Incomplete Iterative Solution of the Subdiffusion Problem

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Abstract

In this work, we develop an efficient incomplete iterative scheme for the numerical solution of the subdiffusion model involving a Caputo derivative of order \( \alpha \in (0,1) \) in time. It is based on piecewise linear Galerkin finite element method in space and backward Euler convolution quadrature in time and solves one linear algebraic system inexactly by an iterative algorithm at each time step. We present theoretical results for both smooth and nonsmooth solutions, using novel weighted estimates of the time-stepping scheme. The analysis indicates that with the number of iterations at each time level chosen properly, the error estimates are nearly identical with that for the exact linear solver, and the theoretical findings provide guidelines on the choice. Illustrative numerical results are presented to complement the theoretical analysis.

Keywords: subdiffusion, finite element method, backward Euler scheme, nonsmooth data, convergence analysis, incomplete iterative scheme

1 Introduction

This work is concerned with efficient iterative solvers for the subdiffusion model. Let \( \Omega \subset \mathbb{R}^d \) \((d = 1, 2, 3)\) be a convex polyhedral domain with a boundary \( \partial \Omega \). The subdiffusion model for the function \( u(t) \) reads:

\[
\begin{align*}
\partial_t^\alpha u(t) + Au(t) &= f(t), \quad \forall 0 < t \leq T, \\
u(0) &= v, \quad \text{in } \Omega,
\end{align*}
\]

where \( T > 0 \) is fixed, \( f : (0, T) \to L^2(\Omega) \) and \( v \in L^2(\Omega) \) are given functions, and \( A = -\Delta : D(A) \equiv H^1_0(\Omega) \cap H^2(\Omega) \to L^2(\Omega) \) denotes the negative Laplacian (with a zero Dirichlet boundary condition). The notation \( \partial_t^\alpha u, \; 0 < \alpha < 1 \), denotes the Caputo derivative of order \( \alpha \) in \( t \), defined by \([15, \text{p. 91}]\)

\[
\partial_t^\alpha u(t) := \frac{1}{\Gamma(1 - \alpha)} \int_0^t (t - s)^{-\alpha} u'(s) \, ds,
\]

where the Gamma function \( \Gamma(\cdot) \) is defined by \( \Gamma(z) := \int_0^\infty s^{z-1} e^{-s} \, ds, \; \Re z > 0. \)

The model (1.1) describes so-called subdiffusion process, in which the mean squared displacement of the particle grows only sublinearly with the time \( t \), in contrast to the linear growth of Brownian motion for normal diffusion. The sublinear growth captures important memory and hereditary effects of the underlying physical process. Many experimental studies show that it can offer a superior fit to experimental data than normal diffusion. The long list of applications includes thermal diffusion in fractal domains, heat conduction with memory effect, and protein transport in cell membrane etc. We refer interested readers to \([22, 21]\) for physical background and mathematical modeling.

Over the last two decades, a number of numerical methods have been developed for the model (1.1), e.g., finite element method, finite difference method and spectral method in space, and convolution quadrature (CQ) and L1 type time-stepping schemes; See \([17, 11, 26, 20, 9, 1, 23, 25]\) for an incomplete list, and \([10]\) for an overview on nonsmooth data analysis, including optimal convergence rates. The error analysis in all existing works requires the exact resolution of resulting linear systems at each time step, which can be
where for the singular behavior. As an example, for optimal error estimate. The number of iterations at initial times should be larger in order to compensate provided that it is large enough. In the absence of smoothness, a uniform iteration number fails to give an estimate and technical proofs. Throughout, the notation results are presented in Section 5 to complement the analysis. In two appendices, we collect useful basic and limited smoothing properties, the analysis in these works does not apply to (1.1).

First, we describe a spatially semidiscrete scheme for problem (1.1) based on the Galerkin FEM. 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 \( h \). Over \( \mathcal{T}_h \), we define a continuous piecewise linear finite element space \( X_h \) by

\[
X_h = \{ v_h \in H^1_0(\Omega) : v_h|_T \text{ is a linear function, } \forall T \in \mathcal{T}_h \}.
\]

We define \( L^2(\Omega) \) projection \( P_h : L^2(\Omega) \to X_h \) and Ritz projection \( R_h : H^1_0(\Omega) \to X_h \) by

\[
(P_h \varphi, \chi) = (\varphi, \chi), \quad \forall \chi \in X_h,
\]

\[
(\nabla R_h \varphi, \nabla \chi) = (\nabla \varphi, \nabla \chi), \quad \forall \chi \in X_h,
\]

respectively, where \( (\cdot, \cdot) \) denotes the \( L^2(\Omega) \) inner product.

The semidiscrete Galerkin FEM for (1.1) is to find \( u_h(t) \in X_h \) such that

\[
(\partial_t^\alpha u_h, \chi) + (\nabla u_h, \nabla \chi) = (f, \chi), \quad \forall \chi \in X_h, \quad t > 0,
\]

2.1 Fully discrete scheme

In this work, we develop an efficient incomplete iterative scheme (IIS) for (1.1), based on the Galerkin finite element method (FEM) in space, backward Euler CQ in time, and an iterative solver for resulting linear systems. We prove nearly optimal error estimates for both smooth and nonsmooth solutions, under a contraction property of the iterative solver, cf. (2.11), which holds for many iterative methods. The IIS can maintain the overall accuracy if the number of iterations at each time level is chosen suitably. Specifically, let \( U_h^{n,M} \) be the solution by the IIS at \( t_n \) obtained with \( M_n \) iterations, and \( u \) the exact solution of (1.1). Then for smooth solutions, e.g., \( u \in C([0,T];D(A)) \cap C^2([0,T];H^1_0(\Omega)) \), there exists a \( \delta > 0 \) such that

\[
\| U_h^{n,m} - u(t_n) \|_{L^2(\Omega)} \leq c(u)(h^2 + \tau), \quad \text{for } c_0 \kappa \leq \delta,
\]

where \( c_0 > 0 \) and \( \kappa \in (0,1) \) are convergence parameters of the iterative method in a weighted energy norm; see Theorem 5.2. That is, the number of iterations at each time level can be chosen uniformly in time provided that it is large enough. In the absence of smoothness, a uniform iteration number fails to give an optimal error estimate. The number of iterations at initial times should be larger in order to compensate for the singular behavior. As an example, for \( v \in D(A) \) and \( f \equiv 0 \), there exists \( \delta > 0 \) such that

\[
\| U_h^{n,m} - u(t_n) \|_{L^2(\Omega)} \leq c(h^2 + \tau \ell_n^{-1}) \| Au \|_{L^2(\Omega)},
\]

provided that \( c_0 \kappa \leq \delta \ell_n^{-1} \min(t_n^{\frac{1}{2}},1) \), where \( \ell_n = \ln(1 + t_n/\tau) \). That is, it requires more iterations at starting time levels, even for smooth initial data, which contrasts sharply with the standard parabolic counterpart [2]. The proof relies crucially on certain new weighted estimates on the time stepping scheme, which differ from known existing nonsmooth data error analysis [9, 13]. The accuracy and efficiency of the scheme are illustrated by extensive numerical experiments.

The idea of incomplete iterations was first proposed for standard parabolic problems with smooth solutions in [5, 3], and then extended in [14, 2, 6]. Bramble et al. [2] proposed an incomplete iterative solver for a discrete scheme based on Galerkin approximation in space and linear multistep backward difference in time, and derived error estimates for nonsmooth initial data. Due to the nonlocality of the model (1.1) and limited smoothing properties, the analysis in these works does not apply to (1.1).

The rest of the paper is organized as follows. In Section 2, we describe the IIS. Then in Sections 3 and 4, we analyze the scheme for smooth and nonsmooth solutions, respectively. Finally, some numerical results are presented in Section 5 to complement the analysis. In two appendices, we collect useful basic estimates and technical proofs. Throughout, the notation \( c \) denotes a generic constant, which may differ at each occurrence, but it is always independent of the time step size \( \tau \) and mesh size \( h \).
with \( u_h(0) = v_h \in X_h \). Let \( A_h : X_h \to X_h \) be the negative discrete Laplacian, i.e., \( (A_h \varphi_h, \chi) = (\nabla \varphi_h, \nabla \chi) \), for all \( \varphi_h, \chi \in X_h \). Then we rewrite (2.1) as
\[
\partial_t^\alpha u_h(t) + A_h u_h(t) = f_h(t), \quad \forall t > 0, \tag{2.2}
\]
with \( u_h(0) = v_h \in X_h \) and \( f_h(t) = P_h f(t) \). The following identity holds
\[
A_h R_h = P_h A. \tag{2.3}
\]

Next we partition the time interval \([0, T]\) uniformly, with grid points \( t_n = n \tau, \ n = 0, \ldots, N \), and a time step size \( \tau = T/N \). Recall the Riemann-Liouville derivative \( R \partial_t^\alpha \varphi(t) = \frac{d}{dt} \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \varphi(s) ds \). The backward Euler CQ for \( R \partial_t^\alpha \varphi(t_n) \) is given by (with \( \varphi^j = \varphi(t_j) \)):
\[
\partial_t^\alpha \varphi^n = \tau^{-\alpha} \sum_{j=0}^{n} b_j^{(\alpha)} \varphi^{n-j}, \quad \text{with } (1-\xi)^\alpha = \sum_{j=0}^{\infty} b_j^{(\alpha)} \xi^j.
\]

An estimate on \( b_j^{(\alpha)} \) is given in Lemma A.2 in Appendix A. Since \( \partial_t^\alpha \varphi = R \partial_t^\alpha (\varphi(t) - \varphi(0)) \) [15, p. 91], the fully discrete scheme for (1.1) reads: Given \( U_h^0 = v_h \in X_h \), find \( U_h^n \in X_h \) such that
\[
\partial_t^\alpha (U_h^n - U_h^0) + A_h U_h^n = f_h^n, \quad n = 1, 2, \ldots, N, \tag{2.4}
\]
with \( f_h^n = P_h f(t_n) \). The solution of (2.4) can be represented by
\[
U_h^n = F_{h,T} v_h + \tau \sum_{j=1}^{n} E_{h,T} f_h^j, \tag{2.5}
\]
where \( F_{h,T} \) and \( E_{h,T} \) are defined by
\[
F_{h,T} = \frac{1}{2\pi i} \int_{\Gamma_{\theta,\delta}} e^{z \tau} \delta_z (e^{-z \tau})^{\alpha-1} (\delta_z (e^{-z \tau}) + A_h)^{-1} dz,
\]
\[
E_{h,T} = \frac{1}{2\pi i} \int_{\Gamma_{\theta,\delta}} e^{z \tau} (\delta_z (e^{-z \tau}) + A_h)^{-1} dz,
\]
respectively, with \( \delta_z (\xi) = (1-\xi)/\tau, \ \Gamma_{\theta,\delta} := \{ z \in \mathbb{C} : |\Im(z)| \leq \pi/\tau \} \), and \( \Gamma_{\theta,\delta} \) (oriented counterclockwise) defined by (for \( \theta \in (\pi/2, \pi) \))
\[
\Gamma_{\theta,\delta} = \{ z \in \mathbb{C} : |z| = \delta, |\arg z| \leq \theta \} \cup \{ z \in \mathbb{C} : z = \rho e^{\pm i \theta}, \rho \geq \delta \}. \tag{2.6}
\]

We have the following smoothing properties, where \( \| \cdot \| \) denotes the operator norm on \( L^2(\Omega) \). The proof is standard, see, e.g., [19, 11], and hence it is omitted.

**Lemma 2.1.** For any \( \beta \in [0, 1] \), there hold
\[
\| A_h^{\beta} F_{h,T} \| \leq c_{n+1}, \quad \| A_h^{\beta} E_{h,T} \| \leq c_{n+1}^{(1-\beta)\alpha-1} \quad \text{and} \quad \| A_h^{\beta} \partial_t^\alpha E_{h,T} \| \leq c_{n+1}^{(1-\beta)\alpha-2}.
\]

### 2.2 Incomplete iterative scheme (IIS)

At each time level, the scheme (2.4) requires solving a linear system. This can be expensive for large-scale problems. Hence, it is of much interest to develop efficient algorithms that solve (2.4) inexactly while maintaining the overall accuracy. In this work, we propose an incomplete iterative BE scheme, by approximately solving the resulting linear systems. Given \( U_h^0, U_h^1, \ldots, U_h^{n-1} \), we use an iterative method to approximate the solution \( U_h^n \) of
\[
(I + \tau^\alpha A_h) \bar{U}_h^n = \tau^\alpha f_h^n - \sum_{j=1}^{n} b_j^{(\alpha)} U_h^{n-j} + \sum_{j=0}^{n} b_j^{(\alpha)} U_h^0, \tag{2.7}
\]
with a starting guess $U_h^{n,0}$. Below we employ a second-order extrapolation:

$$U_h^{n,0} = 2U_h^{n-1} - U_h^{n-2}, \quad n \geq 2. \quad (2.8)$$

At time level $n$, an iterative method gives a sequence $U_h^{n,m}$ convergent to $\bar{U}_h^n$ as the iteration number $m \to \infty$. The IIS is given by setting

$$U_h^n = U_h^{n,M_n}, \quad (2.9)$$

for some parameter $M_n \in \mathbb{N}$, which may vary with $n$ and is to be specified.

The convergence analysis requires a certain contraction condition. We introduce a weighted (energy like) norm $| \cdot |$ on the space $X_h$ defined by

$$| \psi | = \| (I + \tau^n A_h)^n \psi \|_{L^2(\Omega)} \quad \text{for} \quad \psi \in X_h, \quad (2.10)$$

and denote the space by $X$. We assume that there exist $\kappa \in (0,1)$ and $c_0 > 0$:

$$| U_h^{n,m} - \bar{U}_h^n | \leq c_0 \kappa^m | U_h^{n,0} - \bar{U}_h^n | \quad \text{for} \quad m \geq 1. \quad (2.11)$$

The contraction in the weighted norm $| \cdot |$ arises naturally in the study of many iterative solvers, e.g., Krylov subspace methods [24], multigrid methods [8] and domain decomposition methods [28]. The constant $\kappa$ is related to the condition number of preconditioned systems. The nonstandard norm $| \cdot |$ poses the main challenge in the analysis.

### 3 Error analysis for smooth solutions

Now we analyze (2.9) for smooth solutions, to give a first glance into (2.9). The more challenging case of nonsmooth solutions is deferred to Section 4. The analysis below relies on two stability results on (2.4). The IIS is given by setting $U_h^n = U_h^{n,M_n}$.

The following stability estimate of the scheme (2.4) is useful.

**Lemma 3.1.** For the solution $U_h^n$ of (2.4) with $v_h = 0$, there holds

$$\| \bar{v}_h^n \|_{L^2(\Omega)} + \| (A_h \bar{v}_h^n)_{j=1}^n \|_{L^2(\Omega)} \leq c \| (f_{1,1})_{j=1}^n \|_{L^2(\Omega)}, \quad \forall 1 < p < \infty.$$

The following stability estimate of the scheme (2.4) is useful.

**Lemma 3.2.** Let $U_h^n$ be the solution of (2.4) with $v_h = 0$. Then

$$\| U_h^n \|_{L^2(\Omega)} + \| (\nabla U_h^n)_{j=1}^n \|_{L^2(\Omega)} \leq c \| (A_h^{-\frac{1}{2}} f_{1,1})_{j=1}^n \|_{L^2(\Omega)}, \quad \forall q \in (\frac{2}{\alpha}, \infty).$$

**Proof.** By the representation (2.4), we have

$$\| U_h^n \|_{L^2(\Omega)} \leq \tau \sum_{j=1}^n \| E_h^{n,j-1} f_{1,1}^{n,j} \|_{L^2(\Omega)} \leq \tau \sum_{j=1}^n \| A_h^{-\frac{1}{2}} E_h^{n,j} \| \| A_h^{-\frac{1}{2}} f_{1,1} \|_{L^2(\Omega)}.$$

Now for any $q > \frac{2}{\alpha}$, $(\frac{2}{q} - 1) \frac{2-q}{q} > -1$, and thus $\tau \sum_{j=1}^n (t_{n+1} - t_j)^{\frac{2-q}{q}} < \infty$, cf. Lemma A.1 below. Next, by Lemma 2.1 and Young’s inequality,

$$\| U_h^n \|_{L^2(\Omega)} \leq c \tau \sum_{j=1}^n (t_{n+1} - t_j)^{\frac{2-q}{q}} \| A_h^{-\frac{1}{2}} f_{1,1} \|_{L^2(\Omega)} \leq c \| (A_h^{-\frac{1}{2}} f_{1,1})_{j=1}^n \|_{L^2(\Omega)} < \infty.$$

The bound on $\| (\nabla U_h^n)_{j=1}^n \|_{L^2(\Omega)}$ is due to Lemma 3.1.
First, we give an error estimate on (2.4). It serves as a benchmark for (2.9).

**Theorem 3.1.** Let \( u \) be the solution to (1.1), and \( U_h^n \) be the solution of (2.4) with \( v_h = R_h v \). If \( u \in C^2([0, T]; H^1_0(\Omega)) \cap C^1([0, T]; D(A)) \), then

\[
\| U_h^n - u(t_n) \|_{L^2(\Omega)} \leq c(u)(h^2 + \tau).
\]

**Proof.** In a customary way, we split the error \( e^n \equiv U_h^n - u(t_n) \) into

\[
e^n = (U_h^n - R_h u(t_n)) + (R_h u(t_n) - u(t_n)) =: \vartheta^n + \varphi^n.
\]

It suffices to bound the terms \( \vartheta^n \) and \( \varphi^n \). Clearly,

\[
\| \varphi^n \|_{L^2(\Omega)} \leq ch^2 \| u \|_{C([0, T]; H^2(\Omega))}.
\]

(3.1)

It remains to bound \( \vartheta^n \). Note that \( \vartheta^n \) satisfies \( \vartheta^0 = 0 \) and

\[
\partial_t \vartheta^n + A_h \vartheta^n = \partial_t (U_h^n - R_h u(t_n)) + A_h (U_h^n - R_h u(t_n)) \]

\[= (\partial_t U_h^n - v_h) + A_h (U_h^n - R_h u(t_n)) - (\partial_t R_h u(t_n) - v_h) + A_h R_h u(t_n)).
\]

It follows from the identity (2.3), and equations (2.4) and (1.1) that

\[
\partial_t \vartheta^n + A_h \vartheta^n = -\partial_t R_h u(t_n) - v_h + P_h \partial_t u(t_n)
\]

\[= (P_h - R_h) \partial_t u(t_n) - R_h (\partial_t - \partial_t R_h u(t_n) - v).
\]

Since the solution \( u \) is smooth, by the approximation properties of \( R_h \) and \( P_h \),

\[
\| (P_h - R_h) \partial_t u(t_n) \|_{L^2(\Omega)} \leq ch^2 \| u \|_{C^1([0, T]; D(A))},
\]

and by the approximation property of \( \partial_t \) to \( R \partial_t \)

\[
\| R_h (\partial_t - \partial_t R_h u(t_n) - v) \|_{L^2(\Omega)} \leq \| (\partial_t - \partial_t R_h u(t_n) - v) \|_{H^1_0(\Omega)}
\]

\[\leq c\| u \|_{C([0, T]; H^2(\Omega))}.
\]

(3.3)

Now since \( \vartheta^0 = 0 \), the estimate follows from Lemma 3.2. \( \square \)

Next we can state the main result of this part, i.e., convergence rate of the scheme (2.9) for smooth solutions. Thus it can achieve the accuracy of (2.1), if a large enough but fixed number \( m \) of iterations is taken at each time level.

**Theorem 3.2.** Let \( u \) and \( U_h^n \equiv U_h^{n,m} \) be the solutions of (1.1) and (2.8)–(2.9) with \( v_h = R_h v \), respectively, and let \( U_h^1 = U_h^1 \). If \( u \in C^2([0, T]; H^1_0(\Omega)) \cap C^1([0, T]; D(A)) \), then there exists a \( \delta > 0 \) such that

\[
\| U_h^n - u(t_n) \|_{L^2(\Omega)} \leq c(u)(h^2 + \tau), \quad \text{for} \quad c_0 \kappa^m \leq \delta.
\]

**Proof.** In a customary way, we split the error \( e^{n,m} = U_h^{n,m} - u(t_n) \) into

\[
e^{n,m} = (U_h^{n,m} - R_h u(t_n)) + (R_h u(t_n) - u(t_n)) =: \vartheta^{n,m} + \varphi^{n,m}.
\]

In view of (3.3), it suffices to bound \( \vartheta^{n,m} \). We break the proof into three steps.

**Step 1:** Bound \( \vartheta^{n,m} \) by local truncation errors. Note that \( \vartheta^{n,m} \) satisfies \( \vartheta^0 = 0 \) and for \( n = 1, \ldots, N \)

\[
\partial_t \vartheta^{n,m} + A_h \vartheta^{n,m} = (\partial_t (U_h^{n,m} - v_h) + A_h U_h^{n,m}) - (\partial_t R_h u(t_n) - v_h) - A_h R_h u(t_n).
\]

Let the auxiliary function \( \tilde{U}_h^n \in X_h \) satisfy \( \tilde{U}_h^0 = R_h v \) and

\[
\tau^{-\alpha} \left( \tilde{U}_h^n + \sum_{j=1}^{n} b^{(\alpha)}_{n-j} U_h^{j,m} - \sum_{j=0}^{n} b^{(\alpha)}_{n-j} U_h^0 \right) + A_h \tilde{U}_h^n = f_h^n, \quad n = 1, 2, \ldots, N.
\]
This and the identities \([2.3], [1.1]\) and \([2.9]\) imply
\[
\bar{\partial}_\alpha^n \vartheta^n + A_h \vartheta^n = \sigma^n, \quad \text{with } \sigma^n = (I + \tau_h^A A_h)\eta^n + \omega^n, \quad (3.4)
\]
with the errors \(\eta^n\) and \(\omega^n\) given by
\[
\eta^n = \tau^{-\alpha}(U_h^{n,m} - \bar{U}_h^n),
\omega^n = (P_h - R_h)\bar{\partial}_\alpha^n (u(t_n) - v) - R_h(\bar{\partial}_\alpha^n - \partial_\alpha^n)(u(t_n) - v).
\]
By Lemma \([3.2]\) and the triangle inequality, for any \(q \in \left(\frac{2}{\alpha}, \infty\right)\) and \(n = 1, 2, ..., N,\)
\[
\|\vartheta^n\|_{L^q(\Omega)} \leq c\|(A_h^{-\frac{1}{2}}\sigma^n)_{j=1}^n\|_{L^q(\Omega)} + c\|(A_h^{-\frac{1}{2}}\omega^n)_{j=1}^n\|_{L^q(\Omega)}.
\]
Since \(u \in C^2([0, T]; H^1_0(\Omega)) \cap C^1([0, T]; D(A))\), \([2.4]\) and \([3.3]\) imply
\[
\|A_h^{-\frac{1}{2}}\omega^n\|_{L^q(\Omega)} \leq c\|\omega^n\|_{L^q(\Omega)} \leq c(u)(h^2 + \tau).
\]
Further, direct computation gives
\[
\|(I + \tau^A A_h)A_h^{-\frac{1}{2}}\eta^n\|_{L^q(\Omega)} \leq c|\eta^n|. \quad (3.5)
\]
The last three estimates imply (recall \(\| \cdot \|_X = \| \cdot \|_X\)):
\[
\|\vartheta^n\|_{L^q(\Omega)} \leq c\|\eta^n\|_{L^q(X)} + c(u)(h^2 + \tau). \quad (3.6)
\]

**Step 2:** Bound the summand \(|\eta^n|\). Given a tolerance \(\delta > 0\) to be determined, under assumption \([2.11]\), there exists an \(m \in \mathbb{N}\) such that \(c_0\kappa^m \leq \delta\) and by the triangle inequality
\[
|U_h^{n,m} - U_h^n| \leq \delta|U_h^{n,0} - \bar{U}_h^n| \leq \delta\left(|U_h^{n,0} - U_h^{n,m}| + |U_h^{n,m} - U_h^n|\right).
\]
With \(\epsilon = \delta(1 - \delta)^{-1}\), rearranging the inequality gives \(|U_h^{n,m} - U_h^n| \leq c|U_h^{n,0} - U_h^{n,m}|\). Hence,
\[
|\eta^n| = \tau^{-\alpha}|U_h^{n,m} - \bar{U}_h^n| \leq c\tau^{-\alpha}|U_h^{n,0} - U_h^{n,m}|.
\]
Meanwhile, the choice of \(U_h^{n,0}\) in \([2.8]\) implies
\[
U_h^{n,m} - U_h^{n,0} = U_h^{n,m} - 2U_h^{n-1} + U_h^{n-2} = \tau(\bar{\partial}_\tau U_h^{n,m} - \bar{\partial}_\tau U_h^{n-1})
= \tau\bar{\partial}_\tau \theta^n - \tau\bar{\partial}_\tau \theta^{n-1} + \tau^2\bar{\partial}_\tau^2 R_h u(t_n).
\]
The last two estimates together imply
\[
|\eta^n| \leq c\epsilon\epsilon^{-1}\tau^{-\alpha}\left(|\bar{\partial}_\tau \theta^n| + |\bar{\partial}_\tau \theta^{n-1}|\right) + c\epsilon\epsilon^{-2}\alpha|R_h \bar{\partial}_\tau^2 u(t_n)|
\leq c\epsilon\epsilon^{-1}\tau^{-\alpha}\left(|\bar{\partial}_\tau \theta^n| + |\bar{\partial}_\tau \theta^{n-1}|\right) + c\epsilon\epsilon^{-2}\alpha|u|_{C^2([0, T]; H^1_0(\Omega))}. \quad (3.7)
\]
This, \([3.9]\) and the standard inverse inequality in time yield
\[
\|\vartheta^n\|_{L^q(\Omega)} \leq c\epsilon\epsilon^{-1}\tau^{-\alpha}\left(|\bar{\partial}_\tau \theta^n|\right)_{j=1}^n + c(u)(h^2 + \tau)
\leq c\epsilon\epsilon^{-1}\tau^{-\alpha}\left(|\bar{\partial}_\tau \theta^n|\right)_{j=1}^n + c(u)(h^2 + \tau). \quad (3.8)
\]

**Step 3:** Bound \(\|\vartheta^n\|_{L^q(\Omega)}\) explicitly. Let \(I_h = (I + \tau^A A_h)^{-\frac{1}{2}}\). Then the identity \(|\bar{\partial}_\tau \theta^n| = \|(I + \tau^A A_h)\bar{\partial}_\tau I_h \bar{\partial}_\tau\|_{L^q(\Omega)}\) and the triangle inequality imply
\[
\|(\bar{\partial}_\tau \theta^n)_{j=1}^n\|_{L^q(\Omega)} \leq \|(\bar{\partial}_\tau I_h \bar{\partial}_\tau)_{j=1}^n\|_{L^q(\Omega)} + \tau^\alpha\|(\bar{\partial}_\tau A_h I_h \bar{\partial}_\tau)_{j=1}^n\|_{L^q(\Omega)} := I + II.
\]
By Lemma 3.1 we have

\[ I \leq c \|(I_h \sigma^j)_{j=1}^n\|_{L^2(\Omega)}. \]

and similarly, the inverse inequality (in time) and Lemma 3.1 yield

\[ II \leq c \|(A_h I_h \phi^j)_{j=1}^n\|_{L^2(\Omega)} \leq c \|(I_h \sigma^j)_{j=1}^n\|_{L^2(\Omega)}. \]

Combining the last three estimates with (3.2)–(3.4) gives

\[ \|(\bar{\rho}_u^j \phi^j)_{j=1}^n\|_{L^2(X)} \leq c(u)(\tau + h^2) + c\|\rho^j_{j=1}^n\|_{L^2(X)}. \]

Now it follows from (3.7) and (3.9) that

\[ \|(\bar{\rho}_u^j \phi^j)_{j=1}^n\|_{L^2(X)} \leq c(u)(\tau + h^2) + c\|\rho^j_{j=1}^n\|_{L^2(X)}. \]

Thus by choosing a sufficiently small \( \epsilon \), we get

\[ \|(\bar{\rho}_u^j \phi^j)_{j=1}^n\|_{L^2(X)} \leq c(u)(\tau + h^2). \]

This and (3.8) give \( \|q^n\|_{L^2(\Omega)} \leq c(u)(\tau + h^2) \), which completes the proof. \( \square \)

Remark 3.1. The regularity requirement \( u \in C^1([0, T]; D(A)) \cap C^2([0, T]; H^1(\Omega)) \) is restrictive, and it holds only under certain compatibility conditions on the initial data \( v \) and the source term \( f \). It holds if \( v = 0 \), \( f(0) = f'(0) = 0 \) and \( f'' \in L^\infty(0, T; H^1(\Omega)) \) with a small \( \epsilon > 0 \). The proof uses crucially the maximal \( \ell^p \) regularity estimate, which differs greatly from the argument for the case of nonsmooth solutions below.

4 Error analysis for nonsmooth solutions

Now we analyze the case that the solution \( u \) is nonsmooth, and derive error estimates nearly optimal with respect to data regularity. Nonsmooth solutions are characteristic of problem (1.1): with \( f = 0 \) and \( A^\beta v \in L^2(\Omega) \), \( \beta \in [0, 1] \), \( u(t) \) satisfies [10] Theorem 2.1

\[ \|\partial^k u(t)\|_{L^2(\Omega)} \leq c t^{\beta-k} \|A^\beta v\|_{L^2(\Omega)}. \]

Thus, it is important to analyze the scheme for nonsmooth solutions. To this end, we split the error \( \|U_h^n - u(t_n)\|_{L^2(\Omega)} \) into

\[ U_h^n - u(t_n) = (U_h^{n,M_n} - u_h(t_n)) + (u_h(t_n) - u(t_n)), \]

and the spatial error \( \|u(t) - u_h(t)\|_{L^2(\Omega)} \) satisfies (with \( \ell_h = \ln(1/h + 1) \) [10]

\[ \|(u - u_h)(t)\|_{L^2(\Omega)} \leq \begin{cases} c h^2 \|A^\beta v\|_{L^2(\Omega)}, & \text{if } v_h = R_h v, \\ c h^2 t^{-\alpha} \|v\|_{L^2(\Omega)}, & \text{if } v_h = P_h v. \end{cases} \]

Thus, we focus on the temporal error \( \|U_h^{n,M_n} - u_h(t_n)\|_{L^2(\Omega)} \). The analysis below uses certain \( a \ priori \) estimates on the semidiscrete solutions \( u_h \) and its fully discrete approximations \( \bar{\rho}_u^j u_h \). The proofs are deferred to Appendix 4

Lemma 4.1. Let \( u_h \) be the solution to (2.2) with \( f = 0 \). Then for \( \beta \in [0, 1] \)

\[ |\bar{\rho}_u^n u_h(t_n)| \leq c t^{\beta-2} \|A^\beta v_h\|_{L^2(\Omega)}, \quad n > 2. \]

Lemma 4.2. Let \( u_h \) be the solution to (2.2) with \( f = 0 \) and \( y_h(t) = u_h(t) - v_h \). Then for any \( \beta \in [0, 1] \), the following statements hold.
(i) If $Av \in L^2(\Omega)$ and $v_h = R_h v$, then
\[
\|A_h^\beta (\partial_t^\ell y_h(t_n) - \bar{\partial}_t^\ell y_h(t_n))\|_{L^2(\Omega)} \leq c \tau t_n^{1-\beta \alpha} \|Av\|_{L^2(\Omega)}.
\]

(ii) If $v \in L^2(\Omega)$ and $v_h = P_h v$, then
\[
\|A_h^\beta (\partial_t^\ell y_h(t_n) - \bar{\partial}_t^\ell y_h(t_n))\|_{L^2(\Omega)} \leq c \tau t_n^{1-(1-\beta)\alpha} \|v\|_{L^2(\Omega)}.
\]

**Corollary 4.1.** Let $u_h(t)$ be the solution to (2.2) with $f \equiv 0$ and $y_h(t) = u_h(t) - v_h$. If $v \in L^2(\Omega)$ and $v_h = P_h v$, then for any $\beta \in [0,1]$, 
\[
\|A_h^\beta (\partial_t^\ell y_h(t_n) - \bar{\partial}_t^\ell y_h(t_n))\|_{L^2(\Omega)} \leq c \tau t_n^{2-(1-\beta)\alpha} \|v\|_{L^2(\Omega)}.
\]

Below we analyze the homogeneous problem with the smooth and nonsmooth initial data separately, since the requisite estimates differ substantially. The main results of this section, i.e., error estimates for the scheme (2.3) are given in Theorems 4.1 and 4.2.

### 4.1 Smooth initial data

First, we analyze the case of smooth initial data. We begin with a simple weighted estimate of inverse inequality type. The shorthand LHS denotes the left hand side.

**Lemma 4.3.** For any $\varphi^j \in X_h$ (with $\varphi^0 = 0$), and $\gamma \in (0,1)$, there holds
\[
\tau \sum_{j=1}^{n} (t_{n+1} - t_j)^{\gamma-1} \|\bar{\partial}_t^\ell \varphi^j\|_{L^2(\Omega)} \leq c \tau^{-\gamma} \sum_{j=1}^{n} (t_{n+1} - t_j)^{\gamma-1} \|\varphi^j\|_{L^2(\Omega)}.
\]

**Proof.** Since $\varphi^0 = 0$, Lemma A.2 and changing the summation order yield

\[
\text{LHS} \leq c \tau^{1-\gamma} \sum_{j=1}^{n} (t_{n+1} - t_j)^{\gamma-1} \sum_{\ell=0}^{j} (\gamma)^{\ell} \|\varphi^j\|_{L^2(\Omega)}
\]
\[
\leq c \tau^{-\frac{\gamma}{2}} \sum_{\ell=1}^{n} \|\varphi^j\|_{L^2(\Omega)} \sum_{i=0}^{n-\ell} (n - \ell + 1 - i)^{\gamma-1} (i + 1)^{-\gamma-1}.
\]

The desired assertion follows directly from Lemma A.1. \hfill \square

The next result gives a weighted estimate on the scheme (2.4).

**Lemma 4.4.** Let $e^\alpha \in X_h$ satisfy $e^0 = 0$ and 
\[
\bar{\partial}_t^\ell e^\alpha + A_h e^\alpha = \sigma^\alpha, \quad n = 1, \ldots, N.
\]

Then with $\ell_n = \ln(1 + t_n/\tau)$, there holds
\[
\tau \sum_{j=1}^{n} (t_{n+1} - t_j)^{\gamma-1} |\bar{\partial}_t^\ell e^\alpha| \leq c \tau \ell_n \sum_{j=1}^{n} (t_{n+1} - t_j)^{\gamma-1} \|(I + \tau^\alpha A_h)^{-\frac{\ell}{2}} \sigma^j\|_{L^2(\Omega)}.
\]

**Proof.** Let $I_h = (I + \tau^\alpha A_h)^{-\frac{\ell}{2}}$. By the identity $\bar{\partial}_t^\ell e^\alpha = \sigma^\alpha - A_h e^\alpha$, we have
\[
|\bar{\partial}_t^\ell e^\alpha| \leq \|I_h \bar{\partial}_t^\ell e^\alpha\|_{L^2(\Omega)} + \tau^\alpha \|I_h A_h \bar{\partial}_t^\ell e^\alpha\|_{L^2(\Omega)}
\]
\[
\leq \|I_h e^\alpha\|_{L^2(\Omega)} + \|I_h \sigma^\alpha\|_{L^2(\Omega)} + \tau^\alpha \|I_h A_h \bar{\partial}_t^\ell e^\alpha\|_{L^2(\Omega)}.
\]

Then the inverse estimate in Lemma 4.3 implies
\[
\text{LHS} \leq c \tau \sum_{j=1}^{n} (t_{n+1} - t_j)^{\gamma-1} \|(I_h e^\alpha)\|_{L^2(\Omega)} + \|I_h \sigma^\alpha\|_{L^2(\Omega)}
\]

\[ \Delta u \cdot \nabla^\alpha e^j + \tau A h^\alpha e^j \leq c_\tau \sum_{j=1}^n (t_{j+1} - t_j)^{\frac{\alpha}{2}-1} \| I h A h \partial_y e^j \|_{L^2(\Omega)} \]

\[ \leq c_\tau \sum_{j=1}^n (t_{j+1} - t_j)^{\frac{\alpha}{2}-1} \left( \| I h A h e^j \|_{L^2(\Omega)} + \| I h \sigma^j \|_{L^2(\Omega)} \right). \]

Now the representation \( e^j = \tau \sum_{\ell=1}^j E_{h,\tau}^\ell \sigma^\ell \), cf. (2.6), and Lemma 2.1 yield

\[ \| I h A h e^j \|_{L^2(\Omega)} \leq c_\tau \sum_{\ell=1}^n (t_{j+1} - t_\ell)^{-1} \| I h \sigma^\ell \|_{L^2(\Omega)}. \]

Combining the last two estimates and changing the summation order gives

\[ \text{LHS} \leq c_\tau \sum_{j=1}^n (t_{j+1} - t_j)^{\frac{\alpha}{2}-1} \left( \sum_{\ell=1}^j (t_{j+1} - t_\ell)^{-1} \| I h \sigma^\ell \|_{L^2(\Omega)} + \| I h \sigma^j \|_{L^2(\Omega)} \right) \]

\[ = c_\tau \sum_{\ell=1}^n \| I h \sigma^\ell \|_{L^2(\Omega)} \left( \tau \sum_{j=1}^n (t_{j+1} - t_j)^{\frac{\alpha}{2}-1} (t_{j+1} - t_\ell)^{-1} + (t_{n+1} - t_\ell)^{\frac{\alpha}{2}-1} \right). \]

This and Lemma A.1 complete the proof. \( \square \)

Now we can give an error estimate for the scheme (2.4) for smooth initial data, i.e., \( Av \in L^2(\Omega) \). The error bound for (2.9) is identical with that for the exact linear solver, up to a logarithmic factor \( \ell_n \).

**Theorem 4.1.** Let \( Av \in L^2(\Omega) \) and condition (2.11) hold. Let \( u_h^n \equiv U_h^n, M_n \) be the solution of (2.8)-(2.9) with \( f = 0 \) and \( v_h = R_h v \), and let \( U_h^n = \bar{U}_h^n \) for %\( n = 1, 2 \). Then with \( \ell_n = \ln(1 + t_n / \tau) \), there exists a \( \delta > 0 \) such that

\[ \| U_h^n - u_h(t_n) \|_{L^2(\Omega)} \leq c t_{\alpha n} \ell_n \| Av \|_{L^2(\Omega)}, \quad \text{if } c_0 \kappa M_n \leq \delta \ell_n^{-1} \min(\tilde{\epsilon}, 1), \]

for \( n = 1, 2 \), and thus we consider only \( n > 2 \). Note that \( e^n = U_h^n - u_h(t_n) \) satisfies \( e^0 = 0 \) and

\[ \partial_\tau e^n + A_h e^n = \sigma^n := \omega^n + (I + \tau A_h) \eta^n, \]

where \( \omega^n \) and \( \eta^n \) are defined respectively by

\[ \omega^n = - (\partial^\alpha \sigma - \partial^\alpha \eta)(u_h(t_n) - v_h) \quad \text{and} \quad \eta^n = \tau^{-\alpha}(U_h^n - \bar{U}_h^n), \]

where the auxiliary function \( \bar{U}_h^n \in X_h \) satisfies \( \bar{U}_h^0 = R_h v \) and

\[ \tau^{-\alpha} \left( \bar{U}_h^n + \sum_{j=1}^n b_{n-j}^{(0)} U_h^j - \sum_{j=0}^n b_{n-j}^{(0)} U_h^0 \right) + A_h \bar{U}_h^n = f_h, \quad n = 1, 2, \ldots, N. \]

The rest of the proof consists of three steps.

**Step 1:** Bound \( \| e^n \|_{L^2(\Omega)} \) by local truncation errors. Since \( e^0 = 0 \), by the error equation (4.1), (2.5) and Lemma 2.1, \( e^n \) is bounded by

\[ \| e^n \|_{L^2(\Omega)} \leq c_\tau \sum_{j=1}^n (t_{j+1} - t_j)^{\alpha-1} \| \omega^j \|_{L^2(\Omega)} \]

\[ + c_\tau \sum_{j=1}^n (t_{n+1} - t_j)^{\frac{\alpha}{2}-1} \| A_h^{\frac{1}{2}} (I + \tau A_h) \eta^j \|_{L^2(\Omega)} := I + II. \]

It suffices to bound I and II. By Lemmas (4.2) and A.1, I is bounded by

\[ I \leq c_\tau^2 \| Av \|_{L^2(\Omega)} \sum_{j=1}^n (t_{j+1} - t_j)^{\alpha-1} t_j^{-1} \leq c t_{\alpha n} \ell_n \| Av \|_{L^2(\Omega)}. \]

(4.4)
Further, it follows from \((4.5)\) that
\[
\Pi \leq \epsilon r n \sum_{j=1}^{n} (t_{n+1} - t_j) \binom{n}{j} |\eta^j|.
\] (4.5)

**Step 2:** Bound the summand \(|\eta^j|\). By assumption \((4.1)\), for any \(c_0k_n^M \leq \delta \min(t_n^{\omega^2}, 1) \ell_n^{-1},\)
\[
|U_n^k - \bar{U}_n^k| \leq c_0k_n^M \left( \left|U_n^k - U_n^k\right| + |U_n^k - \bar{U}_n^k| \right).
\]
Let \(\epsilon = \frac{\delta}{1 - \delta} \ell_n^{-1}\). Since \(c_0k_n^M/(1 - c_0k_n^M) \leq \epsilon \ell_n^2\), rearranging the terms yields
\[
|U_n^k - \bar{U}_n^k| \leq \epsilon \ell_n^2 |U_n^k - U_n^k|,
\]
and by the definition of \(\eta^n\) in \((4.2)\), \(\eta^1 = \eta^2 = 0\) and for \(n > 2\)
\[
|\eta^n| = \tau^{-\alpha} |U_n^k - \bar{U}_n^k| \leq \epsilon \tau^{-\alpha} \ell_n^2 |U_n^k - U_n^k|,
\]
which together with the choice of \(U_n^k\) in \((4.8)\) implies
\[
|\eta^n| \leq \epsilon \tau^{1 - \alpha} \ell_n^2 \left( |\partial^2 u_k(t_j)| + |\partial^2 e^{-\alpha} + \tau |\partial^2 u_k(t_n)|) \right). \quad (4.6)
\]
By Lemma \((4.1)\) \(|\partial^2 u_k(t_j)| \leq c\epsilon \tau^{\alpha - 2} \|Av\|\). This and Lemma \((4.6)\) give
\[
\tau^{3 - \alpha} \sum_{j=3}^{n} (t_{n+1} - t_j) \binom{n}{j} \ell_n^2 |\partial^2 u_k(t_j)| \leq c\tau^{2 - \alpha} \sum_{j=2}^{n} (t_{n+1} - t_j) \binom{n}{j} \ell_n^2 |\partial^2 u_k(t_n)| \quad (4.7)
\]

**Step 3:** Bound explicitly the term \(\Pi\). The estimates \((4.6)\) and \((4.7)\) imply
\[
\tau \sum_{j=1}^{n} (t_{n+1} - t_j) \binom{n}{j} \ell_n^2 |\partial^2 u_k| \leq c\epsilon \tau^{\alpha - 1} \|Av\|_{L^2(\Omega)} + c\epsilon \tau^{2 - \alpha} \sum_{j=2}^{n} (t_{n+1} - t_j) \binom{n}{j} \ell_n^2 |\partial^2 u_k|.
\]
By the identity \(\partial_j^2 (\partial^2 e) = \partial^2 e\) and Lemma \((4.4)\) we get
\[
\tau^{2 - \alpha} \sum_{j=2}^{n} (t_{n+1} - t_j) \binom{n}{j} \ell_n^2 |\partial^2 u_k| \leq c\tau \sum_{j=2}^{n} (t_{n+1} - t_j) \binom{n}{j} \ell_n^2 |\partial^2 u_k|.
\]
Further, by Lemma \((4.4)\) and \((4.3)\), there holds
\[
\tau \sum_{j=1}^{n} (t_{n+1} - t_j) \binom{n}{j} \ell_n^2 |\partial^2 u_k|
\]
\[
\leq c\epsilon \ell_n \tau \sum_{j=1}^{n} (t_{n+1} - t_j) \binom{n}{j} \ell_n^2 \left( \|I + \tau^\alpha A_k\| \binom{n}{j} \ell_n^2 \right) + \|\eta^n\|_{L^2(\Omega)} \|\eta^n\|_{L^2(\Omega)}
\]
\[
\leq c\epsilon \ell_n \tau \sum_{j=1}^{n} (t_{n+1} - t_j) \binom{n}{j} \ell_n^2 |\eta^n| + c\epsilon \tau^{\alpha - 1} \|Av\|_{L^2(\Omega)}.
\]
The last three estimates together lead to
\[
\tau \sum_{j=1}^{n} (t_{n+1} - t_j) \binom{n}{j} \ell_n^2 |\eta^n| \leq c\epsilon \tau^{\alpha - 1} \ell_n^2 \|Av\|_{L^2(\Omega)} + c\epsilon \ell_n \tau \sum_{j=1}^{n} (t_{n+1} - t_j) \binom{n}{j} \ell_n^2 |\eta^n|,
\]
which upon choosing a sufficiently small \(\delta\) implies
\[
\tau \sum_{j=1}^{n} (t_{n+1} - t_j) \binom{n}{j} \ell_n^2 |\eta^n| \leq c\epsilon \tau^{\alpha - 1} \ell_n^2 \|Av\|_{L^2(\Omega)}.
\]
This, and the estimates \((4.2)\)–\((4.5)\) complete the proof. \(\square\)
4.2 Nonsmooth initial data

Now we turn to nonsmooth initial data, i.e., $v \in L^2(\Omega)$. First we give a weighted estimate on the time stepping scheme (2.4). The weight $t_n$ in the estimate compensates the strong singularity of the summands.

**Lemma 4.5.** If $e^n \in X_h$ satisfies $e^n = 0$ and $\tilde{D}_x e^n + A_h e^n = \sigma^n$, $n = 1, \ldots, N$, then

$$t_n \| e^n \|_{L^2(\Omega)} \leq c\tau \sum_{j=1}^n \| A_h^{-1} \sigma^j \|_{L^2(\Omega)} + (t_{n+1} - t_j)^{\frac{2}{p}-1} t_j \| A_h^{-\frac{2}{p}} \sigma^j \|_{L^2(\Omega)}.$$  

**Proof.** Using (2.5) and the splitting $t_n = (t_n - t_j) + t_j$, we have

$$t_n e^n = \tau \sum_{j=1}^n (t_n - t_j) E_{h,\tau}^{n-j} \sigma^j + \tau \sum_{j=1}^n t_j E_{h,\tau}^{n-j} \sigma^j.$$  

Then from Lemma 2.1 we deduce

$$t_n \| e^n \|_{L^2(\Omega)} \leq \tau \sum_{j=1}^n (t_n - t_j) \| A_h E_{h,\tau}^{n-j} \| \| A_h^{-1} \sigma^j \|_{L^2(\Omega)}$$  

$$+ \tau \sum_{j=1}^n t_j \| A_h \frac{2}{p} E_{h,\tau}^{n-j} \| \| A_h^{-\frac{2}{p}} \sigma^j \|_{L^2(\Omega)}$$  

$$\leq c\tau \sum_{j=1}^n (t_n - t_j)(t_{n+1} - t_j)^{-1} \| A_h^{-1} \sigma^j \|_{L^2(\Omega)}$$  

$$+ c\tau \sum_{j=1}^n t_j (t_{n+1} - t_j)^{\frac{2}{p}-1} \| A_h^{-\frac{2}{p}} \sigma^j \|_{L^2(\Omega)},$$

from which the desired assertion follows. \hfill $\Box$

**Lemma 4.6.** Let $e^n \in X_h$ satisfy $e^0 = 0$ and $\tilde{D}_x e^n + A_h e^n = \sigma^n$, $n = 1, \ldots, N$. Then with $\ell_n = \ln(1 + t_n/\tau)$, there holds

$$\tau^{2-\alpha} \sum_{j=1}^n (t_j + (t_{n+1} - t_j)^{\frac{2}{p}-1} t_j^2) |\tilde{D}_x e^j|$$  

$$\leq c\ell_n t_n \sum_{j=1}^n (1 + t_j (t_{n+1} - t_j)^{\frac{2}{p}-1}) \| (I + \tau^\alpha A_h)^{-\frac{2}{p}} \sigma^j \|_{L^2(\Omega)}.$$  

**Proof.** By the identity $\tilde{D}_x = \tilde{D}_x^{1-\alpha} \tilde{D}_x^\alpha$ and Lemmas A.2 and A.3, we have (with the shorthand $a^\ell = |\tilde{D}_x^\ell e^j|$)

$$\text{LHS} \leq \tau \sum_{j=1}^n t_j \sum_{\ell=1}^j \sum_{j=1}^n |b_{j-\ell}^{(1-\alpha)}| a^\ell + \tau \sum_{j=1}^n (t_{n+1} - t_j)^{\frac{2}{p}-1} t_j^2 \sum_{\ell=1}^j \sum_{j=1}^n |b_{j-\ell}^{(1-\alpha)}| a^\ell$$  

$$\leq c\tau \sum_{\ell=1}^n a^\ell \sum_{j=1}^n j(j+1-\ell)^{\alpha-2}$$  

$$+ c\tau^{2+\frac{3}{2}} \sum_{\ell=1}^n a^\ell \sum_{j=1}^n \sum_{j=1}^n (n+1-j)^{\frac{2}{p}-1} j^2 (j+1-\ell)^{\alpha-2}$$  

$$\leq c\tau t_n \sum_{j=1}^n |\tilde{D}_x^\alpha e^j| + c\tau t_n \sum_{j=1}^n (t_{n+1} - t_j)^{\frac{2}{p}-1} |\tilde{D}_x^\alpha e^j| := I_1 + I_2.$$  

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With \( I_h = (I + \tau^\alpha A_h)^{-\frac{1}{2}} \), the proof of Lemma 4.4 leads to
\[
|\bar{\partial}_r^\alpha e^j| \leq c\|I_h\sigma^j\|_{L^2(\Omega)} + c\tau \sum_{\ell=1}^{j} (t_{j+1} - t_{\ell})^{-1}\|I_h\sigma^\ell\|_{L^2(\Omega)}.
\]

Straightforward computation with Lemma A.1 gives
\[
I_1 \leq c\ell_n t_n \tau \sum_{j=1}^{n} \|I_h\sigma^j\|_{L^2(\Omega)}
\]
\[
I_2 \leq c\ell_n t_n \tau \sum_{j=1}^{n} (1 + (t_{n+1} - t_j)^{\frac{2}{3}} - 1)\|I_h\sigma^j\|_{L^2(\Omega)}.
\]

Collecting the terms gives the desired assertion.

Next, we give a weighted estimate due to the local truncation error \( \omega^k \).

**Lemma 4.7.** Let \( e^n \in X_h \) satisfy \( e^0 = 0 \) and
\[
\bar{\partial}_r^\alpha e^n + A_h e^n = \omega^n, \quad n = 1, \ldots, N,
\]
where \( \omega^n \) defined in [4.2]. Then with \( \ell_n = \ln(1 + t_n/\tau) \), there holds
\[
\tau^{2-\alpha} \sum_{j=1}^{n} t_j |\bar{\partial}_r e^j| + \tau^{2-\alpha} \sum_{j=1}^{n} (t_{n+1} - t_j)^{\frac{2}{3}} t_j^2 |\bar{\partial}_r e^j| \leq c\ell_n \tau^{2-\alpha} \|e\|_{L^2(\Omega)}.
\]

**Proof.** By applying the operator \( \bar{\partial}_r \) to both sides of the defining equation for \( e^n \) and the associativity of CQ, we obtain
\[
\bar{\partial}_r e^n = \tau \sum_{k=1}^{n} E^{n-k}_{h,\tau} \bar{\partial}_r \omega^k.
\]

Let \( w_{j,n} = t_j + (t_{n+1} - t_j)^{\frac{2}{3}} t_j^2 \) be the weight. Then,
\[
\text{LHS} \leq \tau^{2-\alpha} \sum_{j=2}^{n} w_{j,n} \|\bar{\partial}_r e^j\|_{L^2(\Omega)} + \tau^{2} \sum_{j=2}^{n} w_{j,n} \|A_h \bar{\partial}_r e^j\|_{L^2(\Omega)} := I + II.
\]

For the term I, we further split it into two terms (with \( m_j = \lfloor j/2 \rfloor \)):
\[
I \leq \tau^{3-\alpha} \sum_{j=2}^{n} w_{j,n} \|\sum_{k=1}^{m_j} E^{j-k}_{h,\tau} \bar{\partial}_r \omega^k\|_{L^2(\Omega)}
\]
\[
+ \tau^{3-\alpha} \sum_{j=2}^{n} w_{j,n} \|\sum_{k=m_j+1}^{j} E^{j-k}_{h,\tau} \bar{\partial}_r \omega^k\|_{L^2(\Omega)} := I_1 + I_2.
\]

Then by the summation by parts formula
\[
\sum_{i=j}^{k} f_i (g_{i+1} - g_i) + \sum_{i=j+1}^{k} g_i (f_i - f_{i-1}) = f_k g_{k+1} - f_j g_j,
\]
the triangle inequality, and Lemma 2.1, we have
\[
I_1 = \tau^{3-\alpha} \sum_{j=2}^{n} w_{j,n} \|\sum_{k=1}^{m_j-1} \bar{\partial}_r E^{j-k+1}_{h,\tau} \omega^k + \tau^{-1} E^{m_j}_{h,\tau} \omega^j\|_{L^2(\Omega)}.
\]
\begin{align*}
\leq & \tau^{3-\alpha} \sum_{j=2}^n w_{j,n} \sum_{k=1}^{m_j-1} \| \tilde{\partial}_t E_{h,\tau}^{j,k+1} \omega^k \|_{L^2(\Omega)} + \tau^{2-\alpha} \sum_{j=2}^n w_{j,n} \| E_{h,\tau}^{m_j} \omega^j \|_{L^2(\Omega)} \\
\leq & c\tau^{3-\alpha} \sum_{j=2}^n w_{j,n} \sum_{k=1}^{m_j-1} (t_{j+1} - t_k)^{-2} \| A_h^{-1} \omega^k \|_{L^2(\Omega)} \\
+ & c\tau^{2-\alpha} \sum_{j=2}^n w_{j,n} t_{j-1}^{-1} \| A_h^{-1} \omega^j \|_{L^2(\Omega)}.
\end{align*}

By Lemma 4.2 \| A_h^{-1} \omega^j \|_{L^2(\Omega)} \leq c\tau t_j^{-1} \| v \|_{L^2(\Omega)}$, and upon substitution, Lemma A.1 implies
\begin{align*}
I_1 \leq c\tau^{4-\alpha} \sum_{j=2}^n t_j^{-2} w_{j,n} \sum_{k=1}^{m_j-1} t_{k}^{-1} \| v \|_{L^2(\Omega)} + c\tau^{3-\alpha} \sum_{j=2}^n w_{j,n} t_{j-1}^{-2} \| v \|_{L^2(\Omega)} \\
\leq c\tau^{2-\alpha} \ell_n^2 \| v \|_{L^2(\Omega)}.
\end{align*}

Similarly, by Lemma 2.1 Corollary 4.1 and Lemma A.1 we deduce
\begin{align*}
I_2 \leq c\tau^{3-\alpha} \sum_{j=2}^n w_{j,n} \sum_{k=m_j+1}^{j} \| E_{h,\tau}^{j,k} \tilde{\partial}_t \omega^k \|_{L^2(\Omega)} \\
\leq c\tau^{4-\alpha} \sum_{j=2}^n w_{j,n} \sum_{k=m_j+1}^{j} (t_{j+1} - t_k)^{-1} \| A_h^{-1} \tilde{\partial}_t \omega^k \|_{L^2(\Omega)} \\
\leq c\tau^{4-\alpha} \sum_{j=2}^n w_{j,n} \sum_{k=m_j+1}^{j} (t_{j+1} - t_k)^{-1} t_{k}^{-1} \| v \|_{L^2(\Omega)} \leq c\tau^{2-\alpha} \ell_n^2 \| v \|_{L^2(\Omega)}.
\end{align*}

Thus, \( I \leq c\tau^{2-\alpha} \ell_n^2 \| v \|_{L^2(\Omega)} \). In the same manner, we further split II into two terms
\begin{align*}
II \leq & \tau^3 \sum_{j=2}^n w_{j,n} \sum_{k=1}^{m_j-1} E_{h,\tau}^{j,k} A_h \tilde{\partial}_t \omega^k \|_{L^2(\Omega)} \\
& + \tau^3 \sum_{j=2}^n w_{j,n} \sum_{k=m_j+1}^{j} E_{h,\tau}^{j,k} A_h \tilde{\partial}_t \omega^k \|_{L^2(\Omega)} := II_1 + II_2.
\end{align*}

For the term \( II_1 \), we apply summation by parts formula, triangle inequality, Lemmas 2.1, 4.2 and A.1 to obtain
\begin{align*}
II_1 = & \tau^3 \sum_{j=2}^n w_{j,n} \sum_{k=1}^{m_j-1} \tilde{\partial}_t E_{h,\tau}^{j,k+1} A_h \omega^k + \tau^{-1} E_{h,\tau}^{m_j} A_h \omega^j \|_{L^2(\Omega)} \\
\leq & \tau^3 \sum_{j=2}^n w_{j,n} \sum_{k=1}^{m_j-1} \| \tilde{\partial}_t E_{h,\tau}^{j,k+1} A_h \omega^k \|_{L^2(\Omega)} + \tau^2 \sum_{j=2}^n w_{j,n} \| E_{h,\tau}^{m_j} A_h \omega^j \|_{L^2(\Omega)} \\
\leq & c\tau^3 \sum_{j=2}^n w_{j,n} \sum_{k=1}^{m_j-1} (t_{j+1} - t_k)^{-2} \| \omega^k \|_{L^2(\Omega)} + c\tau^2 \sum_{j=2}^n w_{j,n} t_{j-1}^{-1} \| \omega^j \|_{L^2(\Omega)} \\
\leq & c\tau^4 \sum_{j=2}^n t_j^{-2} w_{j,n} \sum_{k=1}^{m_j-1} t_k^{-1-\alpha} \| v \|_{L^2(\Omega)} + c\tau^4 \sum_{j=2}^n t_j^{-1-\alpha} \| v \|_{L^2(\Omega)} \\
\leq & c\tau^{2-\alpha} \ell_n^2 \| v \|_{L^2(\Omega)},
\end{align*}

and likewise by Lemma 2.1 and Corollary 4.1
\begin{align*}
II_2 \leq & \tau^3 \sum_{j=2}^n w_{j,n} \sum_{k=m_j+1}^{j} \| E_{h,\tau}^{j,k} A_h \tilde{\partial}_t \omega^k \|_{L^2(\Omega)}.
\end{align*}
Thus, \( II \leq c \tau^{-\alpha} \ell^2_n \|v\|_{L^2(\Omega)} \), and the desired assertion follows. \( \square \)

Now we can state the error estimate for (2.9) with \( v \in L^2(\Omega) \).

**Theorem 4.2.** Let \( v \in L^2(\Omega) \) and assumption (2.11) hold. Let \( U_h^n = U_h^{n,M_n} \) be the solution to (2.8) with \( f = 0 \) and \( v_h = P_h v \), and let \( U_h^n = \tilde{U}_h^n \) for \( n = 1, 2 \). Then with \( \ell_n = \ln(1 + t_n/\tau) \), there exists a \( \delta > 0 \) such that

\[
\| U_h^n - u_h(t_n) \|_{L^2(\Omega)} \leq c \tau \ell_n \|v\|_{L^2(\Omega)}, \quad \text{if } c_0 \kappa M_n \leq \delta \min(t_n, 1) \ell_n^{-1}.
\]

**Proof.** The proof employs (4.1) - (4.3), and the overall strategy is similar to that for Theorem 3.1. However, due to lower solution regularity, the requisite weighted estimates are different. Below we sketch the main steps.

**Step 1:** Bound \( \| e^n \|_{L^2(\Omega)} \) by \( |\eta|^j \)'s. By (4.1) and Lemma 4.5,

\[
t_n \| e^n \|_{L^2(\Omega)} \leq c \tau \sum_{j=1}^n \| A_h^{-1} \sigma^j \|_{L^2(\Omega)} + c \tau \sum_{j=1}^n (t_{n+1} - t_j)^{1/2} - 1 t_j \| A_h^{-1/2} \sigma^j \|_{L^2(\Omega)}
\]

\[
\leq c \tau \sum_{j=1}^n \| A_h^{-1} \omega^j \|_{L^2(\Omega)} + c \tau \sum_{j=1}^n (t_{n+1} - t_j)^{1/2} - 1 t_j \| A_h^{-1/2} \omega^j \|_{L^2(\Omega)}
\]

\[
+ c \tau \sum_{j=1}^n \| A_h^{-1} \eta^j \|_{L^2(\Omega)} + c \tau \sum_{j=1}^n (t_{n+1} - t_j)^{1/2} - 1 t_j \| A_h^{-1/2} \eta^j \|_{L^2(\Omega)}
\]

\[
:= I + II.
\]

For the term I, Lemmas 4.2 ii) and A.1 lead to \( I \leq c \tau \ell_n \|v\|_{L^2(\Omega)} \). The estimate (3.5) allows simplifying the term II to

\[
II \leq c \tau \sum_{j=2}^n w_{j,n} |\eta|^j \quad \text{with } w_{j,n} = 1 + (t_{n+1} - t_j)^{1/2} - 1 t_j.
\]

(4.8)

The rest of the proof is to explicitly bound II under assumption (2.11).

**Step 2:** Bound the summand \( |\eta|^j \). Under assumption (2.11), for any \( c_0 \kappa M_n \leq \delta \min(t_n, 1) \ell_n^{-1} \),

\[
| U_h^n - \tilde{U}_h^n | \leq c_0 \kappa M_n (| U_h^{n,0} - U_h^n | + | U_h^n - \tilde{U}_h^n |).
\]

Then with \( \epsilon = \frac{\delta}{1 - \delta} \ell_n^{-1} \), we have \( | U_h^n - \tilde{U}_h^n | \leq \epsilon t_n | U_h^{n,0} - U_h^n | \), and hence

\[
|\eta|^n = \tau^{-\alpha} | U_h^n - \tilde{U}_h^n | \leq \epsilon \tau^{-\alpha} t_n | U_h^{n,0} - U_h^n |.
\]

By the choice of \( U_h^{n,0} \) in (2.8), \( \eta^1 = \eta^2 = 0 \) and

\[
|\eta|^n \leq c \tau^{1-\alpha} t_n (|\tilde{\partial}_r e^n| + |\tilde{\partial}_r e^{n-1}| + \tau |\tilde{\partial}_r^2 u_h(t_n)|).
\]

By Lemmas 4.1 and A.1 we have

\[
\tau^{3-\alpha} \sum_{j=3}^n t_j w_{j,n} |\tilde{\partial}_r^2 u_h(t_j)| \leq c \tau^{2-\alpha} \ell_n \|v\|_{L^2(\Omega)}.
\]

(4.9)
**Step 3:** Bound the term II explicitly. It follows from (1.8) and (1.9) that
\[ II \leq c\tau^{2-\alpha} \ell_n \|v\|_{L^2(\Omega)} + c\tau^{2-\alpha} \sum_{j=1}^{n} t_j w_{j,n} |\partial_x e^j|. \]

It follows from Lemmas 4.6 and 4.7 that
\[ \tau^{2-\alpha} \sum_{j=1}^{n} t_j w_{j,n} |\partial_x e^j| \leq c\ell_n \tau \sum_{j=1}^{n} w_{j,n} |\eta^j| + c\tau^{2-\alpha} \ell_n^2 \|v\|_{L^2(\Omega)}. \]

The rest of the proof is identical with Theorem 4.1 and hence omitted. □

**Remark 4.1.** The solution \( U_h^n \) by the scheme (2.4) satisfies [4, Theorem 3.5]
\[ \|U_h^n - u_h(t_n)\| \leq \begin{cases} c\tau_{t_n}^{\alpha-1} \|\nabla v\|_{L^2(\Omega)}, & \text{if } v_h = R_h v, \\ c\tau_{t_n}^{\alpha+1} \|v\|_{L^2(\Omega)}, & \text{if } v_h = P_h v. \end{cases} \]

The error estimates in Theorems 4.7 and 4.8 for (2.9) are comparable, up to a log factor \( \ell_n \). However, the IIS (2.9) does not require the exact solution of the resulting linear systems and thus can be more efficient.

## 5 Numerical experiments and discussions

Now we present numerical results to illustrate the theoretical results. The numerical experiments are performed on the square \( \Omega = (-1,1)^2 \). In the computation, we first divide the interval \((-1,1)\) into \( K \) equally spaced subintervals of length \( h = 2/K \) so that the domain \( \Omega = (-1,1)^2 \) is divided into \( K^2 \) small squares, and then obtain a uniform triangulation by connecting the diagonal of each small square. We divide the time interval \([0,T]\) into a uniform grid with a time step size \( \tau = T/N \). Since the semidiscrete solution \( u_h \) is unavailable in closed form, we compute a reference solution \( u_h(t_n) \) by the corrected CQ generated by BDF3 [11] in time with \( N = 1000 \) and \( K = 256 \) in space. We compute the temporal error at \( t_N = T \) by
\[ e^N = \frac{\|U_h^n - u_h(t_n)\|_{L^2(\Omega)}}{\|u_h(t_N)\|_{L^2(\Omega)}}. \]

In the IIS (2.9), any iterative solver satisfying (2.11) can be employed. In this work, we employ the V-cycle multigrid method with standard Jacobi or Gauss-Seidel smoothers to inexactly solve the linear systems, which is known to satisfy (2.11) [27, Theorem 11.4, p. 199]. Multigrid type methods were employed also in [16, 7], but without error analysis for either smooth or nonsmooth solutions. In the experiments, the spatial mesh size \( h \) is fixed with \( K = 256 \) so that the results focus on the temporal error.

### 5.1 Example 1: smooth solutions

First we consider problem (1.1) with \( A = -5\Delta \), \( T = 1 \), \( v = 0 \) and \( f(x,t) = t^2(1+x_1)(1-x_1)(1+x_2)(1-x_2) \). The source term \( f \) satisfies compatibility conditions: \( f(0) = f'(0) = 0 \) and \( f'' \in C^1([0,T], D(A)) \). Thus the solution \( u \) satisfies the regularity assumption in Theorem 3.2 (see Remark 3.1), and accordingly, the number \( M_n \) of iterations may be taken to be uniform in time, so as to preserve the desired first-order convergence.

We present numerical results for different values of \( \alpha \) and \( M_n \) in Tables 1 and 2 obtained by the IIS (2.9) with point Jacobi and Gauss-Seidel smoothers, respectively. In each small block of the tables, the numbers under the errors denote the log (with a base 2) of the ratio between the errors at consecutive time step sizes, and the theoretical value is one for a first-order convergence. We observe that for all three \( \alpha \) values, a steady convergence for \( M_n = 2 \) and \( M_n = 3 \), however, the results for \( M_n = 1 \) suffer from severe numerical instability, as indicated by large oscillations and big deviation from one. This observation holds for both Jacobi and Gauss-Seidel smoothers, and agrees well with Theorem 3.2 which predicts that a steady convergence of the scheme (2.9) requires a fixed but sufficiently large number of iterations at all time levels for smooth solutions.
Table 1: $L^2$ errors $e^N$ for Example 1 with $K = 128$, point Jacobi smoother.

| $\alpha$ | $M_n \backslash N$ | 10   | 20   | 40   | 80   | 160  | 320  |
|----------|---------------------|------|------|------|------|------|------|
| 0.2      | 1                   | 2.73e-3 | 5.46e-4 | 9.26e-5 | 4.41e-5 | 3.43e-5 | 2.16e-5 |
|          |                     | 2.32 | 2.56 | 1.07 | 0.36 | 0.66 |     |
|          | 2                   | 3.11e-4 | 2.37e-4 | 1.47e-4 | 8.83e-5 | 5.00e-5 | 2.55e-5 |
|          |                     | 0.39 | 0.69 | 0.73 | 0.82 | 0.97 |     |
|          | 3                   | 6.67e-4 | 3.35e-4 | 1.79e-4 | 9.61e-5 | 5.07e-5 | 2.57e-5 |
|          |                     | 0.99 | 0.91 | 0.89 | 0.92 | 0.98 |     |

Table 2: $L^2$ errors $e^N$ for Example 1 with $K = 128$, Gauss-Seidel smoother.

| $\alpha$ | $M_n \backslash N$ | 10   | 20   | 40   | 80   | 160  | 320  |
|----------|---------------------|------|------|------|------|------|------|
| 0.2      | 1                   | 1.43e-3 | 2.06e-4 | 2.93e-4 | 2.10e-4 | 1.24e-4 | 6.64e-5 |
|          |                     | 2.79 | -0.51 | 0.48 | 0.76 | 0.90 |     |
|          | 2                   | 1.70e-3 | 9.41e-4 | 4.99e-4 | 2.66e-4 | 1.39e-4 | 6.98e-5 |
|          |                     | 0.85 | 0.92 | 0.91 | 0.94 | 0.99 |     |
|          | 3                   | 2.07e-3 | 1.04e-3 | 5.31e-4 | 2.74e-4 | 1.39e-4 | 7.02e-5 |
|          |                     | 0.99 | 0.97 | 0.95 | 0.98 | 0.99 |     |
| 0.5      | 1                   | 4.10e-4 | 8.79e-4 | 6.52e-4 | 3.94e-4 | 2.17e-4 | 1.12e-4 |
|          |                     | -1.10 | 0.43 | 0.73 | 0.86 | 0.96 |     |
|          | 2                   | 3.13e-3 | 1.66e-3 | 8.58e-4 | 4.47e-4 | 2.26e-4 | 1.14e-4 |
|          |                     | 0.92 | 0.95 | 0.94 | 0.98 | 0.99 |     |
|          | 3                   | 2.07e-3 | 1.75e-3 | 8.85e-4 | 4.53e-4 | 2.28e-4 | 1.14e-4 |
|          |                     | 1.00 | 0.98 | 0.97 | 0.99 | 1.00 |     |

Table 2: $L^2$ errors $e^N$ for Example 1 with $K = 128$, Gauss-Seidel smoother.

| $\alpha$ | $M_n \backslash N$ | 10   | 20   | 40   | 80   | 160  | 320  |
|----------|---------------------|------|------|------|------|------|------|
| 0.8      | 1                   | 1.31e-3 | 2.75e-4 | 3.50e-4 | 2.30e-4 | 1.28e-4 | 6.75e-5 |
|          |                     | 2.26 | -0.35 | 0.61 | 0.84 | 0.93 |     |
|          | 2                   | 1.80e-3 | 1.02e-3 | 5.39e-4 | 2.76e-4 | 1.40e-4 | 7.03e-5 |
|          |                     | 0.82 | 0.92 | 0.96 | 0.98 | 0.99 |     |
|          | 3                   | 2.16e-3 | 1.11e-3 | 5.59e-4 | 2.81e-4 | 1.41e-4 | 7.05e-5 |
|          |                     | 0.99 | 0.97 | 0.95 | 0.98 | 0.99 |     |
| 0.8      | 1                   | 4.04e-4 | 9.71e-4 | 7.12e-4 | 4.12e-4 | 2.19e-4 | 1.13e-4 |
|          |                     | -1.27 | 0.45 | 0.79 | 0.91 | 0.96 |     |
|          | 2                   | 3.23e-3 | 1.74e-3 | 8.98e-4 | 4.55e-4 | 2.28e-4 | 1.14e-4 |
|          |                     | 0.89 | 0.95 | 0.98 | 0.99 | 1.00 |     |
|          | 3                   | 3.58e-3 | 1.81e-3 | 9.12e-4 | 4.57e-4 | 2.29e-4 | 1.14e-4 |
|          |                     | 0.98 | 0.99 | 1.00 | 1.00 | 1.00 |     |

5.2 Example 2: nonsmooth solutions

Next we consider problem (1.1) with $A = -5\Delta$, $T = 1$, $f = 0$ and $v(x, y) = \chi_{(-1,0) \times (-1,0)}(x, y)$. The initial data $v$ is piecewise constant and hence $v \in H^{1-\epsilon}(\Omega)$ for any small $\epsilon > 0$. The number $M_n$ of iterations in the scheme (2.9) is taken to be (with integers $a, b \geq 0$)

$$M_n = a + b \log_2(t_n^{-1}), \quad n > 2.$$  

The numerical results for the example obtained with the scheme (2.9) with the Jacobi and Gauss-Seidel smoothers are presented in Tables 3 and 4, respectively. With the Jacobi smoother, it is observed that with a fixed number of iterations at each time level (e.g., $M_n = 3$), the IH (2.9) can fail to maintain the first order
Table 3: $L^2$ errors $e^N$ for Example 2 with $a = 3$ and $K = 128$, point Jacobi smoother.

| $\alpha$ | $b$\backslash N | 10   | 20   | 40   | 80   | 160  | 320  |
|------|------------|------|------|------|------|------|------|
| 0.2  | 0          | 1.12e-2 | 5.61e-3 | 2.90e-3 | 1.47e-3 | 6.64e-4 | 3.25e-4 |
|      |            | 1.06  | 0.95  | 0.98  | 1.15  | 1.03  |      |
|      | 3          | 1.17e-2 | 5.71e-3 | 2.90e-3 | 1.57e-3 | 8.15e-4 | 3.67e-4 |
|      |            | 1.03  | 0.98  | 0.89  | 0.94  | 1.14  |      |
|      | 6          | 1.17e-2 | 5.77e-3 | 2.88e-3 | 1.42e-3 | 6.89e-4 | 3.49e-4 |
|      |            | 1.02  | 1.00  | 1.02  | 1.05  | 0.98  |      |

Table 4: $L^2$ errors $e^N$ for Example 2 with $K = 128$, $a = 1$ and $b = 0$, Gauss-Seidel smoother.

| $\alpha$ | $b$\backslash N | 10   | 20   | 40   | 80   | 160  | 320  |
|------|------------|------|------|------|------|------|------|
| 0.2  | 0          | 3.80e-2 | 1.74e-2 | 9.74e-3 | 5.39e-3 | 2.55e-3 | 1.95e-3 |
|      |            | 1.12  | 0.84  | 0.85  | 1.08  | 0.39  |      |
|      | 3          | 3.82e-2 | 1.82e-2 | 9.52e-3 | 5.50e-3 | 2.80e-3 | 1.15e-3 |
|      |            | 1.07  | 0.94  | 0.80  | 0.98  | 1.27  |      |
|      | 6          | 3.84e-2 | 1.87e-2 | 9.36e-3 | 4.40e-3 | 2.20e-3 | 1.17e-3 |
|      |            | 1.04  | 1.00  | 1.09  | 1.00  | 0.90  |      |
| 0.5  | 0          | 7.87e-2 | 3.29e-2 | 2.43e-2 | 1.16e-2 | 4.52e-3 | 4.03e-3 |
|      |            | 1.26  | 0.44  | 1.07  | 1.36  | 0.17  |      |
|      | 3          | 8.00e-2 | 3.70e-2 | 2.14e-2 | 1.12e-2 | 4.94e-3 | 2.54e-3 |
|      |            | 1.11  | 0.79  | 0.94  | 1.18  | 0.96  |      |
|      | 6          | 8.12e-2 | 3.96e-2 | 2.01e-2 | 9.46e-3 | 5.40e-3 | 2.47e-3 |
|      |            | 1.04  | 0.97  | 1.09  | 0.81  | 1.13  |      |

Convergence, especially for $\alpha$ values close to one. In contrast, surprisingly, for $\alpha$ value close to zero, even a fixed number of iterations tend to suffice the desired first-order convergence, despite the low regularity of the solution. However, the precise mechanism of the interesting observation remains elusive. By increasing the number of iterations slightly for small $t_n$, one can restore the convergence rate, which agree well with Theorems 4.1 and 4.2. By changing Jacobi smoother to Gauss-Seidel smoother, the performance of the IIS (2.9) is significantly enhanced, since one iteration at each time level is sufficient to maintain the desired accuracy. The numerical results for Examples 1 and 2 show very clearly the potentials of the scheme (2.9) in speeding up the numerical solution of the subdiffusion model with both smooth and nonsmooth solutions.

6 Conclusions

In this work, we have developed an efficient incomplete iterative scheme for the subdiffusion model. It employs an iterative solver for solving the linear systems inexactly, and is straightforward to implement. Further, we provided theoretical analysis of the scheme under a standard contraction assumption on the iterative solver (in a weighted norm), and proved that it can indeed maintain the accuracy of the time stepping scheme, provided the number of iterations at each time level is properly chosen, on which the analysis has provided useful guidelines. The numerical experiments with the standard multigrid methods fully support the theoretical analysis and indicate that it can significantly reduce the computational cost of the time-stepping scheme.
A Basic estimates

Lemma A.1. For $\beta, \gamma \geq 0$, there holds

$$\sum_{i=1}^{n} (n + 1 - i)^{-\beta} i^{-\gamma} \leq \begin{cases} \frac{cn}{c} \max(1-\gamma,0)^{-\beta}, & 0 \leq \beta < 1, \gamma \neq 1, \\ cn^{-\beta} \ln(1+n), & 0 \leq \beta \leq 1, \gamma = 1, \\ c, & \beta > 1, \gamma > 1. \end{cases}$$

Proof. We denote by $[\cdot]$ the integral part of a real number. Then

$$\sum_{i=1}^{n} (n + 1 - i)^{-\beta} i^{-\gamma} = \sum_{i=1}^{[n/2]} (n + 1 - i)^{-\beta} i^{-\gamma} + \sum_{i=[n/2]+1}^{n} (n + 1 - i)^{-\beta} i^{-\gamma} := I + II.$$

Then, by the trivial inequalities: for $1 \leq i \leq [n/2]$, there holds $(n + 1 - i)^{-\beta} \leq cn^{-\beta}$ and for $[n/2] + 1 \leq i \leq n$, there holds $i^{-\gamma} \leq cn^{-\gamma}$, we deduce

$$I \leq cn^{-\beta} \sum_{i=1}^{[n/2]} i^{-\gamma} \quad \text{and} \quad II \leq cn^{-\gamma} \sum_{i=[n/2]+1}^{n} (n + 1 - i)^{-\beta}.$$

Simple computation gives $\sum_{i=1}^{j} i^{-\gamma} \leq cj^{max(1-\gamma,0)}$ if $\gamma \neq 1$ and $\sum_{i=1}^{j} i^{-1} \leq c \ln(j + 1)$. Combining these estimates yields the desired assertion.

Next we give an upper bound on the CQ weight $b_j^{(\alpha)}$.

Lemma A.2. For the weights $b_j^{(\alpha)}$, $|b_j^{(\alpha)}| \leq e^{2\alpha (j + 1)^{-\alpha - 1}}$.

Proof. The weight $b_j^{(\alpha)}$ is given by $b_0^{(0)} = 1$ and $b_j^{(\alpha)} = -\Pi_{\ell=1}^{j-1} (1 - \frac{1+\alpha}{\ell})$ for any $j \geq 1$. Note the elementary inequality $\ln(1 - x) \leq -x$ for any $x \in (0, 1)$, and the estimate $\sum_{\ell=1}^{j} \ell^{-\alpha} \leq j^{\alpha+1} \int_{1}^{j+1} s^{-\alpha} ds = \ln(j + 1).$ Since $\ln(1 - (1 - \alpha)) \leq \alpha - 1$, for any $j \geq 1$,

$$\ln |b_j^{(\alpha)}| = \ln\alpha + \sum_{\ell=2}^{j} \ln \left(1 - \frac{1+\alpha}{\ell}\right) \leq \ln\alpha - \sum_{\ell=2}^{j} \frac{1+\alpha}{\ell}$$

$$= \ln\alpha + (1 + \alpha) - \sum_{\ell=1}^{j} \frac{1+\alpha}{\ell} \leq 2\alpha - (1 + \alpha) \ln(j + 1).$$

This completes the proof of the lemma.

B Proof of Lemmas 4.1 and 4.2

In this part, we provide the proof of Lemmas 4.1 and 4.2. The proof of Corollary 4.1 is identical with that for Lemma 4.2 and thus it is omitted. The proof relies on the discrete Laplace transform, and the following two well known estimates

\begin{equation}
\frac{c_1}{|z|} \leq |\delta_T(e^{-iz})| \leq c_2 |z| \quad \forall z \in \Gamma_0, \delta, \tag{B.1}
\end{equation}

\begin{equation}
|\delta_T(e^{-iz})| \leq |z| \sum_{k=1}^{\infty} \frac{|z|^k}{k!} \leq |z| e^{|z|^\tau}, \quad \forall z \in \Sigma_\theta, \tag{B.2}
\end{equation}

and the resolvent estimate

$$\|(z + A_h)^{-1}\| \leq c|z|^{-1}, \quad \forall z \in \Sigma_\theta. \tag{B.3}$$

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of Lemma 4.1 By Laplace transform, \( w_h(t_n) = \tilde{\partial}^2 r u_h(t_n) \) is given by

\[
w_h(t_n) = \frac{1}{2\pi i} \int_{\Gamma_{\theta, \delta}} \delta_r(e^{-z\tau})^2 e^{zt_n} K(z) v_h \, dz, \quad \text{with} \quad K(z) = z^{\alpha-1}(z^{\alpha} + A_h)^{-1}.
\]

We split the contour \( \Gamma_{\theta, \delta} \) into \( \Gamma_{\theta, \delta}^+ \) and \( \Gamma_{\theta, \delta}^- \), and denote the corresponding integral by I and II, respectively. We discuss the cases \( v \in L^2(\Omega) \) and \( v \in D(A) \), separately.

Case (i): \( v \in L^2(\Omega) \). By (B.3) and (B.3), \( \|K(z)\| \leq c \) for \( z \in \Gamma_{\theta, \delta}^- \). Then choosing \( \delta = c/t_n \) in \( \Gamma_{\theta, \delta}^- \) gives

\[
\|I\|_{L^2(\Omega)} \leq c \leq c \|v_h\|_{L^2(\Omega)} \left( \int_{\Gamma_{\theta, \delta}^-} e^{zt_n} e^{\theta} \, d\theta + \int_{\theta}^{\delta} t_n^{-1} \, d\theta \right) \leq c t_n^{-2} \|v_h\|_{L^2(\Omega)}.
\]

For any \( z = \rho e^{\pm i\theta} \in \Gamma_{\theta, \delta} \), by the estimates (B.2) and (B.3), \( \|K(z)\| \leq c e^{2\rho \tau} \). By choosing \( \theta \in (\pi/2, \pi) \) sufficiently close to \( \pi \), we deduce

\[
\|I\|_{L^2(\Omega)} \leq c \leq c \|v_h\|_{L^2(\Omega)} \left( \int_{\Gamma_{\theta, \delta}^+} e^{\rho(\cos \theta + 2\rho \tau)} \rho \, d\rho \leq c t_n^{-2} \|v_h\|_{L^2(\Omega)}.
\]

Thus, \( \|\tilde{\partial}^2 r u_h(t_n)\| \leq c t_n^{-2} \|v_h\|_{L^2(\Omega)} \). Next, by the identity \( A_h(z^{\alpha} + A_h)^{-1} = I - z^{\alpha}(z^{\alpha} + A_h) \) and (B.3), \( \|A_hK(z)\| \leq |z|^{\alpha-1} \) for \( z \in \Sigma_\theta \). Then repeating the argument gives

\[
\|A_h \tilde{\partial}^2 r u_h(t_n)\| \leq c t_n^{-2} \|v_h\|_{L^2(\Omega)} \leq c t_n^{-2} \|v_h\|_{L^2(\Omega)}.
\]

Then the assertion for the case \( v \in L^2(\Omega) \) follows from the triangle inequality.

Case (ii): \( v \in D(A) \). Simple computation gives the identity \( K(z) v_h = z^{\alpha-1}(z^{\alpha} + A_h)^{-1} v_h = z^{-1} v_h - z^{-\alpha}(z^{\alpha} + A_h)^{-1} A_h v_h \). Thus, we have

\[
w_h(t_n) = -\frac{1}{2\pi i} \int_{\Gamma_{\theta, \delta}} e^{zt_n} \delta_r(e^{-z\tau})^2 z^{-\alpha} K(z) A_h v_h \, dz,
\]

in which we split the contour \( \Gamma_{\theta, \delta} \) into \( \Gamma_{\theta, \delta}^+ \) and \( \Gamma_{\theta, \delta}^- \), and accordingly the integral. Then the rest of the proof follows from the estimates (B.1), (B.2) and (B.3) as before.

of Lemma 4.2 By Laplace transform and its discrete analogue, we have

\[
\partial^\alpha y_h(t_n) - \tilde{\partial}^r y_h(t_n) = \frac{1}{2\pi i} \int_{\Gamma_{\theta, \delta}} e^{zt_n} K(z) A_h v_h \, dz + \frac{1}{2\pi i} \int_{\Gamma_{\theta, \delta} \setminus \Gamma_{\theta, \delta}^+} e^{zt_n} K(z) A_h v_h \, dz := I + \Pi,
\]

with \( K(z) = (\delta_r(e^{-z\tau}))^\alpha - z^{\alpha} z^{-1}(z^{\alpha} + A_h)^{-1} \). Recall the following estimate:

\[
|\delta_r(e^{-z\tau})^\alpha - z^{\alpha}| \leq c |z|^{1+\alpha}, \quad \forall z \in \Gamma_{\theta, \delta}^-.
\]

Then by choosing \( \delta = c/t_n \) in the contour \( \Gamma_{\theta, \delta} \) and the resolvent estimate (B.3), we obtain

\[
\|I\|_{L^2(\Omega)} \leq c \tau \|A_h v_h\|_{L^2(\Omega)} \left( \int_{\Gamma_{\theta, \delta}^-} e^{-\rho \tau \theta} \, d\rho + \int_{-\theta}^{\theta} c t_n^{-1} \, d\rho \right) \leq c t_n^{-1} \|A v\|_{L^2(\Omega)}.
\]

Further, by (B.2), for any \( z = \rho e^{i\theta} \in \Gamma_{\theta, \delta} \), choosing \( \theta \in (\pi/2, \pi) \) close to \( \pi \),

\[
|e^{zt_n}(\delta_r(e^{-z\tau})^\alpha - z^{\alpha}) z^{-1}| \leq e^{t_n \rho \cos \theta} (c |z|^\alpha e^{\rho \tau} + |z|^\alpha) |z|^{-1} \leq c |z|^{\alpha-1} e^{-\rho \tau}.
\]

Then we deduce

\[
\|I\|_{L^2(\Omega)} \leq c \|A_h v_h\|_{L^2(\Omega)} \int_{\Gamma_{\theta, \delta}^-} e^{-\rho \tau} \, d\rho \leq c t_n^{-1} \|A v\|_{L^2(\Omega)}.
\]
Thus, we show the assertion for $\beta = 0$. For the case $\beta = 1$, the identity $A_h(z\alpha + A_h)^{-1} = I - z\alpha(z\alpha + A_h)$, (B.3) and (B.4) give

$$\|A_hI\|_{L^2(\Omega)} \leq c\tau \|A_hv_h\|_{L^2(\Omega)} \left( \int_0^{c\tau \rho_n} e^{-c\tau \rho_n} \rho^n \, d\rho + \int_0^\rho e^{c\tau \rho^{1-\alpha}} \, d\rho \right)$$

and the bound on $\|A_hII\|_{L^2(\Omega)}$ follows analogously, completing the proof for $\beta = 1$. Then the case $\beta \in (0,1)$ follows by interpolation. This shows part (i). The proof of part (ii) is similar and applies the $L^2(\Omega)$ stability of $P_h$, and hence the detail is omitted.

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