Gamma(\alpha+1)}{\Gamma(j+1)\Gamma(\alpha-j+1)}$. Clearly, for $\alpha = 1$, the scheme (1.3) recovers the classical Crank–Nicolson method [4], and thus it represents a natural extension of the latter to the fractional case, which has long been missing in the literature. For $\alpha \in (0, 1)$, the scheme (1.3) hybridizes the backward Euler CQ with the $\theta$-type method with a weight $\theta = \alpha/2$. This choice was motivated by the fact that it yields a local truncation error $O(\tau^2)$ under certain compatibility conditions; see Section 2.2 for details. The numerical experiments therein show that it is indeed second-order accurate in time if the solution $u$ is sufficiently smooth.

However, the solution $u$ of problem (1.1) can be weakly singular near $t = 0$ even for smooth problem data [26, 27], and thus a straightforward implementation of (1.3) yields only an $O(\tau)$ convergence, cf. Table 2, as for other high-order time stepping schemes. Inspired by [5], we shall correct it at the starting two steps, leading to a novel corrected scheme, cf. (2.4) below. The new scheme has two distinct features, which make it very attractive. (i) Since it employs the backward Euler CQ and changes only the first two steps, it is straightforward to implement. (ii) It is robust with respect to data regularity: it can achieve an $O(\tau^2)$ convergence in time for nonsmooth initial data $v$ and source term $f$ incompatible with $v$ at $t = 0$ (cf. Theorems 3.2 and 3.3). Our numerical experiments in Section 4 fully confirm its accuracy and robustness.

The contributions of the work are threefold. First, we develop essential initial corrections for the scheme (1.3) in order to restore the $O(\tau^2)$ accuracy for nonsmooth data. It presents a new robust second-order scheme for (1.1), competitive with the corrected second-order BDF. Second, we provide a complete convergence analysis of the corrected scheme under realistic regularity conditions on the data. For example, for $v \in L^2(\Omega)$ and $f \equiv 0$, we show in Theorem 3.2 the following error estimate

$$\|u_h(t_n) - U_h^n\|_{L^2(\Omega)} \le c\tau^2 t_n^{-2}\|v\|_{L^2(\Omega)}, \quad n \ge 1,$$

where $u_h$ is the semidiscrete Galerkin solution, cf. (2.1). Some preliminary analysis of the scheme (1.3) was given in [7, Theorem 1] under high regularity assumption on the solution, i.e., $u \in C^4[0,T]$, and restrictive compatibility condition $u^{(i)}(0) = 0$, $i = 0, 1, 2$. We shall derive optimal error estimates that are directly expressed in terms of data regularity. As a by-product, we also give the guideline for constructing initial corrections for other schemes, cf. Remark 3.1. Third, the proof relies on the discrete Laplace transform and a refined analysis of the kernel function, largely inspired by a strategy outlined in [20]. Due to the hybridization of the $\theta$ method with the backward Euler CQ, the scheme lacks a simple convolution structure, leading to a complex kernel, and is challenging to analyze. We shall develop a general strategy in Lemma 3.2 to overcome the challenge. Thus the convergence analysis differs substantially from existing works [5, 12], for which the requisite basic estimates on the kernel are well known.

The rest of the paper is organized as follows. In Section 2 we rederive the scheme (1.3) and develop the initial corrections. Then in Section 3, we present a complete convergence analysis of the corrected scheme. The focus is on the time discretization error, since the error analysis of the semidiscrete Galerkin scheme is well understood. Last, in Section 4 we present extensive numerical experiments to confirm the convergence rates for both smooth and nonsmooth problem data, where a comparative study with CQ generated by the second-order BDF, cf. [12], and the L1-2 scheme, cf. [8], also shows clearly its competitiveness. Throughout, the notation $c$, with or without a subscript, denotes a generic constant which may differ at different occurrences, but it is always independent of the mesh size $h$ and time step size $\tau$.

# 2 The fractional Crank-Nicolson scheme

In this part, we derive a fully discrete scheme for problem (1.1) using a standard Galerkin FEM in space and the fractional Crank-Nicolson approximation in time.

## 2.1 Semidiscrete Galerkin scheme

Let $\mathcal{T}_h$ be a shape regular, quasi-uniform triangulation of the domain $\Omega$ into $d$-simplexes, denoted by $T$, with a mesh size $h$. Then over $\mathcal{T}_h$, we define a continuous piecewise linear finite element space $X_h$ by

$$X_h = \left\{ v_h \in H_0^1(\Omega) : \; v_h|_T \text{ is a linear function}, \; \forall\, T \in \mathcal{T}_h \right\}.$$

We define the $L^2(\Omega)$-projection $P_h : L^2(\Omega) \to X_h$ and the Ritz projection $R_h : H_0^1(\Omega) \to X_h$ by

$$\begin{aligned} (P_h\varphi, \chi_h) &= (\varphi, \chi_h), && \forall\, \chi_h \in X_h, \\ (\nabla R_h\varphi, \nabla\chi_h) &= (\nabla\varphi, \nabla\chi_h), && \forall\, \chi_h \in X_h, \end{aligned}$$

respectively, where $(\cdot,\cdot)$ denotes the inner product of $L^2(\Omega)$. Then the spatially semidiscrete Galerkin FEM scheme for problem (1.1) reads: find $u_h(t) \in X_h$ such that

$$(\partial_t^\alpha u_h, \chi_h) + (\nabla u_h, \nabla\chi_h) = (f, \chi_h), \quad \forall\, \chi_h \in X_h, \tag{2.1}$$

with the initial condition $u_h(0) = v_h \in X_h$. The choice $v_h$ depends on the smoothness of the initial data $v$ ([28]): for $v \in D(\Delta) = H_0^1(\Omega) \cap H^2(\Omega)$, we take $v_h = R_h v$, and for $v \in L^2(\Omega)$, we take $v_h = P_h v$. Upon introducing the discrete Laplacian $\Delta_h : X_h \to X_h$, defined by $-(\Delta_h\varphi_h, \chi_h) = (\nabla\varphi_h, \nabla\chi_h)$ for all $\varphi_h, \chi_h \in X_h$, we can rewrite (2.1) as: with $u_h(0) = v_h \in X_h$ and $f_h(t) = P_h f(t)$

$$\partial_t^\alpha u_h(t) - \Delta_h u_h(t) = f_h(t), \quad \forall\, t > 0. \tag{2.2}$$

The semidiscrete scheme (2.2) has been analyzed in [10, 9, 16, 14], and we refer interested readers to these works for detailed error estimates.

## 2.2 Formal derivation of the fractional Crank-Nicolson scheme

In this part, we formally derive the fractional Crank-Nicolson scheme (1.3). Upon recalling the defining relation of the Caputo derivative $\partial_t^\alpha \varphi$ in terms of the Riemann-Liouville one [15, pp. 91, eq. (2.4.1)], i.e., $\partial_t^\alpha \varphi(t) = {}^R\partial_t^\alpha(\varphi(t) - \varphi(0))$, where the Riemann-Liouville fractional derivative ${}^R\partial_t^\alpha \varphi(t)$, for $0 < \alpha < 1$, is defined by:

$$ {}^R\partial_t^\alpha \varphi(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t (t-s)^{-\alpha} \varphi(s) ds. \tag{2.3} $$

we can rewrite the scheme (2.2) into

$$ {}^R\partial_t^\alpha (u_h(t) - v_h) - \Delta_h u_h(t) = f_h(t), $$

Now consider a uniform partition of $[0, T]$ with time step size $\tau = T/N$, $N \in \mathbb{N}$, so that $0 = t_0 < t_1 < \ldots < t_N = T$, and $t_n = n\tau$, $n = 0, \ldots, N$. The Riemann-Liouville derivative ${}^R\partial_t^\alpha \varphi(t_n)$ can be discretized using the backward Euler CQ (1.4), and it is $O(\tau)$ accurate [25, pp. 204-208]. In order to achieve an $O(\tau^2)$ accuracy, we aim at deriving a $\theta$-type method with a suitable weight $\theta$ by Fourier transform. We denote by $\mathcal{F}_t$ the Fourier transform in $t$ and by $\mathcal{F}_\xi^{-1}$ the inverse Fourier transform in $\xi$. Assuming that the function $\varphi$ is smooth over the domain $\mathbb{R}$ and $\varphi = 0$ for $t \le 0$, then the function

$$ \bar\partial_\tau^\alpha \varphi(t) := \tau^{-\alpha} \sum_{j=0}^\infty b_j \varphi(t - j\tau) $$

coincides with the scheme (1.4) at $t = t_n$ and satisfies

$$ \begin{aligned} \mathcal{F}_t[\bar\partial_\tau^\alpha \varphi(t)](\xi) &= \int_\mathbb{R} \bar\partial_\tau^\alpha \varphi(t) e^{-\mathrm{i}t\xi} dt = \tau^{-\alpha} \sum_{j=0}^\infty \int_\mathbb{R} b_j \varphi(t - j\tau) e^{-\mathrm{i}t\xi} dt \\ &= \tau^{-\alpha}(1 - e^{-\mathrm{i}\tau\xi})^\alpha \mathcal{F}\varphi(\xi) = (\mathrm{i}\xi)^\alpha (1 - \tfrac{\mathrm{i}\alpha}{2}\tau\xi + O(\tau^2\xi^2)) \mathcal{F}\varphi(\xi). \end{aligned} $$

In view of the identity

$$ \mathcal{F}_t[{}^R\partial_t^\alpha \varphi(t-s)](\xi) = (\mathrm{i}\xi)^\alpha e^{-\mathrm{i}s\xi} \mathcal{F}\varphi(\xi) = (\mathrm{i}\xi)^\alpha \big(1 - \mathrm{i}s\xi + O(s^2\xi^2)\big) \mathcal{F}\varphi(\xi), $$

and by the choice $s = \alpha\tau/2$, formally we derive

$$ \begin{aligned} \bar\partial_\tau^\alpha \varphi(t) &= {}^R\partial_t^\alpha \varphi(t - \alpha\tau/2) + \mathcal{F}_\xi^{-1}[O(\tau^2\xi^2)(\mathrm{i}\xi)^\alpha \mathcal{F}\varphi(\xi)] \\ &= {}^R\partial_t^\alpha \varphi(t - \alpha\tau/2) + O(\tau^2) \\ &= (1 - \tfrac{\alpha}{2}) {}^R\partial_t^\alpha \varphi(t) + \tfrac{\alpha}{2} {}^R\partial_t^\alpha \varphi(t - \tau) + O(\tau^2). \end{aligned} $$

By choosing $t = t_n$ in the preceding expression, it intuitively motivates the scheme (1.3).

**Remark 2.1.** *The zero extension to $t < 0$ in the formal derivation implicitly imposes certain compatibility conditions at $t = 0$, i.e., $u^{(i)} = 0$, $i = 0, 1, 2$. The estimate $\bar\partial_\tau^\alpha \varphi(t) = {}^R\partial_t^\alpha \varphi(t - \frac{\alpha}{2}\tau) + O(\tau^2)$ was first observed in [7, Theorem 1]. It implies that despite the $O(\tau)$ convergence at the node $t_n$, the approximation $\bar\partial_\tau^\alpha \varphi^n$ is $O(\tau^2)$ accurate at the point $t = t_n - \frac{\alpha}{2}\tau$.*

We illustrate the scheme (1.3) with one-dimensional numerical examples.

**Example 2.1.** *Consider problem (1.1) on the unit interval $\Omega = (0, 1)$ with $T = 1$.*

(a) *$v = 0$, and $f = 2t^{2-\alpha}x(1-x)/\Gamma(3-\alpha) + 2t^2$. The exact solution $u(x,t) = t^2 x(1-x)$ is smooth.*

(b) *$v = x(1-x)$, and $f = 0$.*

*The mesh size $h$ is fixed at $h = 10^{-4}$ so that the error incurred by spatial discretization is negligible.*

Since the exact solution $u$ is smooth and satisfies the compatibility condition in case 2.1(a), the scheme (1.3) exhibits an $O(\tau^2)$ rate as expected, cf. Table 1, where the $L^2$ error denotes $\|u_h(t_N) - U_h^N\|_{L^2(\Omega)}$. Generally, the solution of problem (1.1) is weakly singular in time near $t = 0$, even for smooth problem data. Thus, a direct implementation of (1.3) can fail to achieve the desired rate. Even though the initial data in case 2.1(b) is smooth, the solution $u$ does not have the requisite temporal regularity, giving only an $O(\tau)$ convergence, cf. Table 2. Nonetheless, with proper corrections at initial steps to be described below, one can restore the desired $O(\tau^2)$ rate, cf. Table 3.

Table 1: The $L^2$ error for Example 2.1(a) at $t_N = 1$, by the scheme (1.3).

| $\alpha\backslash N$ | 10 | 20 | 40 | 80 | 160 | 320 | rate |
|---|---|---|---|---|---|---|---|
| $\alpha = 0.1$ | 6.22e-6 | 1.55e-6 | 3.88e-7 | 9.67e-8 | 2.41e-8 | 5.87e-9 | $\approx 2.01$ |
| $\alpha = 0.5$ | 1.52e-5 | 3.79e-6 | 9.47e-7 | 2.37e-7 | 5.93e-8 | 1.50e-8 | $\approx 2.00$ |
| $\alpha = 0.9$ | 3.84e-6 | 9.63e-7 | 2.42e-7 | 6.08e-8 | 1.54e-8 | 3.95e-9 | $\approx 1.98$ |

Table 2: The $L^2$ error for Example 2.1(b) at $t_N = 1$, by the scheme (1.3).

| $\alpha\backslash N$ | 40 | 80 | 160 | 320 | 640 | 1280 | rate |
|---|---|---|---|---|---|---|---|
| $\alpha = 0.1$ | 1.63e-5 | 8.15e-6 | 4.07e-6 | 2.04e-6 | 1.02e-6 | 5.09e-7 | $\approx 1.00$ |
| $\alpha = 0.5$ | 3.13e-5 | 1.58e-5 | 7.97e-6 | 4.00e-6 | 2.00e-6 | 1.00e-6 | $\approx 0.99$ |
| $\alpha = 0.9$ | 2.04e-6 | 1.35e-6 | 7.55e-7 | 3.98e-7 | 2.05e-7 | 1.03e-7 | $\approx 0.96$ |

Table 3: The $L^2$ error for Example 2.1(b) at $t_N = 1$, by the corrected scheme (2.4).

| $\alpha\backslash N$ | 10 | 20 | 40 | 80 | 160 | 320 | rate |
|---|---|---|---|---|---|---|---|
| $\alpha = 0.1$ | 7.70e-6 | 1.80e-6 | 4.37e-7 | 1.08e-8 | 2.66e-8 | 6.60e-9 | $\approx 2.01$ |
| $\alpha = 0.5$ | 4.24e-5 | 9.91e-6 | 2.40e-6 | 5.89e-7 | 1.46e-7 | 3.61e-8 | $\approx 2.02$ |
| $\alpha = 0.9$ | 4.62e-5 | 9.92e-6 | 2.39e-6 | 5.86e-7 | 1.45e-7 | 3.59e-8 | $\approx 2.03$ |

It is well known that if $\varphi(0) \neq 0$, uncorrected high-order CQs can achieve only an $O(\tau)$ rate, which is also the case for (1.3). Inspired by [5], we correct the scheme (1.3) as follows. To derive the correction, we define $\tilde{f}_h(t) := f_h(t) - f_h(0)$ and rewrite (2.2) into

$$\begin{aligned} {}^R\partial_t^\alpha (u_h(t) - v_h) &= \Delta_h(u_h(t) - v_h) + \Delta_h v_h + \tilde{f}_h(t) + f_h(0) \\ &= \Delta_h(u_h(t) - v_h) + \partial_t \partial_t^{-1} \Delta_h v_h + \tilde{f}_h(t) + \partial_t \partial_t^{-1} f_h(0). \end{aligned}$$

Next we apply (1.3) and approximate $\partial_t \partial_t^{-1}$by $\tilde{\partial}_\tau \partial_t^{-1}$, where $\tilde{\partial}_\tau$ denotes the second-order BDF, i.e.,

$$\begin{aligned} \bar{\partial}_\tau^\alpha (U_h - v_h)^n &= (1 - \tfrac{\alpha}{2})(\Delta_h(U_h - v_h) + \tilde{f}_h)^n + \tfrac{\alpha}{2}(\Delta_h(U_h - v_h) + \tilde{f}_h)^{n-1} \\ &\quad + (1 - \tfrac{\alpha}{2})(\tilde{\partial}_\tau \partial_t^{-1}(\Delta_h v_h + f_h(0)))^n + \tfrac{\alpha}{2}(\tilde{\partial}_\tau \partial_t^{-1}(\Delta_h v_h + f_h(0)))^{n-1}. \end{aligned}$$

The purpose of keeping $\partial_t^{-1}$ intact in the discretization and using the approximation $\tilde{\partial}_\tau \partial_t^{-1}$ instead of $\bar{\partial}_\tau \partial_t^{-1}$ is to maintain the desired $O(\tau^2)$ accuracy. Letting $1_\tau = (0, 3/2, 1, 1, \ldots)$, then $\tilde{\partial}_\tau \partial_t^{-1} 1 = 1_\tau$ on the grid points $t_n$ [5, Section 3], the scheme is given explicitly by

$$\begin{aligned} \bar{\partial}_\tau^\alpha (U_h - v_h)^1 - (1 - \tfrac{\alpha}{2})\Delta_h U_h^1 - (\tfrac{1}{2} - \tfrac{\alpha}{4})\Delta_h v_h &= (1 - \tfrac{\alpha}{2})(F_h^1 + \tfrac{1}{2} F_h^0), \\ \bar{\partial}_\tau^\alpha (U_h - v_h)^2 - (1 - \tfrac{\alpha}{2})\Delta_h U_h^2 - \tfrac{\alpha}{2}\Delta_h U_h^1 - \tfrac{\alpha}{4}\Delta_h v_h &= (1 - \tfrac{\alpha}{2}) F_h^2 + \tfrac{\alpha}{2} F_h^1 + \tfrac{\alpha}{4} F_h^0, \\ \bar{\partial}_\tau^\alpha (U_h - v_h)^n - (1 - \tfrac{\alpha}{2})\Delta_h U_h^n - \tfrac{\alpha}{2}\Delta_h U_h^{n-1} &= (1 - \tfrac{\alpha}{2}) F_h^n + \tfrac{\alpha}{2} F_h^{n-1}, \quad 3 \le n \le N. \end{aligned} \tag{2.4}$$

It is noteworthy that the correction only changes the first two steps.

## 3 Convergence analysis

Now we analyze the corrected scheme (2.4), and discuss homogeneous and inhomogeneous problems separately, and focus on the temporal error.

### 3.1 Solution representations

The convergence analysis relies crucially on the integral representations of the semidiscrete Galerkin solution $w_h(t) := u_h(t) - v_h$ and fully discrete solution $W_h^n := U_h^n - v_h$. First, we derive a representation of the solution $w_h(t)$ by means of Laplace transform. Clearly, the function $w_h(t)$ satisfies

$$\partial_t^\alpha w_h - \Delta_h w_h = \Delta_h v_h + f_h,$$

with $w_h(0) = 0$. Upon Laplace transform, denoted by $\widehat{\ }$, and using the formula $\widehat{\partial_t^\alpha \varphi} = z^\alpha \widehat{\varphi} - z^{\alpha-1}\varphi(0)$ [15, Lemma 2.24, pp. 98], we obtain

$$z^\alpha \widehat{w}_h(z) - \Delta_h \widehat{w}_h(z) = z^{-1}\Delta_h v_h + \widehat{f}_h(z).$$

By inverse Laplace transform, the function $w_h(t)$ can be represented by

$$w_h(t) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\delta}} e^{zt} \left( -K(z)\Delta_h v_h - zK(z)\widehat{f}_h(z) \right) dz, \tag{3.1}$$

with the kernel function

$$K(z) = -z^{-1}(z^\alpha - \Delta_h)^{-1}. \tag{3.2}$$

In the representation (3.1), the contour $\Gamma_{\theta,\delta}$ is defined by

$$\Gamma_{\theta,\delta} = \{z \in \mathbb{C} : |z| = \delta, |\arg z| \le \theta\} \cup \{z \in \mathbb{C} : z = \rho e^{\pm \mathrm{i}\theta}, \rho \ge \delta\},$$

oriented with an increasing imaginary part. Throughout, we choose the angle $\theta \in (\pi/2, \pi)$. Since the discrete Laplacian operator $\Delta_h$ satisfies the following resolvent estimate [28, Chapter 6], [2, Example 3.7.5 and Theorem 3.7.11]

$$\|(z - \Delta_h)^{-1}\| \le cz^{-1}, \quad \forall z \in \Sigma_\theta, \tag{3.3}$$

there exists a constant $c$ which depends only on $\theta$ and $\alpha$ such that

$$\|(z^\alpha - \Delta_h)^{-1}\| \le cz^{-\alpha}, \quad \forall z \in \Sigma_\theta. \tag{3.4}$$

Next, we derive a representation of $W_h^n$ by means of discrete Laplace transform, i.e., generating function. Recall that for a given sequence $(f^n)_{n=0}^\infty$, the generating function $\widetilde{f}(\xi)$ is defined by $\widetilde{f}(\xi) := \sum_{n=0}^\infty f^n \xi^n$. Then we have the following solution representation.

**Proposition 3.1.** *Let $K(z)$ be given by (3.2) and $G_h^n := F_h^n - F_h^0$. Then, there exists a $\delta_0 \in (0, \pi/2)$ (independent of $\tau$) such that for $\delta \in (0, \delta_0]$ and $\theta \in (\pi/2, \pi/2 + \delta_0]$, the fully discrete solution $W_h^n := U_h^n - v_h$ can be represented by*

$$W_h^n = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\delta}^\tau} e^{zt_n} \left( \mu(e^{-z\tau})K(\beta_\tau(e^{-z\tau}))(-\Delta_h v_h - F_h^0) - \beta_\tau(e^{-z\tau})K(\beta_\tau(e^{-z\tau}))\widetilde{G}_h(e^{-z\tau})\tau \right) dz, \tag{3.5}$$

*with the contour (oriented with an increasing imaginary part) defined by $\Gamma_{\theta,\delta}^\tau := \{z \in \Gamma_{\theta,\delta} : |\Im(z)| \le \pi/\tau\}$. The functions $\beta_\tau(\xi)$ and $\mu(\xi)$ are, respectively, given by*

$$\beta_\tau(\xi) = \frac{1-\xi}{\tau(1 - \frac{\alpha}{2} + \frac{\alpha}{2}\xi)^{1/\alpha}} \quad \text{and} \quad \mu(\xi) = \frac{3\xi - \xi^2}{2(1 - \frac{\alpha}{2} + \frac{\alpha}{2}\xi)^{1/\alpha}}. \tag{3.6}$$

*Proof.* It follows from the scheme (2.4) that the function $W_h^n$ satisfies

$$\begin{aligned}\bar\partial_\tau^\alpha W_h^1-(1-\tfrac{\alpha}{2})\Delta_h W_h^1-(\tfrac32-\tfrac34\alpha)\Delta_h v_h&=(1-\tfrac{\alpha}{2})(F_h^1+\tfrac12F_h^0),\\ \bar\partial_\tau^\alpha W_h^2-(1-\tfrac{\alpha}{2})\Delta_h W_h^2-\tfrac{\alpha}{2}\Delta_h W_h^1-(1+\tfrac{\alpha}{4})\Delta_h v_h&=(1-\tfrac{\alpha}{2})F_h^2+\tfrac{\alpha}{2}F_h^1+\tfrac{\alpha}{4}F_h^0,\\ \bar\partial_\tau^\alpha W_h^n-(1-\tfrac{\alpha}{2})\Delta_h W_h^n-\tfrac{\alpha}{2}\Delta_h W_h^{n-1}-\Delta_h v_h&=(1-\tfrac{\alpha}{2})F_h^n+\tfrac{\alpha}{2}F_h^{n-1},\quad 3\le n\le N.\end{aligned}\tag{3.7}$$

with $W_h^0=0$. By multiplying both sides by $\xi^n$ and summing up the results for $n=1,2,\dots$, we obtain

$$\begin{aligned}&\sum_{n=1}^\infty \xi^n\bar\partial_\tau^\alpha W_h^n-\sum_{n=1}^\infty((1-\tfrac{\alpha}{2})\Delta_h W_h^n+\tfrac{\alpha}{2}\Delta_h W_n^{n-1})\xi^n-\Delta_h v_h\left(\sum_{n=1}^\infty\xi^n+(\tfrac12-\tfrac{3\alpha}{4})\xi+\tfrac{\alpha}{4}\xi^2\right)\\ &=\sum_{n=1}^\infty\left((1-\tfrac{\alpha}{2})F_h^n+\tfrac{\alpha}{2}F_h^{n-1}\right)\xi^n+\left((\tfrac12-\tfrac{3\alpha}{4})\xi+\tfrac{\alpha}{4}\xi^2\right)F_h^0.\end{aligned}\tag{3.8}$$

Next we simplify the summations. Since $W_h^0=0$, by the discrete convolution rule, we deduce

$$\begin{aligned}\sum_{n=1}^\infty \xi^n\bar\partial_\tau^\alpha W_h^n=\sum_{n=0}^\infty \xi^n\bar\partial_\tau^\alpha W_h^n&=\tau^{-\alpha}(1-\xi)^\alpha\widetilde{W}_h(\xi),\\ \sum_{n=1}^\infty((1-\tfrac{\alpha}{2})\Delta_h W_h^n+\tfrac{\alpha}{2}\Delta_h W_n^{n-1})\xi^n&=((1-\tfrac{\alpha}{2})+\tfrac{\alpha}{2}\xi)\Delta_h\widetilde{W}_h(\xi).\end{aligned}$$

Meanwhile, by a simple computation, we have $\sum_{n=1}^\infty\xi^n+(\frac12-\frac{3\alpha}{4})\xi+\frac{\alpha}{4}\xi^2=\frac{3\xi-\xi^2}{2(1-\xi)}(1-\frac{\alpha}{2}+\frac{\alpha}{2}\xi)$. Consequently, the definition of $G_h^n$ implies $G_h^0=0$ and

$$\begin{aligned}&\sum_{n=1}^\infty\left((1-\tfrac{\alpha}{2})F_h^n+\tfrac{\alpha}{2}F_h^{n-1}\right)\xi^n+\left((\tfrac12-\tfrac{3\alpha}{4})\xi+\tfrac{\alpha}{4}\xi^2\right)F_h^0\\ =&\sum_{n=1}^\infty\left((1-\tfrac{\alpha}{2})G_h^n+\tfrac{\alpha}{2}G_h^{n-1}\right)\xi^n+\left(\sum_{n=1}^\infty\xi^n+(\tfrac12-\tfrac{3\alpha}{4})\xi+\tfrac{\alpha}{4}\xi^2\right)F_h^0\\ =&(1-\tfrac{\alpha}{2}+\tfrac{\alpha}{2}\xi)\widetilde{G}_h(\xi)+\tfrac{3\xi-\xi^2}{2(1-\xi)}(1-\tfrac{\alpha}{2}+\tfrac{\alpha}{2}\xi)F_h^0.\end{aligned}$$

Substituting the preceding identities into (3.8) yields

$$\left((\beta_\tau(\xi))^\alpha-\Delta_h\right)\widetilde{W}_h(\xi)=\kappa(\xi)\Delta_h v_h+\kappa(\xi)F_h^0+\widetilde{G}_h(\xi),$$

with $\kappa(\xi)=\frac{3\xi-\xi^2}{2(1-\xi)}$. Since $|\xi|\le1$, $\beta_\tau(\xi)^\alpha\in\Sigma_{\theta'}$ for some $\theta'\in(\pi/2,\pi)$ [13, proof of Theorem 6.1], by the resolvent estimate (3.4), we have

$$\widetilde{W}_h(\xi)=((\beta_\tau(\xi))^\alpha-\Delta_h)^{-1}\left(\kappa(\xi)\Delta_h v_h+\kappa(\xi)F_h^0+\widetilde{G}_h(\xi)\right).\tag{3.9}$$

Without loss of generality, we can assume $F_h^n=F_h^0$ (so $G_h^n=0$) for $n>N=T/\tau$. Otherwise we redefine $F_h^n:=F_h^0$ for $n>N=T/\tau$, and this modification does not affect of the value of $W_h^n$ for $n=1,\dots,N$, in view of (3.7). Clearly, the function $\widetilde{W}_h(\xi)$ defined in (3.9) is analytic with respect to $\xi$ in a neighborhood of the origin, and thus Cauchy's integral formula implies that for small $\varrho$

$$W_h^n=\frac{1}{2\pi\mathrm{i}}\int_{|\xi|=\varrho}\xi^{-n-1}\widetilde{W}_h(\xi)d\xi=\frac{\tau}{2\pi\mathrm{i}}\int_{\Gamma^\tau}e^{zt_n}\widetilde{W}_h(e^{-z\tau})\,dz,$$

where the second equality follows by changing the variables $\xi=e^{-z\tau}$, and the contour $\Gamma^\tau$ is given by

$$\Gamma^\tau:=\{z=-\ln(\varrho)/\tau+\mathrm{i}y:\ y\in\mathbb{R}\ \text{and}\ |y|\le\pi/\tau\}.$$

Since both $\kappa(e^{-z\tau})$ and $\widetilde{G}_h(e^{-z\tau})$ are analytic with respect to $z \in \mathbb{C}\backslash\{0\}$, Lemma 3.2 below implies that the function $e^{zt_n}\widetilde{W}_h(e^{-z\tau})$ is analytic with respect to $z$ in the region enclosed by $\Gamma^\tau$, $\Gamma^\tau_{\theta,\delta}$ and the two lines $\Gamma^\tau_\pm := \mathbb{R} \pm \mathrm{i}\pi/\tau$ (oriented from left to right). Then, since the values of $e^{zt_n}\widetilde{W}_h(e^{-z\tau})$ on the two lines $\Gamma^\tau_\pm$ coincide, it follows from Cauchy's theorem that

$$\begin{aligned} W_h^n &= \frac{\tau}{2\pi\mathrm{i}}\int_{\Gamma^\tau} e^{zt_n}\widetilde{W}_h(e^{-z\tau})\,dz = \frac{\tau}{2\pi\mathrm{i}}\int_{\Gamma^\tau_{\theta,\delta}} e^{zt_n}\widetilde{W}_h(e^{-z\tau})\,dz \\ &\quad + \frac{\tau}{2\pi\mathrm{i}}\int_{\Gamma^\tau_+} e^{zt_n}\widetilde{W}_h(e^{-z\tau})\,dz - \frac{\tau}{2\pi\mathrm{i}}\int_{\Gamma^\tau_-} e^{zt_n}\widetilde{W}_h(e^{-z\tau})\,dz = \frac{\tau}{2\pi\mathrm{i}}\int_{\Gamma^\tau_{\theta,\delta}} e^{zt_n}\widetilde{W}_h(e^{-z\tau})\,dz. \end{aligned}$$

This completes the proof of the proposition. □

The next result gives basic estimates on the functions $(1-\frac{\alpha}{2}+\frac{\alpha}{2}e^{-z\tau})^{1/\alpha}$ and $(1-e^{-z\tau})^\alpha$ from Proposition 3.1. These estimates are crucial for the error analysis in Section 3.2 below.

**Lemma 3.1.** *Let $\alpha \in (0,1)$. Then there exists a $\delta_1 > 0$ (independent of $\tau$) such that for $\delta \in (0,\delta_1]$ and $\theta \in (\pi/2, \pi/2+\delta_1]$, there hold for any $z \in \Gamma^\tau_{\theta,\delta}$*

$$c_0 \le |(1-\tfrac{\alpha}{2}+\tfrac{\alpha}{2}e^{-z\tau})^{1/\alpha}| \le c_1, \tag{3.10}$$

$$|(1-\tfrac{\alpha}{2}+\tfrac{\alpha}{2}e^{-z\tau})^{1/\alpha} - (1-\tfrac{z\tau}{2})| \le c\tau^2|z|^2, \tag{3.11}$$

$$|(1-e^{-z\tau})^\alpha - \tau^\alpha z^\alpha(1-\tfrac{\alpha}{2}+\tfrac{\alpha}{2}e^{-z\tau})| \le c|z|^{2+\alpha}\tau^{2+\alpha}, \tag{3.12}$$

*where the constants $c_0$, $c_1$ and $c$ are independent of $\tau$, $\theta$ and $\delta$ (but may depend on $\delta_1$).*

*Proof.* Let $g(z) = (1-\frac{\alpha}{2}+\frac{\alpha}{2}e^{-z\tau})^{1/\alpha}$. First we consider $z \in \Gamma^\tau_{\theta,+}$, and write $z = re^{\mathrm{i}\theta}$, $r \in (\delta, \pi/(\tau\sin\theta)]$. Then with $s = r\tau\sin\theta \in (0,\pi)$ and $\gamma = -\cot\theta > 0$, $\eta = \frac{2}{\alpha}-1 > 1$, there holds

$$|g(z)|^\alpha = \tfrac{\alpha}{2}(\eta^2+e^{2\gamma s}+2\eta e^{\gamma s}\cos s)^{1/2} \ge \tfrac{\alpha}{2}(\eta^2+e^{2\gamma s}-2e^{\gamma s})^{1/2} \ge \tfrac{\alpha}{2}(\eta - e^{\gamma\pi}).$$

Since $\alpha \in (0,1)$, we have $\eta - e^{\gamma\pi} > 0$, for $\theta \in (\pi/2,\pi)$ close to $\pi/2$. Next we consider $z \in \Gamma_\delta$, with $z = \delta e^{\mathrm{i}\varphi}$, $0 \le \varphi \le \theta$ and small $\delta$. Then by letting $\rho = \tau\delta \in (0,1)$ and $s = \rho\cos\varphi \in [-\epsilon,\rho]$, for small $\epsilon > 0$, and $h(s) = (\rho^2-s^2)^{1/2} \le \rho \le 1$, we have $\cos h(s) \ge 0$ and thus

$$|g(z)|^\alpha = \tfrac{\alpha}{2}(\eta^2+2\eta e^{-s}\cos h+e^{-2s})^{1/2} \ge \tfrac{\alpha}{2}(\eta^2+e^{-2s})^{1/2} \ge \tfrac{\alpha}{2}\eta.$$

This shows the lower bound on $|g(z)|$ in (3.10). The upper bound on $|g(z)|$ in (3.10) follows by $|g(z)|^\alpha \le 1-\frac{\alpha}{2}+\frac{\alpha}{2}e^{-\pi\cot\theta} \le c$ for any $z \in \Gamma^\tau_{\theta,+}$, and a similar bound for $z \in \Gamma_\delta$.

For the estimate (3.11), it suffices to show

$$|g(z)-(1-\tfrac{z\tau}{2})|/(|z|^2\tau^2) \le c, \quad \forall z \in \Gamma^\tau_{\theta,\delta}. \tag{3.13}$$

If $|z|\tau \le \epsilon$, where $\epsilon \in (0,1)$ is to be determined, then by Taylor expansion, we deduce

$$g(z)-(1-\tfrac{z\tau}{2}) = \sum_{k=2}^\infty C(\tfrac{1}{\alpha},k)(-\tfrac{\alpha}{2}+\tfrac{\alpha}{2}e^{-z\tau})^k + O(|z|^2\tau^2),$$

with $C(\gamma,k) = \frac{\Gamma(\gamma+1)}{\Gamma(k+1)\Gamma(\gamma-k+1)}$. Meanwhile, we have

$$|-\frac{\alpha}{2}+\frac{\alpha}{2}e^{-z\tau}| \le \frac{\alpha}{2}|z\tau|\sum_{k=0}^\infty \frac{|z\tau|^k}{(k+1)!} \le \frac{\alpha}{2}|z|\tau\frac{e^\epsilon-1}{\epsilon}.$$

Since $f(\epsilon) = \frac{e^\epsilon-1}{\epsilon}$ is increasing in $\epsilon$ for $\epsilon \in (0,\infty)$ and $\lim_{\epsilon\to0^+} f(\epsilon) = 1$, for any $\alpha \in (0,1)$, there exists an $\epsilon \in (0,1)$ such that $\frac{\alpha(e^\epsilon-1)}{2\epsilon} < 1$. By ratio test, $|\sum_{k=2}^\infty C(\frac{1}{\alpha},k)(-\frac{\alpha}{2}+\frac{\alpha}{2}e^{-z\tau})^k| \le c|z|^2\tau^2$, and thus

(3.13) holds. Meanwhile, for $|z|\tau > \epsilon$, there exists a $\delta_1 > 0$ (independent of $\tau$) such that for $\delta \in (0, \delta_1]$ and $\theta \in (\pi/2, \pi/2 + \delta_1]$, $|g(z)| \le c$. Since $|z|\tau \le \pi/\sin\theta$ for $z \in \Gamma^\tau_{\theta,\delta}$, this again yields (3.13), showing the estimate (3.11).

Next we turn to the third estimate (3.12). Since $|z|\tau \le c$ for $z \in \Gamma^\tau_{\theta,\delta}$, like before, it suffices to show (3.12) for $|z|\tau \le 1$. For $|z|\tau \le 1$, by Taylor expansion, we deduce

$$1 - e^{-z\tau} = z\tau \sum_{j=1}^{\infty} \frac{(-z\tau)^{j-1}}{j!} = z\tau + z\tau \sum_{j=2}^{\infty} \frac{(-z\tau)^{j-1}}{j!}.$$

In the identity $\sum_{j=2}^{\infty} \frac{(-z\tau)^{j-1}}{j!} = \frac{-z\tau}{2} + (-z\tau)^2 \sum_{j=3}^{\infty} \frac{(-z\tau)^{j-2}}{j!}$, we have

$$|\sum_{j=3}^{\infty} \frac{(-z\tau)^{j-2}}{j!}| \le \sum_{j=3}^{\infty} \frac{1}{j!} \le e \quad \text{and} \quad |\sum_{j=2}^{\infty} \frac{(-z\tau)^{j-1}}{j!}| \le |z|\tau(e-2) < |z|\tau.$$

Thus we have

$$\begin{aligned}(1 - e^{-z\tau})^\alpha &= z^\alpha\tau^\alpha \big(1 + \sum_{j=2}^{\infty} \frac{(-z\tau)^{j-1}}{j!}\big)^\alpha \\ &= z^\alpha\tau^\alpha + \alpha z^\alpha\tau^\alpha \sum_{j=2}^{\infty} \frac{(-z\tau)^{j-1}}{j!} + z^\alpha\tau^\alpha \sum_{k=2}^{\infty} C(\alpha,k)\big(\sum_{j=2}^{\infty} \frac{(-z\tau)^{j-1}}{j!}\big)^k \\ &= z^\alpha\tau^\alpha - \tfrac{\alpha}{2} z^{\alpha+1}\tau^{\alpha+1} + O(|z|^{\alpha+2}\tau^{\alpha+2}),\end{aligned}$$

and $\tau^\alpha z^\alpha(1 - \frac{\alpha}{2} + \frac{\alpha}{2}e^{-z\tau}) = \tau^\alpha z^\alpha - \frac{\alpha}{2}\tau^{\alpha+1}z^{\alpha+1} + O(|z|^{\alpha+2}\tau^{\alpha+2})$. Combining the last two estimates completes the proof of the lemma. □

The next lemma gives a crucial sector mapping property of the function $\beta_\tau(e^{-z\tau})^\alpha$. The proof relies on the fact that $\beta_\tau(e^{-z\tau})^\alpha$ is very close to $\beta_\tau(e^{-\mathrm{i}s})^\alpha$ for $z \in \Gamma^\tau_{\theta,+}$ (if $\theta \in (\pi/2, \pi)$ is sufficiently close to $\pi/2$) and uses the result $\beta_\tau(e^{-\mathrm{i}s})^\alpha \in \Sigma_{\alpha\pi/2}$ from [13, Theorem 6.1].

**Lemma 3.2.** *For $\alpha \in (0,1)$, let $\phi \in (\alpha\pi/2, \pi)$ be fixed. Then there exists a $\delta_0 > 0$ (independent of $\tau$) such that for $\delta \in (0, \delta_0]$ and $\theta \in (\pi/2, \pi/2 + \delta_0]$, we have*

$$\beta_\tau(e^{-z\tau})^\alpha \in \Sigma_\phi \quad \forall\, z \in \Gamma^\tau_{\theta,\delta} \cup \overline{\Sigma}_{\pi/2}\backslash\{0\}. \tag{3.14}$$

*Moreover, the operator $(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}$ is analytic with respect to $z$ in the region enclosed by the curves $\Gamma^\tau$, $\Gamma^\tau_{\theta,\delta}$ and $\Gamma^\tau_\pm := \mathbb{R} \pm \mathrm{i}\pi/\tau$, and satisfies*

$$\|(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\| \le c|\beta_\tau(e^{-z\tau})|^{-\alpha}, \quad \forall z \in \Gamma^\tau_{\theta,\delta}\,, \tag{3.15}$$

*where the constant $c$ is independent of $\tau$ (but may depend on $\phi$).*

*Proof.* For the proof, we split the contour $\Gamma^\tau_{\theta,\delta}$ into two parts, i.e.,

$$\Gamma^\tau_{\theta,\delta} := \Gamma_\delta \cup \Gamma^\tau_{\theta,\pm} := \{z \in \mathbb{C} : |z| = \delta, |\arg z| \le \theta\} \cup \big\{z \in \mathbb{C} : z = re^{\pm\mathrm{i}\theta},\ \delta \le r \le \pi/(\tau|\sin(\theta)|)\big\}. \tag{3.16}$$

To prove (3.14), we consider the following three cases $z \in \Gamma_\delta$, $z \in \Gamma^\tau_{\theta,\pm}$ and $z \in \overline{\Sigma}_{\pi/2}\backslash\{0\}$, separately. First, for $z \in \Gamma_\delta \subset \Sigma_\theta$, by choosing $\delta > 0$ sufficiently small and using Taylor's expansion, we have

$$\beta_\tau(e^{-z\tau})^\alpha = \frac{(1 - e^{-z\tau})^\alpha}{\tau^\alpha(1 - \frac{\alpha}{2} + \frac{\alpha}{2}e^{-z\tau})} = |z|^\alpha e^{\mathrm{i}\alpha\arg(z)}(1 + O(z\tau)) \in \Sigma_{\alpha\theta+\varepsilon_\delta},$$

for some $\varepsilon_\delta > 0$ with $\lim_{\delta\to 0^+} \varepsilon_\delta = 0$, showing the relation (3.14) for $z \in \Gamma_\delta$. Second, for $z = |z|e^{i\theta} \in \Gamma^\tau_{\theta,+}$, we have $e^{-z\tau} = e^{-s\cot(\theta)}e^{-is}$, $s = |z|\tau\sin(\theta) \in (0,\pi)$. Let $\gamma_\tau(\xi) := \beta_\tau(\xi)^\alpha$. Then there exists some $\sigma(s) \in (0,1)$ such that

$$|\beta_\tau(e^{-z\tau})^\alpha - \beta_\tau(e^{-is})^\alpha| = |\gamma_\tau(e^{-z\tau}) - \gamma_\tau(e^{-is})| \le cs|\cot\theta||\gamma'_\tau(e^{-\sigma(s)s\cot(\theta)}e^{-is})|$$

Straightforward computation gives $\gamma'_\tau(\xi) = -\alpha\tau^{-\alpha}\frac{(1-\xi)^{\alpha-1}(3-\alpha+(\alpha-1)\xi)}{2(1-\frac{\alpha}{2}+\frac{\alpha}{2}\xi)^2}$. For $\theta \in (\pi/2,\pi)$ sufficiently close to $\pi/2$, $e^{-\sigma(s)s\cot(\theta)} \approx 1$. Then Lemma 3.1 implies

$$|\gamma'_\tau(e^{-\sigma(s)s\cot(\theta)}e^{-is})| \le c\tau^{-\alpha}|1 - e^{-\sigma(s)s\cot\theta}e^{-is}|^{\alpha-1}.$$

Combining the preceding two estimates with the inequality $|\cot\theta| \le c|\theta - \pi/2|$ yields

$$|\beta_\tau(e^{-z\tau})^\alpha - \beta_\tau(e^{-is})^\alpha| \le c\tau^{-\alpha}|\theta - \pi/2|s|1 - e^{-\sigma(s)s\cot\theta}e^{-is}|^{\alpha-1}.$$

If $s \in (0,\pi)$ is small, then Taylor's expansion yields $\beta_\tau(e^{-is})^\alpha \approx \tau^{-\alpha}s^\alpha e^{i\alpha\pi/2}$ and $1 - e^{-s\sigma(s)\cot(\theta)}e^{-is} \approx s\sigma(s)\cot(\theta) + is$ asymptotically. Consequently, we have

$$|\beta_\tau(e^{-z\tau})^\alpha - \beta_\tau(e^{-is})^\alpha| \le c\tau^{-\alpha}|\theta - \pi/2|s^\alpha \le c|\theta - \pi/2||\beta_\tau(e^{-is})^\alpha|.$$

Since $\beta_\tau(e^{-is})^\alpha \in \Sigma_{\alpha\pi/2}$ [13, Proof of Theorem 6.1], it follows that $\beta_\tau(e^{-z\tau})^\alpha \in \Sigma_\phi$ when $s$ is sufficiently small. Meanwhile, if $s \in (0,\pi)$ is away from 0, then $|\beta_\tau(e^{-is})^\alpha| \ge c\tau^{-\alpha}$ and so

$$|\beta_\tau(e^{-z\tau})^\alpha - \beta_\tau(e^{-is})^\alpha| \le c|\theta - \pi/2|\tau^{-\alpha} \le c|\theta - \pi/2||\beta_\tau(e^{-is})^\alpha|.$$

By choosing $\theta \in (\pi/2,\pi)$ sufficiently close to $\pi/2$, we again have $\beta_\tau(e^{-z\tau})^\alpha \in \Sigma_\phi$. The proof for the case $z = |z|e^{i\theta} \in \Gamma^\tau_{\theta,-}$ is similar as the case $\Gamma^\tau_{\theta,+}$ and thus omitted. Third and last, for $z \in \overline{\Sigma}_{\pi/2}\backslash\{0\}$, we have $|e^{-z\tau}| \le 1$. In this case, [13, Proof of Theorem 6.1] implies

$$\beta_\tau(e^{-z\tau})^\alpha \in \Sigma_{\alpha\pi/2} \subset \Sigma_\phi.$$

Next we show the analyticity. Since the spectrum of the operator $\Delta_h$ is contained in the negative part of the real line, the result (3.14) (with arbitrary $\delta \in (0,\delta_0]$ and $\theta \in (\pi/2,\pi/2+\delta_0]$) implies that the operator $(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}$ is analytic with respect to $z$ on the right side of the curve $\Gamma^\tau_{\theta_0,\delta_0}$, with $\theta_0 := \pi/2+\delta_0$. The resolvent estimate (3.15) follows immediately from (3.3) and (3.14). □

## 3.2 Error analysis for the homogeneous problem

First we analyze the homogeneous problem, i.e., $f \equiv 0$. By (3.1) and Proposition 3.1, we have

$$w_h(t_n) = -\frac{1}{2\pi i}\int_{\Gamma_{\theta,\delta}} e^{zt_n}K(z)\Delta_h v_h dz \quad \text{and} \quad W_h^n = -\frac{1}{2\pi i}\int_{\Gamma^\tau_{\theta,\delta}} e^{zt_n}\mu(e^{-z\tau})K(\beta_\tau(e^{-z\tau}))\Delta_h v_h dz.$$

Hence, the convergence analysis hinges on properly bounding the approximation error of the kernel $K(\beta_\tau(e^{-z\tau}))$ to $K(z)$ along the contour $\Gamma^\tau_{\theta,\delta}$. The next lemma provides the crucial estimate on $\mu$ and $\beta_\tau$.

**Lemma 3.3.** *Let $\alpha \in (0,1)$ be given, and $\mu(\xi)$, $\beta_\tau(\xi)$ be defined as (3.6) and the constant $\delta_1$ be given in Lemma 3.1. Then for $\delta \in (0,\delta_1]$ and $\theta \in (\pi/2,\pi/2+\delta_1]$, we have for any $z \in \Gamma^\tau_{\theta,\delta}$*

$$|\mu(e^{-z\tau}) - 1| \le c\tau^2|z|^2, \quad |\beta_\tau(e^{-z\tau}) - z| \le c\tau^2|z|^3, \quad \text{and} \quad |\beta_\tau(e^{-z\tau})^\alpha - z^\alpha| \le c\tau^2|z|^{2+\alpha}, \tag{3.17}$$

*and*

$$c_0|z| \le |\beta_\tau(e^{-z\tau})| \le c_1|z|. \tag{3.18}$$

*The constants $c_0$, $c_1$ and $c$ are independent of $\tau$, $\theta$ and $\delta$ (but may depend on $\delta_1$).*

*Proof.* The three estimates in (3.17) are direct consequences of Lemma 3.1. The upper bound in (3.18) follows from Lemma 3.3 and the triangle equality

$$
\begin{aligned}
|\beta_\tau(e^{-z\tau})| &\le (|\beta_\tau(e^{-z\tau}) - z| + |z|) \le (1 + c^2\tau^2|z|^2)|z| \\
&\le \begin{cases} (1 + c^2\tau^2\delta^2)|z|, & \text{for } z \in \Gamma_\delta, \\ (1 + c^2(\pi/\sin\theta)^2)|z|, & \text{for } z \in \Gamma_\theta. \end{cases}
\end{aligned}
$$

Since $c_0|z| \le |\frac{1-e^{-z\tau}}{\tau}| \le c_1|z|$ [11, Lemma 3.1], the lower bound in (3.18) follows from the fact that $|1 - \frac{\alpha}{2} + \frac{\alpha}{2}e^{-z\tau}|$ is uniformly bounded from below in $\tau$ for all $z \in \Gamma^\tau_{\theta,\delta}$, cf. Lemma 3.1. □

Using Lemmas 3.2 and 3.3, we have the following error estimate of the kernel $K(\beta_\tau(e^{-z\tau}))$.

**Lemma 3.4.** *Let $\delta_0$ and $\delta_1$ be defined in Proposition 3.1 and Lemma 3.1, respectively. Then by choosing $\delta = \min(\delta_0, \delta_1)$ and $\theta = \pi/2 + \delta$, we have*

$$
\|\mu(e^{-z\tau})K(\beta_\tau(e^{-z\tau})) - K(z)\| \le c\tau^2|z|^{1-\alpha}, \quad \forall\, z \in \Gamma^\tau_{\theta,\delta},
$$

*where the constant $c$ is independent of $\tau$.*

*Proof.* By the triangle inequality, we obtain

$$
\|\mu(e^{-z\tau})K(\beta_\tau(e^{-z\tau})) - K(z)\| \le |\mu(e^{-z\tau}) - 1|\|K(z)\| + |\mu(e^{-z\tau})|\|K(\beta_\tau(e^{-z\tau})) - K(z)\| =: \mathrm{I} + \mathrm{II}.
$$

The bound on the first term I follows from (3.4) and Lemma 3.3. Appealing to Lemma 3.3 again yields

$$
|\beta_\tau(e^{-z\tau})^{-1} - z^{-1}| = |z - \beta_\tau(e^{-z\tau})||\beta_\tau(e^{-z\tau})|^{-1}|z|^{-1} \le c\tau^2|z|. \tag{3.19}
$$

Similarly, by using (3.4) and (3.15), and Lemma 3.3, and the identity $(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1} - (z^\alpha - \Delta_h)^{-1} = (z^\alpha - \beta_\tau(e^{-z\tau}))(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}(z^\alpha - \Delta_h)^{-1}$, we obtain

$$
\begin{aligned}
&\|(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1} - (z^\alpha - \Delta_h)^{-1}\| \\
\le& |\beta_\tau(e^{-z\tau})^\alpha - z^\alpha|\|(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\|\|(z^\alpha - \Delta_h)^{-1}\| \\
\le& c\tau^2|z|^{2+\alpha}\|(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\|\|(z^\alpha - \Delta_h)^{-1}\| \le c\tau^2|z|^{2-\alpha},
\end{aligned} \tag{3.20}
$$

and hence, the second term II can be bounded by

$$
\mathrm{II} \le c|\beta_\tau(e^{-z\tau})^{-1} - z^{-1}|\|(z^\alpha - \Delta_h)^{-1}\| + c|z|^{-1}\|(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1} - (z^\alpha - \Delta_h)^{-1}\| \le c\tau^2|z|^{1-\alpha},
$$

which completes the proof of the lemma. □

Now we state the temporal error for smooth initial data $v \in D(\Delta)$.

**Theorem 3.1.** *Let $f = 0$, and $u_h$ and $U_h^n$ be the solutions of (2.2) and (2.4), respectively, with $v \in D(\Delta)$ and $U_h^0 = v_h := R_h v$. Then there holds*

$$
\|u_h(t_n) - U_h^n\|_{L^2(\Omega)} \le c\tau^2 t_n^{\alpha-2}\|\Delta v\|_{L^2(\Omega)}, \quad n \ge 1.
$$

*Proof.* With the constants $\delta_0$ and $\delta_1$ given in Proposition 3.1 and Lemma 3.1, respectively, we choose $\delta = \min(\delta_0, \delta_1)$ and $\theta = \pi/2 + \delta$. By (3.1) and Proposition 3.1, we split the error into

$$
\begin{aligned}
u_h(t_n) - U_h^n =& -\frac{1}{2\pi \mathrm{i}}\int_{\Gamma^\tau_{\theta,\delta}} e^{zt_n}\left(K(z) - \mu(e^{-zt})K(\beta_\tau(e^{-z\tau}))\right)\Delta_h v_h\, dz \\
&- \frac{1}{2\pi \mathrm{i}}\int_{\Gamma_{\theta,\delta}\setminus\Gamma^\tau_{\theta,\delta}} e^{zt_n}K(z)\Delta_h v_h dz =: \mathrm{I} + \mathrm{II}.
\end{aligned}
$$

By Lemma 3.4 and choosing $\delta \le 1/t_n$, we bound the first term I by

$$\begin{aligned}\|\mathrm{I}\|_{L^2(\Omega)} &\le c\tau^2\|\Delta_h v_h\|_{L^2(\Omega)}\Big(\int_\delta^{\pi/(\tau\sin\theta)} e^{rt_n\cos\theta} r^{1-\alpha} dr + \int_{-\theta}^{\theta} e^{\delta t_n|\cos\psi|}\delta^{2-\alpha} d\psi\Big)\\ &\le c(t_n^{\alpha-2}+\delta^{2-\alpha})\tau^2\|\Delta_h v_h\|_{L^2(\Omega)} \le c\tau^2 t_n^{\alpha-2}\|\Delta_h v_h\|_{L^2(\Omega)}.\end{aligned}$$

For the second term II, by the estimate (3.4) and the change of variables $s = rt_n$, we obtain

$$\begin{aligned}\|\mathrm{II}\|_{L^2(\Omega)} &\le c\|\Delta_h v_h\|_{L^2(\Omega)}\int_{\pi/(\tau\sin\theta)}^\infty e^{rt_n\cos\theta} r^{-\alpha-1}\,dr\\ &\le c\tau^2\|\Delta_h v_h\|_{L^2(\Omega)}\int_0^\infty e^{rt_n\cos\theta} r^{1-\alpha}\,dr \qquad (\because r \ge \pi/(\tau\sin\theta))\\ &\le c\tau^2 t_n^{\alpha-2}\|\Delta_h v_h\|\int_0^\infty e^{s\cos\theta}s^{1-\alpha}ds \le c\tau^2 t_n^{\alpha-2}\|\Delta_h v_h\|_{L^2(\Omega)},\end{aligned}$$

where the last inequality follows since for $\theta\in(\pi/2,\pi)$ and $\alpha\in(0,1)$, the integral $\int_0^\infty e^{s\cos\theta}s^{1-\alpha}ds < c$. Now the desired estimate follows from the triangle inequality and the identity $\Delta_h R_h = P_h\Delta$. □

Next, we turn to nonsmooth initial data $v \in L^2(\Omega)$. We begin with an estimate on the kernel.

**Lemma 3.5.** *Let $K_s(z) = (z^\alpha - \Delta_h)^{-1}\Delta_h$. By choosing $\delta = \min(\delta_0, \delta_1)$ and $\theta = \pi/2 + \delta$, there exists a $c > 0$ independent of $\tau$ such that*

$$\|\mu(e^{-z\tau})\beta_\tau(e^{-z\tau})^{-1}K_s(\beta_\tau(e^{-z\tau})) - z^{-1}K_s(z)\| \le c\tau^2|z|, \quad \forall\, z\in\Gamma^\tau_{\theta,\delta}.$$

*Proof.* By the triangle inequality and Lemma 3.3, we have

$$\begin{aligned}&\|\mu(e^{-z\tau})\beta_\tau(e^{-z\tau})^{-1}K_s(\beta_\tau(e^{-z\tau})) - z^{-1}K_s(z)\|\\ \le&|\mu(e^{-z\tau})\beta_\tau(e^{-z\tau})^{-1} - z^{-1}|\|K_s(z)\| + |\mu(e^{-z\tau})\beta_\tau(e^{-z\tau})^{-1}|\|K_s(\beta_\tau(e^{-z\tau})) - K_s(z)\|\\ \le&|\mu(e^{-z\tau})\beta_\tau(e^{-z\tau})^{-1} - z^{-1}|\|K_s(z)\| + c|z|^{-1}\|K_s(\beta_\tau(e^{-z\tau})) - K_s(z)\| =: \mathrm{I} + c\mathrm{II}.\end{aligned}$$

The first term I can be bounded directly using Lemma 3.3, (3.19) and the inequality $\|K_s(z)\| = \|I - z^\alpha(z^\alpha-\Delta_h)^{-1}\| \le c$. For the second term II, it suffices to show

$$|z|\mathrm{II} = \|K_s(\beta_\tau(e^{-z\tau})) - K_s(z)\| \le c\tau^2|z|^2.$$

Using (3.4), triangle inequality, Lemma 3.3 and (3.20), we get

$$\begin{aligned}|z|\mathrm{II} &= \|\beta_\tau(e^{-z\tau})^\alpha(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1} - z^\alpha(z^\alpha-\Delta_h)^{-1}\|\\ &\le |z^\alpha - \beta_\tau(e^{-z\tau})^\alpha|\|(z^\alpha-\Delta_h)^{-1}\| + |\beta_\tau(e^{-z\tau})|^\alpha\|(\beta_\tau(e^{-z\tau})^\alpha-\Delta_h)^{-1} - (z^\alpha-\Delta_h)^{-1}\|\\ &\le c|z^\alpha - \beta_\tau(e^{-z\tau})^\alpha|\|(z^\alpha-\Delta_h)^{-1}\| + c|z|^\alpha\|(\beta_\tau(e^{-z\tau})^\alpha-\Delta_h)^{-1} - (z^\alpha-\Delta_h)^{-1}\| \le c\tau^2|z|^2.\end{aligned}$$

Now the triangle inequality completes the proof of the lemma. □

Now we can state the temporal error for nonsmooth initial data $v\in L^2(\Omega)$.

**Theorem 3.2.** *Let $f = 0$, $u_h$ and $U_h^n$ be the solutions of (2.2) and (2.4) with $v\in L^2(\Omega)$, and $U_h^0 = v_h = P_h v$, respectively. Then, there holds*

$$\|u_h(t_n) - U_h^n\|_{L^2(\Omega)} \le c\tau^2 t_n^{-2}\|v\|_{L^2(\Omega)}, \quad n\ge 1.$$

*Proof.* We choose $\delta = \min(\delta_0, \delta_1)$ and $\theta = \pi/2 + \delta$. By Proposition 3.1, we split the error into

$$u_h(t_n) - U_h^n = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\delta}^\tau} e^{zt_n} \left( z^{-1} K_s(z) - \mu(e^{-z\tau}) \beta_\tau(e^{-z\tau})^{-1} K_s(\beta_\tau(e^{-z\tau})) \right) v_h \, dz$$
$$+ \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\delta} \setminus \Gamma_{\theta,\delta}^\tau} e^{zt_n} z^{-1} K_s(z) v_h dz =: \mathrm{I} + \mathrm{II}.$$

By Lemma 3.5 and choosing $\delta \leq 1/t_n$, we bound the first term I by

$$\|\mathrm{I}\|_{L^2(\Omega)} \leq c\tau^2 \|v_h\|_{L^2(\Omega)} \left( \int_\delta^{\pi/(\tau \sin\theta)} e^{rt_n \cos\theta} r dr + \int_{-\theta}^{\theta} e^{\delta t_n |\cos\psi|} \delta^2 d\psi \right) \leq c t_n^{-2} \tau^2 \|v_h\|_{L^2(\Omega)}.$$

For the second term II, we appeal to the resolvent estimate (3.4) and obtain

$$\|\mathrm{II}\|_{L^2(\Omega)} \leq c \|v_h\|_{L^2(\Omega)} \int_{\pi/(\tau \sin\theta)}^\infty e^{rt_n \cos\theta} r^{-1} \, dr \leq c\tau^2 t_n^{-2} \|v_h\|_{L^2(\Omega)}.$$

Now the desired result follows directly from the $L^2(\Omega)$-stability of $P_h$. □

**Remark 3.1.** *The initial correction compensates the solution singularity at $t = 0$, which is crucial to achieve the $O(\tau^2)$ convergence. Otherwise, we can only derive an $O(\tau)$ rate*

$$\|u_h(t_n) - U_h^n\|_{L^2(\Omega)} \leq c\tau t_n^{\alpha-1} \|\Delta v\|_{L^2(\Omega)},$$

*even if the initial data $v$ is smooth. This was numerically verified in Table 2 in Section 2.2. The key of correction is to choose a proper function $\mu$ in (3.6), such that the estimate $|\mu(e^{-z\tau}) - 1| \leq c\tau^2 |z|^2$ from Lemma 3.3 holds. The choice of $\mu$ is clearly nonunique; see Section 4 for another choice. The correction in (2.4) is probably the most practical one, since it only changes the first two steps.*

**Remark 3.2.** *By the proof of Theorems 3.1 and 3.2 and an interpolation argument, we deduce that for $v \in D((-\Delta)^s)$, $s \in [0, 1]$, with $v_h = P_h v$, there holds*

$$\|u_h(t_n) - U_h^n\|_{L^2(\Omega)} \leq c\tau^2 t_n^{s\alpha - 2} \|(-\Delta_h)^s v_h\|_{L^2(\Omega)}.$$

## 3.3 Error analysis for the inhomogeneous problem

Now we turn to the inhomogeneous problem $f \neq 0$ and $v = 0$. By Proposition 3.1, it suffices to analyze the two terms involving $F_h^0 = f_h(0)$ and $\widehat{G}_h$ in the integral representation. First, assume that $f$ is time-independent. Then by (3.1), we have

$$u_h(t_n) - U_h^n = -\frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\delta}} e^{zt_n} K(z) F_h^0 dz + \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\delta}^\tau} e^{zt_n} \mu(e^{-z\tau}) K(\beta_\tau(e^{-z\tau})) F_h^0 \, dz.$$

Then by Lemma 3.4 and repeating the argument in the proof of Theorem 3.2, we deduce

$$\|u_h(t_n) - U_h^n\|_{L^2(\Omega)} \leq c\tau^2 t_n^{\alpha-2} \|F_h^0\|_{L^2(\Omega)} \leq c\tau^2 t_n^{\alpha-2} \|f\|_{L^2(\Omega)}. \tag{3.21}$$

Second, with $f(0) = 0$, by the Taylor expansion of integral form

$$f_h = f_h(0) + t f_h'(0) + t * f_h'' = t f_h'(0) + t * f_h'', \tag{3.22}$$

it suffices to bound the errors for source terms of the form $tg_h$ and $t * g_h$, which is done next. The next lemma gives an error estimate for $tg_h$.

**Lemma 3.6.** *Let $v = 0$, and $u_h$ and $U_h^n$ be the solutions of* (2.2) *with $f_h = tg_h(x) \in X_h$, and* (2.4) *with $F_h^n = f_h(t_n)$, respectively. Then, there holds*

$$\|U_h^n - u_h(t_n)\|_{L^2(\Omega)} \le c\tau^2 t_n^{\alpha-1}\|g_h\|_{L^2(\Omega)}.$$

*Proof.* Like before, we choose $\delta = \min(\delta_0, \delta_1)$ and $\theta = \pi/2 + \delta$. By (3.1) and Proposition 3.1, the semidiscrete Galerkin solution $u_h(t_n)$ and fully discrete solution $U_h^n$ are given by

$$u_h(t_n) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\delta}} e^{zt_n} z^{-2}(z^\alpha - \Delta_h)^{-1} g_h \, dz,$$

and

$$U_h^n = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma^\tau_{\theta,\delta}} e^{zt_n} \frac{\tau^2 e^{-z\tau}}{(1-e^{-z\tau})^2} (\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1} g_h \, dz,$$

respectively. Next, we claim the following estimate on the kernels in the solution representations

$$\|\frac{\tau^2 e^{-z\tau}}{(1-e^{-z\tau})^2}(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1} - z^{-2}(z^\alpha - \Delta_h)^{-1}\| \le c\tau^2|z|^{-\alpha} \quad z \in \Gamma^\tau_{\theta,\delta}. \tag{3.23}$$

This is a direct consequence of Lemmas 3.2 and 3.3 and the following inequality

$$|(1-e^{-z\tau})^2 e^{z\tau}\tau^{-2} - z^2| \le c\tau^2|z|^4 \sum_{n=1}^{\infty} \frac{2}{(2n+2)!}\tau^{2n-2}|z|^{2n-2} \le c\tau^2|z|^4, \quad \forall\, z \in \Gamma^\tau_{\theta,\delta},$$

where the last step holds since $|z|\tau \le c$ for $z \in \Gamma^\tau_{\theta,\delta}$. Next, we split the error into

$$\begin{aligned} u_h(t_n) - U_h^n = &\frac{1}{2\pi \mathrm{i}} \int_{\Gamma^\tau_{\theta,\delta}} e^{zt_n} \left( z^{-2}(z^\alpha - \Delta_h)^{-1} - \frac{\tau^2 e^{-z\tau}}{(1-e^{-z\tau})^2}(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1} \right) g_h \, dz \\ &+ \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\delta}\setminus\Gamma^\tau_{\theta,\delta}} e^{zt_n} z^{-2}(z^\alpha - \Delta_h)^{-1} g_h dz := \mathrm{I} + \mathrm{II}. \end{aligned}$$

Using the estimate (3.23) and choosing $\delta \le 1/t_n$, we bound the first term I by

$$\|\mathrm{I}\|_{L^2(\Omega)} \le c\tau^2\|g_h\|_{L^2(\Omega)} \left( \int_\delta^{\pi/(\tau\sin\theta)} e^{rt_n\cos\theta} r^{-\alpha} dr + \int_{-\theta}^{\theta} e^{\delta t_n|\cos\psi|}\delta^{1-\alpha} d\psi \right) \le c\tau^2 t_n^{\alpha-1}\|g_h\|_{L^2(\Omega)}.$$

Similarly, by appealing to the resolvent estimate (3.4), we obtain

$$\|\mathrm{II}\|_{L^2(\Omega)} \le c\|g_h\|_{L^2(\Omega)} \int_{\pi/(\tau\sin\theta)}^{\infty} e^{rt_n\cos\theta} r^{-2-\alpha} \, dr \le c\tau^2 t_n^{\alpha-1}\|g_h\|_{L^2(\Omega)}.$$

Now the desired result follows from the triangle inequality. □

The next lemma gives an error estimate for $t * g_h$.

**Lemma 3.7.** *Let $v_h = 0$, $u_h$ and $U_h^n$ be the solutions of* (2.2) *with $f_h = t * g_h \in X_h$ and* (2.4) *with $F_h^n = f_h(t_n)$, respectively. Then, there holds*

$$\|U_h^n - u_h(t_n)\|_{L^2(\Omega)} \le c\tau^2 \int_0^{t_n} (t_n - s)^{\alpha-1}\|g_h(s)\|_{L^2(\Omega)} \, ds.$$

*Proof.* We choose $\delta = \min(\delta_0, \delta_1)$ and $\theta = \pi/2 + \delta$ like before. First, we introduce the operator $\mathcal{E}(t)$ defined by $\mathcal{E}(t) = \frac{1}{2\pi\mathrm{i}} \int_{\Gamma_{\theta,\delta}} e^{zt}(z^\alpha - \Delta_h)^{-1}\, dz$. Then, the semidiscrete Galerkin solution $u_h(t_n)$ can be represented by

$$u_h(t_n) = (\mathcal{E} * f_h)(t_n) = (\mathcal{E} * (t * g_h))(t_n) = ((\mathcal{E} * t) * g_h)(t_n).$$

Next we derive the representation of the fully discrete solution $U_h^n$. Using the generating function $\widetilde{f}_h(\xi) = \sum_{n=0}^\infty f_h(t_n)\xi^n$, and $\widetilde{U}_h(\xi) = (\beta_\tau(\xi)^\alpha - \Delta_h)^{-1}\widetilde{f}_h(\xi) =: \widetilde{\mathcal{E}}(\beta_\tau(\xi))\widetilde{f}_h(\xi)$, we represent $U_h^n$ by

$$U_h^n = \sum_{j=0}^n \mathcal{E}_\tau^{n-j} f_h(t_j) \qquad \text{with} \qquad \widetilde{\mathcal{E}}(\beta_\tau(\xi)) = \sum_{n=0}^\infty \mathcal{E}_\tau^n \xi^n.$$

Simple computation yields the following integral representation

$$\mathcal{E}_\tau^n = \frac{\tau}{2\pi\mathrm{i}} \int_{\Gamma_{\theta,\delta}^\tau} e^{zn\tau}(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\, dz.$$

Using Lemma 3.3, we have the following estimate

$$\|\mathcal{E}_\tau^n\| \le c\tau t_n^{\alpha-1}. \tag{3.24}$$

Let $\mathcal{E}_\tau(t) = \sum_{n=0}^\infty \mathcal{E}_\tau^n \delta_{t_n}(t)$, with $\delta_{t_n}$ being the Dirac-delta function at $t_n$ (from the left side). Then we have

$$U_h^n = (\mathcal{E}_\tau * f_h)(t_n) = (\mathcal{E}_\tau * (t * g_h))(t_n) = ((\mathcal{E}_\tau * t) * g_h)(t_n).$$

By the discrete convolution rule, we have

$$\widetilde{(\mathcal{E}_\tau * t)}(\xi) = \sum_{n=0}^\infty \sum_{j=0}^n \mathcal{E}_\tau^{n-j} t_j \xi^n = \big(\sum_{j=0}^\infty \mathcal{E}_\tau^j \xi^j\big)\big(\sum_{j=0}^\infty t_j \xi^j\big) = \widetilde{\mathcal{E}}(\beta_\tau(\xi))\frac{\tau\xi}{(1-\xi)^2},$$

and consequently, by repeating the argument in the proof of Lemma 3.6, we deduce

$$\|((\mathcal{E}_\tau - \mathcal{E}) * t)(t_n)\| \le c\tau^2 t_n^{\alpha-1}.$$

Next, we derive that for $t > 0$

$$\|((\mathcal{E}_\tau - \mathcal{E}) * t)(t)\| \le c\tau^2 t^{\alpha-1}, \quad \forall t \in (t_{n-1}, t_n). \tag{3.25}$$

To see the claim, we recall the Taylor expansion of $\mathcal{E}(t)$ at $t = t_n$

$$(\mathcal{E} * t)(t) = (\mathcal{E} * t)(t_n) + (t - t_n)(\mathcal{E} * 1)(t_n) + \int_{t_n}^t (t - s)\mathcal{E}(s)\, ds.$$

This expansion holds also for $(\mathcal{E}_\tau * t)(t)$. Then the preceding argument yields

$$\|((\mathcal{E} - \mathcal{E}_\tau) * t)(t_n)\| \le c\tau^2 t_n^{\alpha-1} \quad \text{and} \quad \|(\mathcal{E} - \mathcal{E}_\tau) * 1)(t_n)\| \le c\tau t_n^{\alpha-1}.$$

Meanwhile, by the resolvent estimate (3.4), we have $\|\mathcal{E}(t)\| \le ct^{\alpha-1}$, and consequently, there holds

$$\Big\| \int_{t_n}^t (t - s)\mathcal{E}(s)\, ds \Big\| \le c \int_t^{t_n} (s - t)s^{\alpha-1}\, ds \le c\tau^2 t^{\alpha-1}.$$

Similarly, appealing to (3.24), we deduce

$$\Big\| \int_{t_n}^t (t - s)\mathcal{E}_\tau(s)\, ds \Big\| \le \tau \|\mathcal{E}_\tau^n\| \le c\tau^2 t_n^{\alpha-1}.$$

Then (3.25) follows directly by $t_n^{\alpha-1} \le t^{\alpha-1}$ for $t \in (t_{n-1}, t_n)$ and $\alpha \in (0, 1)$, concluding the proof. $\square$

By (3.21) and Lemmas 3.6 and 3.7, we obtain the error estimate for the inhomogeneous problem.

**Theorem 3.3.** *Let $v = 0$, $f \in W^{1,\infty}(0,T;L^2(\Omega))$, $\int_0^t (t-s)^{\alpha-1}\|f''(s)\|_{L^2(\Omega)}ds \in L^\infty(0,T)$, and $u_h$ and $U_h^n$ be the solutions of (2.2) with $f_h = P_h f$ and (2.4) with $F_h^n = P_h f(t_n)$, respectively. Then, there holds*

$$\|u_h(t_n) - U_h^n\|_{L^2(\Omega)} \le c\tau^2 \left( t_n^{\alpha-2}\|f(0)\|_{L^2(\Omega)} + t_n^{\alpha-1}\|f'(0)\|_{L^2(\Omega)} + \int_0^{t_n} (t_n - s)^{\alpha-1}\|f''(s)\|_{L^2(\Omega)}\,ds \right).$$

**Remark 3.3.** *The estimate in Theorem 3.3 agrees with the regularity theory for (1.1). In case $v = 0$, following the splitting (3.22), one can show that the solution $u$ of problem (1.1) satisfies*

$$\|\partial_t^2 u(t)\|_{L^2(\Omega)} \le c\left( t^{\alpha-2}\|f(0)\|_{L^2(\Omega)} + t^{\alpha-1}\|f'(0)\|_{L^2(\Omega)} + \int_0^t (t-s)^{\alpha-1}\|f''(s)\|_{L^2(\Omega)}\,ds \right).$$

*Hence, in order to have an $O(\tau^2)$ rate, we require $f(0)$, $f'(0) \in L^2(\Omega)$ and a certain integrability of $f''(t)$. Otherwise, the scheme (2.4) might lose its second-order accuracy.*

# 4 Numerical experiments and discussions

Now we present examples on the unit square $\Omega = (0,1)^2$ to illustrate the scheme (2.4). In the computations, we divide the unit interval $(0,1)$ into $M$ equally spaced subintervals, with a mesh size $h = 1/M$, which partitions the domain $\Omega$ into $M^2$ small squares. Then we get a symmetric mesh by connecting the diagonal of each small square. We fix the time step size $\tau$ at $\tau = t/N$, where $t$ is the time of interest. To examine the temporal convergence rates, we always fix the mesh size $h$ at $h = 1/500$, and employ a time step size $\tau = t/1000$ to compute the reference solution $u_h(t)$. Throughout, we measure the error $e^n = u_h(t_n) - U_h^n$ by the normalized $L^2(\Omega)$ error $\|e^n\|_{L^2(\Omega)}/\|v\|_{L^2(\Omega)}$. Since the spatial discretization error has been examined in [10, 9], we shall focus on the temporal error below.

We consider the following four examples to illustrate the convergence analysis.

(a) $v = xy(1-x)(1-y) \in D(\Delta)$ and $f = 0$;

(b) $v = \chi_{(0,1/2]\times(0,1)}(x,y) \in D((-\Delta)^{1/4-\epsilon})$ with $\epsilon \in (0,1/4)$ and $f = 0$;

(c) $v = 0$, and $f = (1 + t^{1.5})\chi_{(0,1/2]\times(0,1)}(x,y)$;

(d) $v = 0$, and $f = t^\beta \chi_{(0,1/2]\times(0,1)}(x,y)$ with $\beta \in (0,1)$;

First we examine the convergence for the homogenous problem. The numerical results for cases (a) and (b) at the time $t = 1$ are given in Tables 4 and 5, where `rate` in the last column refers to the empirical convergence rate, and the numbers in the bracket denote theoretical predictions from Section 3. It is observed that the corrected scheme (2.4) exhibits a steady $O(\tau^2)$ convergence for both smooth and nonsmooth data, which shows clearly its robustness. In Tables 4 and 5, we also include the numerical results by CQ generated by the second-order BDF (SBD) and L1-2 scheme. In theory, SBD is $O(\tau^2)$ accurate for both smooth and nonsmooth problem data [12], but a complete convergence analysis of the L1-2 scheme is still to be developed, with a local truncation error $O(\tau^{3-\alpha})$ [8]. The L1-2 scheme exhibits only an $O(\tau)$ convergence, due to the insufficient solution regularity even for smooth problem data, which contrasts sharply with the scheme (2.4) and SBD. Numerically, with the same time step size $\tau$, the scheme (2.4) is slightly more accurate than SBD.

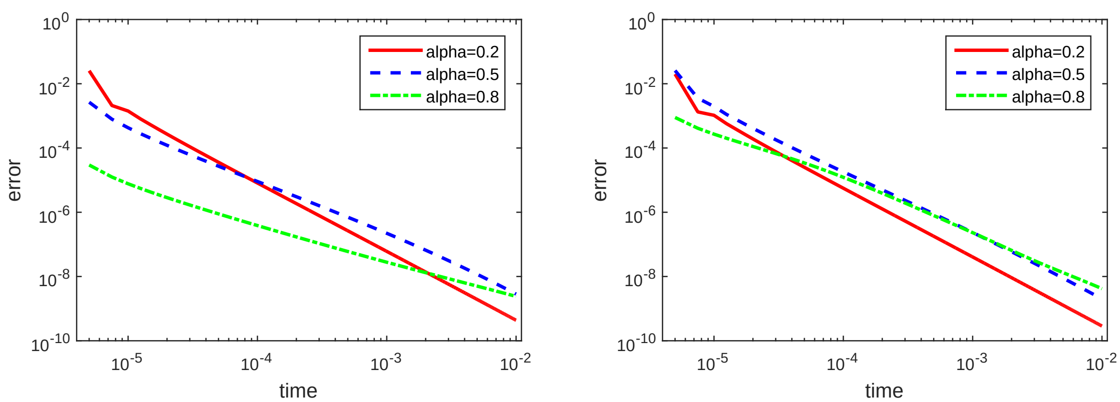
Due to the insufficient regularity in time for problem (1.1), the temporal error deteriorates as the time $t_n \to 0$ irrespective of the data regularity; see Fig. 1 for the evolution of the $L^2$ errors with time for cases (a) and (b). For both smooth and nonsmooth initial data, the error increases as $t$ tends to $t = 0$, and the rate is larger for smaller $\alpha$, concurring with the analysis in Section 3.2. Next we verify the sharpness of the prefactor in the error estimates for small $t_n$. By Remark 3.2, the $L^2(\Omega)$ error decays at a rate like $O(t_n^\alpha)$ and $O(t_n^{\alpha/4-\alpha\epsilon})$ for $v \in D(\Delta)$ and $v \in D((-\Delta)^{1/4-\epsilon})$, for any $\epsilon \in (0,1/4)$, respectively. Hence,

Table 4: The $L^2$-error for Example (a) at $t = 1$ with $h = 1/500$.

| Scheme | $\alpha\backslash N$ | 10 | 20 | 40 | 80 | 160 | rate |
|---|---|---|---|---|---|---|---|
| CN | 0.2 | 4.87e-5 | 1.14e-5 | 2.76e-6 | 6.73e-7 | 1.62e-7 | $\approx$ 2.06 (2.00) |
| | 0.5 | 1.19e-4 | 2.78e-5 | 6.70e-6 | 1.63e-6 | 3.93e-7 | $\approx$ 2.06 (2.00) |
| | 0.8 | 1.22e-4 | 2.68e-5 | 6.46e-6 | 1.57e-6 | 3.78e-7 | $\approx$ 2.05 (2.00) |
| SBD | 0.2 | 7.78e-5 | 1.82e-5 | 4.38e-6 | 1.07e-6 | 2.64e-7 | $\approx$ 2.02 (2.00) |
| | 0.5 | 1.44e-4 | 3.34e-5 | 8.03e-6 | 1.96e-6 | 4.82e-7 | $\approx$ 2.05 (2.00) |
| | 0.8 | 1.67e-4 | 3.88e-5 | 9.26e-6 | 2.26e-6 | 5.52e-7 | $\approx$ 2.05 (2.00) |
| L1-2 | 0.2 | 5.02e-4 | 2.49e-4 | 1.23e-4 | 6.00e-5 | 2.87e-5 | $\approx$ 1.03 (2.80) |
| | 0.5 | 1.57e-3 | 7.72e-4 | 3.73e-4 | 1.78e-4 | 8.29e-5 | $\approx$ 1.06 (2.50) |
| | 0.8 | 1.63e-3 | 9.42e-4 | 4.67e-4 | 2.23e-4 | 1.04e-4 | $\approx$ 1.00 (2.20) |

Table 5: The $L^2$-error for Example (b) for $\alpha = 0.5$ with $h = 1/500$.

| scheme | $t\backslash N$ | 10 | 20 | 40 | 80 | 160 | rate |
|---|---|---|---|---|---|---|---|
| CN | 1 | 7.48e-5 | 1.74e-5 | 4.18e-6 | 1.02e-6 | 2.45e-7 | $\approx$ 2.05 (2.00) |
| | 0.01 | 4.74e-4 | 1.10e-4 | 2.66e-5 | 6.51e-6 | 1.56e-6 | $\approx$ 2.05 (2.00) |
| | 0.001 | 5.45e-4 | 1.28e-4 | 3.09e-5 | 7.55e-6 | 1.82e-6 | $\approx$ 2.05 (2.00) |
| SBD | 1 | 8.98e-5 | 2.08e-5 | 5.00e-6 | 1.22e-6 | 3.00e-7 | $\approx$ 2.05 (2.00) |
| | 0.01 | 5.23e-4 | 1.22e-4 | 2.94e-5 | 7.22e-6 | 1.77e-6 | $\approx$ 2.04 (2.00) |
| | 0.001 | 5.46e-4 | 1.29e-4 | 3.10e-5 | 7.63e-6 | 1.88e-6 | $\approx$ 2.04 (2.00) |
| L1-2 | 1 | 3.52e-4 | 1.73e-4 | 8.43e-5 | 4.04e-5 | 1.90e-5 | $\approx$ 1.05 (2.50) |
| | 0.01 | 2.29e-3 | 1.14e-3 | 5.53e-4 | 2.66e-4 | 1.25e-4 | $\approx$ 1.05 (2.50) |
| | 0.001 | 3.32e-3 | 1.65e-3 | 8.11e-4 | 3.93e-4 | 1.97e-4 | $\approx$ 1.04 (2.50) |




(a) case (a): smooth data

(b) case (b): nonsmooth data

Figure 1: The $L^2$-error versus the time $t$ with $\alpha = 0.2$, 0.5 and 0.8, $\tau = 2 \times 10^{-6}$, for cases (a) and (b).

Table 6: The $L^2$-error for Examples (a) and (b) for $\alpha = 0.5$ as $t \to 0$ with $h = 1/500$ and $N = 10$.

| $t$ | 1e-3 | 1e-4 | 1e-5 | 1e-6 | 1e-7 | 1e-8 | rate |
|---|---|---|---|---|---|---|---|
| (a) | 5.24e-4 | 2.07e-4 | 6.90e-5 | 2.22e-5 | 7.06e-6 | 2.24e-6 | 0.49 (0.50) |
| (b) | 5.43e-4 | 4.06e-4 | 2.97e-4 | 2.23e-4 | 1.67e-4 | 1.24e-4 | 0.13 (0.13) |

for a fixed $N$ and with $\alpha = 1/2$, the error should behave like $O(t_n^{1/2})$ and $O(t_n^{1/8})$ for cases (a) and (b), respectively, which are fully confirmed by Table 6, verifying the sharpness of the error analysis.

Next we examine the scheme (2.4) for inhomogeneous problems. In case (c), $f \in L^\infty(0,T;L^2(\Omega))$ and $\int_0^t (t-s)^{\alpha-1}\|f''(s)\|_{L^2(\Omega)}\,ds \in L^\infty(0,T)$ for any $\alpha\in(0,1)$. Theorem 3.3 predicts an $O(\tau^2)$ convergence, which is fully confirmed by the results in Table 7. The preceding observations on the SBD and L1-2 scheme remain valid for the inhomogeneous problem: the SBD is $O(\tau^2)$ accurate, but the L1-2 scheme can only achieve an $O(\tau)$ rate. The purpose of case (d) is to explore the limit of the scheme (2.4): In case (d), for small exponent $\beta>0$, the source term $f$ is not smooth enough to apply Theorem 3.3, and the $O(\tau^2)$ convergence does not hold. To see the possible convergence rate, consider the fractional ODE $\partial_t^\alpha u(t) = t^\beta$ with $u(0)=0$, whose solution is given by $u(t)=\frac{\Gamma(\alpha+1)}{\Gamma(\alpha+\beta+1)}t^{\alpha+\beta}$. The temporal regularity of the solution lies in $H^{\alpha+\beta+1/2-\epsilon}(0,T)$, from which one can expect at best a rate $O(\tau^{\min(\alpha+\beta+1/2,2)})$. The empirical rate is of order $O(\tau^{\min(1+\beta,2)})$ for the case $\alpha=1/2$, cf. Table 8, which agrees well with the expected solution regularity, thereby further verifying the robustness of the scheme (2.4).

Table 7: The $L^2$-error for Example (c) at $t=1$ with $h=1/500$.

| Scheme | $\alpha\backslash N$ | 10 | 20 | 40 | 80 | 160 | rate |
|---|---|---|---|---|---|---|---|
| CN | 0.2 | 1.66e-6 | 3.93e-7 | 9.55e-8 | 2.34e-8 | 5.64e-9 | $\approx$ 2.05 (2.00) |
| | 0.5 | 3.52e-6 | 8.23e-7 | 1.99e-7 | 4.86e-8 | 1.17e-8 | $\approx$ 2.05 (2.00) |
| | 0.8 | 4.49e-6 | 6.80e-7 | 1.63e-7 | 3.97e-8 | 9.54e-9 | $\approx$ 2.06 (2.00) |
| SBD | 0.2 | 1.97e-6 | 4.65e-7 | 1.13e-7 | 2.78e-8 | 6.83e-9 | $\approx$ 2.04 (2.00) |
| | 0.5 | 4.32e-6 | 1.00e-6 | 2.42e-7 | 5.91e-8 | 1.45e-8 | $\approx$ 2.05 (2.00) |
| | 0.8 | 3.49e-6 | 8.03e-7 | 1.90e-7 | 4.61e-8 | 1.13e-8 | $\approx$ 2.07 (2.00) |
| L1-2 | 0.2 | 9.79e-6 | 4.85e-6 | 2.39e-6 | 1.16e-6 | 5.49e-7 | $\approx$ 1.04 (2.80) |
| | 0.5 | 1.67e-5 | 8.16e-6 | 3.96e-6 | 1.90e-6 | 8.87e-7 | $\approx$ 1.06 (2.50) |
| | 0.8 | 1.05e-5 | 4.70e-6 | 2.06e-6 | 8.91e-7 | 3.84e-7 | $\approx$ 1.19 (2.20) |

Table 8: The $L^2$-error for Example (d) at $t=1$ with $h=1/500$ and $\alpha=0.5$.

| $\beta\backslash N$ | 10 | 20 | 40 | 80 | 160 | rate |
|---|---|---|---|---|---|---|
| 0.2 | 9.12e-6 | 3.98e-6 | 1.73e-6 | 7.44e-7 | 3.15e-7 | $\approx$ 1.21 (−−) |
| 0.5 | 2.83e-6 | 9.90e-7 | 3.47e-7 | 1.22e-7 | 4.22e-8 | $\approx$ 1.52 (−−) |
| 0.8 | 1.07e-6 | 2.97e-7 | 8.28e-8 | 2.31e-8 | 6.43e-9 | $\approx$ 1.85 (−−) |

Last, we revisit the correction at starting steps. As indicated in Remark 3.1, there are many possible corrections to the scheme (1.3) in order to restore the $O(\tau^2)$ accuracy. According to the convergence analysis in Section 3, the only requirement on the correction is to choose an auxiliary function $\mu(\xi)$ in (3.5) such that the estimate on $\mu$ in Lemma 3.3 holds and the resulting scheme only changes the first few steps (and thus easy to implement). For example, the following choice satisfies the estimate

$$\mu_0(\xi) = (4\xi - 3\xi^2 + \xi^3)/[2(1-\tfrac{\alpha}{2}+\tfrac{\alpha}{2}\xi)^{1/\alpha}]. \tag{4.1}$$

Then the corresponding fully discrete scheme modifies the first three steps:

$$\begin{aligned}
\bar\partial_\tau^\alpha(U_h-v_h)^1 - (1-\tfrac{\alpha}{2})\Delta_h U_h^1 - (1-\tfrac{\alpha}{2})\Delta_h v_h &= (1-\tfrac{\alpha}{2})(F_h^1+F_h^0),\\
\bar\partial_\tau^\alpha(U_h-v_h)^2 - (1-\tfrac{\alpha}{2})\Delta_h U_h^2 - \tfrac{\alpha}{2}\Delta_h U_h^1 - (\tfrac{3\alpha}{4}-\tfrac{1}{2})\Delta_h v_h &= (1-\tfrac{\alpha}{2})F_h^2 + \tfrac{\alpha}{2}F_h^1 + (\tfrac{3\alpha}{4}-\tfrac{1}{2})F_h^0,\\
\bar\partial_\tau^\alpha(U_h-v_h)^3 - (1-\tfrac{\alpha}{2})\Delta_h U_h^3 - \tfrac{\alpha}{2}\Delta_h U_h^2 + \tfrac{\alpha}{4}\Delta_h v_h &= (1-\tfrac{\alpha}{2})F_h^3 + \tfrac{\alpha}{2}F_h^2 - \tfrac{\alpha}{4}F_h^0.
\end{aligned}$$

Then the error estimates in Section 3 hold also for the correction (4.1). Numerically, the scheme also achieves a very steady second-order convergence, cf. Table 9.

Table 9: The $L^2$-error for Examples (b) and (c) at $t = 0.1$, with $h = 1/500$, by the correction (4.1).

| Case | $\alpha\backslash N$ | 10 | 20 | 40 | 80 | 160 | rate |
|---|---|---|---|---|---|---|---|
| (b) | 0.2 | 4.61e-5 | 1.08e-5 | 2.61e-6 | 6.37e-7 | 1.53e-7 | $\approx$ 2.05 (2.00) |
| | 0.5 | 2.20e-4 | 5.14e-5 | 1.24e-5 | 3.03e-6 | 7.28e-7 | $\approx$ 2.04 (2.00) |
| | 0.8 | 8.47e-4 | 1.86e-4 | 4.49e-5 | 1.09e-5 | 2.63e-6 | $\approx$ 2.05 (2.00) |
| (c) | 0.2 | 2.16e-6 | 5.09e-7 | 1.22e-7 | 2.92e-8 | 6.97e-9 | $\approx$ 2.07 (2.00) |
| | 0.5 | 1.03e-5 | 2.42e-6 | 5.82e-7 | 1.41e-7 | 3.31e-8 | $\approx$ 2.06 (2.00) |
| | 0.8 | 3.92e-5 | 9.07e-6 | 2.17e-6 | 5.28e-7 | 1.24e-7 | $\approx$ 2.05 (2.00) |

# 5 Conclusion

In this work, we have analyzed a fractional Crank-Nicolson scheme for discretizing the subdiffusion model, which naturally generalizes the classical Crank-Nicolson scheme for the heat equation to the fractional case. We have developed essential initial corrections to robustify the scheme which changes only the starting two steps so that it is easy to implement and meanwhile can achieve the desired second-order convergence for both smooth and nonsmooth problem data. A complete convergence analysis was provided, and optimal error estimates in time directly with respect to the data regularity were established. The accuracy, efficiency and robustness of the corrected scheme were fully confirmed by extensive numerical experiments, and a comparative study was included to indicate its competitiveness with existing schemes in terms of the accuracy and efficiency.

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