ERROR ANALYSIS OF THE L1 METHOD ON GRADED AND UNIFORM MESHES FOR A FRACTIONAL-DERIVATIVE PROBLEM IN TWO AND THREE DIMENSIONS

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Abstract. An initial-boundary value problem with a Caputo time derivative of fractional order \( \alpha \in (0, 1) \) is considered, solutions of which typically exhibit a singular behaviour at an initial time. For this problem, we give a simple framework for the analysis of the error of L1-type discretizations on graded and uniform temporal meshes in the \( L_\infty \) and \( L_2 \) norms. This framework is employed in the analysis of both finite difference and finite element spatial discretizations. Our theoretical findings are illustrated by numerical experiments.

1. Introduction

The purpose of this paper is to give a simple framework for the analysis of the error in the \( L_\infty (\Omega) \) and \( L_2 (\Omega) \) norms for L1-type discretizations of the fractional-order parabolic problem

\[ \begin{aligned}
D_\alpha^t u + L u &= f(x, t) \quad \text{for } (x, t) \in \Omega \times (0, T], \\
u(x, t) &= 0 \quad \text{for } (x, t) \in \partial \Omega \times (0, T], \\
u(x, 0) &= u_0(x) \quad \text{for } x \in \Omega.
\end{aligned} \tag{1.1} \]

This problem is posed in a bounded Lipschitz domain \( \Omega \subset \mathbb{R}^d \) (where \( d \in \{1, 2, 3\} \)).

The operator \( D_\alpha^t \), for some \( \alpha \in (0, 1) \), is the Caputo fractional derivative in time defined \([2]\) by

\[ D_\alpha^t u(\cdot, t) := \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \partial_s u(\cdot, s) \, ds \quad \text{for } 0 < t \leq T, \tag{1.2} \]

where \( \Gamma(\cdot) \) is the Gamma function, and \( \partial_s \) denotes the partial derivative in \( s \). The spatial operator \( L \) is a linear second-order elliptic operator:

\[ Lu := \sum_{k=1}^d \left\{-\partial_{x_k} (a_k(x) \partial_{x_k} u) + b_k(x) \partial_{x_k} u \right\} + c(x) u, \tag{1.3} \]

with sufficiently smooth coefficients \( \{a_k\}, \{b_k\} \) and \( c \) in \( C(\bar{\Omega}) \), for which we assume that \( a_k > 0 \) in \( \bar{\Omega} \), and also either \( c \geq 0 \) or \( c - \frac{1}{2} \sum_{k=1}^d \partial_{x_k} b_k \geq 0 \).

Throughout the paper, it will be assumed that there exists a unique solution of this problem in \( C(\bar{\Omega} \times [0, T]) \) such that \( |\partial_t^l u(\cdot, t)| \lesssim 1 + t^{\alpha-1} \) for \( l = 0, 1, 2 \) (the notation \( \lesssim \) is rigorously defined in the final paragraph of this section). This is a realistic assumption, satisfied by typical solutions of problem (1.1), in contrast to a stronger assumption \( |\partial_t^l u(\cdot, t)| \lesssim 1 \) frequently made in the literature (see, e.g.,

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Indeed, Theorem 2.1 shows that if a solution $u$ of (1.1) is less singular than we assume (in the sense that $|\partial^l u(\cdot,t)| \lesssim 1 + t^{-\gamma}$ for $l = 0, 1, 2$ with any $\gamma > \alpha$), then the initial condition $u_0$ is uniquely defined by the other data of the problem, which is clearly too restrictive. At the same time, our results can be easily applied to the case of $u$ having no singularities or exhibiting a somewhat different singular behaviour at $t = 0$.

We consider L1-type schemes for problem (1.1), which employ the discretization of $D_t^\alpha u$ defined, for $m = 1, \ldots, M$, by

\begin{equation}
\delta_t^\alpha U^m := \frac{1}{\Gamma(1-\alpha)} \sum_{j=1}^m \delta_t U^j \int_{t_{j-1}}^{t_j} (t_m - s)^{-\alpha} \, ds, \quad \delta_t U^j := \frac{U^j - U^{j-1}}{t_j - t_{j-1}},
\end{equation}

when associated with the temporal mesh $0 = t_0 < t_1 < \ldots < t_M = T$ on $[0,T]$. Similarly to [17], our main interest will be in graded temporal meshes as they offer an efficient way of computing reliable numerical approximations of solutions singular at $t = 0$. We shall also consider uniform temporal meshes, as although the latter have lower convergence rates near $t = 0$, they have been shown to be first-order accurate for $t \gtrsim 1$ [4, 8].

Novelty. We present a simple framework for the estimation of the temporal-discretization error whenever an L1 scheme is used on graded or uniform temporal meshes. This framework is employed in the analysis of both finite difference and finite element spatial discretizations. For the former, we obtain, in a substantially more concise way, the maximum norm error bounds of [17] for the case $d = 1$, as well as extend them to $d = 2, 3$. For finite element spatial discretizations, the errors on uniform temporal meshes in the $L^2(\Omega)$ norm have been estimated in [8], while all our error bounds on graded meshes, as well as those in the $L^\infty(\Omega)$ norm on uniform temporal meshes, appear to be entirely new.

Outline. We start by presenting, in §2, a paradigm for the temporal-error analysis using a simplest example without spatial derivatives. This error analysis is extended in §3 to temporal semidiscretizations of (1.1). Full discretizations that employ finite differences and finite elements are respectively addressed in §4 and §5. Finally, the assumptions on the derivatives of the exact solution are discussed in §6 and our theoretical findings are illustrated by numerical experiments in §7.

Notation. We write $a \simeq b$ when $a \lesssim b$ and $a \gtrsim b$, and $a \lesssim b$ when $a \leq C b$ with a generic constant $C$ depending on $\Omega$, $T$, $u_0$, and $f$, but not on the total numbers of degrees of freedom in space or time. Also, for $1 \leq p \leq \infty$, and $k \geq 0$, we shall use the standard norms in the spaces $L^p(\Omega)$ and the related Sobolev spaces $W^{k}_p(\Omega)$, while $H^1_0(\Omega)$ is the standard space of functions in $W^1_2(\Omega)$ vanishing on $\partial \Omega$. 

2. Paradigm for the temporal-discretization error analysis

2.1. Graded temporal mesh. Throughout the paper, we shall frequently consider the graded temporal mesh $\{t_j = T(j/M)^r\}_{j=0}^M$ with some $r \geq 1$ (while $r = 1$ generates a uniform mesh). For this mesh, a calculation shows that

\begin{equation}
\tau_j := t_j - t_{j-1} \simeq M^{-1} \frac{1}{j^{1-1/r}} \quad \text{for } j = 1, \ldots, M.
\end{equation}

This follows from $\tau_1 = t_1 \simeq M^{-r}$ for $j = 1$, and $t_j \leq 2^r t_{j-1}$ for $j \geq 2$. 

2. Stability properties of the discrete fractional operator $\delta_t^\alpha$. The definition (2.1.4) of $\delta_t^\alpha$ can be rewritten as

\[(2.2a) \quad \delta_t^\alpha V^m = \kappa_{m,m} V^m - \sum_{j=1}^{m} (\kappa_{m,j} - \kappa_{m,j-1}) V^{j-1},\]

\[(2.2b) \quad \kappa_{m,j} := \frac{\tau_j^{-1}}{\Gamma(1-\alpha)} \int_{t_{j-1}}^{t_j} (t_m - s)^{-\alpha} ds \quad \text{for} \quad j = 1, \ldots, m, \quad \kappa_{m,0} := 0.\]

Here $\kappa_{m,j}$ for $j \geq 1$ is the average of the function $\{\Gamma(1-\alpha)\}^{-1}(t_m - s)^{-\alpha}$ on the interval $s \in (t_{j-1}, t_j)$, so $\kappa_{m,j} \leq \kappa_{m,j}$ for all admissible $j$ and $m$.

**Lemma 2.1.** (i) For any $\{V^j\}_{j=0}^M$ on an arbitrary mesh $\{t_j\}_{j=0}^M$, one has

$$|V^m - V^0| \lesssim \max_{j=1,\ldots,m} \left\{ \delta_t^\alpha |V^j| \right\} \quad \text{for} \quad m = 1, \ldots, M.$$  

(ii) If $V^0 = 0$ and $\delta_t^\alpha |V^j| \leq |F^j|$ for $j = 1, \ldots, M$, then $|V^m| \lesssim \max_{j=1,\ldots,m} \{ \delta_t^\alpha |F^j| \}$ for $m = 1, \ldots, M$.

**Proof.** (i) Let $W^j := V^j - V^0$; then $W^0 = 0$, while $\delta_t^\alpha W^j = \delta_t^\alpha V^j =: F^j$, so we need to prove that $|W^m| \lesssim \max_{j\leq m} \{ \delta_t^\alpha |F^j| \}$. Let $\max_{j\leq m} |W^j| = |W^n|$ for some $1 \leq n \leq m$. Then, by (2.2a) combined with $W^0 = 0$, one gets

\[(2.3) \quad \kappa_{n,n} |W^n| - \sum_{j=2}^{n} (\kappa_{n,j} - \kappa_{n,j-1}) |W^j| \leq |F^n| \quad \Rightarrow \quad |W^n| \leq \kappa_{n,1}^{-1} |F^n|.\]

Next, recalling (2.2b), and also using $(t_n - s)^{-\alpha} \geq t_n^{-\alpha}$ on $(0, t_1)$, one concludes that $\kappa_{n,1} \gtrsim t_n^{-\alpha}$. So $|W^n| \leq t_n^{-\alpha} |F^n|$, which immediately implies the desired assertion.

(ii) Let $W^0 = 0$ and $\delta_t^\alpha W^j = |F^j|$ for $j = 1, \ldots, M$. Then $0 \leq |V^m| \leq W^m$ (as $\delta_t^\alpha$ is associated with an $M$-matrix), while $|V^m| \lesssim \max_{j=1,\ldots,m} \{ \delta_t^\alpha |F^j| \}$ by the result of part (i). The desired assertion follows. \[\square\]

To deal with uniform temporal meshes, we employ a more subtle stability result.

**Lemma 2.1** (4). Let $r = 1$ and $\tau := TM^{-1}$. Given $\gamma \in (0, \alpha]$, if $V^0 = 0$ and $|\delta_t^\alpha V^j| \lesssim \tau^\gamma t_j^{-\alpha - \gamma}$ for $j = 1, \ldots, M$, then $|V^j| \lesssim \tau^\gamma t_j^{-\alpha}$ for $j = 1, \ldots, M$.

**Proof.** The desired assertion follows from [4, Lemma 3] with $\beta = 1 + \gamma$. We give an alternative proof in Appendix [B]. \[\square\]

The next lemma will be useful when dealing with Ritz projections while estimating the errors of finite element discretizations in [5].

**Lemma 2.2.** Let $\{V^j\}_{j=0}^M \in \mathbb{R}^{M+1}$ and $\{\lambda^j\}_{j=1}^M \in \mathbb{R}^M$, and $\tilde{\lambda} = \tilde{\lambda}(t)$ be a piecewise-constant left-continuous function defined by $\tilde{\lambda}(t) = \lambda^j$ for $t \in (t_{j-1}, t_j)$, $j = 1, \ldots, M$. Then, with the notation $J^{1-\alpha} \lambda(t) := \{\Gamma(1-\alpha)\}^{-1} \int_0^t (t-s)^{-\alpha} \lambda(s) \, ds$,

\[(2.4) \quad \delta_t^\alpha V^j \lesssim J^{1-\alpha} \lambda(t_j) \quad \forall \, j \geq 1 \quad \Rightarrow \quad V^m - V^0 \lesssim \sum_{j=1}^{m} \tau_j \lambda^j \quad \forall \, m \geq 0.\]

**Proof.** Let $\lambda^j := V^0 + \int_0^{t_j} \tilde{\lambda} dt$ so that $\lambda^j = \delta_t^\alpha \lambda^j$. Now, $J^{1-\alpha} \lambda(t_j) = \delta_t^\alpha \lambda^j$, so we get $M$ equations $\delta_t^\alpha V^j \lesssim \delta_t^\alpha \lambda^j$ for $j = 1, \ldots, M$. Augmenting these equations by $V^0 = \lambda^0$, we get the matrix relation $A \vec{V} \lesssim \tilde{A} \vec{\lambda}$ for the column vectors $\vec{V} := \{V^j\}_{j=0}^M$. 

and $\bar{\Lambda} := \{\Lambda^j\}_{j=0}^M$ with an inverse-monotone $(M+1) \times (M+1)$ matrix $A$. (The latter follows from $A$ being diagonally dominant, with the entries $A_{ij} \leq 0$ for $i \neq j$ in view of \eqref{2.2a}.) Consequently, $\bar{V} \leq \bar{\Lambda}$, which immediately yields the desired assertion. \hfill $\square$

2.3. Error estimation for a simplest example (without spatial derivatives). It is convenient to illustrate our approach to the estimation of the temporal-discretization error using a very simple example. Consider a fractional-derivative problem without spatial derivatives together with its discretization:

\begin{align}
(2.5a) \quad & D_t^\alpha u(t) = f(t) \quad \text{for } t \in (0, T), \quad u(0) = u_0, \\
(2.5b) \quad & \delta_j^\alpha U^j = f(t_j) \quad \text{for } j = 1, \ldots, M, \quad U^0 = u_0.
\end{align}

Throughout this subsection, with slight abuse of notation, $\partial_s$ will be used for $\frac{d}{dt}$, while $\delta_t u(t_j) := \tau^{-1}_j[u(t_j) - u(t_{j-1})]$ (similarly to $\delta_t$ in \eqref{1.4}).

**Lemma 2.3.** Let $\{t_j = T(j/M)^r\}_{j=0}^M$ for some $r \geq 1$. Then for $u$ and $U^j$ that satisfy (2.5), one has

$$|u(t_m) - U^m| \lesssim \max_{j=1,\ldots,m} \psi^j,$$

where $m = 1, \ldots, M$, and

\begin{align}
(2.6a) \quad & \psi^1 := \tau^{-\alpha}_1 \sup_{s \in (0, t_1)} (s^{1-\alpha}[\delta_t u(t_1) - \partial_s u(s)]), \\
(2.6b) \quad & \psi^j := \tau^{-\alpha}_j t^{-\alpha}_j \sup_{s \in (t_{j-1}, t_j)} \partial_s^2 u(s) \quad \text{for } j \geq 2.
\end{align}

**Proof.** Using the standard piecewise-linear Lagrange interpolant $u^I$ of $u$, let

$$\chi := u - u^I \quad \Rightarrow \quad |\chi(s)| \leq \tau^{-\alpha}_j (t_j - s) \sup_{s \in (t_{j-1}, t_j)} \partial_s^2 u \quad \text{for } s \in [t_{j-1}, t_j].$$

Comparing this with (2.6b), one concludes that

\begin{align}
(2.7a) \quad & |\chi(s)| \leq \psi^j \tau^{-\alpha}_j t_j^{-\alpha} \min\{1, (m - s)/r_m\} \quad \text{for } s \in (t_{j-1}, t_j), \quad j \geq 2.
\end{align}

On $(0, t_1)$, combining (2.6a) with the definition of $\chi$ yields

\begin{align}
(2.7b) \quad & |\chi(s)| \leq \psi^1 \tau^{-\alpha}_1 \int_{t_1}^{t_j} \zeta^{-\alpha-1} d\zeta \lesssim \psi^1 \tau^{-\alpha}_1 s^{-1}(t_1 - s) \quad \text{for } s \in (0, t_1).
\end{align}

We now proceed to estimating the error $e^j := u(t_j) - U^j$, for which (2.5) implies

\begin{align}
(2.8) \quad & \delta_j^\alpha e^j = \delta_j^\alpha u(t_j) - D_t^\alpha u(t_j) \quad \text{for } j = 1, \ldots, M, \quad e^0 = 0.
\end{align}

For $r_m$, recalling the definitions \eqref{1.2} and \eqref{1.4} of $D_t^\alpha$ and $\delta_j^\alpha$, we arrive at

$$\Gamma(1-\alpha) r_m = \sum_{j=1}^{m} \int_{(m - s) - \alpha}^{(m - s)} \delta_j^\alpha (u(t_j) - \partial_s u(s)) \, ds \leq \alpha \sum_{j=1}^{m} \int_{(m - s) - \alpha}^{(m - s)} \psi^j \, ds.$$

(In particular, for the interval $(t_{m-1}, t_m)$, to check the validity of the above integration by parts, with $\epsilon \to 0^+$, one can integrate by parts over $(t_{m-1}, t_m - \epsilon)$.)
Next, combining the above representation of $r^m$ with the bounds (2.7) on $\chi$, one can check that
\begin{equation}
|r^m| \lesssim \hat{J}^m (\tau_1/t_m) \psi^1 + J^m \max_{j=2,\ldots,m} \{ \nu_{m,j} \psi^j \},
\end{equation}
where (with the use, when deriving $J^m$, of $1 \leq t_j^{\alpha/r} s^{-\alpha/r}$ for $s \in (t_{j-1}, t_j)$)
\begin{align*}
\hat{J}^m &:= \tau_1^{-\alpha} (t_m/t_1) \int_0^{t_1} s^{\alpha-1} (t_1 - s) (t_m - s)^{-\alpha-1} ds, \\
J^m &:= \tau_m t_m^{-\alpha(1-1/r)} \int_0^{t_m} s^{-\alpha/r} (t_m - s)^{-\alpha-1} \min\{1, (t_m - s)/\tau_m\} ds,
\end{align*}
\begin{equation}
\nu_{m,j} := (\tau_j/\tau_m)^{\alpha} (t_j/t_m)^{-\alpha(1-1/r)} \simeq 1.
\end{equation}
Here, the bound on $\nu_{m,j}$ follows from $\tau_j/\tau_m \simeq (t_j/t_m)^{-1-1/r}$ (in view of (2.1)). For $J^m$, the observation that $(t_1 - s)/(t_m - s) \leq t_1/t_m$ for $s \in (0, t_1)$ implies
\begin{equation}
\hat{J}^m \leq t_1^{-\alpha} \int_0^{t_1} s^{\alpha-1} (t_1 - s)^{-\alpha} ds = t_1^{-\alpha} \int_0^1 \hat{s}^{\alpha-1} (1 - \hat{s})^{-\alpha} d\hat{s} \lesssim t_1^{-\alpha},
\end{equation}
where $\hat{s} := s/t_1$. For $J^m$, it is helpful to employ another substitution $\hat{s} := s/t_m$ and $\hat{\tau}_m := \tau_m/t_m$, so, for $m \geq 2$, one gets
\begin{equation}
J^m = t_m^{-\alpha} \hat{\tau}_m \int_0^1 \hat{s}^{\alpha/(1-\hat{\tau}_m)} (1 - \hat{s})^{-\alpha-1} \min\{1, (1 - \hat{s})/\hat{\tau}_m\} d\hat{s} \lesssim t_m^{-\alpha}.
\end{equation}
Here we also used $1 - \hat{\tau}_m \gtrsim 2^{-r}$ combined with $\alpha/r \in (0, 1)$ (so one may consider the intervals $(0, 2^{-r})$, $(2^{-r}, 1 - \hat{\tau}_m)$ and $(1 - \hat{\tau}_m, 1)$ separately).

Finally, we combine (2.9) with the above bounds on $\hat{J}^m$ and $J^m$, and arrive at
\begin{equation}
|r^m| \lesssim t_1^{-\alpha} \{ (\tau_1/t_m) \psi^1 + \max_{j=2,\ldots,m} \psi^j \},
\end{equation}
while $|\delta^m e^m| = |r^m|$. As $\tau_1/t_m \leq 1$, the desired assertion follows by an application of Lemma 2.1. \hfill \square

**Corollary 2.4.** Under the conditions of Lemma 2.3, suppose $|\partial_t^i u(t)| \lesssim 1 + t^{\alpha-i}$ for $i = 1, 2$ and $t \in [0, T]$. Then $|u(t_m) - U^m| \lesssim M^{-\min\{\alpha, 2-\alpha\}}$ for $m = 1, \ldots, M$.

**Proof.** It suffices to show that $\psi^j \lesssim M^{-\min\{\alpha, 2-\alpha\}}$ for $j \geq 1$. As $t \leq T$, we have $|\partial_t^j u(t)| \lesssim t^{\alpha-1}$. For $\psi^1$ of (2.6a), note that $s^{1-\alpha}|\partial_t u(t_1)| \lesssim \tau_1^{-\alpha} \int_0^{\tau_1} s^{\alpha-1} ds \simeq 1$, while $s^{1-\alpha}|\partial_s u(s)| \lesssim 1$, so $\psi^1 \lesssim \tau_1^{-\alpha} \simeq M^{-\alpha}$. For any other $\psi^j$, defined in (2.6b), in view of $t_{j-1} \geq 2^{-2j} t_j$, one gets $|\partial_t^j u(s)| \lesssim t_j^{-\alpha} \lesssim t_j^{-2}$ for $s \in (t_{j-1}, t_j)$, so $\psi^j \lesssim (\tau_j/t_j)^{2-\alpha} t_j^2$. Now, set $\gamma := \min\{\alpha, 2-\alpha\}$. Then $(\tau_j/t_j)^{2-\alpha} \leq (\tau_j/t_j)^{\gamma} \lesssim M^{-\gamma} t_j^{-\gamma/r}$, by (2.1). Combining this with $t_j^{-\gamma/r} \lesssim 1$ yields $\psi^j \lesssim M^{-\gamma} = M^{-\min\{\alpha, 2-\alpha\}}$ for $j \geq 2$. \hfill \square

**Remark 2.5** (Optimal mesh grading $r$). The optimal error bound $O(M^{-2-\alpha})$ in Corollary 2.4 is attained when $r = (2 - \alpha)/\alpha$. For any larger $r$, one also enjoys the optimal rate of convergence; however, increased temporal mesh widths near $t = T$ (for example, $\tau_M \approx r TM^{-1}$) lead to larger errors. See also [17] Remark 5.6.
2.4. Analysis on the uniform mesh. Let us now consider the case of a uniform
temporal mesh (i.e. \( r = 1 \)). If \( u \) is smooth on \([0, T]\) in the sense that \( |\partial_l^\gamma u| \lesssim 1 \) for \( l = 1, 2 \), then an application of Lemma 2.3 immediately yields for the error
to be \( \lesssim M^{-(2-\alpha)} \). However, we are interested in a more realistic case of \( u \) being singular at \( t = 0 \).

We start with a shaper version of Lemma 2.3

**Lemma 2.3.** Under the conditions of Lemma 2.3, let \( r = 1 \) and \( \tau := TM^{-1} \), and set \( \gamma = \min\{\alpha, 1-\alpha\} \). Then

\[
|v(t_m) - V_m^\gamma| \lesssim t_m^{\alpha-1} \max_{j=1,\ldots,m} \{\tau^{-\gamma} t_j^{1-\alpha+\gamma} \psi_j \}.
\]

**Proof.** An inspection of the proof of Lemma 2.3 shows that one can replace the
term \( J_m^\gamma \max_{j=2,\ldots,m}(nu_{m,j} \psi_j) \) in (2.9) (where recall that \( n_{m,j} \simeq 1 \)) by

\[
\tilde{J}_m := \int_{t_1}^{t_m} s^{-\alpha/r-1}(t_m - s)^{-\alpha-1} \min\{1, (t_m - s)/\tau_m \} ds.
\]

where (with the use of \( 1 \leq (t_j/s)^{-1-\alpha/r} \) for \( s \in (t_{j-1}, t_j) \))

\[
\tilde{J}_m := \tau_m^{-\alpha} \int_{t_1}^{t_m} s^{-\alpha/r-1}(1 - s)^{-\alpha-1} \min\{1, (1 - s)/\hat{\tau}_m \} d\hat{s} \lesssim t_m^{-\alpha}.
\]

Here, for convenience, the terms that differ from \( J_m^\gamma \) are framed.

Next, note that \( J_m \lesssim t_m^m \) for \( m \geq 2 \). Indeed, imitating the estimation of \( J_m^\gamma \) in the proof of Lemma 2.3, we employ the substitution \( \hat{s} := s/t_m \) and the notation \( \hat{t}_j := t_j/t_m \) to get

\[
\tilde{J}_m = t_m^{-\alpha} \int_{\hat{t}_1}^{1} \hat{s}^{-\alpha/r-1}(1 - \hat{s})^{-\alpha-1} \min\{1, (1 - \hat{s})/\hat{\tau}_m \} d\hat{s} \lesssim t_m^{-\alpha}.
\]

Finally set \( r = 1 \), and an application of Lemma 2.1 yields the desired assertion. \( \square \)

**Corollary 2.6 (Uniform temporal mesh).** Under the conditions of Lemma 2.3 let \( r = 1 \) and \( \tau := TM^{-1} \), and suppose \( |\partial_l^\gamma u(t)| \lesssim 1 + t^{\alpha-l} \) for \( l = 1, 2 \) and \( t \in (0, T) \). Then \( |u(t_m) - U_m^\gamma| \lesssim t_m^{-\alpha} M^{-1} \lesssim M^{-\alpha} \) for \( m = 1, \ldots, M \).

**Proof.** We imitate the proof of Corollary 2.3, only now employ Lemma 2.3. So it suffices to show that \( \tau^{-\gamma} t_j^{1-\alpha+\gamma} \psi_j \lesssim \tau \). For \( j = 1 \), this follows from \( \psi_1 \lesssim \tau^\alpha \), while for \( j \geq 2 \), from \( \psi_j \lesssim \tau^{2-\alpha} t_j^{\alpha+2} \). Thus \( \tau^{1+\gamma} t_j^{\alpha-\gamma} \) (as \( \tau \leq t_j \) and \( \gamma \leq 1-\alpha \)). \( \square \)
3. Error analysis for the L1 semidiscretization in time

Consider the semidiscretization of our problem (1.1) in time using the L1-method:

\[(1.1) \quad \delta_t^\alpha U^j + LU^j = f(\cdot, t_j) \text{ in } \Omega, \quad U^j = 0 \text{ on } \partial\Omega \text{ for } j = 1, \ldots, M; \quad U^0 = u_0.\]

**Theorem 3.1.** (i) Given \(p \in \{2, \infty\}, \) let \(\{t_j = T(j/M)^r\}_{j=0}^M\) for some \(r \geq 1,\) and \(u\) and \(U^j\) respectively satisfy (1.1), (1.3) and (3.1). Then, under the condition \(c - p^{-1} \sum k=1^d \partial_x b_k \geq 0,\) one has

\[(3.2) \quad \|u(\cdot, t_m) - U^m\|_{L_p(\Omega)} \lesssim \max_{j=1,\ldots,m} \|\psi^j\|_{L_p(\Omega)} \quad \text{for } m = 1, \ldots, M,\]

where \(\psi^j = \psi^j(x)\) is defined by (2.6), in which \(u(\cdot)\) is understood as \(u(x, \cdot)\) when evaluating \(\delta_u, \delta_u^2\) and \(\delta_u.\)

(ii) Furthermore, if \(r = 1,\) a sharper \(\max_{j=1,\ldots,m} \{\tau^{-1} t_j^{1-\alpha+\gamma} \|\psi^j\|_{L_p(\Omega)}\}\) can replace the right-hand side in (3.2), where \(\tau = TM^{-1}\) and \(\gamma = \min(\alpha, 1 - \alpha).\)

**Corollary 3.2.** (i) Under the conditions of Theorem 3.1, suppose \(\|\partial_t u(\cdot, t)\|_{L_p(\Omega)} \lesssim 1 + t^{\alpha-1}\) for \(l = 1, 2, t \in (0, T].\) Then \(\|u(\cdot, t_m) - U^m\|_{L_p(\Omega)} \lesssim M^{-\min\{\alpha, 2 - \alpha\}}\) for \(m = 1, \ldots, M.\)

(ii) If, additionally, \(r = 1,\) then \(\|u(\cdot, t_m) - U^m\|_{L_p(\Omega)} \lesssim t_m^{\alpha-1} M^{-1}\) for \(m = 1, \ldots, M.\)

**Proof.** Imitate the proofs of Corollaries 2.4 and 2.6 for parts (i) and (ii), respectively.

**Proof of Theorem 3.1.** For the error \(e^m := u(\cdot, t_m) - U^m,\) using (1.1) and (3.1), one easily gets a version of (2.8):

\[\delta_t^\alpha e^m + Le^m = \delta_t^\alpha u(\cdot, t_m) - D_t^\alpha u(\cdot, t_m) \quad \text{for } m = 1, \ldots, M, \quad e^0 = 0.\]

Note that the bound (2.10) on \(r^m\) obtained in the proof of Lemma 2.3 implies that \(\|r^m\|_{L_p(\Omega)} \lesssim t_m^{\alpha-1} \max_{j=1,\ldots,m} \|\psi^j\|_{L_p(\Omega)}\). Hence, to complete the proof of part (i), it suffices to show that

\[(3.3) \quad \delta_t^\alpha \|e^m\|_{L_p(\Omega)} \leq \|r^m\|_{L_p(\Omega)} \quad \text{for } m = 1, \ldots, M.\]

Then, indeed, (3.2) immediately follows by an application of Lemma 2.4 (obtained in the proof of Lemma 2.3) with (3.3) and then applying Lemma 2.1 yields the assertion of part (ii).

We now proceed to establishing (3.3). Rewrite the equation \(\delta_t^\alpha e^m + Le^m = r^m\) using (2.2a) as

\[(3.4) \quad \kappa_{m,m} e^m + \sum_{j=1}^m (\kappa_{m,j} - \kappa_{m,j-1}) e^j - r^m,\]

and address the cases \(p = 2, p = \infty\) separately.

For \(p = 2,\) consider the \(L_2(\Omega)\) inner product (denoted \(\langle \cdot, \cdot \rangle\)) of (3.4) with \(e^m\). As \(c - \frac{1}{2} \sum_{k=1}^d \partial_x b_k \geq 0\) implies \(\langle Le^m, e^m \rangle \geq 0,\) so for \(p = 2\) one gets

\[(3.5) \quad \kappa_{m,m} \|e^m\|_{L_p(\Omega)} \leq \sum_{j=1}^m (\kappa_{m,j} - \kappa_{m,j-1}) \|e^j\|_{L_p(\Omega)} + \|r^m\|_{L_p(\Omega)}.\]

By (2.2a), this implies (3.3) for \(p = 2.\)
For \( p = \infty \), let \( \max_{x \in \Omega} |e^m(x)| = |e^m(x^*)| \) for some \( x^* \in \Omega \). Suppose that \( e^m(x^*) \geq 0 \) (the case \( e^m(x^*) < 0 \) is similar). Then \( c \geq 0 \) implies \( L e^m(x^*) \geq 0 \), so (3.4) at \( x = x^* \) yields \( \kappa_{m,m} e^m(x^*) \leq \sum_{j=1}^m (\kappa_{m,j} - \kappa_{m,j-1}) e^{j-1}(x^*) + r^m(x^*) \) and then (3.5) for \( p = \infty \). By (2.2a), the desired assertion (3.3) follows for \( p = \infty \). \( \square \)

4. Maximum norm error analysis for finite difference discretizations

Consider our problem (1.1)–(1.3) in the spatial domain \( \Omega = (0,1)^d \subset \mathbb{R}^d \). Let \( \Omega_h \) be the tensor product of \( d \) uniform meshes \( \{ih\}_{i=0}^N \), with \( \Omega_h := \Omega \setminus \partial \Omega \) denoting the set of interior mesh nodes. Now, consider the finite difference discretization

\[
\| \cdot \|_\Omega = (0 \leq \| \cdot \|_\Omega \leq \infty) \text{ is defined by (1.4). The discrete spatial operator } L_h \text{ is a standard finite difference operator defined, using the standard orthonormal basis } \{i_k\}_{k=1}^d \text{ in } \mathbb{R}^d \text{ (such that } z = (z_1, \ldots, z_d) = \sum_{k=1}^d z_k i_k \text{ for any } z \in \mathbb{R}^d),
\]

by

\[
L_h V(z) := \sum_{k=1}^d h^{-2} \{ u_k(z + \frac{1}{2} i_k) \left[ U(z) - U(z + i_k) \right] + u_k(z - \frac{1}{2} i_k) \left[ U(z) - U(z - i_k) \right] \}
+ \sum_{k=1}^d \frac{1}{2} h^{-1} b_k(z) \left[ U(z + i_k) - U(z - i_k) \right] + c(z) U(z) \text{ for } z \in \Omega_h.
\]

(Here the terms in the first and second sums respectively discretize \( -\partial_{x_k}(a_k \partial_{x_k} u) \) and \( b_k \partial_{x_k} u \) from (1.3).) The error of this method will be bounded in the nodal maximum norm, denoted \( \| \cdot \|_\infty,\Omega_h := \max_{\Omega_h} | \cdot | \).

**Theorem 4.1.** (i) Let \( \{t_j = T(j/M)\}_{j=0}^M \) for some \( r \geq 1 \), and \( u \) satisfy (1.1)–(1.3) in \( \Omega = (0,1)^d \) with \( c \geq 0 \). Then, under the condition

\[
h^{-1} \geq \max_{k=1,\ldots,d} \left\{ \frac{1}{2} \| b_k \|_{L^\infty(\Omega)} \| a_K^{-1} \|_{L^\infty(\Omega)} \right\},
\]

there exists a unique solution \( \{U^j\}_{j=0}^M \) of (4.1), and

\[
\| u(-,t_m) - U^m \|_{\infty,\Omega_h} \lesssim \max_{j=1,\ldots,M} \| \psi_j \|_{L^\infty(\Omega)} + t_m^a \| (L_h - L) u(-,t_m) \|_{\infty,\Omega_h},
\]

where \( m = 1, \ldots, M \), and \( \psi_j = \psi_j(x) \) is defined by (2.6), in which \( u(\cdot) \) is understood as \( u(x,\cdot) \) when evaluating \( \partial_x u, \partial^2_x u \) and \( \delta_t u \).

(ii) If \( r = 1 \), then \( \max_{j=1,\ldots,m} \| \psi_j \|_{L^\infty(\Omega)} \) in (4.3) can be replaced by a sharper

\[
\max_{j=1,\ldots,m} \left\{ \tau^{-\gamma} \| \psi_j \|_{L^\infty(\Omega)} \right\}, \text{ where } \tau = TM^{-1} \text{ and } \gamma = \min \{ \alpha, 1 - \alpha \}.
\]

**Corollary 4.2.** (i) Under the conditions of Theorem 4.1, suppose \( \| \partial^l_t u(-,t) \|_{L^\infty(\Omega)} \lesssim 1 + t^{\alpha-1} \) for \( l = 1, 2 \) and \( t \in (0,T] \), and also \( \| \partial^l_{x_k} u(-,t) \|_{L^\infty(\Omega)} \lesssim 1 \) for \( l = 3, 4, k = 1, \ldots, d \) and \( t \in (0,T] \). Then

\[
\| u(-,t_m) - U^m \|_{\infty,\Omega_h} \lesssim M^{-\min \{ \alpha r, 2 - \alpha \}} + t_m^a h^2 \text{ for } m = 1, \ldots, M.
\]

(ii) If, additionally, \( r = 1 \), then

\[
\| u(-,t_m) - U^m \|_{\infty,\Omega_h} \lesssim t_m^{\alpha-1} M^{-1} + t_m^a h^2 \text{ for } m = 1, \ldots, M.
\]
Proof. Imitate the proofs of Corollaries 2.4 and 2.6 for parts (i) and (ii), respectively, to show that $|\psi| \lesssim M^{-\min\{\alpha,2-\alpha\}}$ and $\tau^{-\gamma} t_j^{\alpha-\gamma} |\psi| \lesssim \tau$. Combine these bounds with the standard truncation error estimate $|\langle \mathcal{L}_h - \mathcal{L} \rangle u| \lesssim h^2$.

Remark 4.3. In the case $d = 1$, error bounds similar to those of Corollary 2.2 can be found in [17, Theorem 5.2] and [4, Theorem 1] for parts (i) and (ii), respectively. Note also that the assumptions made in this corollary on the derivatives of $u$ are realistic; see §6.1 and Example A in [4, 2.2]

Proof of Theorem 4.1. For the error $e_m(z) := u(z,t_m) - U^m(z)$, using (1.1) and (4.1), one easily gets a version of (2.8):

$$\delta^a e_m + \mathcal{L} e_m = R^m := \delta^a u(\cdot,t_m) - D_t^2 u(\cdot,t_m) + (\mathcal{L}_h - \mathcal{L}) u(\cdot,t_m) \quad \text{in } \Omega_h \text{ for } m \geq 1,$$

subject to $e^0 = 0$ in $\Omega_h$, and $e^m = 0$ on $\Omega_h \cap \partial \Omega$. Recall that the bound (2.10) on $r^m$ obtained in the proof of Lemma 2.3 implies that $|e^m| \lesssim t_j^{-\alpha} \max_{j=1,\ldots,m} \|\psi^j\|_{L^\infty(\Omega)}$. Hence, to complete the proof of part (i), it suffices to show that

$$(4.4) \quad \delta_t^a |e_m|\infty_{\Omega_h} \leq \|R^m\|_{\infty,\Omega_h} \quad \text{for } m = 1, \ldots, M.$$ 

Then, indeed, (4.3) immediately follows by an application of Lemma 2.1.

For $r = 1$, when dealing with the component $r^m$ of $R^m$, we combine the bound (2.12) (obtained in the proof of Lemma 2.3) with (4.4) and then employ Lemma 2.1, which yields the assertion of part (ii).

To prove (4.4), let $\max_{z \in \Omega_h} |e_m(z)| = |e_m(z^*)|$ for some $z^* \in \Omega_h$. Suppose that $e_m(z^*) \geq 0$ (the case $e_m(z^*) < 0$ is similar). Then (4.2) combined with $c \geq 0$ implies that $\mathcal{L}_h e_m(z^*) \geq 0$, so $\delta^a e_m + \mathcal{L} e_m = R^m$ at $z = z^*$ yields $\delta^a e_m(z^*) \leq R^m(z^*)$. In view of (2.2a), our assertion (4.4) follows.

5. Error analysis for finite element discretizations

In this section, we discretize (1.1)–(1.3), posed in a general bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$, by applying a standard finite element spatial approximation to the temporal semidiscretization (3.1). Let $S_h \subset H^1_0(\Omega) \cap C(\Omega)$ be a Lagrange finite element space of fixed degree $\ell \geq 1$ relative to a quasiform simplicial triangulation $\mathcal{T}$ of $\Omega$. (To simplify the presentation, it will be assumed that the triangulation covers $\Omega$ exactly.) Now, for $m = 1, \ldots, M$, let $u^m_h \in S_h$ satisfy

$$(5.1) \quad \langle \delta_t^a u^m_h,v_h \rangle + \mathcal{A}_h(u^m_h,v_h) = \langle f(\cdot,t_m),v_h \rangle \quad \forall v_h \in S_h$$

with $u^0_h = u_0$ or some $u^0_h \approx u_0$.

With $\langle \cdot, \cdot \rangle$ denoting the exact $L^2(\Omega)$ inner product, (5.1) employs a possibly approximate inner product $\langle \cdot, \cdot \rangle_h$. To be more precise, either $\langle \cdot, \cdot \rangle_h = \langle \cdot, \cdot \rangle$, or $\langle v, w \rangle_h := \sum_{T \in \mathcal{T}} Q_T[vw]$ results from an application of a linear quadrature formula $Q_T$ for $f_T$ with positive weights. Let $\mathcal{A}$ be the standard bilinear form associated with the elliptic operator $\hat{\mathcal{L}} := \mathcal{L} - c$ (i.e. $\mathcal{A}(v,w) = \langle \mathcal{L} v - cv, w \rangle$) for smooth $v$ and $w$ in $H^1_0(\Omega)$). The bilinear form $\mathcal{A}_h$ in (5.1) is related to $\mathcal{A}$ and defined by $\mathcal{A}_h(v,w) := \mathcal{A}(v,w) + \langle cv, w \rangle_h$.

Our error analysis will invoke the Ritz projection $\mathcal{R}_h u(t) \in S_h$ of $u(\cdot,t)$ associated with our discretization of the operator $\hat{\mathcal{L}}$ and defined by $\hat{\mathcal{A}}(\mathcal{R}_h u,v_h) = \langle \hat{\mathcal{L}} u, v_h \rangle \forall v_h \in S_h$ and $t \in [0,T]$. 


When estimating the error in the $L_p(\Omega)$ norm for $p \in \{2, \infty\}$, an additional assumption $A_p$ will be made, which we now describe. The set of interior mesh nodes is denoted by $\mathcal{N}$, with the corresponding piecewise-linear hat functions $\{\phi_z\}_{z \in \mathcal{N}}$.

$A_2$ Let $\langle \cdot, \cdot \rangle_h = \langle \cdot, \cdot \rangle$. (Otherwise, see Remark 5.2.)

$A_\infty$ Let $\ell = 1$ (i.e. linear finite elements are employed), and let the stiffness matrix associated with $A_h(\cdot, \cdot) + \kappa_{m,m}(\cdot, \cdot)_h$ have non-positive off-diagonal entries, i.e. $K_{zz} := A_h(\phi_z, \phi_z) + \kappa_{m,m}(\phi_z, \phi_z)_h \leq 0$ for any two interior nodes $z \neq z'$, where $m = 1, \ldots, M$.

(It suffices to check $K_{zz} \leq 0$ for $m = 1$ only, as $Q_T$ uses positive weights, while $\kappa_{1,1} = \max_{m=1,\ldots,M} \{\kappa_{m,m}\} = \tau_1^{1-\alpha}/\Gamma(2-\alpha)$.)

Sufficient conditions for $A_\infty$ will be discussed in §5.2–5.3. Note that an assumption similar to $A_\infty$ has been shown to be both necessary and sufficient for non-negativity preservation in finite element discretizations of equations of type (1.1) [9].

**Theorem 5.1.** (i) Given $p \in \{2, \infty\}$, let $\{t_j = T(j/M)^r\}_{j=0}^M$ for some $r \geq 1$, and $u$ satisfy (1.1)–(1.3) with $c - p^{-1} \sum_{j=1}^d \partial_x \psi_j \geq 0$. Then, under the condition $A_p$, there exists a unique solution $\{u^m\}_{m=0}^M$ of (5.1) and, for $m = 1, \ldots, M$,

$$\|u(\cdot, t_m) - u_h^m\|_{L_p(\Omega)} \leq \|u_0 - u_h^0\|_{L_p(\Omega)} + \max_{j=1,\ldots,m} \|\psi_j\|_{L_p(\Omega)} \int_0^{s_m} \|\rho(\cdot, t)\|_{L_p(\Omega)} \, dt,$$

where $\rho(\cdot, t) := \mathcal{R}_h u(t) - u(\cdot, t)$, while $\psi_j := \psi_j(x)$ is defined by (2.6), in which $u(\cdot)$ is understood as $u(x, \cdot)$ when evaluating $\partial_x u$, $\partial_x^2 u$ and $\partial_t u$.

(ii) If $r = 1$, then max$_{j=1,\ldots,m} \|\psi_j\|_{L_p(\Omega)}$ in (5.2) can be replaced by a sharper max$_{j=1,\ldots,m} \|\psi_j\|_{L_\infty(\Omega)}$, where $\tau = TM^{-1}$ and $\gamma = \min\{\alpha, 1-\alpha\}$.

Proof. Let $e_h^m := \mathcal{R}_h u(t_m) - u_h^m \in S_h$. Then $u(\cdot, t_m) - u_h^m = e_h^m - \rho(\cdot, t_m)$, so it suffices to prove the desired bounds for $e_h^m$. Now, a standard calculation using (5.1) and (1.1) yields

$$\langle \delta_t^m e_h^m, v_h \rangle_h + A_h(e_h^m, v_h)$$

$$= \langle \delta_t^m \mathcal{R}_h u(t_m), v_h \rangle_h + \langle \mathcal{A}(\mathcal{R}_h u(t_m), v_h) \rangle_h + \langle c \mathcal{R}_h u(t_m) - f(\cdot, t_m), v_h \rangle_h$$

$$= \langle \delta_t^m \rho(\cdot, t_m) + c\rho(\cdot, t_m) + \delta_t^m u(\cdot, t_m) - D_t^m u(\cdot, t_m), v_h \rangle_h \forall v_h \in S_h,$$
with \( \delta^\alpha \rho \). For the latter, Lemma 2.2 is applied with \( \lambda^j \) := \( \|\delta^\alpha \rho(\cdot, t_j)\|_{L^p(\Omega)} \). Then \( \|\delta^\alpha \rho(\cdot, t_m)\|_{L^p(\Omega)} \leq J^{1-\alpha} \lambda(t_m) \), while \( \tau_j \lambda^j \leq J^{T_j-1} \|\partial_t \rho(\cdot, t)\|_{L^p(\Omega)} \), so the resulting contribution to the bound on \( \|e^m_h\|_{L^p(\Omega)} \) will be \( \sum_{j=1}^m \tau_j \lambda^j \leq J^{T_m} \|\partial_t \rho(\cdot, t)\|_{L^p(\Omega)} \).

If \( r = 1 \), when dealing with the component \( r^m \) or \( R^m \) in (5.4), we recall the bound (2.12) (obtained in the proof of Lemma 2.3) and then apply Lemma 2.1, which yields the assertion of part (ii).

To prove (5.4), consider the cases \( p = 2 \) and \( p = \infty \) separately.

For \( p = 2 \), set \( v_h := e^m_h \) in (5.3) and note that condition \( A_2 \) combined with \( c - \frac{1}{2} \sum_{k=1}^d \partial_x b_k \geq 0 \) implies \( A_h(e^m_h, e^m_h) \geq 0 \), and then \( \delta^\alpha e^m_h, e^m_h \leq \langle R^m, e^m_h \rangle \). The bound (5.4) follows in view of (2.2a).

For \( p = \infty \), let \( \max_{x \in \Omega} |e^m_h(x)| = |e^m_h(z^*)| \) for some node \( z^* \in N \). Now, set \( v_h := \phi_{z^*} \) in (5.3) and note that condition \( A_\infty \) implies

\[
|A_h(e^m_h, \phi_{z^*}) + \kappa_{m,m}(e^m_h, \phi_{z^*})| \geq \{A_h(1, \phi_{z^*}) + \kappa_{m,m}(1, \phi_{z^*})\} |e^m_h(z^*)|.
\]

(Here we used the representation \( e^m_h = e^m_h(z^*) - \sum_{z \neq z^*} [e^m_h(z^*) - e^m_h(z)] \phi_{z^*} \). Note also that (in view of the definition of \( A_h \) related to \( L \) of (1.3)) for any \( z \in N \)

\[
A_h(1, \phi_{z^*}) + \kappa_{m,m}(1, \phi_{z^*}) = (c + \kappa_{m,m}, \phi_{z^*}) \geq \kappa_{m,m}(1, \phi_{z^*})
\]

Combining these two observations with (5.3) and (2.2a), we arrive at

\[
\kappa_{m,m}(1, \phi_{z^*})\|e^m_h(z^*)\| \leq \sum_{j=1}^m \left(\kappa_{m,j} - \kappa_{m,j-1}\right) (e^m_j, \phi_{z^*}) + \{R^m, \phi_{z^*}\}.
\]

Now, recall that \( Q_T \) has positive weights so \( |\langle v, \phi_{z^*}\rangle| \leq \|v\|_{L_\infty(\Omega)} \langle 1, \phi_{z^*}\rangle \) for any \( v \). With this observation, dividing the above relation by \( \langle 1, \phi_{z^*}\rangle \) and again using (2.2a), we finally get (5.4) for \( p = \infty \).

Remark 5.2 (Case \( \langle \cdot, \cdot \rangle \neq \langle \cdot, \cdot \rangle \): error in the \( L_2(\Omega) \) norm. Suppose that \( Q_T[1] = |T| \) and the Lagrange element nodes in each \( T \) are included in the set of quadrature points for \( Q_T \), while \( h := \max_{T \in T(\Omega)} \{\text{diam } T\} \) is sufficiently small. Then a version of Theorem 5.1 is valid for \( p = 2 \) (with condition \( A_2 \) dropped) with \( \|\cdot\|_{L^p(\Omega)} \) replaced by \( \|\cdot\|_{L^2(\Omega)} \). Indeed, the proof of Theorem 5.1 applies to this case with \( A_h(e^m_h, e^m_h) \geq 0 \) for sufficiently small \( h \), in view of

\[
\|c e^m_h, e^m_h\| \leq h\|\nabla e^m_h\|_{L^2(\Omega)}.
\]

Note also that \( \|\cdot\|_{L^2(\Omega)} \) in \( S_h \) as \( \langle \cdot, \cdot \rangle_h \) is an inner product in \( S_h \); for the latter, note that \( Q_T[\langle v, w\rangle] \) generates an inner product for \( v_h, w_h \in S_h \) restricted to \( T \).

5.1. Application of Theorem 5.1 to the error analysis in the \( L_2(\Omega) \) norm.

Let \( \Omega \subset \mathbb{R}^d \) (for \( d \in \{2, 3\} \)) be a domain of polyhedral type as defined in [12] §4.1.1. To be more precise, for \( d = 3 \), the boundary \( \partial \Omega \) consists of a finite number of open smooth faces, open smooth edges and vertices, the latter being cones with edges. Also, the angle between any two faces not exceed \( \theta^* \). (These conditions are satisfied, for example, by a convex domain of polyhedral type, as well as by a smooth domain). Then \( \|v\|_{H^2(\Omega)} \lesssim \|L^2(\Omega) \), for any \( 1 < p < 2 + \epsilon \). (where \( \epsilon = \epsilon(\Omega) > 0 \)). In the case \( a_{k} = 1 \) for \( k = 1, \ldots, d \) in (1.3), see [12] Theorem 4.3.2. Note that for a convex polygonal domain, this result follows from [10] Theorem 5.1 if \( p = 2 \), and is obtained in [5] Chapter 4 for any \( p < 2 + \epsilon \). The treatment of variable smooth coefficients \( \{a_k\} \) was addressed in [10] §2.
Consequently, for the error of the Ritz projection $\rho(\cdot, t) = \mathcal{R}_h u(t) - u(\cdot, t)$ one has
\begin{equation}
\|\partial_t^l \rho(\cdot, t)\|_{L^2(\Omega)} \lesssim h \inf_{v_h \in \mathcal{S}_h} \|\partial_t^l u(\cdot, t) - v_h\|_{W^j_{2}(\Omega)} \quad \text{for } l = 0, 1, t \in (0, T].
\end{equation}

For $l = 0$, see, e.g., [11 (8.5.5)]. A similar result for $l = 1$ follows as $\partial_t \rho(\cdot, t) = \mathcal{R}_h \dot{u}(t) - \dot{u}(\cdot, t)$, where $\dot{u} := \partial_t u$.

**Corollary 5.3.** (i) Under the conditions of Theorem 5.1 for $p = 2$, suppose that $\|\partial_t^l u(\cdot, t)\|_{W^j_{2}(\Omega)} \lesssim 1 + t^\alpha$ for $l = 0, 1$ and $\|\partial_t^2 u(\cdot, t)\|_{L^2(\Omega)} \lesssim 1 + t^{\alpha-2}$, where $t \in (0, T]$. Then
\begin{equation}
\|u(\cdot, t_m) - u_h^m\|_{L^2(\Omega)} \lesssim M^{-\min\{\alpha, 2 - \alpha\}} + h^{\ell+1} \quad \text{for } m = 1, \ldots, M.
\end{equation}

(ii) If, additionally, $r = 1$, then
\begin{equation}
\|u(\cdot, t_m) - u_h^m\|_{L^2(\Omega)} \lesssim t_m^{\alpha-1} M^{-1} + h^{\ell+1} \quad \text{for } m = 1, \ldots, M.
\end{equation}

**Proof.** Imitate the proofs of Corollaries 2.4 and 2.6 for parts (i) and (ii), respectively, to show that $\|\nabla u\|_{L^2(\Omega)} \lesssim M^{-\min\{\alpha, 2 - \alpha\}}$ and $\tau^{-\gamma} t_m^{1-\alpha+\gamma} \|\nabla u\|_{L^2(\Omega)} \lesssim \tau \lesssim M^{-1}$. Combine these bounds with $\|\partial_t^l \rho(\cdot, t)\|_{L^2(\Omega)} \lesssim h^{\ell+1}(1 + t^\alpha)$ for $l = 0, 1$ (the latter follows from (5.5)). \qed

**Remark 5.4.** The errors of finite element discretizations of type $(5.1)$ are also estimated in the $L^2(\Omega)$ norm in a recent paper [8], where the authors particularly address the non-smooth data. In the case of a uniform temporal mesh and $f = 0$, an error bound similar to that of Corollary 5.3(ii) is given in [8, Theorem 3.16(a)]. Note also that the assumptions made in Corollary 5.3 on the derivatives of $u$ are realistic; see [6.1] and Example B in [6.2].

**Remark 5.5 (Convergence in positive time in the $W^j_{2}(\Omega)$ semi-norm for $r = 1$).** Under condition $A_2$, one has $A_\ell(e_h^m, e_h^n) \geq \|\nabla e_h^m\|_{L^2(\Omega)}^2$. Now, imitating the proof of (5.4) for $p = 2$, one gets $\delta^2 (\kappa_{m,n}^{-1} \|\nabla e_h^m\|_{L^2(\Omega)}^2 / e_h^n) \leq \|R^m\|_{L^2(\Omega)}$ for $m \geq 1$. Consequently, $\kappa_{m,n}^{-1} \|\nabla e_h^m\|_{L^2(\Omega)}^2 / e_h^n \leq \|R^m\|_{L^2(\Omega)}$ (as well as $\|e_h^n\|_{L^2(\Omega)}$) is bounded similarly to the error in Corollary 5.3(ii), while, by (2.2b), $\kappa_{m,m} \approx M^\alpha$. Combining this with the standard error bound on $\|\nabla u\|_{L^2(\Omega)}$ (see, e.g., [11 (8.5.4)]) yields convergence of $(5.1)$ in the $W^j_{2}(\Omega)$ semi-norm for $t_m \gtrsim 1$.

5.2. Lumpred-mass linear finite elements: application of Theorem 5.1 to the error analysis in the $L^\infty(\Omega)$ norm.

In this section we restrict our consideration to the case $a_k = 1$ and $b_k = 0$ in (1.3) for $k = 1, \ldots, d$, and lumped-mass linear finite-element discretizations, i.e. $\ell = 1$ and $\langle \cdot, \cdot \rangle_h$ is defined using the quadrature rule $Q_T[v] := \int_T v^t$, where $v^t$ is the standard linear Lagrange interpolant.

For the error of the Ritz projection $\rho(\cdot, t) = \mathcal{R}_h u(t) - u(\cdot, t)$, one has
\begin{equation}
\|\partial_t^l \rho(\cdot, t)\|_{L^\infty(\Omega)} \lesssim h^{2-q-|\ln h|} \left\{ \|\partial_t^l u(\cdot, t)\|_{W^j_{2}(\Omega)} + \|\partial_t^l \mathcal{L} u(\cdot, t)\|_{W^{j-\alpha}_{2,2}(\Omega)} \right\},
\end{equation}
where $l = 0, 1, q = 0, 1$ and $t \in (0, T]$. Consider (5.6) for $l = 0$ (while the case $l = 1$ is similar as $\partial_t \rho(\cdot, t) = \mathcal{R}_h \dot{u}(t) - \dot{u}(\cdot, t)$, where $\dot{u} = \partial_t u$). If $\langle \cdot, \cdot \rangle_h = \langle \cdot, \cdot \rangle$, the terms involving $\mathcal{L} u$ disappear; this version of (5.6) immediately follows from the quasi-optimality of the Ritz projection in the $L^\infty$ norm; see, e.g., [14 Theorem 2], [11 Theorem 3.1] and [17 Theorem 5.1], for, respectively, polygonal,
convex polyhedral and smooth domains. The lumped-mass quadrature $\langle \cdot, \cdot \rangle_h \neq \langle \cdot, \cdot \rangle$ induces an additional component $\hat{\rho}_h \in S_h$ in $\rho$, defined by $\langle \nabla \hat{\rho}_h, \nabla \psi \rangle_h = \langle \mathcal{L} u, \psi \rangle_h - \langle \mathcal{L} u, \nu \rangle_h \forall \psi \in S_h$. For completeness, the bound of type (5.6) (with $l = 0$) for $\hat{\rho}_h$ is proved in Appendix A.

As we intend to apply Theorem 5.1 under condition $A_{\infty}$, note that the latter is satisfied under the following assumptions on the triangulation. For $\Omega \subset \mathbb{R}^2$, let $T$ be a Delaunay triangulation, i.e., the sum of the angles opposite to any interior edge is less than or equal to $\pi$. In the case $\Omega \subset \mathbb{R}^3$, for any interior edge $E$, let $\omega_E := \{T \in T : \partial T \supset E\}$, and impose that $\sum_{T \subset \omega_E} |E_T| \cot \theta_E^2 \geq 0$, where $\theta_E^2$ is the angle between the faces of $T$ not containing $E$, and the edge $E_T$ is their intersection. Under these conditions on $T$, the stiffness matrix for $-\sum_{k=1}^d \partial_x^2$ is an $M$-matrix (see, e.g., [19, Lemma 2.1]), while the mass matrix is positive diagonal. So indeed, $A_{\infty}$ is satisfied. Note also that it is sufficient, but clearly not necessary, for the triangulation to be non-obtuse (i.e. with no interior angle in any mesh element exceeding $\frac{\pi}{2}$).

**Corollary 5.6.** (i) Under the conditions of Theorem 5.1 for $p = \infty$, suppose that $\|\partial_t^l u(\cdot, t)\|_{W^{2,1}(\Omega)} \lesssim 1 + t^{\alpha - 1}$ and $\|\partial_t^l \mathcal{L} u(\cdot, t)\|_{W^{2,1}(\Omega)} \lesssim 1 + t^{\alpha - 1}$ for $l = 0, 1$, and also $\|\partial_t^l u(\cdot, t)\|_{L^\infty(\Omega)} \lesssim 1 + t^{\alpha - 2}$, where $\in (0, T)$. Then

$$\|u(\cdot, t_m) - u_h^m\|_{L^\infty(\Omega)} \lesssim M^{-\min(\alpha, 2 - \alpha)} + h^2 |\ln h| \quad \text{for} \ m = 1, \ldots, M.$$  

(ii) If, additionally, $r = 1$, then

$$\|u(\cdot, t_m) - u_h^m\|_{L^\infty(\Omega)} \lesssim t_m^{\alpha - 1} M^{-1} + h^2 |\ln h| \quad \text{for} \ m = 1, \ldots, M.$$  

**Proof.** Imitate the proofs of Corollaries 2.4 and 2.6 for parts (i) and (ii), respectively, to show that $\|\partial_t^l \psi\|_{L^\infty(\Omega)} \lesssim M^{-\min(\alpha r, 2 - \alpha)}$ and $\tau^{1 - \alpha + \gamma} \|\partial_t^l \psi\|_{L^\infty(\Omega)} \lesssim \tau \lesssim M^{-1}$. Combine these bounds with $\|\partial_t^l \rho(\cdot, t)\|_{L^\infty(\Omega)} \lesssim h^2 |\ln h|(1 + t^{\alpha - 1})$ for $l = 0, 1$ (the latter follows from (5.6)). \hfill $\Box$

**Remark 5.7.** The assumptions made in Corollary 5.6 on the derivatives of $u$ are realistic; see §6.1 and Example C in §6.2.

### 5.3. Linear finite elements without quadrature: a comment on the the error analysis in the $L^\infty(\Omega)$ norm.

Suppose $a_k = 1$ in (1.3) for $k = 1, \ldots, d$, and $\langle \cdot, \cdot \rangle_h = \langle \cdot, \cdot \rangle$. Then the mass matrix is not diagonal and contains positive off-diagonal entries. Still, condition $A_{\infty}$ is satisfied (and so Theorem 5.1 with $p = \infty$ can be applied) if $h^2 \tau_1^{-\alpha} \leq C_T$ for a sufficiently small constant $C_T$ that we specify below, and, additionally, the triangulation is non-obtuse and $\min_{T \subset \omega_E} \theta_T^2 \leq \theta^*$ for some fixed positive $\theta^* < \frac{\pi}{2}$ (for the notation, see §5.2). Indeed, for such a triangulation, not only the stiffness matrix for $-\sum_{k=1}^d \partial_x^2$ is an $M$-matrix, but its contribution to $A_{zz'}^m$, for any two nodes $x \neq x'$ connected by an interior edge $E$, will be strictly negative and equal to $-\sum_{T \subset \omega_E} |E_T| \cot \theta_E^2 / (d(d - 1))$ (with $E_T$, in the case $d = 2$, being a node and the notational convention $|E_T| = 1$ used); see [19, Lemma 2.1]. A calculation also shows that the contribution of $\langle \partial_t \phi^{x'}, \phi_x \rangle$ to $A_{zz'}^m$ does not exceed $(\tau_1^{-\alpha} / \Gamma(2 - \alpha) + \|\cdot\|_{L^\infty(\Omega)} |\omega_E| / (d + 1)(d + 2))$. Furthermore, the contribution of $\langle \partial_t \phi(x) \partial_x \phi^{x'}, \phi_x \rangle$ to $A_{zz'}^m$ is $\lesssim h - 1 |\omega_E|$. As the triangulation is quasi-uniform, these
observations imply that there is a positive constant $C'_T$ such that for any interior edge $E$, one has

$$\frac{(d + 1)(d + 2)}{d(d - 1)} |\omega_E|^{-1} \sum_{T \in \omega_E} |E'_T| \cot \theta^E_T \geq C'_T h^{-2}.$$  

Now, $h^2 \tau_1^{-\alpha} \leq C_T$, with any fixed constant $C_T < C'_T \Gamma(2 - \alpha)$, implies $A_\infty$ (assuming that $h$ is sufficiently small; in fact, one can use $C_T = C'_T \Gamma(2 - \alpha)$ if $c = 0$ and $b_k = 0$ for $k = 1, \ldots, d$ in (1.3)). To avoid computing $C'_T$, one can instead impose $h^2 |\ln h| \tau_1^{-\alpha} \leq C_T$ with any fixed $C_T > 0$ and $h$ sufficiently small. Note that although the above triangulation condition is somewhat restrictive, it is satisfied by mildly structured meshes with all mesh elements close to equilateral triangles/regular tetrahedra.

Note also that in most practical situations, the convergence rates do not deteriorate because of the restriction $\tau_1^\alpha \geq h^2$. To be more precise, as long as $r \leq (2 - \alpha)/\alpha$ (including the optimal $r = (2 - \alpha)/\alpha$), the error in part (i) of Corollary 5.6 is $\lesssim M^{-\alpha} + h^2 |\ln h| \approx \tau_1^\alpha + h^2 |\ln h|$. Similarly, in part (ii) for $t_m \geq 1$, the error is $\lesssim \tau_1 + h^2 |\ln h|$, so a reasonable choice $\tau_1 \approx h^2$ is clearly within the restriction $\tau_1^\alpha \geq h^2$.

6. Estimation of derivatives of the exact solution $u$

The purpose of this section is to show that the assumptions made in §§3.3, 3.4 on the derivatives of the exact solution $u$ of (1.1) are realistic, and give examples of when they are satisfied. The discussion will be mainly restricted to the case of the operator $L$ being self-adjoint (i.e. $b_k = 0$ for $k = 1, \ldots, d$ in (1.3)); for the non-self-adjoint case, see Remark 6.1 below. For simplicity, we also assume that $\Omega$ is either a convex domain of polyhedral type or a smooth domain. Hence, we shall be able to invoke $\|v\|_{W^2_2(\Omega)} \lesssim \|Lv\|_{L_2(\Omega)}$ when $v = 0$ on $\partial \Omega$, as well as the consequent property $\|v\|_{L_\infty(\Omega)} \lesssim \|Lv\|_{L_2(\Omega)}$ (in view of the Sobolev embedding theorem).

The approach that we consider here employs the method of separation of variables, in which the eigenvalues and eigenfunctions of the self-adjoint operator $L$ (see, e.g., [5] §6.5) for their existence and properties) are used to get an explicit eigenfunction expansion of $u$. Note that the time-dependent coefficients in this expansion are represented using Mittag-Leffler functions. This approach was used in [13] for smooth domains, [6] §2.2 and §3.4] for polygonal/polyhedral domains, and [14] §2] for $\Omega = (0, 1)$.

6.1. Temporal derivatives of $u$. The assumptions made in Corollary 3.2 on temporal derivatives of $u$ (that $\|\partial_t^l u(\cdot, t)\|_{L_p(\Omega)} \lesssim 1 + t^{\alpha - l}$ for $l = 1, 2$, and $p \in \{2, \infty\}$) are realistic. For example, for the case $p = \infty$, $d = 1$ and $L = -\partial_x^2 + c(x_1)$, they are satisfied under certain regularity assumptions on $u_0$ and $f$ (including $L^1 f(\cdot, t) = L^q u_0 = 0$ on $\partial \Omega$ for $l = 0, 1$ and $q = 0, 1, 2$) by [17] Theorem 2.1. The proof relies on the term-by-term differentiation with respect to $t$ of the eigenfunction expansion of $u$. Note that this proof cannot be directly extended to $d > 1$ (as the eigenfunctions are not necessarily uniformly bounded, while the eigenvalues exhibit a different asymptotic behaviour in higher dimensions).

These difficulties are avoided by the following modification. A term-by-term application of $L^1 \partial_t^l$ to the eigenfunction expansion of $u$ yields $\|L^1 \partial_t^l u(\cdot, t)\|_{L_p(\Omega)} \lesssim 1 + t^{\alpha - l}$ for $l = 1, 2$ and $q = 0, 1$. Now, setting $q = 0$ and $q = 1$ implies the desired bounds on the temporal derivatives for $p = 2$ and $p = \infty$, respectively.
It should be noted that this approach relies on the regularity assumptions that $\|u_0\|_{L_2} + \|\partial_t f(t, \cdot)\|_{L_2} \leq 1$ for $l = 0, 1, 2$ (where the assumptions of the temporal derivatives of $f$ may, in fact, be weakened). Here (similar to [1, 13, 17]), we used the norm $\|v\|_{L^2} := \{\sum_{i=1}^{\infty} \lambda_i^{2\gamma} (v, \psi_i)^2\}^{1/2}$, where $0 < \lambda_1 < \lambda_2 = \lambda_3 \leq \ldots$ are the eigenvalues of $L$, while $\{\psi_i\}_{i=1}^{\infty}$ are the corresponding normalized eigenfunctions satisfying $\|\psi_i\|_{L_2} = 1$.

### 6.2. Spatial and mixed derivatives of $u$

In §4.5 (see Corollaries 4.2, 5.3, 5.6), a number of additional assumptions were made that involve spatial derivatives of $u$. Here the situation is more delicate, as if $\Omega$ has any corners, $u$ may exhibit corner singularities.

**Example A.** Consider $\Omega = (0, 1)^2$ and $L = -[\partial_{x_1}^2 + \partial_{x_2}^2] + c(x_1, x_2)$ under the assumption $\|u_0\|_{L_2} + \|f(\cdot, t)\|_{L_2} \leq 1$. Note that the latter implies that the elliptic corner compatibility conditions up to order 2 are satisfied. Hence, [18, Theorem 3.1] combined with the Sobolev embedding theorem yields $\|u\|_{W_2^2(\Omega)} \leq \|u\|_{L_2^2(\Omega)}$ for any $t \in (0, T)$. Similarly, $\|Lu\|_{W_2^2(\Omega)} \leq \|L^2 u\|_{W_2^2(\Omega)} \leq \|L^3 u\|_{L_2(\Omega)}$, while one can show (by an application of $L^3$ to the eigenfunction expansion of $u$) that $\|L^3 u\|_{L_2(\Omega)} \leq 1$. Combining these observations, one gets $\|u\|_{W_2^2(\Omega)} \leq 1$, so the assumptions made in Corollary 4.2 on the spatial derivatives of $u$ are satisfied.

**Example B.** It is assumed in Corollary 5.3 that $\|\partial_t^l u(\cdot, t)\|_{W_2^{l+1} (\Omega)} \leq 1 + t^\alpha - l$ for $l = 0, 1$ and $t \in (0, T)$. For linear finite elements, i.e. $l = 1$, these bounds follow from $\|\partial_t^l u\|_{W_2^2(\Omega)} \leq \|L\partial_t^l u\|_{L_2(\Omega)}$ combined with the bound on $\|L\partial_t^l u(\cdot, t)\|_{L_2(\Omega)}$ obtained in §6.1 (see the case $q = 1$). For $l > 1$, a similar argument can be used (under additional data regularity assumptions) if $\Omega$ is smooth.

**Example C.** If $\Omega$ is smooth, then both $\|\partial_t^l u(\cdot, t)\|_{W_2^2(\Omega)}$ and $\|\partial_t^l u(\cdot, t)\|_{W_2^2(\Omega)}$ are $\leq \|L\partial_t^l u(\cdot, t)\|_{W_2^2(\Omega)}$. For the latter, using the argument of Example B, one can show that $\|\partial_t^l u(\cdot, t)\|_{W_2^2(\Omega)} \leq 1 + t^\alpha - l$ under the regularity assumption $\|u_0\|_{L_2} + \|\partial_t^l f(\cdot, t)\|_{L_2} \leq 1$. So for this example, the assumptions made in Corollary 5.6 on $u$ are satisfied.

**Remark 6.1 (Non-self-adjoint $L$).** Even if some coefficient(s) $b_k \neq 0$ in (1.3), one can sometimes employ the eigenfunction expansion after reducing the problem (1.1) to the self-adjoint case. For example, if the coefficients $\{a_k\}$ and $\{b_k\}$ in (1.3) are constant, it suffices to rewrite (1.1) for the unknown function $\tilde{u} := u \exp\{-\sum_{k=1}^{d} \frac{1}{2} (b_k/a_k) x_k\}$. A similar trick for the case of variable coefficients and $d = 1$ is described in §2.

### 7. Numerical results

Our model problem is (1.1) with $L = -[\partial_{x_1}^2 + \partial_{x_2}^2]$, posed in the domain $\Omega \times [0, 1]$ (see Fig.1 left) with $\partial \Omega$ parameterized by $x_1(l) := \frac{3}{2} R \cos \theta$ and $x_2(l) := R \sin \theta$, where $R(l) := 0.4 + 0.5 \cos^2 l$ and $\theta(l) := l + e^{(l-5)/2} \sin(l/2) \sin l$ for $l \in [0, 2\pi]$. We choose $f$, as well as the initial and non-homogeneous boundary conditions, so that the unique exact solution $u = t^a \cos(xy)$. This problem is discretized by (5.1) (with an obvious modification for the case of non-homogeneous boundary conditions) using lumped-mass linear finite elements (described in §5.2) on quasiuniform Delaunay triangulations of $\Omega$ (with DOF denoting the number of degrees of freedom in space).
Table 1. Maximum nodal errors (odd rows) and computational rates \( q \) in \( M^{-q} \) (even rows) for \( r = (2 - \alpha) / \alpha \) and spatial DOF=398410

| \( M \) | 64  | 128  | 256  | 512  | 1024 | 2048 |
|------|-----|------|------|------|------|------|
| \( \alpha = 0.3 \) | 4.157e-4 | 1.428e-4 | 4.750e-5 | 1.558e-5 | 5.053e-6 | 1.624e-6 |
|       | 1.542 | 1.588 | 1.608 | 1.624 | 1.637 |
| \( \alpha = 0.5 \) | 7.824e-4 | 3.109e-4 | 1.173e-4 | 4.301e-5 | 1.555e-5 | 5.582e-6 |
|       | 1.331 | 1.407 | 1.447 | 1.468 | 1.478 |
| \( \alpha = 0.7 \) | 1.236e-3 | 5.924e-4 | 2.693e-4 | 1.181e-4 | 5.045e-5 | 2.120e-5 |
|       | 1.061 | 1.137 | 1.190 | 1.226 | 1.251 |

The errors in the maximum nodal norm \( \max_{z \in N, m=1,...,M} |u_h^m(z) - u(z, t_m)| \) are shown in Fig. 1 (right) and Table 1 for, respectively, a large fixed \( M \) and DOF. In the latter case, we also give computational rates of convergence. The graded temporal mesh \( \{t_j = T(j/M)^r\}_{j=0}^M \) was used with the optimal \( r = (2 - \alpha) / \alpha \) (see Remark 2.5).

By Corollary 5.6(i), the errors are expected to be \( \lesssim M^{-q} + \ln h \) for \( q = 0, 1 \). Our numerical results clearly confirm the sharpness of this corollary for the considered case. For more extensive numerical experiments, we refer the reader to [17], where, in particular, the influence of \( r \) on the errors is numerically investigated, as well as [4, 8] for numerical results on uniform temporal meshes.

**APPENDIX A. LUMPED-MASS QUADRATURE ERROR IN THE MAXIMUM NORM**

The lumped-mass quadrature \( \langle \cdot, \cdot \rangle_h \neq \langle \cdot, \cdot \rangle \) induces an additional component \( \hat{\rho}_h \in S_h \) in the error of the Ritz projection \( \rho(\cdot, t) = R_h u - u \), defined by \( \langle \nabla \hat{\rho}_h, \nabla v_h \rangle = \langle \hat{L}u, v_h \rangle - \langle L u, v_h \rangle \forall v_h \in S_h \). We claim that

\[
\| \hat{\rho}_h \|_{L^\infty(\Omega)} \lesssim h^{2-q} \ln h \| \hat{L}u(\cdot, t) \|_{W^{2-\gamma}_{d/2}(\Omega)} \quad \text{for} \quad q = 0, 1.
\]

The desired bound of type (5.6) (with \( l = 0 \)) for \( \hat{\rho}_h \) follows in view of \( \hat{L}c = L - c \).

To prove (A.1), a standard calculation yields, for any \( v_h \in S_h \) and \( q = 0, 1 \),

\[
|\langle \nabla \hat{\rho}_h, \nabla v_h \rangle| \lesssim h^{2-q} \left\{ \| \hat{L}u \|_{W^{2-\gamma}_{d/2}(\Omega)} \| v_h \|_{L_{d/(d-2)}(\Omega)} + \| \hat{L}u \|_{W^{1-\gamma}_{d}(\Omega)} \| \nabla v_h \|_{L_{d/(d-1)}(\Omega)} \right\}.
\]

Figure 1. Delaunay triangulation of \( \Omega \) with DOF=172 (left), maximum nodal errors for \( \alpha = 0.5 \), \( r = (2 - \alpha) / \alpha \) and \( M = 10^4 \).
In view of the Sobolev embedding \( \| \hat{\mathcal{L}}u \|_{W_{d,q}^{1-q}(\Omega)} \lesssim \| \mathcal{L}u \|_{W_{d,2}^{2-q}(\Omega)} \), one arrives at
\begin{equation}
(A.2) \quad | \langle \nabla \hat{\rho}_h, \nabla v_h \rangle | \lesssim h^{2-q} \left\{ \| v_h \|_{L_d/(d-2)(\Omega)} + \| \nabla v_h \|_{L_d/(d-1)(\Omega)} \right\} \| \hat{\mathcal{L}}u \|_{W_{d,2}^{2-q}(\Omega)}.
\end{equation}

Next, consider the cases \( d = 2, 3 \) separately.

For \( d = 2 \), one has \( d/(d-2) = \infty \) and \( d/(d-1) = 2 \). Set \( v_h := \hat{\rho}_h \) in (A.2), and recall the discrete Sobolev inequality \( \| \hat{\rho}_h \|_{L_\infty(\Omega)} \lesssim | \ln h |^{1/2} \| \nabla \hat{\rho}_h \|_{L_2(\Omega)} \), so \( \| \nabla \hat{\rho}_h \|_{L_2(\Omega)} \lesssim h^{2/| \ln h |} \| \hat{\mathcal{L}}u \|_{W_{d,2}^{2-q}(\Omega)} \), so (A.1) follows.

For \( d = 3 \), with \( \| \hat{\rho}_h \|_{L_\infty(\Omega)} = | \hat{\rho}_h(x^*) | \) for some interior node \( x^* \in \Omega \), let \( g_h \in \mathcal{S}_h \) be a discrete version of the Green’s function \( g_h \in \mathcal{S}_h \) associated with \( x^* \) and defined by \( \langle \nabla g_h, \nabla v \rangle = v_h(x^*) \forall v \in \mathcal{S}_h \). Now set \( v_h := g_h \) in (A.2), so
\[
| \langle \nabla \hat{\rho}_h, \nabla g_h \rangle | \lesssim h^{2-q} \left\{ \| g_h \|_{L_3(\Omega)} + \| \nabla g_h \|_{L_3/(2)(\Omega)} \right\} \| \hat{\mathcal{L}}u \|_{W_{d,2}^{2-q}(\Omega)},
\]
where we employed the bounds on \( \| g_h \|_{L_3(\Omega)} \) and \( \| \nabla g_h \|_{L_3/(2)(\Omega)} \) from (11), (3.10), (3.11) and the final formula in §3. So we again get (A.1).

**Appendix B. Proof of Lemma 2.1**

**Proof.** (i) First, consider \( \gamma = \alpha \). As the operator \( \delta^\alpha_t \) is associated with an \( M \)-matrix, it suffices to construct a barrier function \( 0 \leq B^j \lesssim t^\alpha_j \) such that \( \delta^\alpha_t B^j \geq \tau^\alpha t^{\alpha_j - 1} \). Fix a sufficiently large number \( 2 \leq p \lesssim 1 \), and then set \( \beta := 1 - \alpha \) and \( B(s) := \min \{ (s/t_p)^{1-p}, s^{-\beta} \} \), and also \( B^j := B(t_j) \). Note that, when using the notation of type \( \lesssim \), the dependence on \( p \) will be shown explicitly.

For \( j \leq p \), a straightforward calculation shows that \( \delta^\alpha_t B^j = D^\alpha_t B(t_j) \approx t^\beta_j t^{-\beta - 1} \lesssim p^{-\beta - 1}(\tau^\alpha t^{\alpha_j - 1}) \). Next, for \( D^\alpha_t B(t) \) with \( t > t_p \) one has
\[
\Gamma(1-\alpha) D^\alpha_t B(t) = \int_0^{t_p} t_p^{-\beta - 1}(t-s)^{-\alpha} ds - \beta \int_{t_p}^{t} s^{-\beta - 1}(t-s)^{-\alpha} ds.
\]

Here, using \( \hat{s} := s/t \) and \( \hat{t}_p := t_p/t \), and noting that \( \alpha + \beta = 1 \), one gets
\[
I = \beta \int_{\hat{t}_p}^{1} \hat{s}^{-\beta - 1}(1-\hat{s})^{-\alpha} d\hat{s} = \hat{t}_p^{-\beta}(1-\hat{t}_p)^{\beta} \leq \hat{t}_p^{-\beta}(1-\beta t_p).
\]

Now, using \( t^{-\beta} \hat{t}_p^{-\beta} = t^{-\beta} t^{-\alpha} \), one concludes for \( t > t_p \) that
\begin{equation}
(B.1) \quad \Gamma(1-\alpha) D^\alpha_t B(t) \geq t^{-\beta} t^{-\alpha} (\beta t_p/t) = \beta t_p^{\alpha} t^{1-\alpha - 1} = \beta p^\alpha (\tau^\alpha t^{\alpha_j - 1}).
\end{equation}

So, to complete the proof, it remains to show that \( \frac{1}{2}D^\alpha_t B(t_m)^2 \geq | \delta^\alpha_t B^m - D^\alpha_t B(t_m) | \) for any \( m > p \). For the latter, with the notation \( F(s) := \beta^{-1}(t_m - s)^{\beta} \), note that \( \delta^\alpha_t B^m \) involves \( \sum_{j=1}^m \) of the terms
\[
\delta^\alpha_t B^j \left\{ \int_{t_{j-1}}^{t_j} (t_m - s)^{-\alpha} ds = \delta^\alpha_t F^{j} \int_{t_{j-1}}^{t_j} B(s) ds \right\}.
\]

Note also that the component \( \sum_{j=1}^p \) is identical in \( \delta^\alpha_t B^m \) and \( D^\alpha_t B(t_m) \). Now, subtracting one of the above representations from the corresponding components.
\[
\int_{t_{j-1}}^{t_j} B'(s) F'(s) \, ds \text{ of } D_t^p B(t_m) \text{ yields }
\]
\[
|\delta_t^\alpha B^m - D_t^p B(t_m)| \lesssim \tau \int_{t_p}^{t_m} s^{-\beta-1} (t_m-s)^{-\alpha-1} \, ds + \tau \int_{t_n}^{t_m} (s-\tau)^{-\beta-2} (t_m-s)^{-\alpha} \, ds,
\]
where \( n := \max\{p, \lfloor m/2 \rfloor \} \), and \( n \leq m-2 \) whenever \( n > p \). Here, when dealing with \( s \in (t_{j-1}, t_j) \), we also used \( |\delta_t F^j - F'(s)| \leq \tau |F''(t_j)| \lesssim \tau (t_m-s)^{-\alpha-1} \) for \( j \leq n \), and \( |\delta_t B^j - B'(s)| \leq \tau |B''(t_{j-1})| \lesssim \tau (s-\tau)^{-\beta-2} \) for \( j > n \). Estimating the above integrals \( \int_{t_p}^{t_m} \) and \( \int_{t_n}^{t_m} \) similarly to \( I \) and respectively using \( (t_m-s)^{-1} \leq 2(t_m-s)^{-1} \) and \( (s-\tau)^{-1} \leq 2(s-\tau)^{-1} \), one finally gets
\[
|\delta_t^\alpha B^m - D_t^p B(t_m)| \lesssim \tau t_m^{-2} (t_p/t_m)^{-\beta} \simeq p^{-\beta} (\tau^\alpha t_m^{-\alpha}).
\]
Combining this with \( (B.1) \) and choosing \( p \) sufficiently large yields the desired assertion \( \delta_t^\alpha B^m \gtrsim \tau^\alpha t_m^{-\alpha} \).

(ii) It remains to consider \( \gamma \in (0, \alpha) \). Set \( p_m := 2^m p \) and \( c_m := 2^{-m} \gamma \). Now, set \( B_0(s) := \min\{st_m^{-\beta-1}, s^{-\beta}\} \) (i.e. \( B_0(s) = B(s) \)), and \( B_m^j := B_m(t_j) \), and then \( B^j := \sum_{m=0}^{\infty} c_m B_m^j \). Here \( p \) is from part (i), and, when using the notation of type \( \lesssim \), the dependence on \( \gamma \) and \( m \), but not on \( p \), will be shown explicitly.

Imitating the argument used in part (i), one gets \( \delta_t^\alpha B_m^j \gtrsim 0 \) for \( j \geq 0 \), while for \( j > p_m \) one has \( \delta_t^\alpha B_m^j \gtrsim t_p^{-\alpha} t_j^{\gamma-1} \) (compare with \( (B.1) \)). The latter implies \( c_m (\delta_t^\alpha B_m^j) \gtrsim c_m t_p^{-\alpha} t_j^{\gamma-1} \gtrsim \tau^\gamma t_j^{\gamma-1} \) for \( p_m < j \leq p_{m+1} \). Combining this with \( c_0 = 1 \) and \( \delta_t^\alpha B_0^j \gtrsim \tau^\alpha t_j^{\gamma-1} \gtrsim \tau^\gamma t_j^{\gamma-1} \) for \( 1 \leq j \leq p_0 \), one concludes that \( \delta_t^\alpha B^j \gtrsim \tau^\gamma t_j^{\gamma-1} \). Finally, note that \( \sum_{m=0}^{\infty} c_m = C_\gamma := (1-2^{-\gamma})^{-1} \), so \( B^j \lesssim C_\gamma t_j^{-\beta} = C_\gamma t_j^{-\gamma} \), which completes the proof. \( \square \)

References

[1] S. C. Brenner and L. R. Scott, The mathematical theory of finite element methods, Springer-Verlag, New York, third ed., 2008.
[2] K. Diethelm, The analysis of fractional differential equations, Lecture Notes in Mathematics, Springer-Verlag, Berlin, 2010.
[3] L. C. Evans, Partial Differential Equations, American Mathematical Society, 1998.
[4] J. L. Gracia, E. O’Riordan and M. Stynes, Convergence in positive time for a finite difference method applied to a fractional convection-diffusion problem, Comput. Methods Appl. Math. (2017), doi: https://doi.org/10.1515/cmam-2017-0019.
[5] P. Grisvard, Elliptic problems in nonsmooth domains, Pitman, Boston, MA, 1985.
[6] B. Jin, R. Lazarov and Z. Zhou, Error estimates for a semidiscrete finite element method for fractional order parabolic equations, SIAM J. Numer. Anal. 51 (2013), 445–466.
[7] B. Jin, R. Lazarov and Z. Zhou, Two fully discrete schemes for fractional diffusion and diffusion-wave equations with nonsmooth data, SIAM J. Sci. Comput. 38 (2016), A146–A170.
[8] B. Jin, R. Lazarov and Z. Zhou, An analysis of the L1 scheme for the subdiffusion equation with nonsmooth data, IMA J. Numer. Anal. 36 (2016), 197–221.
[9] B. Jin, R. Lazarov, V. Thomée and Z. Zhou, On nonnegativity preservation in dinite element methods for subdiffusion equations, Math. Comp. 86 (2017), 2239–2270.
[10] V. A. Kondrat’ev, Boundary value problems for elliptic equations in domains with conical or angular points, Trudy Moskov. Mat. Obsch. 16 (1967) 209–292, English transl. in: Trans. Moscow Math. Soc. 16 (1967) 227–313.
[11] D. Leykekhman and B. Vexler, Finite element pointwise results on convex polyhedral domains, SIAM J. Numer. Anal. 54 (2016), 561–587.
[12] V. Maz’ya and J. Rossmann, Elliptic equations in polyhedral domains, American Mathematical Society, Providence, RI, 2010.
[13] K. Sakamoto and M. Yamamoto, Initial value/boundary value problems for fractional diffusion-wave equations and applications to some inverse problems, J. Math. Anal. Appl. 382 (2011), 426–447.
[14] A. H. Schatz, A weak discrete maximum principle and stability of the finite element method in $L_\infty$ on plane polygonal domains. I, Math. Comp. 34 (1980), 77–91.
[15] A. H. Schatz and L. B. Wahlbin, On the quasi-optimality in $L_\infty$ of the $H^1$-projection into finite element spaces, Math. Comp. 38 (1982), 1–22.
[16] M. Stynes, Too much regularity may force too much uniqueness, Fract. Calc. Appl. Anal. 19 (2016), 1554–1562.
[17] M. Stynes, E. O’Riordan and J. L. Gracia, Error analysis of a finite difference method on graded meshes for a time-fractional diffusion equation, SIAM J. Numer. Anal. 55 (2017), 1057–1079.
[18] E. A. Volkov, Differentiability properties of solutions of boundary value problems for the Laplace and Poisson equations on a rectangle, Trudy Mat. Inst. Steklov. 77 (1965) 89–112.
[19] J. Xu and L. Zikatanov, A monotone finite element scheme for convection-diffusion equations, Math. Comp. 68 (1999), 1429–1446.

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