Sharp $H^1$-norm error estimates of two time-stepping schemes for reaction-subdiffusion problems

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Abstract

Due to the intrinsically initial singularity of solution and the discrete convolution form in numerical Caputo derivatives, the traditional $H^1$-norm analysis (corresponding to the case for a classical diffusion equation) to the time approximations of a fractional subdiffusion problem always leads to suboptimal error estimates (a loss of time accuracy). To recover the theoretical accuracy in time, we propose an improved discrete Grönwall inequality and apply it to the well-known $L^1$ formula and a fractional Crank-Nicolson scheme. With the help of a time-space error-splitting technique and the global consistency analysis, sharp $H^1$-norm error estimates of the two nonuniform approaches are established for a reaction-subdiffusion problems. Numerical experiments are included to confirm the sharpness of our analysis.

Keywords: reaction-subdiffusion problems, initial singularity, discrete Grönwall inequality, time-space error-splitting technique, sharp $H^1$-norm error estimate

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1 Introduction

Sharp $H^1$-norm error estimates are established for two nonuniform time approximations to a linear reaction-subdiffusion problems \[ \mathcal{D}_t^\alpha u + Lu = c(x) u + f(x,t) \quad \text{for } x \in \Omega \text{ and } 0 < t \leq T, \]
\[ u = u_b(t,x) \quad \text{for } x \in \partial \Omega \text{ and } 0 < t < T, \]
\[ u = u_0(x) \quad \text{for } x \in \Omega \text{ when } t = 0, \]

where $L$ is a linear, second-order, strongly-elliptic partial differential operator in the spatial variable $x$, and $c(x)$ is a reaction coefficient satisfying $|c(x)| \leq \kappa$ for a positive constant $\kappa$. Here,

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\( D_t^\alpha = \frac{C}{0} D_t^\alpha \) denotes the Caputo fractional derivative of order \( \alpha \) with respect to time \( t \),

\[
(D_t^\alpha v)(t) := (I^{1-\alpha} v')(t) = \int_0^t \omega_{1-\alpha}(t-s)v'(s) \, ds \quad \text{for} \quad 0 < \alpha < 1 \quad \text{and} \quad t > 0,
\]

involving the Riemann–Liouville fractional integral operator of order \( \beta > 0 \), defined by

\[
(I^\beta v)(t) := \int_0^t \omega_\beta(t-s)v(s) \, ds \quad \text{for} \quad t > 0, \quad \text{where} \quad \omega_\beta(t) := \frac{t^{\beta-1}}{\Gamma(\beta)}.
\]

An important and key consideration \([4, 6, 7, 19–22, 26]\) in solving subdiffusion problems is that the solution \( u(x,t) \) is typically non-smooth near the initial time, i.e., \( \partial u/\partial t = O(1 + t^{\alpha-1}) \) as \( t \to 0 \), see \([18,24,25]\). Among many approaches, one way to handle initial time singularity is to use nonuniform time steps, see \([2,3,11,15,18,22,26,28]\). The main reason is that the nonuniform mesh is simple and flexible to deal with not only the singular behavior near the initial time, but also the possible rapid growth of the solution far away from \( t = 0 \).

For the classical parabolic equation, the numerical analysis of the widespread backward Euler and Crank-Nicolson schemes on general nonuniform meshes for approximating the first-order time derivative would be almost the same as the uniform case, and has been well understood. For the subdiffusion problems considered here, the numerical analysis on nonuniform meshes is much more complicates due to the convolution integral form of Caputo derivative (1.2). Recently, Liao et al. developed a theoretical framework in \([12–15]\) for the numerical analysis of nonuniform time approximations, including the L1 formula \([6,12,16,27]\), two-level fast L1 formula \([15]\) and the fractional Crank-Nicolson (FracCN) scheme \([1,11,14]\), to reaction-subdiffusion problems. This framework involves three novel tools: a complementary discrete convolution kernel, a discrete fractional Grönwall inequality and a global consistency analysis. The stability and sharp \( L^2 \)-norm error estimates are obtained on general nonuniform meshes by taking into the initial singularity account. However, it seems that the framework is not straightforward to obtain the optimal \( H^1 \)-norm estimates of nonuniform time discretizations for problem (1.1). This motivates us to extend the framework to deal with the optimal \( H^1 \)-norm error estimate in this paper.

Actually, due to the nonlocal property of fractional time derivative and the lack of smoothness near the initial time, the traditional \( H^1 \)-norm analysis (for the parabolic problems corresponding to \( \alpha \to 1 \)) always leads to a suboptimal \( H^1 \)-norm error estimate. The goal of this paper is to achieve the optimal \( H^1 \)-norm error estimates of both L1 and FracCN schemes on a general nonuniform mesh \( 0 = t_0 < t_1 < t_2 < \cdots < t_N = T \). Denote the time-step size \( \tau_k := t_k - t_{k-1} \), the adjoint step ratio \( \rho_k := \tau_k/\tau_{k+1} \) for \( k \geq 1 \), and the maximum step size \( \tau := \max_{1 \leq k \leq N} \tau_k \). Our focus is on the time discretization of problems (1.1), for simplicity, we only consider the finite difference method for the spatial discretization in one dimension with \( \Omega := (x_l, x_r) \).

\[
\mathcal{L} := -\partial_x(\mu(x)\partial_x) \quad \text{and} \quad 0 < \mu_0 \leq \mu(x) \leq \mu_1 \quad \text{for} \quad \text{two positive constants} \quad \mu_0 \quad \text{and} \quad \mu_1.
\]

Nevertheless, the theoretical results in time approximations together with their proofs here are also valid for multi-dimensional problems, and are extendable for some other spatial discretization such as the spectral method. To make the present analysis extendable (such as for multi-term subdiffusion equations in Caputo’s sense), let \( \sigma \in (0,1) \cup (1,2) \) be a regularity parameter and assume that \( u(\cdot,t) \in C_\sigma^m((0,T]) \), where the space \( C_\sigma^m((0,T]) \) is defined by

\[
C_\sigma^m((0,T]) := \left\{ u \left| u \in C([0,T]) \cap C^m((0,T]) \quad \text{and} \quad |u^{(\ell)}| \leq C_\alpha(1 + t^{\sigma-\ell}) \right| \text{for} \quad \ell = 1, \cdots, m \quad \text{and} \quad 0 < t \leq T \right\}.
\]

Generally, the convergence rates of numerical Caputo derivatives are always limited by the nonsmoothness near the initial time. It is reasonable to use a nonuniform mesh that concentrates grid points near \( t = 0 \). Let \( \gamma \geq 1 \) be a user-chosen parameter, and assume that \([14,15,19]\).
M-conv. There is a constant \( C_\gamma > 0 \), independent of \( k \), such that 
\[
\tau_k \leq C_\gamma \tau \min\{1, t_k^{1-1/\gamma}\}
\]
for \( 1 \leq k \leq N \), \( t_k \leq C_\gamma t_{k-1} \) and \( \tau_k/t_k \leq C_\gamma \tau_{k-1}/t_{k-1} \) for \( 2 \leq k \leq N \).

Since \( \tau_1 = t_1 \), M-conv implies that \( \tau_1 = O(\tau^\gamma) \), while for those \( t_k \) bounded away from \( t = 0 \) one has \( \tau_k = O(\tau) \). The parameter \( \gamma \) controls the extent to which the grid points are concentrated near \( t = 0 \). A practical example satisfying M-conv is an initially graded grid [2, 3, 12, 19, 20, 26]

\[
t_k = (k/N_0)^\gamma T_0 \quad \text{for} \quad 0 \leq k \leq N_0 \quad \text{and} \quad t_k = T_0 + (k - N_0)\tau \quad \text{for} \quad N_0 < k \leq N,
\]

with
\[
N_0 := \left\lceil \frac{\gamma N T_0}{T + (\gamma - 1)T_0} \right\rceil \quad \text{for a small user-chosen} \quad T_0 \leq T.
\]

Throughout the paper, any subscripted \( C \), such as \( C_\Omega \), \( C_\gamma \), \( C_v \) and \( C_u \), denotes a generic positive constant, not necessarily the same at different occurrences, which is always dependent on the given data and the solution, but independent of temporal and spatial mesh sizes. The rest of this paper is organized as follows. In Section 2 we present an unified implicit time-stepping approach for subdiffusion problems and some preliminary results. In Section 3 we investigate the \( H^1 \)-norm error bound for the L1 scheme, while the second-order FracCN scheme with unequal time-steps is studied in Section 4. Two numerical examples in Section 5 are given to demonstrate the sharpness of our analysis.

## 2 An unified time-stepping scheme and \( H^1 \)-norm stability

Assume that approximate the Laplacian \( \mathcal{L} \) by the usual second-order difference operator \( \mathcal{L}_h \) on a discrete grid \( \Omega_h := \{ x_i + ih | 0 \leq i \leq M \} \) with \( h := (x_i - x_{i-1})/M \). For any function \( v_h \) on \( \Omega_h \), we define \( \partial_h v_h(x_{i-1/2}) := (v_h(x_i) - v_h(x_{i-1}))/h \) and

\[
(\mathcal{L}_h v_h)(x_i) := -\partial_h (\mu(x_i) \partial_h v_h(x_i)) = -\left( \mu(x_{i+1/2}) \partial_h v_h(x_{i+1/2}) - \mu(x_{i-1/2}) \partial_h v_h(x_{i-1/2}) \right)/h.
\]

We put \( \Omega_h := \Omega \cap \Omega_h \) and \( \partial \Omega_h := \partial \Omega \cap \partial \Omega_h \). For any functions \( v_h \) and \( w_h \) belonging to the space \( \mathbb{V}_h \) of grid functions that vanish on the boundary \( \partial \Omega_h \), we introduce the discrete inner product \( \langle v_h, w_h \rangle := h \sum_{x \in \Omega_h} v_h(x) w_h(x) \), the \( L_2 \) norm \( \| v_h \| := \sqrt{\langle v_h, v_h \rangle} \) and the \( H^1 \) semi-norm

\[
\| v_h \|_1 := \sqrt{\langle v_h, \mathcal{L}_h v_h \rangle} = \sqrt{h \sum_{x \in \Omega_h} \mu(x) (\partial_h v_h(x))^2}.
\]

There exists a positive constant \( C_\Omega \) only dependent on the domain \( \Omega \), the constants \( \mu_0 \) and \( \mu_1 \) such that \( \| v_h \| \leq C_\Omega |v_h|_1 \). The \( H^1 \) semi-norm \( |v_h|_1 \) is equivalent to the discrete \( H^1 \) norm \( \| v_h \|_1 := \sqrt{\| v_h \|^2 + |v_h|_1^2} \). So, in general, the estimates of \( |v_h|_1 \) are called \( H^1 \)-norm estimates.

### 2.1 A time-weighted difference scheme

Let \( \nu \in [0, 1/2) \) be an offset parameter and denote \( t_{n-\nu} := \nu t_{n-1} + (1 - \nu) t_n \). For any mesh function \( v_k \approx v(t_k) \), define \( v^{k-\nu} := \nu v^{k-1} + (1 - \nu) v^k \) and \( \nabla_\tau v^{k} := v^k - v^{k-1} \) for \( k \geq 1 \). The Caputo derivative [1, 2] of the function \( v \) can always be approximated by a convolution-like summation,

\[
(D_\tau^n v)(t_{n-\nu}) \approx (D_\tau^{\alpha} v)^{n-\nu} := \sum_{k=1}^{n} A_{n-k}^{(n, \nu)} \nabla_\tau v^k \quad \text{for} \quad 1 \leq n \leq N,
\]

with the local consistence error

\[
\Upsilon^{n-\nu} := (D_\tau^{\alpha} v)(t_{n-\nu}) - (D_\tau^{\nu} v)^{n-\nu} \quad \text{for} \quad 1 \leq n \leq N.
\]
Here, the corresponding discrete kernels, writing as $A_{n-k}^{(n,\nu)}$ to reflect the convolution structure of the integral in $\left[D_{\tau}^\alpha \right]$, will be determined later. Our discrete solution, $u_h^n \approx u(x,t_n)$ for $x \in \Omega_h$, is defined by a time-weighted time-stepping scheme

$$(D_{\tau}^\alpha u_h)^{n-\nu} + L_h u_h^{n-\nu} = c(x) u_h^{n-\nu} + f(x,t_{n-\nu}) \quad \text{for } x \in \Omega_h \text{ and } 1 \leq n \leq N,$$

$$u_h^0 = u_0(x) \quad \text{for } x \in \Omega_h.$$  \hspace{1cm} (2.3)

In this paper, we will focus on two different cases of $\left(D_{\tau}^\alpha v\right)^{n-\nu}$: one is the widespread L1 formula [12,16,26,27] with $\nu = 0$, and the other is the recently suggested nonuniform Alikhanov formula [14] with $\nu = \theta := \alpha/2$. For simplicity, the above scheme (2.3) is called the L1 and FracCN method, respectively, corresponding to the offset parameter $\nu = 0$ and $\nu = \theta$.

The present approach would be fit for general nonuniform time meshes and applicable for any discrete fractional derivatives having the form (2.1), provided $A_{n-k}^{(n,\nu)}$ satisfy three criteria:

A1. The discrete kernels are monotone, that is, $A_{k-2}^{(n,\nu)} \geq A_{k-1}^{(n,\nu)} > 0$ for $2 \leq k \leq n \leq N$, and the first one is properly large so that $(1-2\nu)A_0^{(n,\nu)} - (1-\nu)A_1^{(n,\nu)} \geq 0$ for $\nu \in [0,1/2]$.

A2. There is a constant $\pi_A > 0$, $A_{n-k}^{(n,\nu)} \geq \frac{1}{\pi_A} \int_{k-1}^k \omega_{1-\alpha}(t_n-s) \, ds$ for $1 \leq k \leq n \leq N$.

A3. There is a constant $\rho > 0$ such that the local step ratio $\rho_k \leq \rho$ for $1 \leq k \leq N-1$.

As noted in [13], the assumptions A1–A2 on the discrete convolution kernels $A_{n-k}^{(n,\nu)}$ are valid for the most frequently used discrete Caputo derivatives, at least if assumption A3 is satisfied for appropriate $\rho$. Actually, the local mesh parameter $\rho$ in A3 will also appear in our discrete fractional Grönwall inequality and the $H^1$-norm stability estimate.

### 2.2 An $H^1$-norm stability

Always, the $H^1$-norm stability and convergence analysis on (general) nonuniform meshes makes use of a discrete fractional Grönwall inequality and a global consistency analysis, which involve a complementary discrete convolution kernel $P_{n-k}^{(n,\nu)}$ introduced by Liao et al. [12,13] and having the identical property

$$\sum_{j=k}^n P_{n-j}^{(n,\nu)} A_{j-k}^{(n,\nu)} \equiv 1 \quad \text{for } 1 \leq k \leq n \leq N.$$  \hspace{1cm} (2.4)

In fact, rearranging this identity yields a recursive formula (in effect, a definition)

$$P_0^{(n,\nu)} := \frac{1}{A_0^{(n,\nu)}}, \quad P_{n-j}^{(n,\nu)} := \frac{1}{A_{j-k}^{(n,\nu)}} \sum_{k=j+1}^n \left( A_{k-j-1}^{(k,\nu)} - A_{k-j}^{(k,\nu)} \right) P_{n-k}^{(n,\nu)} \quad \text{for } 1 \leq j \leq n - 1.$$  \hspace{1cm} (2.5)

Actually, it has been shown [13] Lemma 2.2] that $P_{n-k}^{(n,\nu)}$ is well-defined and non-negative if the assumption A1 holds. Furthermore, if the assumption A2 holds, then

$$\sum_{j=1}^n P_{n-j}^{(n,\nu)} \omega_{1+m\alpha}(t_n) \leq \pi_A \omega_{1+m\alpha}(t_n) \quad \text{for } 1 \leq n \leq N \text{ and } m = 0,1.$$  \hspace{1cm} (2.6)

Next we give a discrete fractional Grönwall inequality [13] Theorem 3.4], which should be fit for the classical $H^1$-norm stability analysis.
Theorem 2.1. Let the assumptions A1–A3 hold, let $0 \leq \nu < 1/2$, and let $(g^n)_n^{N}$ and $(\lambda_l)_l^{N-1}$ be given non-negative sequences. Assume further that there exists a constant $\Lambda$ (independent of the time-step sizes) such that $\Lambda \geq \sum_{l=0}^{N-1} \lambda_l$, and that the maximum step size satisfies

$$\tau \leq \frac{1}{\sqrt{2\pi A \Gamma(2 - \alpha) \Lambda}}.$$  

For any non-negative sequence $(v^k)_{k=0}^{N}$ such that

$$\sum_{k=1}^{n} A^{(n,\nu)}_{n-k} \nabla \tau v^k \leq \sum_{k=1}^{n} \lambda_{n-k} v^{k-\nu} + g^n \quad \text{for } 1 \leq n \leq N,$$

or

$$v^n \leq v^0 + \sum_{j=1}^{n} P^{(n,\nu)}_{n-j} \sum_{k=1}^{j} \lambda_{j-k} v^{k-\nu} + \sum_{j=1}^{n} P^{(n,\nu)}_{n-j} g^j \quad \text{for } 1 \leq n \leq N,$$

then it holds that

$$v^n \leq 2E_\alpha \left( 2 \max \{1, \rho\} \pi A \Lambda t^n_\alpha \right) \left( v^0 + \max_{1 \leq k \leq n} \sum_{j=1}^{k} P^{(k,\nu)}_{j-k} g^j \right)$$

$$\leq 2E_\alpha \left( 2 \max \{1, \rho\} \pi A \Lambda t^n_\alpha \right) \left( v^0 + \pi \alpha \Gamma(1 - \alpha) \max_{1 \leq k \leq n} \left\{ t^n_k g^k \right\} \right) \quad \text{for } 1 \leq n \leq N.$$

In the subsequent discrete energy approach, we also need the following lemma, which can be verified by a similar proof of [13, Lemma 4.1].

Lemma 2.1. If the condition A1 holds, the discrete Caputo formula (2.1) satisfies

$$v^{n-\nu} \left( D_\tau^\alpha v \right)^{n-\nu} \geq \frac{1}{2} \sum_{k=1}^{n} A^{(n,\nu)}_{n-k} \nabla \tau \left( |v^k|^2 \right) \quad \text{for } 1 \leq n \leq N.$$

We now consider the stability of the unified scheme (2.3) by assuming that $u_b(x, t_n) = 0$. By taking the inner product of the first equation in (2.3) with $2 \left( D_\tau^\alpha u_h \right)^{n-\nu}$, one has

$$2 \left\| \left( D_\tau^\alpha u_h \right)^{n-\nu} \right\|^2 + 2 \left\langle \mathcal{L}_h u_h^{n-\nu}, \left( D_\tau^\alpha u_h \right)^{n-\nu} \right\rangle = 2 \left\langle c u_h^{n-\nu}, \left( D_\tau^\alpha u_h \right)^{n-\nu} \right\rangle + 2 \left\langle f^{n-\nu}, \left( D_\tau^\alpha u_h \right)^{n-\nu} \right\rangle$$

$$\leq 2 \left\| \left( D_\tau^\alpha u_h \right)^{n-\nu} \right\|^2 + \kappa^2 \left\| u_h^{n-\nu} \right\|^2 + \left\| f^{n-\nu} \right\|^2.$$

Therefore, applying Lemma 2.1 ($v := L_{h_1}^{1/2} u_h$) and the embedding inequality, one gets

$$\sum_{k=1}^{n} A^{(n,\nu)}_{n-k} \nabla \tau \left( |u_h^k|^2 \right) \leq 2\kappa^2 C_{\Omega} \left( (1 - \nu)^2 |u_h^0|^2 + \nu^2 |u_h^{n-1}|^2 \right) + \left\| f^{n-\nu} \right\|^2$$

$$\leq 2\kappa^2 C_{\Omega} \left( (1 - \nu)^2 |u_h^0|^2 + \nu |u_h^{n-1}|^2 \right) + \left\| f^{n-\nu} \right\|^2, \quad 1 \leq n \leq N,$$

which has the form of (2.7) with $\lambda_l = 0$ for $l \geq 1$,

$$\lambda_0 := 2\kappa^2 C_{\Omega}, \quad v^k := |u_h^k|^2 \quad \text{and} \quad g^n := \left\| f^{n-\nu} \right\|^2.$$

Theorem 2.2 says that the weighted time-stepping method (2.3) is stable in the following sense.

Theorem 2.2. If A1–A3 hold with the maximum time-step size $\tau \leq 1 / \sqrt{4\pi A \Gamma(2 - \alpha) \kappa^2 C_{\Omega}}$, then the time-stepping scheme (2.3) with $u_b(x, t_n) = 0$ is stable in the $H^1$-norm, that is,

$$\left\| u_h^n \right\|^2 \leq 2E_\alpha \left( 4\pi A \max \{1, \rho\} \kappa^2 C_{\Omega} t^n_\alpha \right) \left( |u_h^0|^2 + \max_{1 \leq k \leq n} \sum_{j=1}^{k} P^{(k,\nu)}_{j-k} \left\| f^{j-\nu} \right\|^2 \right)$$

$$\leq 2E_\alpha \left( 4\pi A \max \{1, \rho\} \kappa^2 C_{\Omega} t^n_\alpha \right) \left( |u_h^0|^2 + \pi \alpha \Gamma(1 - \alpha) \max_{1 \leq k \leq n} \left\{ t^n_k \left\| f^{k-\nu} \right\|^2 \right\} \right) \quad \text{for } 1 \leq n \leq N.$$
2.3 An improved Grönwall inequality

It is easy to check that, the solution error, $\tilde{u}_h^n := u(x, t_n) - u^n_h$ for $x \in \Omega_h$, satisfies the zero-valued initial and boundary conditions, and the governing equation

$$(D^\nu_t \tilde{u}_h)^{n-\nu} + \mathcal{L}_h \tilde{u}_h^{n-\nu} = c(x) \tilde{u}_h^{n-\nu} + \Upsilon_h^{n-\nu}[u] + R_w^{n-\nu} + R_s^{n-\nu} \quad \text{for } x \in \Omega_h \text{ and } 1 \leq n \leq N,$$  \hfill (2.9)

where $\Upsilon_h^{n-\nu}[u]$ is defined by (2.2),

$$R_w^{n-\nu} := (c(x) - \mathcal{L})[u^{n-\nu} - u(t_{n-\nu})] \quad \text{and} \quad R_s^{n-\nu} := (\mathcal{L} - \mathcal{L}_h)u^{n-\nu}. \hfill (2.10)$$

Nonetheless, it always yields a suboptimal $H^1$-norm error estimate if the a priori estimate in Theorem 2.2 is directly applied to the above error system, because the global consistency error $\sum_{j=1}^k P_{k-j}^{(k,\nu)} \| \Upsilon_h^{j-\nu}[u] \|^2$ has a loss of time accuracy, see an example in the next section.

To end this section, we present an extension of the fractional Grönwall inequality in [13, Theorem 3.1]. This result will be useful to obtain the optimal time accuracy in the $H^1$-norm.

**Theorem 2.3.** Let the assumptions A1–A3 hold, let $0 \leq \nu < 1/2$, and let $(\xi^n)_{n=1}^N$, $(\eta^n)_{n=1}^N$ and $(\lambda_l)_{l=0}^{N-1}$ be given non-negative sequences. Assume further that there exists a constant $\Lambda$ (independent of the step sizes) such that $\Lambda \geq \sum_{l=0}^{N-1} \lambda_l$, and that the maximum step size satisfies

$$\tau \leq \frac{1}{\sqrt[3]{2\pi \Lambda}}.$$

For any non-negative sequence $(v^k)_{k=0}^N$ such that

$$\sum_{k=1}^n A_{n-k}^{(n,\nu)} \nabla \tau (v^k)^2 \leq \sum_{k=1}^n \lambda_{n-k} (v^{k-\nu})^2 + v^{n-\nu} \xi^n + (\eta^n)^2 \quad \text{for } 1 \leq n \leq N, \hfill (2.11)$$

or

$$(v^n)^2 \leq (v^0)^2 + \sum_{j=1}^n P_{n-j}^{(n,\nu)} \sum_{j=1}^n \lambda_{j-k} (v^{j-\nu})^2 + \sum_{j=1}^n P_{n-j}^{(n,\nu)} v^{j-\nu} \xi^j + \sum_{j=1}^n P_{n-j}^{(n,\nu)} (\eta^j)^2. \hfill (2.12)$$

Then it holds that, for $1 \leq n \leq N$,

$$v^n \leq 2E_{\alpha} \left( \max \{1, \rho \} \pi_A \alpha \right) \left( v^0 + \max_{1 \leq k \leq n} \sum_{j=1}^k P_{k-j}^{(k,\nu)} \xi^j + \sqrt{\pi \Lambda} \left( \alpha \right) \max_{1 \leq k \leq n} \left\{ l_k^{\alpha/2} \eta^k \right\} \right). \hfill (2.13)$$

**Proof.** Two different cases are considered with a notation $E_{\alpha} := 2E_\alpha \left( \max \{1, \rho \} \pi_A \alpha \right)$. If

$$v^n \leq \eta^n := \sqrt{\pi \Lambda} \left( \alpha \right) \max_{1 \leq k \leq n} \left\{ l_k^{\alpha/2} \eta^k \right\},$$

then the claimed inequality (2.13) follows because $E_{\alpha} \geq 2$ for any $0 < \alpha < 1$ and $n \geq 0$. Otherwise, if $v^n > \eta^n$, then $v^n > \sqrt{\pi \Lambda} \left( \alpha \right) \frac{2}{n} \eta^n$ and the inequality (2.11) becomes

$$\sum_{k=1}^n A_{n-k}^{(n,\nu)} \nabla \tau (v^k)^2 \leq \sum_{k=1}^n \lambda_{n-k} (v^{k-\nu})^2 + v^{n-\nu} \xi^n + v^n \frac{\eta^n}{\sqrt{\pi \Lambda} \left( \alpha \right) l_n \eta^n} \quad \text{for } 1 \leq n \leq N. \hfill (2.14)$$

Therefore, following the proof of [13, Theorem 3.1] with

$$g^n = \xi^n + \frac{\eta^n}{\sqrt{\pi \Lambda} \left( \alpha \right) l_n \eta^n},$$
one can apply (2.10) to obtain that

\[ v^n \leq E^\alpha_n \left( v^0 + \max_{1 \leq k \leq n} \sum_{j=1}^k P^{(k,\nu)}_{k-j} \xi_j + \max_{1 \leq k \leq n} \sum_{j=1}^k P^{(k,\nu)}_{k-j} \frac{\eta_j}{\pi A \Gamma(1-\alpha)} \right) \]

\[ \leq E^\alpha_n \left( v^0 + \max_{1 \leq k \leq n} \sum_{j=1}^k P^{(k,\nu)}_{k-j} \xi_j + \sqrt{\Gamma(1-\alpha)/\pi_A} \max_{1 \leq k \leq n} \left\{ t^{\alpha/2}_k \right\} \max_{1 \leq k \leq n} \left\{ \sum_{j=1}^k P^{(k,\nu)}_{k-j} \omega_1-\omega_2(t_j) \right\} \right) \]

\[ \leq E^\alpha_n \left( v^0 + \max_{1 \leq k \leq n} \sum_{j=1}^k P^{(k,\nu)}_{k-j} \xi_j + \sqrt{\pi_A \Gamma(1-\alpha)} \max_{1 \leq k \leq n} \left\{ t^{\alpha/2}_k \eta^k \right\} \right). \]

It completes the proof. \( \square \)

Remark 1. One may use the inequality (2.6) to bound the summation \( \sum_{j=1}^k P^{(k,\nu)}_{k-j} \xi_j \), that is,

\[ \sum_{j=1}^k P^{(k,\nu)}_{k-j} \xi_j \leq \sum_{j=1}^k P^{(k,\nu)}_{k-j} \omega_1-\omega_2(t_j) \frac{\xi_j}{\omega_1-\omega_2(t_j)} \leq \pi_A \max_{1 \leq j \leq k} \xi_j. \]

So the discrete solution of (2.11) can also be bounded by

\[ v^n \leq 2E^\alpha \left( 2\max\{1,\rho\} \pi A \Lambda t_n^\alpha \right) \left( v^0 + \pi A \Gamma(1-\alpha) \max_{1 \leq k \leq n} \left\{ t^{\alpha/2}_k \right\} + \sqrt{\pi A \Gamma(1-\alpha)} \max_{1 \leq k \leq n} \left\{ t^{\alpha/2}_k \eta^k \right\} \right). \]

On the other hand, if the given sequence \((\lambda_i)_{i=0}^{N-1}\) is non-positive and the constant \(\Lambda \leq 0\), a similar argument will show that the discrete inequality (2.13) holds in a simpler form, requiring only the assumptions A1-A2 but no restrictions on time steps,

\[ v^n \leq v^0 + \max_{1 \leq k \leq n} \sum_{j=1}^k P^{(k,\nu)}_{k-j} \xi_j + \sqrt{\pi A \Gamma(1-\alpha)} \max_{1 \leq k \leq n} \left\{ t^{\alpha/2}_k \eta^k \right\} \]

\[ \leq v^0 + \pi A \Gamma(1-\alpha) \max_{1 \leq j \leq n} \left\{ t^{\alpha/2}_j \right\} + \sqrt{\pi A \Gamma(1-\alpha)} \max_{1 \leq k \leq n} \left\{ t^{\alpha/2}_k \eta^k \right\} \quad \text{for } 1 \leq n \leq N. \] (2.15)

3 Sharp \(H^1\)-norm error estimate for L1 scheme

In this section, assume that the solution \(u \in C([0,T]; H^1(\Omega)) \cap C^2_0((0,T]; H^1(\Omega))\). The Caputo’s derivative \(D^\nu_t v\) is approximated by the L1 formula \((D^\nu_t v)^n\), the case of \(\nu = 0\) in (2.1), with unequal time-steps. The corresponding discrete convolution kernel \(A_{n-k}^{(n,0)}\) is defined by

\[ A_{n-k}^{(n,0)} := \int_{t_{k-1}}^{t_k} \omega_1-\omega_2(t_n-s) \frac{ds}{\tau_k}, \quad 1 \leq k \leq n. \] (3.1)

Obviously, A2 holds for \(\pi_A = 1\), and next Lemma implies that A1 is valid.

Lemma 3.1. [33, Lemma 2.1] For fixed \(n \geq 2\), the discrete kernel \(A_{n-k}^{(n,0)}\) in (3.1) satisfies

\[ A_{n-k}^{(n,0)} = A_{n-k-1}^{(n,0)} + \frac{1}{2} \int_{t_{k-1}}^{t_k} d\omega_1-\omega_2(t_n-s) > 0 \quad \text{for } 1 \leq k \leq n-1. \]

Hence we can use the complementary discrete convolution kernel \(P_{n-k}^{(n,0)}\), see (2.4)-(2.6), in the subsequent analysis. Also, Lemma 3.1 and Theorem 2.2 imply the unconditional stability of L1 scheme for the linear problem (1.1).
Corollary 3.1. The L1 method \([2\text{.}3]\) with \(\nu = 0\) is stable in the discrete \(H^1\) norm.

For the L1 scheme \([2\text{.}1]\) with the discrete convolution kernels \([5\text{.}1]\), we have the following estimate on the consistency error.

Lemma 3.2. For \(v \in C^2_\sigma((0, T])\), the local consistency error of the L1 formula \((D^\nu v)^n\) satisfies

\[
|\Upsilon^n[v]| \leq A_0(n, 0)G^n + \sum_{k=1}^{n-1} (A_{n-k-1}^{(n, 0)} - A_{n-k}^{(n, 0)})G^k \text{ for } n \geq 1,
\]

where \(G^k\) is defined by \(G^k := 2\int_{t_{k-1}}^{t_k} |v''(t)| \, dt\). Thus the global consistency error

\[
\sum_{j=1}^{n} P_{n-j}^{(n, 0)} |\Upsilon^j[v]| \leq \frac{C_v}{\sigma} \tau_1 + \frac{C_v}{1 - \alpha} \max_{2 \leq k \leq n} t_k \tau_k^{\sigma - 2 \alpha} \text{ for } n \geq 1.
\]

Moreover, if the time mesh satisfies \(\text{M-conv}\), then

\[
\sum_{j=1}^{n} P_{n-j}^{(n, 0)} |\Upsilon^j[v]| \leq \frac{C_v}{\sigma(1 - \alpha)} \tau^{\min(2 - \alpha, \gamma \sigma)} \text{ for } 1 \leq n \leq N.
\]

Proof. See the proof of Lemmas 3.1 and 3.3 (taking \(\epsilon = 0\)) in [15].

3.1 Suboptimal estimate by traditional \(H^1\)-norm analysis

In this subsection, we show that the traditional \(H^1\)-norm analysis together with the discrete Grönwall inequality in Theorem \([2\text{.}1]\) always yields a suboptimal estimate in the \(H^1\)-norm, if the solution is nonsmooth near the initial time. Without losing the generality, we consider the error equation \([2\text{.}9]\) with \(\nu = 0\), that is,

\[
(D^\nu \tilde{u}^n_h) + L_h \tilde{u}^n_h = c(x) \tilde{u}^n_h + \Upsilon^n_h[u] + R^n_s \text{ for } x \in \Omega_h \text{ and } 1 \leq n \leq N,
\]

where \(\Upsilon^n_h[u]\) and \(R^n_s\) are defined by \([2\text{.}2]\) and \([2\text{.}10]\), respectively. Taking the inner product of the error equation in \([3\text{.}2]\) with \(2(D^\nu \tilde{u}^n_h)^n\), one has

\[
2\| (D^\nu \tilde{u}^n_h)^n \|^2 + 2\langle L_h \tilde{u}^n_h, (D^\nu \tilde{u}^n_h)^n \rangle = 2\langle c\tilde{u}^n_h, (D^\nu \tilde{u}^n_h)^n \rangle + 2\langle \Upsilon^n_h[u] + R^n_s, (D^\nu \tilde{u}^n_h)^n \rangle \
\leq 2\| (D^\nu \tilde{u}^n_h)^n \|^2 + \kappa^2\|\tilde{u}^n_h\|^2 + \|\Upsilon^n_h[u] + R^n_s\|^2.
\]

Lemma \[3\text{.}1\] ensures \(\text{A1}\), so we apply Lemma \([2\text{.}1]\) and the embedding inequality to get

\[
\sum_{k=1}^{n} A_{n-k}^{(n, 0)} \| (\tilde{u}^n_h)^2 \|_{1, h} \leq \kappa^2 C_\Omega \|\tilde{u}^n_h\|^2 + \|\Upsilon^n_h[u] + R^n_s\|^2,
\]

which takes the form of \([2\text{.}7]\) with \(\nu^k = \|\tilde{u}^k_h\|^2\) and \(g^n = \|\Upsilon^n_h[u] + R^n_s\|^2\). So Theorem \([2\text{.}1]\) together with the upper bound \([2\text{.}0]\) yields the following estimate

\[
\|\tilde{u}^n_h\|^2 \leq 2E_{\alpha} \left( 2 \max(1, \rho) \kappa^2 C_\Omega t^n \right) \left( \max_{1 \leq k \leq n} \sum_{j=1}^{k} P_{k-j}^{(k, 0)} \|\Upsilon^j_h[u]\|^2 + \Gamma(1 - \alpha) \max_{1 \leq k \leq n} \tau_k^{\alpha \|R^n_s\|^2} \right),
\]

if the maximum time-step size \(\tau \leq 1/\sqrt[\nu]{2\Gamma(2 - \alpha)\kappa^2 C_\Omega}\). To continue the error analysis, one requires the following result, which takes advantage of the discrete convolution structure of local truncation error in Lemma \([3\text{.}2]\).
Lemma 3.3. If \( v \in C^2_\sigma((0,T)) \) for \( \sigma \in (\frac{\alpha}{2},1) \cup (1,2) \) and the maximum step ratio \( \rho \leq 1 \), then
\[
\sum_{j=1}^{n} P_{n-j}^{(n,0)} |\mathcal{T}^j[v]|^2 \leq \frac{C_v}{\sigma^2} \tau_1^{2\alpha} + \frac{C_v}{1-\alpha} \max_{2 \leq k \leq n} t_k \tau_k^{4-2\alpha} \quad \text{for } 1 \leq n \leq N.
\]
Moreover, if the time mesh satisfies \textbf{M-conv}, then
\[
\sum_{j=1}^{n} P_{n-j}^{(n,0)} |\mathcal{T}^j[v]|^2 \leq \frac{C_v}{\sigma^2 (1-\alpha)} \tau^{2\min\{2-\alpha, \gamma(\sigma-\alpha/2)\}} \quad \text{for } 1 \leq n \leq N.
\]

Proof. Applying Lemma 3.2 and the Cauchy-Schwarz inequality, one has
\[
|\mathcal{T}^j[v]|^2 \leq \left( 2A_0^{(j,0)} - A_{j-1}^{(j,0)} \right) \left[ A_0^{(j,0)} (G^j)^2 + \sum_{k=1}^{j-1} (A_{j-k-1}^{(j,0)} - A_{j-k}^{(j,0)}) (G^k)^2 \right]
\leq 2 \left( A_0^{(j,0)} G^j \right)^2 + 2 \sum_{k=1}^{j-1} A_0^{(j,0)} (A_{j-k-1}^{(j,0)} - A_{j-k}^{(j,0)}) (G^k)^2.
\]
The definition (3.1) gives \( A_0^{(j,0)} = \tau_j^{-\alpha}/\Gamma(2-\alpha) \) such that \( \max_{k+1 \leq j \leq n} A_0^{(j,0)} = A_0^{(k,0)} \) if the maximum ratio \( \rho \leq 1 \). Multiplying the above inequality by \( P_{n-j}^{(n,0)} \) and summing the index \( j \) from 1 to \( n \), we exchange the order of summation and apply the definition (2.5) of \( P_{n-j}^{(n,0)} \) to get
\[
\sum_{j=1}^{n} P_{n-j}^{(n,0)} |\mathcal{T}^j[v]|^2 \leq 2 \sum_{j=1}^{n} P_{n-j}^{(n,0)} (A_0^{(j,0)} G^j)^2 + 2 \sum_{j=1}^{n} P_{n-j}^{(n,0)} \sum_{k=1}^{j-1} A_0^{(j,0)} (A_{j-k-1}^{(j,0)} - A_{j-k}^{(j,0)}) (G^k)^2.
\]
\[
= 2 \sum_{j=1}^{n} P_{n-j}^{(n,0)} (A_0^{(j,0)} G^j)^2 + 2 \sum_{k=1}^{n-1} (G^k)^2 \sum_{j=k+1}^{n} P_{n-j}^{(n,0)} A_0^{(j,0)} (A_{j-k-1}^{(j,0)} - A_{j-k}^{(j,0)})
\leq 2 \sum_{j=1}^{n} P_{n-j}^{(n,0)} (A_0^{(j,0)} G^j)^2 + 2 \sum_{k=1}^{n-1} (G^k)^2 A_0^{(k,0)} \sum_{j=k+1}^{n} P_{n-j}^{(n,0)} (A_{j-k-1}^{(j,0)} - A_{j-k}^{(j,0)})
\]
\[
= 2 \sum_{j=1}^{n} P_{n-j}^{(n,0)} (A_0^{(j,0)} G^j)^2 + 2 \sum_{k=1}^{n-1} P_{n-k}^{(n,0)} (A_0^{(k,0)} G^k)^2 \quad \text{for } 1 \leq n \leq N. \quad (3.4)
\]

Now, following the proof of Lemma 3.3 in [12], one can apply the definition (3.1) to find that
\[
\frac{A_0^{(k,0)}}{A_0^{(k-2,0)}} < \frac{\omega_{2-\alpha}(\tau_k)}{\tau_k \omega_{1-\alpha}(t_k - t_1)} = \frac{(t_k - t_1)^\alpha}{\tau_k^\alpha}, \quad 2 \leq k \leq n.
\]
The regularity assumption implies that
\[
G^j \leq C_v \tau_j^\sigma / \sigma \quad \text{and} \quad G^k \leq C_v t_k^{\sigma-2} \tau_k^2 \quad \text{for } 2 \leq k \leq n.
\]
Furthermore, the property (2.4) shows that \( P_{n-1}^{(n,0)} A_0^{(1,0)} \leq 1 \) and \( \sum_{k=2}^{n} P_{n-k}^{(n,0)} A_0^{(k,0)} = 1. \) Thus it
follows from (3.4) that
\[
\sum_{j=1}^{n} P_{n-j}^{(n,0)} |\mathcal{Y}^{j}[u]|^2 \leq 4P_{n-1}^{(n,0)} (A_0^{(1,0)}G^1)^2 + 4 \sum_{k=2}^{n} P_{n-k}^{(n)} (A_0^{(k,0)}G^k)^2 \\
\leq 4A_0^{(1,0)} (G^1)^2 + \frac{4}{1-\alpha} \sum_{k=2}^{n} P_{n-k}^{(n,0)} t_k^{\alpha} \tau_k^{-\alpha} A_0^{(k,0)} (G^k)^2 \\
\leq C_v \tau_1^{2-\alpha/\sigma^2} + \frac{C_u}{1-\alpha} \sum_{k=2}^{n} P_{n-k}^{(n,0)} t_k^{\alpha} t_k^{-\alpha} \tau_k^{-\alpha} \\
\leq C_v \tau_1^{2-\alpha/\sigma^2} + \frac{C_u}{1-\alpha} \max_{2 \leq k \leq n} t_k^{\alpha} t_k^{-\alpha} \tau_k^{-\alpha} \text{ for } 1 \leq n \leq N.
\]

If the mesh fulfills \textbf{M-conv}, then \( \tau_1 \leq C_\gamma \tau^\gamma \) and, with \( \beta := 2 \min\{2-\alpha, \gamma(\sigma-\alpha/2)\} \),
\[
t_k^{\alpha} t_k^{-\alpha} \tau_k^{-\alpha} \leq C_\gamma t_k^{2-\alpha} \tau_k^{-\alpha} \leq C_\gamma (t_k^{1-\alpha}) \beta \text{ for } 2 \leq k \leq n.
\]

It leads to the desired estimate and completes the proof. \( \square \)

Since \( u \in C([0,T]; H^4(\Omega)) \), one has the spatial error estimate \( \|R_n^k\| \leq C_u h^2 \). Applying the zero-valued initial data and Lemma 3.3 one derive from (3.3) that
\[
|\tilde{u}_h^n|_{1} \leq C_u \max_{1 \leq k \leq n} \sum_{j=1}^{k} P_{k-j}^{(k,0)} |\mathcal{Y}^{j}[u]|^2 + C_u \Gamma(1-\alpha) \max_{1 \leq k \leq n} t_k^{\alpha} \|R_n^k\| \\
\leq C_u \sigma^2 \|\mathcal{Y}[u]\| \left( \tau^{\min\{2-\alpha, \gamma(\sigma-\alpha/2)\}} + t_n^{\alpha} h^2 \right)
\]
or
\[
|\tilde{u}_h^n|_{1} \leq C_u \sigma \left( \tau^{\min\{2-\alpha, \gamma(\sigma-\alpha/2)\}} + t_n^{\alpha} h^2 \right) \text{ for } 1 \leq n \leq N. \quad (3.5)
\]

It is optimal only when the regularity parameter \( \sigma \geq 2-\alpha/2 \), see previous studies \cite{11,28} by assuming the solution is smooth near the initial time; however, there is always a loss of theoretical accuracy \( O(\tau^{-\alpha/2}) \) in time under the realistic assumption.

**Remark 2.** As similar to the ordinary diffusion case corresponding to \( \alpha = 1 \), the standard \( L^2 \)-norm error analysis \cite{12} leads to the sharp estimate for a weighted \( H^1 \) norm, but always gives a suboptimal estimate for the \( H^1 \)-norm error at any time \( t_n \), see also \cite{16,17,27} for the analysis considering the smooth solutions. Actually, by taking the inner product of the error equation in (3.2) with \( \tilde{u}_h^n \) and applying the Cauchy-Schwarz inequality, one has
\[
\langle (P_{\tau}^\alpha \tilde{u}_h^n, \tilde{u}_h^n) + |\tilde{u}_h^n|_{1}^2 \leq \kappa \|\tilde{u}_h^n\|^2 + \|\tilde{u}_h^n\| |\mathcal{Y}^{j}[u]| + R_n^j \rangle.
\]

Therefore, applying Lemma 2.7 we have
\[
\sum_{k=1}^{j} A_{j-k}^{(j,0)} \mathcal{Y}^{j}(\|\tilde{u}_h^n\|^2) + 2 |\tilde{u}_h^n|_{1}^2 \leq 2 \kappa \|\tilde{u}_h^n\|^2 + 2 \|\tilde{u}_h^n\| |\mathcal{Y}^{j}[u]| + R_n^j.
\]

Multiplying the above inequality by \( P_{n-j}^{(n,0)} \) and summing the index \( j \) from 1 to \( n \), we get
\[
\|\tilde{u}_h^n\|^2 + 2 \sum_{j=1}^{n} P_{n-j}^{(n,0)} |\tilde{u}_h^n|_{1}^2 \leq 2 \kappa \sum_{j=1}^{n} P_{n-j}^{(n,0)} |\tilde{u}_h^n|^2 + 2 \|\tilde{u}_h^n\| |\mathcal{Y}^{j}[u]| + R_n^j.
\]
or, with $\|\tilde{u}_h^n\| := \sqrt{\|\tilde{u}_h^n\|^2 + 2\sum_{j=1}^n P_{n-j}^{(n,0)} \|\tilde{u}_h^j\|^2}$,

$$\|\tilde{u}_h^n\|^2 \leq \|\tilde{u}_h^0\|^2 + 2\kappa \sum_{j=1}^n P_{n-j}^{(n,0)} \|\tilde{u}_h^j\|^2 + 2\sum_{j=1}^n P_{n-j}^{(n,0)} \|\tilde{u}_h^j\| \|\tilde{Y}_h^j[u] + R_s^n\|,$$

which takes the form of (2.12) with $v^n = \|\tilde{u}_h^n\|$, $\xi^j = 2\|\tilde{Y}_h^j[u] + R_s^n\|$ and $\eta^j = 0$. So the discrete Grönwall inequality in Theorem 2.3 yields

$$\|\tilde{u}_h^n\| \leq 4E_\alpha \left(2\max(1,\rho)\kappa t_n^\alpha \right) \left(\|\tilde{u}_h^0\| + \max_{1\leq k\leq n} \sum_{j=1}^k P_{k-j}^{(k,0)} \|\tilde{Y}_h^k[u] + R_s^n\| \right),$$

if the maximum step size $\tau \leq 1/ \sqrt{4\Gamma(2-\alpha)\kappa}$. Applying the spatial error estimate $\|R_s^n\| \leq C_u h^2$ and Lemma 3.2 we have the sharp estimate for a weighted $H^1$-norm

$$\sqrt{\|\tilde{u}_h^n\|^2 + \sum_{j=1}^n P_{n-j}^{(n,0)} \|\tilde{u}_h^j\|^2} \leq \frac{C_u}{\sigma(1-\alpha)} (\tau^{\min(2-\alpha,\gamma)\sigma} + t_n^\alpha h^2) \quad \text{for} \quad 1 \leq n \leq N.$$

However, a loss of accuracy $O(\tau_n^{-\frac{\alpha}{2}})$ will be seen in the $H^1$-norm error at any time $t_n$, $|\tilde{u}_h^n|_1 \leq \sqrt{A_0^{(n,0)} \sum_{j=1}^n P_{n-j}^{(n,0)} \|\tilde{u}_h^j\|_1^2} \leq \frac{C_u}{\sigma(1-\alpha)} \tau_n^{-\frac{\alpha}{2}} (\tau^{\min(2-\alpha,\gamma)\sigma} + t_n^\alpha h^2) \quad \text{for} \quad 1 \leq n \leq N.$$

Compared with (3.5), the loss of accuracy appears both in time and space.

### 3.2 Sharp $H^1$-norm error estimate

A sharp $H^1$-norm error estimate reflecting the initial singularity is obtained by applying the improved discrete Grönwall inequality in Theorem 2.3 and treating the temporal truncation error specially. We will redefine the time truncation error uniformly over the closed space domain, that is, $\tilde{Y}_h^n[u]$ in (3.2) can be redefined as follows, see Remark 3 below,

$$\tilde{Y}_h^n[u] := (D^\alpha_t u_h)(t_n) - (D^\alpha_t u_h)^n \quad \text{for} \quad x \in \tilde{\Omega}_h \text{ and } 1 \leq n \leq N.$$  \hspace{1cm} (3.6)

Then the error equation (3.2) can be formulated as

$$(D^\alpha_t \tilde{u}_h)^n = -L_h \tilde{u}_h^n + c(x) \tilde{u}_h^n + \tilde{Y}_h^n[u] + R_s^n \quad \text{for} \quad x \in \Omega_h \text{ and } 1 \leq n \leq N.$$

By taking the inner product of the error equation in (3.7) with $L_h \tilde{u}_h^n$, one applies the discrete first Green formula to find

$$\langle (D^\alpha_t \tilde{u}_h)^n, L_h \tilde{u}_h^n \rangle = -\|L_h \tilde{u}_h^n\|^2 + \langle c\tilde{u}_h^n, L_h \tilde{u}_h^n \rangle + \langle \mu \partial_h \tilde{Y}_h^n[u], \partial_h \tilde{u}_h^n \rangle + \langle R_s^n, L_h \tilde{u}_h^n \rangle \leq \frac{1}{2} \kappa^2 \|\tilde{u}_h^n\|^2 + \|\tilde{u}_h^n\|_1 \|\tilde{Y}_h^n[u]\|_1 + \frac{1}{2} \|R_s^n\|^2 \leq \frac{1}{2} \kappa^2 C_\Omega \|\tilde{u}_h^n\|_1^2 + \|\tilde{u}_h^n\|_1 \|\tilde{Y}_h^n[u]\|_1 + \frac{1}{2} \|R_s^n\|^2,$$

where the Cauchy-Schwarz inequality and the embedding inequality have been used. We apply Lemma 2.1 to obtain

$$\sum_{k=1}^n A^{(n,0)}_{n-k} \nabla_\tau (\|\tilde{u}_h^k\|^2) \leq \kappa^2 C_\Omega \|\tilde{u}_h^n\|_1^2 + 2 \|\tilde{u}_h^n\|_1 \|\tilde{Y}_h^n[u]\|_1 + \|R_s^n\|^2, \quad 1 \leq n \leq N,$$
which has the form of (2.11) with \( \lambda_0 := \kappa^2 C_\Omega \), \( \nu^k := |\bar{u}_h^k|_1 \), \( \xi^n := 2|\mathcal{T}_h[u]|_1 \) and \( \eta^n := \|R_s^n\| \). Therefore, applying Theorem 2.3 we see that

\[
|\bar{u}_h^n|_1 \leq 4E_{\alpha}(2\max\{1, \rho\}\kappa^2 C_\Omega t^n_\alpha) \max_{1 \leq k \leq n} \left( \sum_{j=1}^{k} P^{(k,0)}_{k-j} |\mathcal{T}_h[u]|_1 + \sqrt{\Gamma(1-\alpha)t_k^{\alpha/2}}\|R_s^k\| \right),
\]

(3.8)

if the maximum time-step size \( \tau \leq 1/\sqrt{2\Gamma(2-\alpha)\kappa^2 C_\Omega} \). It remains to evaluate the right-hand side of (3.8) by taking the initial singularity into account. Note that, the formula of Taylor expansion with integral expansion gives

\[
\partial_h(\mathcal{T}_h[u])(x_i-h^\alpha) = \int_0^1 (\mathcal{D}^\alpha_t \partial_x u(x_i-h^\alpha))(t) - (\mathcal{D}^\alpha_t \partial_x u(x_i-h^\alpha))^n \, \mathrm{d}\lambda
\]

for \( x \in \Omega_h \) and 1 \( \leq n \leq N \). Then Lemma 3.2 with \( v = \partial_x u \) gives the global consistency error

\[
\sum_{j=1}^{k} P^{(k,0)}_{k-j} |\mathcal{T}_h[u]|_1 \leq \frac{C_u}{\sigma(1-\alpha)\tau_{\text{min}(2-\alpha,\gamma\sigma)}} \quad \text{for} \quad 1 \leq k \leq N,
\]

and, obviously, \( \|R_s^k\| \leq C_u h^2 \). So the inequality (3.8) shows that

\[
|\bar{u}_h^n|_1 \leq \frac{C_u}{\sigma(1-\alpha)} E_{\alpha}(2\max\{1, \rho\}\kappa^2 C_\Omega t^n_\alpha) \left( \tau_{\text{min}(2-\alpha,\gamma\sigma)}^\alpha + t_n^{\alpha/2}h^2 \right) \quad \text{for} \quad 1 \leq n \leq N.
\]

It yields the following \( H^1 \)-norm error estimate.

**Theorem 3.1.** Assume that the subdiffusion solution \( u \in \mathcal{C}([0, T]; H^4(\Omega)) \cap \mathcal{C}_2^0([0, T]; H^1(\Omega)) \). If the maximum time-step size \( \tau \leq 1/\sqrt{2\Gamma(2-\alpha)\kappa^2 C_\Omega} \), then the solution of the L1 method (2.3) with \( \nu = 0 \) on the nonuniform mesh satisfying A3 and M-conv, is unconditionally convergent in the discrete \( H^1 \)-norm,

\[
|u(t_n) - u^n_h|_1 \leq \frac{C_u}{\sigma(1-\alpha)} E_{\alpha}(2\max\{1, \rho\}\kappa^2 C_\Omega t^n_\alpha) \left( \tau_{\text{min}(2-\alpha,\gamma\sigma)}^\alpha + t_n^{\alpha/2}h^2 \right),
\]

(3.9)

where \( C_u \) may depend on \( u \) and \( T \), but is uniformly bounded with respect to \( \alpha \) and \( \sigma \). It achieves an optimal time accuracy of order \( O(\tau^{2-\alpha}) \) if \( \gamma \geq \max\{1, (2-\alpha)/\sigma\} \).

**Remark 3.** The special treatment of consistency error in time is motivated by the time-space error-splitting technique proposed originally in [8–10] for obtaining the maximum norm error estimate via the discrete energy approach, see also [15] for a recent application in the numerical analysis of a nonlinear subdiffusion problem. To see it more clearly, we introduce \( w = (c(x) - \mathcal{L})u \) and reformulate the subdiffusion problem (1.1) into

\[
w = \mathcal{D}^\alpha_t u - f(x, t) \quad \text{for} \quad x \in \Omega \quad \text{and} \quad 0 < t \leq T,
\]

\[
w = (c(x) - \mathcal{L})u \quad \text{for} \quad x \in \Omega \quad \text{and} \quad 0 < t \leq T.
\]

The fully discrete system follows as

\[
w^n_h = (\mathcal{D}^\alpha_t u^n_h) - f(x, t_n) \quad \text{for} \quad x \in \Omega_h \quad \text{and} \quad 1 \leq n \leq N,
\]

\[
w^n_h = (c(x) - \mathcal{L}_h)u^n_h \quad \text{for} \quad x \in \Omega_h \quad \text{and} \quad 0 \leq n \leq N.
\]

Then the solution errors, \( \tilde{u}_h^n := w(x, t_n) - w^n_h \) and \( \bar{u}_h^n := u(x, t_n) - u^n_h \) for \( x \in \Omega_h \) satisfy

\[
\tilde{u}_h^n = (\mathcal{D}^\alpha_t \bar{u}_h^n) - \mathcal{T}_h^n[u] \quad \text{for} \quad x \in \Omega_h \quad \text{and} \quad 1 \leq n \leq N,
\]

\[
\bar{u}_h^n = (c(x) - \mathcal{L}_h)\bar{u}_h^n + R_s^n \quad \text{for} \quad x \in \Omega_h \quad \text{and} \quad 0 \leq n \leq N.
\]
We see that, the time and space truncation errors are redefined directly via this coupled error system. This is, the time truncation error is defined uniformly over the closed space domain and the spatial truncation error is defined uniformly over all time levels.

For the $H^1$-norm error estimate considered here, it needs only to redefine the time consistency error as done in [33]. It also motivates that we can obtain an optimal $H^1$-norm error estimate via two stages: a time-discrete system is considered in the first stage so that the time truncation error is defined uniformly with respect to the spatial domain. As the spatial approximation of an elliptic problem, the fully-discrete system can be treated traditionally in the second stage and an optimal $H^1$-norm error estimate would be achieved because it does not involve the time consistency error. We will illuminate the two-stage process in the next section for a second-order scheme although it seems unusual in finite difference method.

4 Sharp $H^1$-norm error estimate for FracCN scheme

To present an alternative approach for a sharp $H^1$-norm error estimate, we recall the usual inner product $(v, w) = \int_\Omega v(x) w(x) \, dx$ with the associated $L^2(\Omega)$ norm $\|v\|_{L^2(\Omega)} = \sqrt{(v, v)}$. For any functions $v$ and $w$ belonging to the space of grid functions that vanish on the boundary $\partial \Omega$, define the $H^1$-seminorm $|v|_{H^1(\Omega)} = \sqrt{(\mu \partial_x v, \partial_x v)}$. There exists a positive constant $C_\Omega$ is dependent on the domain $\Omega$, the constants $\mu_0$ and $\mu_1$, such that $\|v\|_{L^2(\Omega)} \leq C_\Omega \|v\|_{H^1(\Omega)}$. Moreover, one has

$$|v|_1 \leq C_\Omega \|v\|_{H^1(\Omega)} \quad (4.1)$$

which can be checked by the Cauchy-Schwarz inequality with $\partial \Omega v(x_i) = \frac{1}{h} \int_{x_{i-1}}^{x_i} v'(x) \, dx$.

4.1 Nonuniform Alikhanov approximation

Now we recall the nonuniform Alikhanov approximation, see also [23]. Let $\Pi_{1,k} v$ denote the linear interpolant of a function $v$ with respect to the nodes $t_{k-1}$ and $t_k$, and let $\Pi_{2,k} v$ denote the quadratic interpolant with respect to $t_{k-1}$, $t_k$ and $t_{k+1}$. It is easy to find that

$$\Pi_{1,k}'(t) = \frac{\nabla_\tau v^k}{\tau_k} \quad \text{and} \quad \Pi_{2,k}'(t) = \frac{\nabla_\tau v^k}{\tau_k} + \frac{2(t - t_{k-1/2})}{\tau_k} \left( \rho_k \nabla_\tau v^{k+1} - \nabla_\tau v^k \right).$$

The nonuniform Alikhanov formula to the Caputo derivative $({\mathcal{D}}_\tau^\alpha v)(t_{n-\theta})$ is defined by

$$(D_\tau^\alpha v)^{n-\theta} := \int_{t_{n-1}}^{t_{n-\theta}} \omega_{1-\alpha}(t_{n-\theta} - s) (\Pi_{1,n} v)'(s) \, ds + \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \omega_{1-\alpha}(t_{n-\theta} - s) (\Pi_{2,k} v)'(s) \, ds$$

$$= a_0^{(n)} \nabla_\tau v^n + \sum_{k=1}^{n-1} \left( a_{n-k}^{(n)} \nabla_\tau v^k + \rho_k b_{n-k}^{(n)} \nabla_\tau v^{k+1} - b_{n-k}^{(n)} \nabla_\tau v^k \right), \quad (4.2)$$

where the discrete coefficients $a_{n-k}^{(n)}$ and $b_{n-k}^{(n)}$ are defined by

$$a_{n-k}^{(n)} := \int_{t_{n-1}}^{t_{n-\theta}} \frac{\omega_{1-\alpha}(t_{n-\theta} - s)}{\tau_n} \, ds \quad \text{and} \quad a_{n-k}^{(n)} := \int_{t_{k-1}}^{t_k} \frac{\omega_{1-\alpha}(t_{n-\theta} - s)}{\tau_n} \, ds, \quad 1 \leq k \leq n - 1; \quad \tag{4.3}$$

$$b_{n-k}^{(n)} := \frac{2}{\tau_k} \int_{t_{k-1}}^{t_k} (s - t_{k-1/2}) \omega_{1-\alpha}(t_{n-\theta} - s) \, ds, \quad 1 \leq k \leq n - 1. \quad \tag{4.4}$$

Notice that while $\alpha \to 1$, we have $\omega_{2-\alpha}(t) \to 1$ and $\omega_{1-\alpha}(t) \to 0$, uniformly for $t$ in any compact subinterval of the open half-line $(0, \infty)$. Thus, $a_0^{(n)} = \omega_{2-\alpha}((1 - \theta)\tau_n) / \tau_n \to 1 / \tau_n$. 

whereas $a_{n-k}^{(n)} \to 0$ and $b_{n-k}^{(n)} \to 0$ for $1 \leq k \leq n-1$. It follows that $(D^\alpha_T v)^{n-\theta} \to \nabla_T v^n/\tau_k$ and $\theta = \alpha/2 \to 1/2$ so the time-stepping scheme (2.3) with $\nu = \theta$ tends to the classical second-order Crank–Nicolson method for a (classical) linear reaction-diffusion equation. This is why we also call (2.3) for the case $\nu = \theta$ as a fractional Crank–Nicolson method.

Rearranging the terms in (4.2), we obtain the compact form (2.3) with $\nu = \theta$, where the discrete convolution kernel $A_{n-k}^{(n,\theta)}$ is defined as follows: $A_0^{(1,\theta)} := a_0^{(1)}$ if $n = 1$ and, for $n \geq 2$,

$$A_{n-k}^{(n,\theta)} := \begin{cases} a_0^{(n)} + \rho_{n-1} b_1^{(n)}, & \text{for } k = n, \\ a_n^{(n)} + \rho_{k-1} b_{k-1}^{(n)} - b_{n-k}^{(n)}, & \text{for } 2 \leq k \leq n-1, \\ a_{n-1}^{(n)} - b_{n-1}^{(n)}, & \text{for } k = 1. \end{cases}$$ (4.5)

Some useful properties of $A_{n-k}^{(n,\theta)}$ have been established recently by assuming that

**A3r.** The parameter $\theta = \alpha/2$, and the maximum time-step ratio $\rho = 7/4$.

**Theorem 4.1.** \([14, \text{Theorem 2.2}]\) If A3r holds, then the discrete kernels in (4.5) fulfills

(I) The discrete kernels $A_{n-k}^{(n,\theta)}$ are positive and monotone,

$$A_{n-k-1}^{(n,\theta)} - A_{n-k}^{(n,\theta)} \geq (1 + \rho_k) b_{n-k}^{(n)} - \frac{1}{5\tau_k} \int_{t_{k-1}}^{t_k} (t_k - s) \omega_{-\alpha}(t_{n-\theta} - s) \, ds > 0 \quad \text{for } 1 \leq k \leq n-1;$$

(II) And, $A_0^{(n,\theta)} - A_1^{(n,\theta)} > \theta (2A_0^{(n,\theta)} - A_1^{(n,\theta)})$ for $n \geq 2$;

(III) The discrete kernels $A_{n-k}^{(n,\theta)}$ are bounded, $A_{n-k}^{(n,\theta)} \leq A_0^{(n,\theta)} \leq \frac{24}{11\tau_k} \int_{t_{n-1}}^{t_n} \omega_{1-\alpha}(t_{n-s}) \, ds$ and

$$A_{n-k}^{(n,\theta)} \geq \frac{4}{11\tau_k} \int_{t_{k-1}}^{t_k} \omega_{1-\alpha}(t_{n-s}) \, ds \quad \text{for } 1 \leq k \leq n.$$ 

The first two parts (I)-(II) ensures that A1 is valid, and the last part (III) implies that A2 holds with $\pi_A = \frac{11}{4}$. Hence we can use the complementary discrete convolution kernel $P_{n-k}^{(n,\theta)}$, see (2.4)-(2.6), in this section. They allow us to apply Lemma 2.1 and Theorem 2.1 and establish the stability of the FracCN scheme (2.3). Actually, Theorems 4.1 and 2.2 imply the $H^1$-norm stability of the FracCN scheme for the linear problem (1.1).

**Corollary 4.1.** If the local mesh restriction A3r holds, then the FracCN method (2.3) with $\nu = \theta$ is unconditionally stable in the discrete $H^1$-norm.

To derive a sharp $H^1$-norm error estimate, we need the following two Lemmas.

**Lemma 4.1.** Let $v \in C^3((0,T])$ with $\sigma \in (0,1) \cup (1,2)$. If the mesh condition A3r holds, then the local consistency error $\Upsilon^{n-\theta} v$ of the nonuniform Alikhanov formula $(D^\sigma_T v)^{n-\theta}$ in (1.2) with the discrete convolution kernels (4.5) satisfies

$$|\Upsilon^{n-\theta} v| \leq A_0^{(n,\theta)} C_{lloc}^{n-1} + \sum_{k=1}^{n-1} (A_{n-k-1}^{(n,\theta)} - A_{n-k}^{(n,\theta)}) G_{\text{his}}^k$$ for $1 \leq n \leq N$

where

$$G_{lloc}^k := \frac{3}{2} \int_{t_{k-1}}^{t_{k-1/2}} (s - t_{k-1})^2 |v''(s)| \, ds + \frac{3\tau_k}{2} \int_{t_{k-1/2}}^{t_k} (t_k - s) |v''(s)| \, ds,$$

$$G_{\text{his}}^k := \frac{5}{2} \int_{t_{k-1}}^{t_{k}} (s - t_{k-1})^2 |v''(s)| \, ds + \frac{5}{2} \int_{t_{k}}^{t_{k+1}} (t_{k+1} - s)^2 |v''(s)| \, ds.$$
Thus the global consistency error can be bounded by
\[
\sum_{j=1}^{n} p^{(n,\nu)}_{n-j} |\mathbf{\Upsilon}^{j-\nu}[v]| \leq C_{v} \left( \tau_{1}/\sigma + t_{1}^{\nu-3} \tau_{2}^{3} + \frac{1}{1-\alpha} \max_{2 \leq k \leq n} t_{k}^{\nu-3} \tau_{k-1}^{3}/\tau_{k-1}^{\nu} \right).
\]

**Proof.** See Theorem 3.4 and Lemma 3.6 in [14].

Next Lemma suggests that the time weighted operator will not lead to any loss of the temporal accuracy in the $H^{1}$-norm error analysis, although the solution is non-smooth near $t = 0$.

**Lemma 4.2.** Let $v \in C^{2}_{\sigma}((0, T])$ with $\sigma \in (0, 1) \cup (1, 2)$. The truncation error of $v^{n-\nu}$ satisfies
\[
|v(t_{j-\theta}) - v^{1-\nu}| \leq C_{v} \tau_{1}^{\sigma}/\sigma \quad \text{and} \quad |v(t_{j-\theta}) - v^{j-\nu}| \leq C_{v} t_{j}^{\nu-2} \tau_{j}^{2} \quad \text{for } 2 \leq j \leq N
\]
such that
\[
\max_{1 \leq j \leq n} \left\{ t_{j}^{\nu/2} |v(t_{j-\theta}) - v^{j-\nu}| \right\} \leq C_{v} \tau_{1}^{\sigma+\nu/2}/\sigma + C_{v} \max_{2 \leq k \leq n} t_{k}^{\nu/2} \tau_{k-1}^{2} \quad \text{for } 1 \leq n \leq N.
\]

**Proof.** The Taylor expansion with the integral remainder gives, see also [11] Lemma 2.5,
\[
v^{j-\nu} - v(t_{j-\theta}) = \theta \int_{t_{j-1}}^{t_{j}} (s - t_{j-1}) v''(s) \, ds + (1 - \theta) \int_{t_{j-\theta}}^{t_{j}} (t_{j} - s) v''(s) \, ds, \quad 1 \leq j \leq N.
\]
The claimed results then follow immediately.

### 4.2 Two-stage convergence analysis

Now we describe an alternative two-stage process for obtaining a sharp $H^{1}$-norm error estimate for the second-order FracCN method (2.23) with $\nu = \theta$ by assuming that the subdiffusion problem (1.1) has a unique solution $u \in C([0, T]; H^{1}(\Omega)) \cap C^{2}_{\sigma}((0, T]; H^{2}(\Omega)) \cap C^{3}_{\sigma}((0, T]; H^{3}(\Omega))$.

**Temporal error analysis via a time-discrete system.** We apply the nonuniform Alikhanov formula $(\mathcal{D}_{\nu}^{\alpha} u)^{n-\nu}$ with the discrete convolution kernels (4.5) to approximate the problem (1.1),
\[
(\mathcal{D}_{\nu}^{\alpha} u)^{n-\nu} + \mathcal{L} u^{n-\nu} = c(x) u^{n-\nu} + f(x, t_{n-\nu}) \quad \text{for } x \in \Omega \text{ and } 1 \leq n \leq N,
\]
\[
u^{n} = u_{b}(x, t_{n}) \quad \text{for } x \in \partial \Omega \text{ and } 1 \leq n \leq N,
\]
\[
u^{0} = u_{0}(x) \quad \text{for } x \in \Omega.
\]
Then the solution error, $e^{n} = u(x, t_{n}) - u^{n}$ for $x \in \Omega$, satisfies the zero-valued initial-boundary conditions and the governing equation
\[
(\mathcal{D}_{\nu}^{\alpha} e)^{n-\nu} + \mathcal{L} e^{n-\nu} = c(x) e^{n-\nu} + \mathbf{\Upsilon}^{n-\nu}[u] + R_{w}^{n-\nu} \quad \text{for } x \in \Omega \text{ and } 1 \leq n \leq N,
\]
where $\mathbf{\Upsilon}^{n-\nu}[u]$ is defined by (2.2) and $R_{w}^{n-\nu} := (c(x) - \mathcal{L}) [u^{n-\nu} - u(t_{n-\nu})]$ for $x \in \Omega$.

By taking the (continuous) inner product of the error equation in (4.7) with $\mathcal{L} e^{n-\nu}$, one applies the first Green formula to find
\[
\left( (\mathcal{D}_{\nu}^{\alpha} e)^{n-\nu}, \mathcal{L} e^{n-\nu} \right) = - \| \mathcal{L} e^{n-\nu} \|_{L^{2}(\Omega)}^{2} + (ce^{n-\nu}, \mathcal{L} e^{n-\nu}) + (R_{w}^{n-\nu}, \mathcal{L} e^{n-\nu})
\]
\[
+ \left( \mu \partial_{x} \mathbf{\Upsilon}^{n-\nu}[u], \partial_{x} e^{n-\nu} \right)
\]
\[
\leq \frac{1}{2} \kappa^{2} \| e^{n-\nu} \|_{L^{2}(\Omega)}^{2} + \frac{1}{2} \| R_{w}^{n-\nu} \|_{L^{2}(\Omega)}^{2} + \| e^{n-\nu} \|_{H^{1}(\Omega)}^{2} \| \mathbf{\Upsilon}^{n-\nu}[u] \|_{H^{1}(\Omega)}
\]
\[
\leq \frac{1}{2} \kappa^{2} C_{\Omega} \| e^{n-\nu} \|_{H^{1}(\Omega)}^{2} + \| e^{n-\nu} \|_{H^{1}(\Omega)} \| \mathbf{\Upsilon}^{n-\nu}[u] \|_{H^{1}(\Omega)} + \frac{1}{2} \| R_{w}^{n-\nu} \|_{L^{2}(\Omega)}^{2},
\]

Thus the solution error in the $H^{1}$-norm can be bounded by
\[
\| e^{n-\nu} \|_{H^{1}(\Omega)} \leq \frac{1}{2} \kappa^{2} C_{\Omega} \| e^{n-\nu} \|_{H^{1}(\Omega)}^{2} + \| e^{n-\nu} \|_{H^{1}(\Omega)} \| \mathbf{\Upsilon}^{n-\nu}[u] \|_{H^{1}(\Omega)} + \frac{1}{2} \| R_{w}^{n-\nu} \|_{L^{2}(\Omega)}^{2}.
\]
where the Cauchy-Schwarz inequality and the embedding inequality have been used. We apply Lemma 2.1 together with $\nu = \theta$ and Theorem 4.1 to obtain

$$\sum_{k=1}^{n} A_{n-k}^{(n,\theta)} \| e^k \|^2_{H^1(\Omega)} \leq \kappa^2 C_\Omega \| e^{n-\theta} \|^2_{H^1(\Omega)} + 2 \| e^{n-\theta} \|_{H^1(\Omega)} \| \mathcal{Y}^{n-\theta}[u] \|_{H^1(\Omega)} + \| R_{w}^{n-\theta} \|_{L^2(\Omega)}^2,$$

which has the form of (2.11) with $\lambda_0 := \kappa^2 C_\Omega$, $\lambda_l := 0$ ($l \geq 1$),

$$\nu^k := \| e^k \|^2_{H^1(\Omega)}, \quad \xi^n := 2 \| \mathcal{Y}^{n-\theta}[u] \|_{H^1(\Omega)} \quad \text{and} \quad \eta^n := \| R_{w}^{n-\theta} \|_{L^2(\Omega)}.$$

Therefore, applying Theorem 2.3 with $\pi_A = 11/4$, we get

$$\| e^n \|^2_{H^1(\Omega)} \leq 4E_\alpha \left( 10\kappa^2 C_\Omega t_n^\alpha \right) \max_{1 \leq k \leq n} \int_{0}^{1} \int_{0}^{1} \left| \mathcal{Y}^{j-\theta}[u] \right|^2_{H^1(\Omega)}$$

$$+ 4 \sqrt{1 - \alpha} \int_{0}^{1} \int_{0}^{1} \left| \mathcal{Y}^{j-\theta}[u] \right|^2_{H^1(\Omega)} \leq \| R_{w}^{n-\theta} \|_{L^2(\Omega)}^2$$

if the local assumption $A3r$ holds with the maximum time-step size $\tau \leq 1/ \sqrt{6(2 - \alpha)} \kappa^2 C_\Omega$.

Then, applying Lemma 4.1 (with $\nu = \partial_x u$) and Lemma 4.2, one obtains

$$\| u(t_n) - u^n \|^2_{H^1(\Omega)} \leq \frac{C_u}{\sigma(1 - \alpha)} \left\{ \frac{1}{2} \| e^n \|^2_{H^1(\Omega)} + \frac{1}{2} \| R_{w}^{n-\theta} \|_{L^2(\Omega)}^2 \right\}.$$

**Spatial error analysis via the fully-discrete system** Now return to the fully-discrete system (2.3) with $\nu = \theta$, which can be viewed as the spatial approximation of time-discrete system (4.6). Under our priori assumptions to the problem (1.1), this system has a unique solution $u^n \in H^4(\Omega)$ for $1 \leq n \leq N$. Thus the solution error, $z^n_h := u^n - u^n$ for $x \in \Omega_h$, satisfies the zero-valued initial-boundary conditions, and the governing equation

$$(D_{tau}^n z^n_h)_{\theta} + L_h z^n_h = c(x) z^n_h + R_{wa}^{n-\theta} \quad \text{for} \quad x \in \Omega_h \quad \text{and} \quad 1 \leq n \leq N,$$

where $R_{wa}^{n-\theta}$ is defined by (2.10). We will proceed to apply the standard $H^1$-norm analysis, as done in the subsection 2.2. By taking the inner product of (4.9) with $(D_{tau}^n z^n_h)_{\theta}$, one has

$$\langle L_h z^n_h, (D_{tau}^n z^n_h)_{\theta} \rangle = -\| (D_{tau}^n z^n_h)_{\theta} \|^2 + \langle c z^n_h, (D_{tau}^n z^n_h)_{\theta} \rangle + \langle R_{wa}^{n-\theta}, (D_{tau}^n z^n_h)_{\theta} \rangle$$

$$\leq \frac{1}{2} \| z^n_h \|^2 + \| R_{wa}^{n-\theta} \|^2.$$

Therefore, applying Lemma 2.1 and the embedding inequality, one gets

$$\sum_{k=1}^{n} A_{n-k}^{(n,\theta)} \| z^k_h \|^2_{H^1(\Omega)} \leq \kappa^2 C_\Omega \left\{ (1 - \theta) \| z^n_h \|_{H^1(\Omega)} + \theta \| z^{n-1}_h \|_{H^1(\Omega)} \right\}^2 + \| R_{wa}^{n-\theta} \|^2$$

for $1 \leq n \leq N$, which has the form of (2.11) with $\lambda_0 := \kappa^2 C_\Omega$, $\lambda_l := 0$ ($l \geq 1$), $\nu^k := \| z^k_h \|_{H^1(\Omega)}$, $\xi^n := 0$ and $

\eta^n := \| R_{wa}^{n-\theta} \|$. Then the fractional Grönwall inequality in Theorem 2.3 (taking $\rho = 7/4$ and $\pi_A = 11/4$) and the error estimate $\| R_{w}^{k-\theta} \| \leq C_u h^2$ yield

$$\| u^n - u^n \|_{H^1(\Omega)} \leq 4E_\alpha \left( 10\kappa^2 C_\Omega t_n^\alpha \right) \sqrt{\Gamma(1 - \alpha)} \max_{1 \leq k \leq n} \{ t_k^{\alpha/2} \| R_{w}^{k-\theta} \| \}$$

$$\leq C_u E_\alpha \left( 10\kappa^2 C_\Omega t_n^\alpha \right) \sqrt{\Gamma(1 - \alpha)} t_n^{\alpha/2} h^2,$$

if the assumption $A3r$ holds with the maximum time-step size $\tau \leq 1/ \sqrt{6(2 - \alpha)} \kappa^2 C_\Omega$. 


We are in the position to complete the error estimate. Combining (4.8) with (4.10), one can apply the triangle inequality and the relationship (4.11) to find
\[ |u(t_n) - u^n|_1 \leq |u(t_n) - u^n|_1 + |u^n - u^n_h| \leq C_\Omega |u(t_n) - u^n|_{H^1(\Omega)} + |u^n - u^n_h|_1 \] (4.11)
where \( C_\Omega \) may depend on \( u \) and \( T \), but is uniformly bounded with respect to \( \alpha \) and \( \sigma \). If the mesh assumption \( \text{M-conv} \) holds, then \( \tau_1 \leq C \gamma \tau^\gamma \) and
\[ t_k^{\alpha/2} \tau_k^{3/2} \leq C t_k^{\alpha/2} \max(0, \sigma - (3 - \alpha)/\gamma) \tau_k^\gamma, \quad 2 \leq k \leq n; \] (4.12)
where \( \beta := \min\{2, \gamma \sigma\} \). In addition,
\[ t_k^{\alpha/2} \tau_k^{3/2} \leq C t_k^{\alpha/2} \max(0, \sigma - (3 - \alpha)/\gamma) \tau_k^\gamma, \quad 2 \leq k \leq n; \] (4.13)

So the following result is achieved by inserting (4.12) and (4.13) into (4.11).

**Theorem 4.2.** Suppose that the initial-boundary value problem (1.1) of the subdiffusion equation has a solution \( u \in C([0, T]; H^1(\Omega)) \cap C^\sigma_2([0, T]; H^2(\Omega)) \cap C^3_\sigma((0, T]; H^1(\Omega)) \), and consider the fractional Crank-Nicolson method (2.3) using the Alikhanov formula \( (D^\tau_v)^n v \) with the discrete convolution kernels (4.5). If the local mesh condition \( \text{A3r} \) holds with the maximum time-step size \( \tau \leq 1/ \sqrt[6]{10(2 - \alpha)^2 \Omega} \), then the discrete solution \( u^n \) is convergent in the discrete \( H^1 \)-norm,
\[ |u(t_n) - u^n|_1 \leq \frac{C_u}{\sigma(1 - \alpha)} \left( \tau_1^{\gamma} + \max_{2 \leq k \leq n} t_k^{\alpha/2} \tau_k^{3/2} \max_{2 \leq k \leq n} t_k^{\alpha/2} \tau_k^{3/2} + t_n^{\alpha/2} h^2 \right). \]

In particular, if the mesh assumption \( \text{M-conv} \) holds, then
\[ |u(t_n) - u^n|_1 \leq \frac{C_u}{\sigma(1 - \alpha)} \left( \tau^{\min(\gamma, \sigma)} + h^2 \right) \quad \text{for} \ 1 \leq n \leq N, \]
where \( C_u \) may depend on \( u \) and \( T \), but is uniformly bounded with respect to \( \alpha \) and \( \sigma \).

**Remark 4.** As noted early in (4.7), by an argument similar to that in (4.12), it is not difficult to show that \( \tau_k^{\alpha/2} \tau_k^{3/2} \leq C \gamma \tau_k^{\gamma}, \) which means that the Alikhanov formula \( (D^\tau_v)^n v \) approximates \( (D^\tau_v)^n v \) to order \( \mathcal{O}(\tau^\gamma) \) if \( \gamma \geq (3 - \alpha)/\sigma \). However, the term (4.13) arising from \( R^{n-\theta}_v \) would still limit the convergence rate for the overall scheme to order \( \mathcal{O}(\tau^2) \).

From the point of view of different spatial discretization methods, the two-stage analysis would be more general that the direct error splitting technique in subsection 3.2. On the other hand, the traditional \( H^1 \)-norm analysis in subsection 3.1 will yield a suboptimal error estimate because the global consistency error \( \sum_{j=1}^k P_{k-j}^{(k, \theta)}\| Y_{j-\theta}^j[u] \|^2 \) also has a loss of time accuracy. Actually, by using the discrete convolution bound of the local consistency error in Lemma 4.1, one can present an proof similar to that of Lemma 4.3 and find the following estimate.

**Lemma 4.3.** If \( v \in C^2_\sigma((0, T]) \) for \( \sigma \in (\frac{3}{2}, 1) \cup (1, 2) \) and the maximum step ratio \( \rho \leq 1 \), then the global consistency error of the nonuniform Alikhanov formula \( (D^\tau_v)^n v \) in (4.2) with the discrete convolution kernels (4.5) satisfies
\[ \sum_{j=1}^n P_{n-j}^{(n, \theta)}\| Y_{j-\theta}^j[v] \|^2 \leq \frac{C_v}{\gamma^2} \tau_1^{\sigma - \gamma} + t_1^{\sigma - \gamma} \tau_1^\gamma + \frac{C_v}{\sigma - \gamma} \max_{2 \leq k \leq n} t_k^{\alpha/2} \tau_k^{3/2} \max_{2 \leq k \leq n} t_k^{\alpha/2} \tau_k^{3/2} f_{k-1}^2 \quad \text{for} \ 1 \leq n \leq N. \]
Moreover, if the time mesh satisfies $\textbf{M-conv}$, then
\[
\sum_{j=1}^{n} P_{n-j}^{(n,\theta)} |\tau^{j-\theta}[v]|^2 \leq \frac{C_v}{\sigma^2(1-\alpha)} \tau^{2\min\{2,\gamma(\sigma-\alpha/2)\}} \quad \text{for } 1 \leq n \leq N.
\]

5 Numerical examples

We present some numerical results to verify our error estimates. Always, consider the reaction-subdiffusion problem (1.1) in the spatial domain $\Omega = (0, \pi)$ and the time interval $[0, T]$ with $T = 1$. In the computations, the domain $(0, \pi)$ is divided into $M$ equally spaced subintervals with a mesh length $h = \pi/M$, and the time interval $[0,1]$ is divided into $N$ parts by an initially graded grid (1.4) with $T_0 = \min\{\gamma^{-1}, 2^{-\gamma}\}$. Throughout our tests, we measure the discrete $H^1$-seminorm solution error $e(M,N) = \max_{1 \leq n \leq N} |u(t_n) - u_n^h|$. Since the convergence behavior of the spatial discretization is well understood, we focus on the temporal convergence here by setting a sufficiently large $M$ such that the time error dominates the spatial error in each run and $e(M,N) \approx e(N)$. The experimental rate (listed as “Order” in tables) in temporal direction is estimated by using $\text{Order} = \log_2(e(N)/e(2N))$.

**Example 1. Numerical results for the fully discrete L1 scheme.** We set a diffusive coefficient $\mu(x) = \exp(x)$, a reaction coefficient $c(x) = 2\sin(x) + 1$, and a specific source term $f(x, t)$ such that the exact solution $u(x, t) = \omega_1 + \sigma(t) \sin(x)$. It is seen that this solution fulfills the assumption $u \in C^2_{2\sigma}(0, T; H^1(\Omega))$ for the regularity parameter $\sigma \in (0, 1) \cup (1, 2)$.

| $N$ | $\alpha = 0.1, \sigma = 1.9$ | $\alpha = 0.5, \sigma = 1.5$ | $\alpha = 0.9, \sigma = 1.1$ |
|-----|-----------------------------|-----------------------------|-----------------------------|
|     | $e(M,N)$ Order              | $e(M,N)$ Order              | $e(M,N)$ Order              |
| 100 | 3.84e-06 1.83               | 1.71e-04 1.38               | 1.03e-03 0.94               |
| 200 | 1.08e-06 1.84               | 6.56e-05 1.40               | 5.36e-04 0.96               |
| 400 | 3.02e-07 1.84               | 2.48e-05 1.42               | 2.75e-04 0.98               |
| 800 | 8.46e-08 1.84               | 9.27e-06 1.43               | 1.40e-04 0.99               |
| 1600| 2.37e-08 *                  | 3.43e-06 *                  | 7.04e-05 *                  |

To test the sharpness of our error estimate Theorem 3.1, we consider four different scenarios, respectively, in Tables 2 and 3. Setting the fixed and sufficiently big $M = 20000$, the sufficiently small value of $h$ can guarantee that the dominated errors arise from the L1 approximation of Caputo derivative. By taking $\sigma = 2 - \alpha$ and $\gamma = 1$, the computational results of the scheme for different $\alpha = 0.1, 0.5, 0.9$ are presented in Table 2. It is observed that the scheme has the temporal order $O(\tau^{2-\alpha})$, which is consistent with our theoretical analysis.

| $N$ | $\gamma = 1$ | $\gamma = 3$ | $\gamma = 3.75$ |
|-----|--------------|--------------|-----------------|
|     | $e(M,N)$ Order | $e(M,N)$ Order | $e(M,N)$ Order |
| 100 | 2.57e-02 0.45 | 6.34e-04 1.43 | 4.66e-04 1.47 |
| 200 | 1.88e-02 0.46 | 2.34e-04 1.45 | 1.68e-04 1.48 |
| 400 | 1.37e-02 0.47 | 8.56e-05 1.47 | 6.01e-05 1.49 |
| 800 | 9.88e-03 0.47 | 3.10e-05 1.48 | 2.14e-05 1.49 |
| 1600| 7.11e-03 *     | 1.11e-05 *     | 7.63e-06 *     |

\[\text{min}\{\gamma\sigma, 2 - \alpha\}\]

\[0.50\]

\[1.50\]

\[1.50\]
Table 3: Numerical accuracy for Example 1 with $\alpha = 0.5$, $\sigma = 0.75$ and $\gamma_{\text{opt}} = 2$.

| $N$  | $\gamma = 1$ | $\gamma = 2$ | $\gamma = 2.5$ |
|------|--------------|--------------|----------------|
|      | $e(M,N)$     | Order        | $e(M,N)$       | Order        | $e(M,N)$       | Order        |
| 100  | 3.70e-03     | 0.70         | 2.26e-04       | 1.41         | 1.47e-04       | 1.47         |
| 200  | 2.28e-03     | 0.71         | 8.48e-05       | 1.43         | 5.30e-05       | 1.48         |
| 400  | 1.39e-03     | 0.72         | 3.14e-05       | 1.45         | 1.90e-05       | 1.48         |
| 800  | 8.46e-04     | 0.72         | 1.15e-05       | 1.46         | 6.79e-06       | 1.49         |
| 1600 | 5.12e-04     | *            | 1.47e-05       | *            | 2.42e-06       | *            |

min\{\gamma\sigma, 2 - \alpha\} = 0.75, 1.50, 1.50

Table 4: Numerical accuracy for Example 1 with $\alpha = 0.5$, $\sigma = 1.25$ and $\gamma_{\text{opt}} = 1.2$.

| $N$  | $\gamma = 1$ | $\gamma = 1.2$ | $\gamma = 1.8$ |
|------|--------------|---------------|---------------|
|      | $e(M,N)$     | $e(M,N)$      | $e(M,N)$      |
| 100  | 2.75e-04     | 1.18e-04      | 7.76e-05      |
| 200  | 1.22e-04     | 4.52e-05      | 2.75e-05      |
| 400  | 5.33e-05     | 1.70e-05      | 9.55e-06      |
| 800  | 2.31e-05     | 6.34e-06      | 3.14e-06      |
| 1600 | 9.92e-06     | *             | 9.96e-07      |

min\{\gamma\sigma, 2 - \alpha\} = 1.25, 1.50, 1.50

Numerical results in Tables 3-4 (with $\alpha = 0.5$ and $\sigma < 2 - \alpha$) support the predicted time accuracy in Theorem 3.1. In the case of uniform mesh $\gamma = 1$, the solution is accurate of order $O(\tau^\gamma\sigma)$, and nonuniform meshes improve the numerical precision and convergence rate of solution. When the grid parameter $\gamma \geq \gamma_{\text{opt}}$, the optimal time accuracy $O(\tau^{2-\alpha})$ is observed. Thus the $H^1$-norm error estimate (3.9) is sharp.

**Example 2.** Numerical results for the fully discrete FracCN scheme. We choose $\mu(x) = \cos(x) + 2$, $c(x) = 2\sin(x) + 1$, $u^0 = \sin(x)$, and a forcing source $f(x,t)$ such that the problem has a solution $u(x,t) = (1 + \omega_{1+\sigma}(t))\sin(x)$.

Table 5: Numerical accuracy for Example 2 with $\sigma = 1 + \alpha$ and $\gamma = 1$.

| $N$  | $\alpha = 0.4, \sigma = 1.4$ | $\alpha = 0.6, \sigma = 1.6$ | $\alpha = 0.8, \sigma = 1.8$ |
|------|-----------------------------|-----------------------------|-----------------------------|
|      | $e(M,N)$     | Order        | $e(M,N)$     | Order        | $e(M,N)$     | Order        |
| 128  | 3.42e-05     | 1.63         | 3.43e-05     | 1.97         | 2.65e-05     | 1.97         |
| 256  | 1.10e-05     | 1.57         | 8.73e-06     | 1.96         | 6.76e-06     | 1.96         |
| 512  | 3.73e-06     | 1.54         | 2.23e-06     | 1.90         | 1.73e-06     | 1.92         |
| 1024 | 1.28e-06     | 1.51         | 5.40e-07     | 1.71         | 4.61e-07     | 1.86         |
| 2048 | 4.50e-07     | 1.49         | 1.33e-07     | 1.71         | 1.27e-07     | 1.83         |
| 4096 | 1.60e-07     | *            | 5.02e-08     | *            | 3.57e-08     | *            |

min\{\gamma\sigma, 2\} = 1.40, 1.60, 1.80

The solution is approximated by the FracCN scheme (2.3) with $\nu = \alpha/2$. For different fractional order $\alpha$, the numerical results are computed with varying temporal stepsizes and fixed sufficiently large spatial points $M = 20000$. Like before, for fixed $M$, the computational errors and numerical convergence orders in the $H^1$-norm are given in Tables 5-8 with different temporal step sizes, from which, the $O(\tau^{\min\{\gamma\sigma,2\}})$ convergence of the difference scheme (2.3) is apparent, indicating the sharpness of our estimate in Theorem 4.2.
Table 6: Numerical accuracy for Example 2 with $\sigma = 1.2$ and $\alpha = 0.4$.

| $N$ | $\gamma = 1$ | Order | $\gamma = 5/3 = \gamma_{\text{opt}}$ | Order | $\gamma = 2$ | Order |
|-----|--------------|--------|----------------------------------|--------|--------------|--------|
| 128 | 6.17e-05     | 1.36   | 1.32e-05                         | 2.05   | 1.39e-05     | 2.04   |
| 256 | 2.40e-05     | 1.34   | 3.19e-06                         | 2.00   | 3.36e-06     | 2.04   |
| 512 | 9.49e-06     | 1.31   | 7.98e-07                         | 2.06   | 8.16e-07     | 2.06   |
| 1024| 3.83e-06     | 1.29   | 1.91e-07                         | 2.05   | 1.96e-07     | 2.06   |
| 2048| 1.57e-06     | *      |                                  | *      |              | *      |

$\min\{\gamma \sigma, 2\}$

1.20   2.00   2.00

Table 7: Numerical accuracy for Example 2 with $\sigma = 0.8$ and $\alpha = 0.4$.

| $N$ | $\gamma = 2$ | Order | $\gamma = 5/2 = \gamma_{\text{opt}}$ | Order | $\gamma = 3$ | Order |
|-----|--------------|--------|----------------------------------|--------|--------------|--------|
| 128 | 2.43e-05     | 2.12   | 2.49e-05                         | 2.12   | 2.75e-05     | 2.12   |
| 256 | 5.59e-06     | 1.69   | 5.72e-06                         | 2.15   | 6.35e-06     | 2.15   |
| 512 | 1.74e-06     | 1.61   | 1.29e-06                         | 2.35   | 1.43e-06     | 2.33   |
| 1024| 5.69e-07     | 1.61   | 2.53e-07                         | 2.43   | 2.84e-07     | 2.33   |
| 2048| 1.87e-07     | *      |                                  | *      |              | *      |

$\min\{\gamma \sigma, 2\}$

1.60   2.00   2.00

Table 8: Numerical accuracy for Example 2 with $\sigma = 0.4$ and $\alpha = 0.4$.

| $N$ | $\gamma = 2$ | Order | $\gamma = 5/2 = \gamma_{\text{opt}}$ | Order | $\gamma = 5 = \gamma_{\text{opt}}$ | Order |
|-----|--------------|--------|----------------------------------|--------|----------------------------------|--------|
| 128 | 3.35e-03     | 0.81   | 1.50e-03                         | 1.01   | 4.56e-04                         | 2.17   |
| 256 | 1.91e-03     | 0.81   | 7.41e-04                         | 1.00   | 1.01e-04                         | 2.20   |
| 512 | 1.09e-03     | 0.81   | 3.71e-04                         | 1.00   | 2.20e-05                         | 2.17   |
| 1024| 6.21e-04     | 0.80   | 1.85e-04                         | 1.00   | 4.90e-06                         | 2.14   |
| 2048| 3.56e-04     | *      |                                  | *      |                                  | *      |

$\min\{\gamma \sigma, 2\}$

0.80   1.00   2.00

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