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_∞ and L_2 norms. This framework is employed in the analysis of both finite difference and finite element spatial discretiztions. 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

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

This problem is posed in a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$ (where $d \in \{1, 2, 3\}$). The operator D_t^α, for some $\alpha \in (0, 1)$, is the Caputo fractional derivative in time defined [2] by

$$
(1.2) \qquad D_t^\alpha u(\cdot, t) := \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \, \partial_s u(\cdot, s) \, ds \qquad \text{for} \ \ 0 < t \le T,
$$

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

$$
(1.3) \qquad \mathcal{L}u := \sum_{k=1}^d \Big\{ -\partial_{x_k}(a_k(x) \, \partial_{x_k} u) + b_k(x) \, \partial_{x_k} u \Big\} + c(x) \, u,
$$

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 $c \ge 0$ or $c - \frac{1}{2} \sum_{k=1}^d \partial_{x_k} b_k \ge 0$. All our results also apply to the case $\mathcal{L} = \mathcal{L}(t)$, while some remain valid for a more general uniformly-elliptic $\mathcal{L}$ (i.e., with mixed second-order derivatives); see Remark 3.3.

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 $|\partial_t^l u(\cdot, t)| \lesssim 1 + t^{\alpha - l}$ for $l = 0, 1, 2$ (the notation $\lesssim$ is rigourously 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 $|\partial^l u(\cdot, t)| \lesssim 1$ frequently made in the literature (see, e.g., references in [8, Table 1.1]). Indeed, [21, Theorem 2.1] shows that if a solution u of (1.1) is less singular than we assume (in the sense that $|\partial_t^l u(\cdot, t)| \lesssim 1 + t^{\gamma - l}$ 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

$$(1.4) \quad \delta_t^\alpha U^m := \frac{1}{\Gamma(1 - \alpha)} \sum_{j=1}^m \delta_t U^j \int_{t_{j-1}}^{t_j} (t_m - s)^{-\alpha} \, ds, \qquad \delta_t U^j := \frac{U^j - U^{j-1}}{t_j - t_{j-1}},$$

when associated with the temporal mesh $0 = t_0 < t_1 < \ldots < t_M = T$ on $[0, T]$. Similarly to [22], our main interest will be in graded temporal meshes as they offer an efficient way of computing reliable numerical approximations of solutions that are 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 $t \gtrsim 1$ [5, 9].

Novelty. We present a new framework for the estimation of the error whenever an L1 scheme is used on graded or uniform temporal meshes. This framework is simple, applies to both finite difference and finite element spatial discretizations, and works for error estimation in both $L_2(\Omega)$ and $L_\infty(\Omega)$ norms. It easily extends to general elliptic operators $\mathcal{L} = \mathcal{L}(t)$, as well as quasi-uniform and quasi-graded temporal meshes. Naturally, it yields versions of some previously-known error bounds as particular cases. It is also used here to establish entirely new results.

Graded meshes for problems of type (1.1) for the case $d = 1$ were recently considered in [22], where maximum norm error bounds are obtained for finite difference discretizations. In comparison, our analysis deals with temporal-discretization errors on graded meshes in an entirely different and substantially more concise way. To be more precise, we use more intuitive integral representations of the temporal truncation errors; see Lemma 2.3. Once error bounds on graded meshes are established for a paradigm problem without spatial derivatives, they seamlessly extend to finite difference and finite element spatial discretizations of (1.1) for any $d \geq 1$. Our results on graded meshes are new for finite element discretizations, as well as for finite difference discretizations for $d > 1$.

The convergence behaviour of the L1 method on uniform temporal meshes is well understood. In particular, for finite element spatial discretizations, the errors in the $L_2(\Omega)$ norm have been estimated in [9] using Laplace transform techniques (for $\mathcal{L} = -\triangle$ and $f = 0$). For finite difference discretizations for $d = 1$, a similar error bound in the maximum norm was established in [5]. Within our theoretical framework, we easily get versions of error bounds of [9] and [5]. Furthermore, we give error bounds for finite element discretizations in the $L_\infty(\Omega)$ norm on uniform temporal meshes, which appear to be entirely new. (Some error bounds in the L_∞ norm for linear-finite-element spatial semidiscretizations are given in [12].)

Our approach to uniform meshes is very similar to the case of graded meshes. The main difference is in that now we employ a more subtle stability property of the discrete fractional-derivative operator δ_t^α from [5], a version of which is also given in [11]; see Lemma 2.1*. Additionally, we give a considerably shorter and more intuitive proof of this stability result. This new proof relies on a simple barrier function, and may be of independent interest; see Appendix A.

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 $a \leq Cb$ with a generic constant C depending on Ω, 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 $W_p^k(\Omega)$, while $H_0^1(\Omega)$ is the standard space of functions in $W_2^1(\Omega)$ 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

$$(2.1) \qquad \tau_j := t_j - t_{j-1} \simeq M^{-1}\, t_j^{1-1/r} \qquad \text{for } j = 1, \ldots, M.$$

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

Note that all results of the paper immediately apply to a quasi-graded mesh defined by $\{t_j = T(\xi_j)^r\}_{j=0}^M$, where $\{\xi_j\}_{j=0}^M$ is a quasi-uniform mesh on $[0,1]$.

2.2. **Stability properties of the discrete fractional operator δ_t^α.** The definition (1.4) of δ_t^α can be rewritten as

$$(2.2\text{a}) \quad \delta_t^\alpha V^m = \underbrace{\kappa_{m,m}}_{>0} V^m - \sum_{j=1}^m \underbrace{(\kappa_{m,j} - \kappa_{m,j-1})}_{>0}\, V^{j-1},$$

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

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 $\kappa_{m,j-1} \leq \kappa_{m,j}$ 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*

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

(ii) *If $V^0 = 0$ and $\delta_t^\alpha |V^j| \leq |F^j|$ for $j = 1, \ldots, M$, then*

$$|V^m| \lesssim \max_{j=1,\ldots,m} \left\{ t_j^\alpha\, |F^j| \right\} \qquad \text{for } m = 1, \ldots, M.$$

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 $|W^m| \lesssim \max_{j \leq m} \{t_j^\alpha |F^j|\}$. 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

$$(2.3) \qquad \underbrace{\kappa_{n,n}}_{>0} |W^n| - \sum_{j=2}^n \underbrace{(\kappa_{n,j} - \kappa_{n,j-1})}_{>0} |W^n| \leq |F^n| \quad \Rightarrow \quad |W^n| \leq \kappa_{n,1}^{-1} |F^n|.$$

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 $|W^n| \lesssim t_n^\alpha |F^n|$, which immediately implies the desired assertion.

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

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

Lemma 2.1* ([5]). *Let $r = 1$ and $\tau := TM^{-1}$. Given $\gamma \in (0, \alpha]$, if $V^0 = 0$ and $|\delta_t^\alpha V^j| \lesssim \tau^\gamma t_j^{-\gamma-1}$ for $j = 1, \dots, M$, then $|V^j| \lesssim t_j^{\alpha-1}$ for $j = 1, \dots, M$.*

Proof. The desired assertion follows from [5, Lemma 3] with $\beta = 1 + \gamma$; see also [11, Theorem 3.3] for a similar result. We give an alternative (substantially shorter) proof in Appendix A.   □

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 let $\bar\lambda = \bar\lambda(t)$ be a piecewise-constant left-continuous function defined by $\bar\lambda(t) = \lambda^j$ for $t \in (t_{j-1}, t_j]$, $j = 1, \dots, M$. Then, with the notation $J^{1-\alpha} v(t) := \{\Gamma(1-\alpha)\}^{-1} \int_0^t (t-s)^{-\alpha} v(s)\, ds$,*

$$(2.4) \qquad \delta_t^\alpha V^j \leq J^{1-\alpha} \bar\lambda(t_j) \quad \forall j \geq 1 \quad \Rightarrow \quad V^m - V^0 \leq \sum_{j=1}^m \tau_j \lambda^j \quad \forall m \geq 0.$$

Proof. Let $\Lambda^j := V^0 + \int_0^{t_j} \bar\lambda\, dt$ so that $\lambda^j = \delta_t \Lambda^j$. Now, $J^{1-\alpha} \bar\lambda(t_j) = \delta_t^\alpha \Lambda^j$, so we get M equations $\delta_t^\alpha V^j \leq \delta_t^\alpha \Lambda^j$ for $j = 1, \dots, M$. Augmenting these equations by $V^0 = \Lambda^0$, we get the matrix relation $A\vec{V} \leq A\vec{\Lambda}$ for the column vectors $\vec{V} := \{V^j\}_{j=0}^M$ and $\vec{\Lambda} := \{\Lambda^j\}_{j=0}^M$ 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 (2.2a).) Consequently, $\vec{V} \leq \vec{\Lambda}$, which immediately yields the desired assertion.   □

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:

$$(2.5a) \qquad D_t^\alpha u(t) = f(t) \qquad \text{for } t \in (0, T], \qquad\qquad u(0) = u_0,$$

$$(2.5b) \qquad \delta_t^\alpha U^j = f(t_j) \qquad \text{for } j = 1, \dots, M, \qquad U^0 = u_0.$$

Throughout this subsection, with slight abuse of notation, ∂_t will be used for $\frac{d}{dt}$, while $\delta_t u(t_j) := \tau_j^{-1}[u(t_j) - u(t_{j-1})]$ (similarly to δ_t in (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*

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

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

(2.6a) $$\psi^1 := \tau_1^\alpha \sup_{s \in (0,t_1)} \left(s^{1-\alpha} |\delta_t u(t_1) - \partial_s u(s)| \right),$$

(2.6b) $$\psi^j := \tau_j^{2-\alpha} t_j^\alpha \sup_{s \in (t_{j-1},t_j)} |\partial_s^2 u(s)| \qquad \text{for } j \geq 2.$$

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

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

As χ will appear in the truncation error, it is useful to note that, in view of (2.6b),

(2.7a) $$|\chi(s)| \leq \psi^j \tau_j^\alpha t_j^{-\alpha} \min\{1, (t_j - s)/\tau_j\} \quad \text{for } s \in (t_{j-1}, t_j), \; j \geq 2.$$

On $(0, t_1)$, one has $\chi'(s) = \partial_s u(s) - \delta_t u(t_1)$, which, combined with (2.6a), yields

(2.7b) $$|\chi(s)| \leq \psi^1 \tau_1^{-\alpha} \underbrace{\int_s^{t_1} \zeta^{\alpha-1} \, d\zeta}_{\lesssim s^{\alpha-1}(t_1-s)} \lesssim \psi^1 \tau_1^{-\alpha} s^{\alpha-1} (t_1 - s) \quad \text{for } s \in (0, t_1).$$

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

(2.8) $$\delta_t^\alpha e^j = \underbrace{\delta_t^\alpha u(t_j) - D_t^\alpha u(t_j)}_{=:r^j} \quad \text{for } j = 1, \dots, M, \qquad e^0 = 0.$$

For r^m, recalling the definitions (1.2) and (1.4) of D_t^α and δ_t^α, we arrive at

$$\Gamma(1-\alpha) \, r^m = \sum_{j=1}^m \int_{t_{j-1}}^{t_j} (t_m - s)^{-\alpha} \underbrace{[\delta_t u(t_j) - \partial_s u(s)]}_{=-\chi'(s)} \, ds = \alpha \sum_{j=1}^m \int_{t_{j-1}}^{t_j} (t_m - s)^{-\alpha-1} \chi(s) \, ds.$$

(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 χ, we claim that

(2.9) $$|r^m| \lesssim \mathring{\mathcal{J}}^m \, (\tau_1/t_m) \, \psi^1 + \mathcal{J}^m \max_{j=2,\dots,m} \{\nu_{m,j} \, \psi^j\},$$

where

$$\mathring{\mathcal{J}}^m := \tau_1^{-\alpha} \, (t_m/\tau_1) \int_0^{t_1} s^{\alpha-1} (t_1 - s) \, (t_m - s)^{-\alpha-1} ds,$$

$$\mathcal{J}^m := \tau_m^\alpha \, t_m^{-\alpha(1-1/r)} \int_{t_1}^{t_m} s^{-\alpha/r} \, (t_m - s)^{-\alpha-1} \min\{1, (t_m - s)/\tau_m\} \, ds,$$

$$\nu_{m,j} := (\tau_j/\tau_m)^\alpha \, (t_j/t_m)^{-\alpha(1-1/r)} \simeq 1.$$

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)). To check the bound (2.9), note that the two terms in its right-hand side are, respectively, associated with $\int_0^{t_1}$ and $\sum_{j=2}^m \int_{t_{j-1}}^{t_j}$ in r^m. Note also that for $j = 2, \dots, m-1$, it is convenient to use a version of (2.7a) with $\min\{1, (t_j - s)/\tau_j\} \leq 1$ replaced by

$\min\{1, (t_m - s)/\tau_m\} \geq 1$. So a calculation using (2.7a) and the definition of $\nu_{m,j}$ implies for $j = 2, \ldots, m$ that

$$|\chi(s)| \leq \{\nu_{m,j}\,\psi^j\}\,\tau_m^\alpha\,t_m^{-\alpha(1-1/r)}\,\underbrace{t_j^{-\alpha/r}}_{\lesssim s^{-\alpha/r}}\,\min\{1, (t_m - s)/\tau_m\} \quad \text{for } s \in (t_{j-1}, t_j).$$

This observation leads to the definition of $\mathcal{J}^m$ in (2.9).

For $\mathring{\mathcal{J}}^m$, the observation that $(t_1 - s)/(t_m - s) \leq t_1/t_m$ for $s \in (0, t_1)$ implies

$$\mathring{\mathcal{J}}^m \leq t_m^{-\alpha} \int_0^{t_1} s^{\alpha-1}(t_1 - s)^{-\alpha}\,ds = t_m^{-\alpha} \int_0^1 \hat{s}^{\alpha-1}(1 - \hat{s})^{-\alpha}\,d\hat{s} \lesssim t_m^{-\alpha},$$

where $\hat{s} := s/t_1$. For $\mathcal{J}^m$, it is helpful to employ another substitution $\hat{s} := s/t_m$ and $\hat{\tau}_j := \tau_j/t_m$, so, for $m \geq 2$, one gets

$$\mathcal{J}^m = t_m^{-\alpha}\,\hat{\tau}_m^\alpha\,\underbrace{\int_{\hat{\tau}_1}^1 \hat{s}^{-\alpha/r}(1 - \hat{s})^{-\alpha-1}\min\{1, (1 - \hat{s})/\hat{\tau}_m\}\,d\hat{s}}_{\lesssim \hat{\tau}_m^{-\alpha}} \lesssim t_m^{-\alpha}.$$

Here, when bounding the integral, it is convenient to replace the lower limit $\hat{\tau}_1$ by 0, and then consider the intervals $(0, 2^{-r})$, $(2^{-r}, 1 - \hat{\tau}_m)$, and $(1 - \hat{\tau}_m, 1)$ separately (in view of $1 - \hat{\tau}_m \geq 2^{-r}$). On these intervals, the integrand is, respectively, $\lesssim \hat{s}^{-\alpha/r}$, $\lesssim (1 - \hat{s})^{-\alpha-1}$, and $\lesssim (1 - \hat{s})^{-\alpha}/\hat{\tau}_m$, so the corresponding integrals are, respectively, $\lesssim 1$ (in view of $\alpha/r \in (0, 1)$), $\lesssim \hat{\tau}_m^{-\alpha}$, and $\lesssim \hat{\tau}_m^{-\alpha}$. So the above bound on $\mathcal{J}^m$ is indeed true.

Finally, we combine (2.9) with the above bounds on $\mathring{\mathcal{J}}^m$ and $\mathcal{J}^m$, and arrive at

$$(2.10) \qquad\qquad |r^m| \lesssim t_m^{-\alpha}\big\{(\tau_1/t_m)\psi^1 + \max_{j=2,\ldots,m}\psi^j\big\},$$

while $|\delta_t^\alpha e^m| = |r^m|$. As $\tau_1/t_m \leq 1$, the desired assertion follows by an application of Lemma 2.1. $\qquad\square$

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

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

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, $\tau_M \approx rTM^{-1}$) lead to larger errors. See also [22, 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 $|\partial_t^l u| \lesssim 1$ 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 sharper 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*

$$|u(t_m) - U^m| \lesssim t_m^{\alpha-1} \max_{j=1,\ldots,m} \{\tau^{-\gamma} t_j^{1-\alpha+\gamma} \psi^j\}.$$

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

$$(2.11) \qquad \widetilde{\mathcal{J}}^m \max_{j=2,\ldots,m} \{(t_j/t_m) \psi^j\},$$

where (with the use of $t_j^{-1} \le s^{-1}$ for $s \in (t_{j-1}, t_j)$)

$$\widetilde{\mathcal{J}}^m := \tau_m^\alpha \, t_m^{-\alpha(1-1/r) + \boxed{1}} \int_{t_1}^{t_m} s^{-\alpha/r - \boxed{1}} (t_m - s)^{-\alpha-1} \min\{1, (t_m - s)/\tau_m\} \, ds.$$

Here, for convenience, the terms that differ from $\mathcal{J}^m$ are framed.

Next, set $r = 1$ and $\tau_j = \tau$. We claim that $\widetilde{\mathcal{J}}^m \lesssim t_m^{-\alpha}$ for $m \ge 2$. Indeed, imitating the estimation of $\mathcal{J}^m$ in the proof of Lemma 2.3, we employ the substitution $\hat{s} := s/t_m$ and the notation $\hat{\tau} := \tau/t_m$ to get

$$\widetilde{\mathcal{J}}^m = t_m^{-\alpha} \hat{\tau}^\alpha \underbrace{\int_{\hat{\tau}}^1 \hat{s}^{-\alpha-1}(1 - \hat{s})^{-\alpha-1} \min\{1, (1 - \hat{s})/\hat{\tau}\} \, d\hat{s}}_{\lesssim \hat{\tau}^{-\alpha}} \lesssim t_m^{-\alpha}.$$

Here $\hat{\tau} \le \frac{1}{2} \le 1 - \hat{\tau}$, so one may consider the intervals $(\hat{\tau}, \frac{1}{2})$, $(\frac{1}{2}, 1 - \hat{\tau})$, and $(1 - \hat{\tau}, 1)$ separately.

Now, using (2.11) in (2.9), we arrive at a version of (2.10):

$$(2.12) \qquad |r^m| \lesssim t_m^{-\alpha-1} \max_{j=1,\ldots,m} \{t_j \psi^j\} \lesssim t_m^{-\gamma-1} \max_{j=1,\ldots,m} \{t_j^{1-\alpha+\gamma} \psi^j\}.$$

Finally, 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 $|\partial_t^l u(t)| \lesssim 1 + t^{\alpha-l}$ for $l = 1, 2$ and $t \in (0, T]$. Then $|u(t_m) - U^m| \lesssim t_m^{\alpha-1} M^{-1} \lesssim M^{-\alpha}$ for $m = 1, \ldots, M$.*

Proof. We imitate the proof of Corollary 2.4, only now we 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 $j \ge 2$, from $\psi^j \lesssim \tau^{2-\alpha} t_j^{\alpha+(\alpha-2)} \lesssim \tau^{1+\gamma} t_j^{\alpha-1-\gamma}$ (as $\tau \le t_j$ and $\gamma \le 1 - \alpha$). $\square$

3. Error analysis for the L1 semidiscretization in time

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

$$(3.1) \quad \delta_t^\alpha U^j + \mathcal{L} U^j = f(\cdot, t_j) \text{ in } \Omega, \quad U^j = 0 \text{ on } \partial\Omega \text{ for } j = 1, \ldots, M; \quad U^0 = u_0.$$

Theorem 3.1.

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

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

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

(ii) *Furthermore, if $r = 1$, a sharper $\max_{j=1,\ldots,m}\{\tau^{-\gamma}\,t_j^{1-\alpha+\gamma}\,\|\psi^j\|_{L_p(\Omega)}\}$ 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 $\|\partial_t^l u(\cdot, t)\|_{L_p(\Omega)} \lesssim 1 + t^{\alpha-l}$ for $l = 1, 2$ and $t \in (0, T]$. Then $\|u(\cdot, t_m) - U^m\|_{L_p(\Omega)} \lesssim M^{-\min\{\alpha r, 2-\alpha\}}$ 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):

$$(3.3) \quad \delta_t^\alpha e^m + \mathcal{L}e^m = \underbrace{\delta_t^\alpha u(\cdot, t_m) - D_t^\alpha u(\cdot, t_m)}_{=:r^m} \quad \text{for } m = 1, \ldots, M, \qquad e^0 = 0.$$

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

$$(3.4) \qquad \qquad \delta_t^\alpha \|e^m\|_{L_p(\Omega)} \leq \|r^m\|_{L_p(\Omega)} \qquad \text{for } m = 1, \ldots, M.$$

Then, indeed, (3.2) immediately follows by an application of Lemma 2.1.

If $r = 1$, combining (2.12) (obtained in the proof of Lemma 2.3*) with (3.4) and then applying Lemma 2.1* yields the assertion of part (ii).

We now proceed to establishing (3.4). Rewrite the equation $\delta_t^\alpha e^m + \mathcal{L}e^m = r^m$ using (2.2a) as

$$(3.5) \qquad \underbrace{\kappa_{m,m}}_{>0} e^m + \mathcal{L}e^m = \sum_{j=1}^m \underbrace{(\kappa_{m,j} - \kappa_{m,j-1})}_{>0} e^{j-1} + r^m,$$

and address the cases $p = 2$ and $p = \infty$ separately.

For $p = 2$, consider the $L_2(\Omega)$ inner product (denoted $\langle \cdot, \cdot \rangle$) of (3.5) with e^m. As $c - \frac{1}{2}\sum_{k=1}^d \partial_{x_k} b_k \geq 0$ implies $\langle \mathcal{L}e^m, e^m \rangle \geq 0$, so for $p = 2$ one gets

$$(3.6) \qquad \kappa_{m,m}\|e^m\|_{L_p(\Omega)} \leq \sum_{j=1}^m (\kappa_{m,j} - \kappa_{m,j-1})\|e^{j-1}\|_{L_p(\Omega)} + \|r^m\|_{L_p(\Omega)}.$$

By (2.2a), this implies (3.4) 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 $\mathcal{L}e^m(x^*) \geq 0$, so (3.5) 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 (3.6) for $p = \infty$. By (2.2a), the desired assertion (3.4) follows for $p = \infty$.

Note that in our proof of (3.4) for $p = \infty$, we relied on $\mathcal{L}e^m$ being well-defined in the classical sense. More generally, (3.3) implies that e^m solves an elliptic equation with the operator $\mathcal{L} + \kappa_{m,m}$. Now, $\{r^j\} \in L_\infty(\Omega)$ implies that $e^m \in C(\bar{\Omega})$. So one can modify the above argument by using a more general result $\kappa_{m,m}\|e^m\|_{L_\infty(\Omega)} \leq \|(\mathcal{L} + \kappa_{m,m})e^m\|_{L_\infty(\Omega)}$ (the latter follows from the maximum principle for functions in $C(\bar{\Omega})$ [4, Corollary 3.2].)
□

Remark 3.3 (More general $\mathcal{L}$). The results of this section also apply to a general uniformly-elliptic $\mathcal{L}$ defined by $\mathcal{L}u := \sum_{k=1}^{d}\{-\sum_{n=1}^{d}\partial_{x_k}(a_{kn}\,\partial_{x_n}u)+b_k\,\partial_{x_k}u\}+c\,u$, where the coefficients $a_{kn}(x)$ form a symmetric uniformly-positive-definite matrix. Indeed, when establishing (3.4), we still have $\langle\mathcal{L}e^m, e^m\rangle \geq 0$ and $\kappa_{m,m}\|e^m\|_{L_\infty(\Omega)} \leq \|(\mathcal{L}+\kappa_{m,m})e^m\|_{L_\infty(\Omega)}$ for, respectively, $p=2$ and $p=\infty$. For fully discrete finite-element discretizations, Theorem 5.1 remains valid, but condition A_p for $p=\infty$ may be problematic. Similarly, finite difference discretizations that satisfy the discrete maximum principle are not readily available in this more general case.

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 $\bar{\Omega}_h$ be the tensor product of d uniform meshes $\{ih\}_{i=0}^{N}$, with $\Omega_h := \bar{\Omega}_h\backslash\partial\Omega$ denoting the set of interior mesh nodes. Now, consider the finite difference discretization

(4.1)
$$\delta_t^\alpha U^j(z) + \mathcal{L}_h U^j(z) = f(z, t_j) \quad \text{for } z \in \Omega_h, \ \ j = 1, \dots, M,$$
$$U^j = 0 \quad \text{in } \bar{\Omega}_h \cap \partial\Omega, \ \ j = 1, \dots, M, \qquad U^0 = u_0 \quad \text{in } \bar{\Omega}_h.$$

Here δ_t^α is defined by (1.4). The discrete spatial operator $\mathcal{L}_h$ is a standard finite difference operator defined, using the standard orthonormal basis $\{\mathbf{i}_k\}_{k=1}^{d}$ in $\mathbb{R}^d$ (such that $z = (z_1, \dots, z_d) = \sum_{k=1}^{d} z_k\,\mathbf{i}_k$ for any $z \in \mathbb{R}^d$), by

$$\mathcal{L}_h V(z)$$
$$:= \sum_{k=1}^{d} h^{-2}\Big\{a_k(z+\tfrac{1}{2}h\mathbf{i}_k)\,\big[U(z)-U(z+h\mathbf{i}_k)\big]+a_k(z-\tfrac{1}{2}h\mathbf{i}_k)\,\big[U(z)-U(z-h\mathbf{i}_k)\big]\Big\}$$
$$+ \sum_{k=1}^{d} \tfrac{1}{2}h^{-1}\,b_k(z)\,\big[U(z+h\mathbf{i}_k)-U(z-h\mathbf{i}_k)\big] + c(z)\,U(z) \qquad \text{for } z \in \Omega_h.$$

(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 $\{t_j = T(j/M)^r\}_{j=0}^{M}$ 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*

(4.2)
$$h^{-1} \geq \max_{k=1,\dots,d}\big\{\tfrac{1}{2}\|b_k\|_{L_\infty(\Omega)}\,\|a_k^{-1}\|_{L_\infty(\Omega)}\big\},$$

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

(4.3) $$\|u(\cdot, t_m) - U^m\|_{\infty\,;\Omega_h} \lesssim \max_{j=1,\dots,m}\|\psi^j\|_{L_\infty(\Omega)} + t_m^\alpha\,\|(\mathcal{L}_h - \mathcal{L})u(\cdot, t_m)\|_{\infty\,;\Omega_h},$$

where $m = 1, \dots, M$, and $\psi^j = \psi^j(x)$ is defined by (2.6), in which $u(\cdot)$ is understood as $u(x, \cdot)$ when evaluating $\partial_s u$, $\partial_s^2 u$, and $\delta_t u$.

(ii) *If $r = 1$, then $\max_{j=1,\dots,m}\|\psi^j\|_{L_\infty(\Omega)}$ in (4.3) can be replaced by a sharper $\max_{j=1,\dots,m}\{\tau^{-\gamma}\,t_j^{1-\alpha+\gamma}\,\|\psi^j\|_{L_\infty(\Omega)}\}$, where $\tau = TM^{-1}$ and $\gamma = \min\{\alpha, 1-\alpha\}$.*

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

$$\|u(\cdot, t_m) - U^m\|_{\infty\,;\Omega_h} \lesssim M^{-\min\{\alpha r, 2-\alpha\}} + t_m^\alpha\,h^2 \qquad \text{for } m = 1, \dots, M.$$

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

$$\|u(\cdot, t_m) - U^m\|_{\infty;\Omega_h} \lesssim t_m^{\alpha-1}M^{-1} + t_m^\alpha h^2 \qquad \text{for } m = 1, \ldots, M.$$

Proof. Imitate the proofs of Corollaries 2.4 and 2.6 for parts (i) and (ii), respectively, to show that $|\psi^j| \lesssim M^{-\min\{\alpha r, 2-\alpha\}}$ and $\tau^{-\gamma} t_j^{1-\alpha+\gamma} |\psi^j| \lesssim \tau$. Combine these bounds with the standard truncation error estimate $|(\mathcal{L}_h - \mathcal{L})u| \lesssim h^2$. $\qquad\square$

Remark 4.3. In the case $d = 1$, error bounds similar to those of Corollary 4.2 can be found in [22, Theorem 5.2] and [5, 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 §6.2.

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):

$$\delta_t^\alpha e^m + \mathcal{L}_h e^m = R^m := \underbrace{\delta_t^\alpha u(\cdot, t_m) - D_t^\alpha u(\cdot, t_m)}_{=:r^m} + (\mathcal{L}_h - \mathcal{L})u(\cdot, t_m) \quad \text{in } \Omega_h \text{ for } m \geq 1,$$

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

$$(4.4) \qquad \delta_t^\alpha \|e^m\|_{\infty;\Omega_h} \leq \|R^m\|_{\infty;\Omega_h} \qquad \text{for } m = 1, \ldots, M.$$

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 $\max_{z\in\Omega_h} |e^m(x)| = |e^m(z^*)|$ for some $z^* \in \Omega_h$. Suppose that $e^m(z^*) \geq 0$ (the case $e^m(z^*) < 0$ is similar). As (4.2) combined with $c \geq 0$ implies that the spatial discrete operator $\mathcal{L}_h$ is associated with a diagonally-dominant M-matrix, so $\mathcal{L}_h e^m(z^*) \geq 0$, so $\delta_t^\alpha e^m + \mathcal{L}_h e^m = R^m$ at $z = z^*$ yields $\delta_t^\alpha e^m(z^*) \leq R^m(z^*)$. In view of (2.2a), our assertion (4.4) follows. $\qquad\square$

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 $S_h \subset H_0^1(\Omega) \cap C(\bar\Omega)$ be a Lagrange finite element space of fixed degree $\ell \geq 1$ relative to a quasi-uniform simplicial triangulation $\mathcal{T}$ of Ω. (To simplify the presentation, it will be assumed that the triangulation covers Ω exactly.) Now, for $m = 1, \ldots, M$, let $u_h^m \in S_h$ satisfy

$$(5.1) \qquad \langle \delta_t^\alpha u_h^m, v_h \rangle_h + \mathcal{A}_h(u_h^m, v_h) = \langle f(\cdot, t_m), v_h \rangle_h \qquad \forall v_h \in S_h$$

with $u_h^0 = u_0$ or some $u_h^0 \approx u_0$.

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 $\int_T$ with positive weights. Let $\mathring{\mathcal{A}}$ be the standard bilinear form associated with the elliptic operator $\mathring{\mathcal{L}} := \mathcal{L} - c$ (i.e., $\mathring{\mathcal{A}}(v, w) = \langle \mathcal{L}v - cv, w \rangle$ for smooth v and w in $H_0^1(\Omega)$). The bilinear form $\mathcal{A}_h$ in (5.1) is related to $\mathring{\mathcal{A}}$ and defined by $\mathcal{A}_h(v, w) := \mathring{\mathcal{A}}(v, w) + \langle cv, w \rangle_h$.

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 $\mathring{\mathcal{L}}$ and defined by $\mathring{\mathcal{A}}(\mathcal{R}_h u, v_h) = \langle \mathring{\mathcal{L}} u, v_h \rangle_h$ $\forall v_h \in S_h$ 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_∞ Let $\ell = 1$ (i.e., linear finite elements are employed), and let the stiffness matrix associated with $\mathcal{A}_h(\cdot, \cdot) + \kappa_{m,m} \langle \cdot, \cdot \rangle_h$ have non-positive off-diagonal entries, i.e., $\mathbb{A}_{zz'}^m := \mathcal{A}_h(\phi_{z'}, \phi_z) + \kappa_{m,m} \langle \phi_{z'}, \phi_z \rangle_h \leq 0$ for any two interior nodes $z \neq z'$, where $m = 1, \ldots, M$.

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

Sufficient conditions for A_∞ will be discussed in §§5.2–5.3. Note that an assumption similar to A_∞ has been shown to be both necessary and sufficient for non-negativity preservation in finite element discretizations of equations of type (1.1) [10].

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 $c - p^{-1} \sum_{k=1}^d \partial_{x_k} b_k \geq 0$. Then, under the condition A_p, there exists a unique solution $\{u_h^m\}_{m=0}^M$ of (5.1) and, for $m = 1, \ldots, M$,*

$$(5.2) \quad \|u(\cdot, t_m) - u_h^m\|_{L_p(\Omega)} \lesssim \|u_0 - u_h^0\|_{L_p(\Omega)} + \max_{j=1,\ldots,m} \|\psi^j\|_{L_p(\Omega)}$$

$$+ \max_{t \in \{0, t_m\}} \|\rho(\cdot, t)\|_{L_p(\Omega)} + \int_0^{t_m} \|\partial_t \rho(\cdot, t)\|_{L_p(\Omega)}\, dt,$$

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 $\partial_s u$, $\partial_s^2 u$, and $\delta_t u$.

(ii) *If $r = 1$, then $\max_{j=1,\ldots,m} \|\psi^j\|_{L_\infty(\Omega)}$ in (5.2) can be replaced by a sharper $\max_{j=1,\ldots,m} \{\tau^{-\gamma} t_j^{1-\alpha+\gamma} \|\psi^j\|_{L_\infty(\Omega)}\}$, 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

$$(5.3) \quad \langle \delta_t^\alpha e_h^m, v_h \rangle_h + \mathcal{A}_h(e_h^m, v_h)$$

$$= \langle \delta_t^\alpha \underbrace{\mathcal{R}_h u}_{=\rho+u}(t_m), v_h \rangle_h + \underbrace{\mathring{\mathcal{A}}(\mathcal{R}_h u(t_m), v_h)}_{=\langle \mathring{\mathcal{L}} u(\cdot, t_m), v_h \rangle_h} + \langle c \mathcal{R}_h u(t_m) - f(\cdot, t_m), v_h \rangle_h$$

$$= \langle \delta_t^\alpha \rho(\cdot, t_m) + c\rho(\cdot, t_m) + \underbrace{\delta_t^\alpha u(\cdot, t_m) - D_t^\alpha u(\cdot, t_m)}_{=:r^m}, v_h \rangle_h \quad \forall v_h \in S_h,$$

for $m \geq 1$, with $e_h^0 = [u_0 - u_h^0] + \rho(\cdot, 0)$.

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

$$(5.4) \quad \delta_t^\alpha \|e_h^m\|_{L_p(\Omega)} \leq \| \underbrace{\delta_t^\alpha \rho(\cdot, t_m) + c\rho(\cdot, t_m) + r^m}_{=:R^m} \|_{L_p(\Omega)} \quad \text{for } m = 1, \ldots, M.$$

Note that δ_t^α is associated with an M-matrix, so we can deal with the terms $|\delta_t^\alpha \rho|$ and $|c\rho + r^m|$ in the right-hand side of (5.4) separately. With this observation, indeed, (5.2) immediately follows by an application of Lemma 2.1 when dealing with the term $c\rho + r^m$ in the right-hand side of (5.4), and Lemma 2.2 when dealing with $\delta_t^\alpha \rho$. For the latter, Lemma 2.2 is applied with $\lambda^j := \|\delta_t \rho(\cdot, t_j)\|_{L_p(\Omega)}$. Then $\|\delta_t^\alpha \rho(\cdot, t_m)\|_{L_p(\Omega)} \leq J^{1-\alpha} \bar\lambda(t_m)$, while $\tau_j \lambda^j \lesssim \int_{t_{j-1}}^{t_j} \|\partial_t \rho(\cdot, t)\|_{L_p(\Omega)}$, so the resulting contribution to the bound on $\|e_h^m\|_{L_p(\Omega)}$ will be $\sum_{j=1}^m \tau_j \lambda^j \lesssim \int_0^{t_m} \|\partial_t \rho(\cdot, t)\|_{L_p(\Omega)}$.

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 $v_h := e_h^m$ in (5.3) and note that condition A_2 combined with $c - \frac{1}{2} \sum_{k=1}^d \partial_{x_k} b_k \geq 0$ implies $\mathcal{A}_h(e_h^m, e_h^m) \geq 0$, and then $\langle \delta_t^\alpha e_h^m, e_h^m \rangle \leq \langle R^m, e_h^m \rangle$. The bound (5.4) follows in view of (2.2a).

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

$$|\mathcal{A}_h(e_h^m, \phi_{z^*}) + \kappa_{m,m} \langle e_h^m, \phi_{z^*} \rangle_h| \geq \{\mathcal{A}_h(1, \phi_{z^*}) + \kappa_{m,m} \langle 1, \phi_{z^*} \rangle_h\} |e_h^m(z^*)|.$$

(Here we used the representation $e_h^m = e_h^m(z^*) - \sum_{z \neq z^*} [e_h^m(z^*) - e_h^m(z)] \phi_z$.) Note also that (in view of the definition of $\mathcal{A}_h$ related to $\mathcal{L}$ of (1.3)) for any $z \in \mathcal{N}$

$$\mathcal{A}_h(1, \phi_z) + \kappa_{m,m} \langle 1, \phi_z \rangle_h = \langle c + \kappa_{m,m}, \phi_z \rangle_h \geq \kappa_{m,m} \langle 1, \phi_z \rangle_h.$$

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

$$\kappa_{m,m} \langle 1, \phi_{z^*} \rangle_h \, |e_h^m(z^*)| \leq \sum_{j=1}^m \underbrace{(\kappa_{m,j} - \kappa_{m,j-1})}_{>0} \langle e_h^{j-1}, \phi_{z^*} \rangle_h + \langle R^m, \phi_{z^*} \rangle_h.$$

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

Remark 5.2 (Case $\langle \cdot, \cdot \rangle_h \neq \langle \cdot, \cdot \rangle$: error in the $L_2(\Omega)$). 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 $h := \max_{T \in \mathcal{T}} \{\operatorname{diam} T\}$ is sufficiently small. Then a version of Theorem 5.1 is valid for $p = 2$ (with condition A_2 dropped) with $\|\cdot\|_{L_2(\Omega)}$ replaced by $\|\cdot\|_{h;2} := \langle \cdot, \cdot \rangle_h^{1/2}$. Indeed, the proof of Theorem 5.1 applies to this case with $\mathcal{A}_h(e_h^m, e_h^m) \geq 0$ for sufficiently small h, in view of $|\langle c\,e_h^m, e_h^m \rangle_h - \langle c\,e_h^m, e_h^m \rangle)| \lesssim h\|\nabla e_h^m\|_{L_2(\Omega)}$. Note also that $\|\cdot\|_{h;2} \simeq \|\cdot\|_{L_2(\Omega)}$ in S_h (as $\langle \cdot, \cdot \rangle_h$ is an inner product in S_h; for the latter, note that $Q_T[v_h w_h]$ 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 [15, §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, let the angle between any two faces not exceed $\theta^* < \pi$. (These conditions are satisfied, for example, by a convex domain of polyhedral-type, as well as by a smooth domain.) Then $\|v\|_{W_2^2(\Omega)} \lesssim \|\mathcal{L}v\|_{L_2(\Omega)}$; see [15, Theorem 4.3.2] in the case

$a_k = 1 \ \forall \, k$ in (1.3), as well as [13, Theorem 5.1] and [6, Chapter 4] for $d = 2$. The treatment of variable smooth coefficients $\{a_k\}$ was addressed in [13, §2].

Consequently, for the error of the Ritz projection $\rho(\cdot, t) = \mathcal{R}_h u(t) - u(\cdot, t)$ one has

$$(5.5) \quad \|\partial_t^l \rho(\cdot, t)\|_{L_2(\Omega)} \lesssim h \inf_{v_h \in S_h} \|\partial_t^l u(\cdot, t) - v_h\|_{W_2^1(\Omega)} \quad \text{for } l = 0, 1, \ t \in (0, T].$$

For $l = 0$, see, e.g., [1, Theorem 5.7.6]. 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* $\|\partial_t^l u(\cdot, t)\|_{W_2^{\ell+1}(\Omega)}$ $\lesssim 1 + t^{\alpha - l}$ *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*

$$\|u(\cdot, t_m) - u_h^m\|_{L_2(\Omega)} \lesssim M^{-\min\{\alpha r, 2 - \alpha\}} + h^{\ell + 1} \quad \text{for } m = 1, \ldots, M.$$

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

$$\|u(\cdot, t_m) - u_h^m\|_{L_2(\Omega)} \lesssim t_m^{\alpha - 1} M^{-1} + h^{\ell + 1} \quad \text{for } m = 1, \ldots, M.$$

Proof. Imitate the proofs of Corollaries 2.4 and 2.6 for parts (i) and (ii), respectively, to show that $\|\psi^j\|_{L_2(\Omega)} \lesssim M^{-\min\{\alpha r, 2 - \alpha\}}$ and $\tau^{-\gamma} t_j^{1 - \alpha + \gamma} \|\psi^j\|_{L_2(\Omega)} \lesssim \tau \lesssim M^{-1}$. Combine these bounds with $\|\partial_t^l \rho(\cdot, t)\|_{L_2(\Omega)} \lesssim h^{\ell + 1}(1 + t^{\alpha - l})$ for $l = 0, 1$ (the latter follows from (5.5)). $\square$

Remark 5.4. 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. The errors of finite element discretizations of type (5.1) are also estimated in the $L_2(\Omega)$ norm in a recent paper [9], 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 [9, Theorem 3.16(a)].

Remark 5.6 (Convergence in positive time in the $W_2^1(\Omega)$ seminorm for $r = 1$). Under condition A$_2$, one has $\mathcal{A}_h(e_h^m, e_h^m) \geq \|\nabla e_h^m\|_{L_2(\Omega)}^2$. Now, imitating the proof of (5.4) for $p = 2$, one gets $\delta_t^\alpha \big(\kappa_{m,m}^{-1} \|\nabla e_h^m\|_{L_2(\Omega)}^2 / \|e_h^m\|_{L_2(\Omega)} + \|e_h^m\|_{L_2(\Omega)} \big) \leq \|R^m\|_{L_2(\Omega)}$ for $m \geq 1$. Consequently, $\kappa_{m,m}^{-1} \|\nabla e_h^m\|_{L_2(\Omega)}^2 / \|e_h^m\|_{L_2(\Omega)}$ (as well as $\|e_h^m\|_{L_2(\Omega)}$) is bounded similarly to the error in Corollary 5.3(ii), while, by (2.2b), $\kappa_{m,m} \simeq M^\alpha$. Combining this with the standard error bound on $\|\nabla \rho\|_{L_2(\Omega)}$ (see, e.g., [1, (8.5.4)]) yields convergence of (5.1) in the $W_2^1(\Omega)$ seminorm for $t_m \gtrsim 1$.

5.2. Lumped-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 $Q_T[v] := \int_T v^I$, where v^I 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

$$(5.6) \quad \|\partial_t^l \rho(\cdot, t)\|_{L_\infty(\Omega)} \lesssim h^{2 - q} |\ln h| \Big\{ \|\partial_t^l u(\cdot, t)\|_{W_\infty^{2 - q}(\Omega)} + \|\partial_t^l \mathcal{L} u(\cdot, t)\|_{W_{d/2}^{2 - q}(\Omega)} \Big\},$$

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_∞ norm; see, e.g., [19, Theorem 2], [14, Theorem 3.1], and [20, 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 ρ, defined by $\langle\nabla\hat{\rho}_h,\nabla v_h\rangle = \langle\mathring{\mathcal{L}}u,v_h\rangle_h - \langle\mathring{\mathcal{L}}u,v_h\rangle \; \forall v_h \in S_h$. For completeness, the bound of type (5.6) (with $l = 0$) for $\hat{\rho}_h$ is proved in Appendix B.

As we intend to apply Theorem 5.1 under condition A_∞, note that the latter is satisfied under the following assumptions on the triangulation. For $\Omega \subset \mathbb{R}^2$, let $\mathcal{T}$ be a Delaunay triangulation, i.e., the sum of the angles opposite to any interior edge is less than or equal to π. In the case $\Omega \subset \mathbb{R}^3$, for any interior edge E, let $\omega_E := \{T \in \mathcal{T} : \partial T \supset E\}$, and impose that $\sum_{T \subset \omega_E} |E_T'| \cot\theta_T^E \geq 0$, where θ_T^E is the angle between the faces of T not containing E, and the edge E_T' is their intersection. Under these conditions on $\mathcal{T}$, the stiffness matrix for $-\sum_{k=1}^d \partial_{x_k}^2$ is an M-matrix (see, e.g., [24, Lemma 2.1]), while the mass matrix is positive diagonal. So indeed, A_∞ 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 5.7.

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

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

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

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

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

Remark 5.8. The assumptions made in Corollary 5.7 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 error analysis in the $L_\infty(\Omega)$ norm.** We shall start by checking condition A_∞, used in Theorem 5.1, for the simplest case of $d = 1$ and $\mathcal{L} = -\partial_{x_1}^2$. A straightforward calculation shows that the stiffness matrix associated with $\mathcal{A}_h(\cdot,\cdot) + \kappa_{1,1}\langle\cdot,\cdot\rangle$ will be a tridiagonal matrix with diagonal entries $\frac{2}{h} + \frac{2}{3}h\kappa_{1,1}$ and off-diagonal entries $-\frac{1}{h} + \frac{1}{6}h\kappa_{1,1}$. So, for off-diagonal entries to be non-positive, one needs to impose $\kappa_{1,1} \leq 6h^{-2}$, i.e., $\tau_1^{-\alpha} \leq 6\Gamma(2-\alpha)h^{-2}$. Note that exactly the same condition is required for the discrete maximum principle in the classical parabolic case of (1.1) with $\alpha = 1$ assuming the backward Euler discretization in time is combined with linear finite elements without quadrature.

A similar condition is true if $a_k = 1$ 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_∞ is satisfied (and so Theorem 5.1 with $p = \infty$ can be applied) if $h^2\tau_1^{-\alpha} \leq C_{\mathcal{T}}$ for a sufficiently small constant $C_{\mathcal{T}}$ that we specify below, and, additionally, the triangulation is non-obtuse and $\min_{T \subset \omega_E}\theta_T^E \leq \theta^*$ 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 $-\sum_{k=1}^{d} \partial_{x_k}^2$ is an M-matrix, but its contribution to $\mathbb{A}_{zz'}^m$, for any two nodes $z \neq z'$ connected by an interior edge E, will be strictly negative and equal to $-\sum_{T \subset \omega_E} |E_T'| \cot \theta_T^E / \{d(d-1)\}$ (with E_T', in the case $d = 2$, being a node and the notational convention $|E_T'| = 1$ used); see [24, Lemma 2.1]. A calculation also shows that the contribution of $\langle (\kappa_{1,1} + c)\phi_{z'}, \phi_z \rangle$ to $\mathbb{A}_{zz'}^m$ does not exceed $(\tau_1^{-\alpha}/\Gamma(2 - \alpha) + \|c\|_{L_\infty(\Omega)})|\omega_E|/\{(d+1)(d+2)\}$. Furthermore, the contribution of $\langle b_k(x)\, \partial_{x_k}\phi_{z'}, \phi_z \rangle$ to $\mathbb{A}_{zz'}^m$ is $\lesssim h^{-1}|\omega_E|$. As the triangulation is quasi-uniform, these observations imply that there is a positive constant $C_{\mathcal{T}}'$ such that for any interior edge E, one has

$$\frac{(d+1)(d+2)}{d(d-1)}\ |\omega_E|^{-1}\sum_{T \subset \omega_E} |E_T'| \cot \theta_T^E \geq C_{\mathcal{T}}' h^{-2}.$$

Now, $h^2\tau_1^{-\alpha} \leq C_{\mathcal{T}}$, with any fixed constant $C_{\mathcal{T}} < C_{\mathcal{T}}'\Gamma(2 - \alpha)$, implies A_∞ (assuming that h is sufficiently small; in fact, one can use $C_{\mathcal{T}} = C_{\mathcal{T}}'\Gamma(2 - \alpha)$ if $c = 0$ and $b_k = 0$ for $k = 1, \ldots, d$ in (1.3)). To avoid computing $C_{\mathcal{T}}'$, one can instead impose $h^2|\ln h|\,\tau_1^{-\alpha} \leq C_{\mathcal{T}}$ with any fixed $C_{\mathcal{T}} > 0$ 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 $\tau_1^\alpha \gtrsim h^2$. 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 5.7 is $\lesssim M^{-\alpha r} + h^2|\ln h| \simeq \tau_1^\alpha + h^2|\ln h|$. Similarly, in part (ii) for $t_m \gtrsim 1$, the error is $\lesssim \tau_1 + h^2|\ln h|$, so a reasonable choice $\tau_1 \simeq h^2$ is clearly within the restriction $\tau_1^\alpha \gtrsim h^2$.

6. Estimation of derivatives of the exact solution u

The purpose of this section is to show that the assumptions made in §§3–5 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 $\mathcal{L}$ 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 Ω is either a convex domain of polyhedral-type or a smooth domain. Hence, we shall be able to invoke $\|v\|_{W_2^2(\Omega)} \lesssim \|\mathcal{L}v\|_{L_2(\Omega)}$ when $v = 0$ on $\partial\Omega$, as well as the consequent property $\|v\|_{L_\infty(\Omega)} \lesssim \|\mathcal{L}v\|_{L_2(\Omega)}$ (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 $\mathcal{L}$ (see, e.g., [3, §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 [18] for smooth domains, [7, §2.2 and §3.4] for polygonal/polyhedral domains, and [22, §2] for $\Omega = (0, 1)$. Eigenfunction expansions are frequently used to establish regularity estimates for fractional-derivative problems; see, e.g., [16, 17], where somewhat different problems were considered. In particular, the bounds [16, (1.6) and (1.7)] are somewhat similar to those we obtain below.

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 $\mathcal{L} = -\partial_{x_1}^2 + c(x_1)$, they are satisfied under certain regularity assumptions on u_0 and f (including $\mathcal{L}^l f(\cdot, t) = \mathcal{L}^q u_0 = 0$ on $\partial\Omega$ for $l = 0, 1$ and $q = 0, 1, 2$) by [22, 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 $\mathcal{L}^q \partial_t^l$ to the eigenfunction expansion of u yields $\|\mathcal{L}^q \partial_t^l u(\cdot, t)\|_{L_2(\Omega)} \lesssim 1 + t^{\alpha-l}$ 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 $\|u_0\|_{\mathcal{L}^{q+2}} + \|\partial_t^l f(\cdot, t)\|_{\mathcal{L}^{q+1}} \lesssim 1$ for $l = 0, 1, 2$ (where the assumptions of the temporal derivatives of f may, in fact, be weakened). Here (similarly to [7, 18, 22]) we used the norm $\|v\|_{\mathcal{L}^\gamma} := \left\{\sum_{i=1}^\infty \lambda_i^{2\gamma} \langle v, \psi_i \rangle^2\right\}^{1/2}$, where $0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \ldots$ are the eigenvalues of $\mathcal{L}$, while $\{\psi\}_{i=1}^\infty$ are the corresponding normalized eigenfunctions satisfying $\|\psi_i\|_{L_2(\Omega)} = 1$.

6.2. **Spatial and mixed derivatives of** u**.** In §§4–5 (see Corollaries 4.2, 5.3, and 5.7), a number of additional assumptions were made that involve spatial derivatives of u. Here the situation is more delicate, as if Ω has any corners, u may exhibit corner singularities.

Example A. Consider $\Omega = (0, 1)^2$ and $\mathcal{L} = -[\partial_{x_1}^2 + \partial_{x_2}^2] + c(x_1, x_2)$ under the assumption $\|u_0\|_{\mathcal{L}^3} + \|f(\cdot, t)\|_{\mathcal{L}^{5/2}} \lesssim 1$. Note that the latter implies that the elliptic corner compatibility conditions up to order 2 are satisfied. Hence, [23, Theorem 3.1] combined with the Sobolev embedding theorem yields $\|u\|_{W_\infty^4(\Omega)} \lesssim \|\mathcal{L}u\|_{W_\infty^{2+\epsilon}(\Omega)} \lesssim \|\mathcal{L}u\|_{W_2^4(\Omega)}$ for any $t \in (0, T]$. Similarly, $\|\mathcal{L}u\|_{W_2^4(\Omega)} \lesssim \|\mathcal{L}^2 u\|_{W_2^2(\Omega)} \lesssim \|\mathcal{L}^3 u\|_{L_2(\Omega)}$, while one can show (by an application of $\mathcal{L}^3$ to the eigenfunction expansion of u) that $\|\mathcal{L}^3 u\|_{L_2(\Omega)} \lesssim 1$. Combining these observations, one gets $\|u\|_{W_\infty^4(\Omega)} \lesssim 1$, 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 $\|\partial_t^l u(\cdot, t)\|_{W_2^{\ell+1}(\Omega)} \lesssim 1 + t^{\alpha-l}$ for $l = 0, 1$ and $t \in (0, T]$. For linear finite elements, i.e., $\ell = 1$, these bounds follow from $\|\partial_t^l u\|_{W_2^2(\Omega)} \lesssim \|\mathcal{L}\partial_t^l u\|_{L_2(\Omega)}$ combined with the bound on $\|\mathcal{L}\partial_t^l u(\cdot, t)\|_{L_2(\Omega)}$ obtained in §6.1 (see the case $q = 1$). For $\ell > 1$, a similar argument can be used (under additional data regularity assumptions) if Ω is smooth.

Example C. If Ω is smooth, then both $\|\partial_t^l u(\cdot, t)\|_{W_\infty^2(\Omega)}$ and $\|\mathcal{L}\partial_t^l u(\cdot, t)\|_{W_{d/2}^2(\Omega)}$ are $\lesssim \|\mathcal{L}\partial_t^l u(\cdot, t)\|_{W_2^2(\Omega)}$. For the latter, using the argument of Example B, one can show that $\|\mathcal{L}\partial_t^l u(\cdot, t)\|_{W_2^2(\Omega)} \lesssim 1 + t^{\alpha-l}$ for $l = 0, 1$ under the regularity assumption $\|u_0\|_{\mathcal{L}^3} + \|\partial_t^l f(\cdot, t)\|_{\mathcal{L}^2} \lesssim 1$. So for this example, the assumptions made in Corollary 5.7 on u are satisfied.

Remark 6.1 (Non-self-adjoint $\mathcal{L}$). 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 $\widetilde{u} :=$
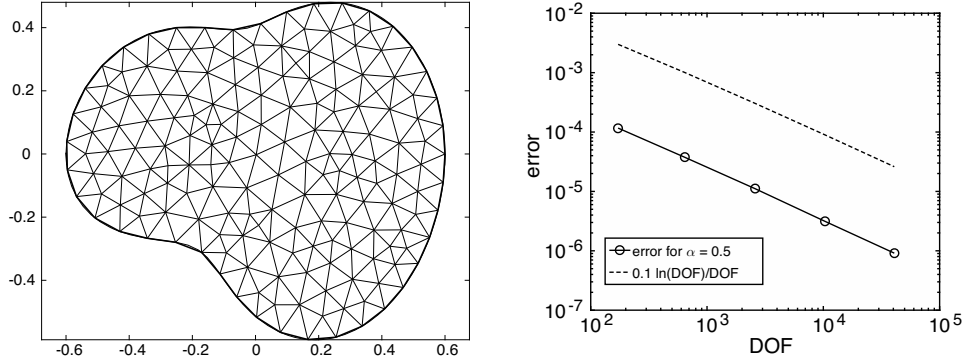
FIGURE 1. Delaunay triangulation of Ω with DOF=172 (left), maximum nodal errors for $\alpha = 0.5$, $r = (2 - \alpha)/\alpha$, and $M = 10^4$.

$u \exp\left\{-\sum_{k=1}^{d} \frac{1}{2}(b_k/a_k)x_k\right\}$. A similar trick for the case of variable coefficients and $d = 1$ is described in [5, §2].

7. NUMERICAL RESULTS

Our model problem is (1.1) with $\mathcal{L} = -(\partial_{x_1}^2 + \partial_{x_2}^2)$, posed in the domain $\Omega \times [0, 1]$ (see Figure 1, left) with $\partial\Omega$ parameterized by $x_1(l) := \frac{2}{3}R\cos\theta$ 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 $u = t^\alpha \cos(xy)$. 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 quasi-uniform Delaunay triangulations of Ω (with DOF denoting the number of degrees of freedom in space).

The errors in the maximum nodal norm $\max_{z\in\mathcal{N},\, m=1,\ldots,M} |u_h^m(z) - u(z, t_m)|$ are shown in Figure 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 5.7(i), the errors are expected to be $\lesssim M^{-(2-\alpha)} + h^2|\ln h|$. Our numerical results clearly confirm the sharpness of this corollary for the considered case. For more extensive numerical experiments, we refer the reader to [22],

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

	$M = 64$	$M = 128$	$M = 256$	$M = 512$	$M = 1024$	$M = 2048$
$\alpha = 0.3$	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	

where, in particular, the influence of r on the errors is numerically investigated, as well as [5, 9] for numerical results on uniform temporal meshes.

APPENDIX A. PROOF OF LEMMA 2.1*

Proof.

(i) First, consider $\gamma = \alpha$. As the operator δ_t^α is associated with an M-matrix, it suffices to construct a barrier function $0 \le B^j \lesssim t_j^{\alpha-1}$ such that $\delta_t^\alpha B^j \gtrsim \tau^\alpha t_j^{-\alpha-1}$. Fix a sufficiently large number $2 \le p \lesssim 1$, and then set $\beta := 1 - \alpha$ and $B(s) := \min\{(s/t_p)t_p^{-\beta}, s^{-\beta}\}$, 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 $j \le p$, a straightforward calculation shows that $\delta_t^\alpha B^j = D_t^\alpha B(t_j) \simeq t_j^\beta t_p^{-\beta-1} \gtrsim p^{-\beta-1}(\tau^\alpha t_j^{-\alpha-1})$. Next, for $D_t^\alpha B(t)$ with $t > t_p$ one has

$$\Gamma(1-\alpha) \, D_t^\alpha B(t) = \underbrace{\int_0^{t_p} t_p^{-\beta-1}(t-s)^{-\alpha}\,ds}_{\ge t_p^{-\beta}t^{-\alpha}} - \beta \underbrace{\int_{t_p}^t s^{-\beta-1}(t-s)^{-\alpha}\,ds}_{=:t^{-1}I} \,.$$

Here, using $\hat{s} := s/t$ and $\hat{t}_p := t_p/t$, and noting that $\alpha + \beta = 1$, one gets

$$I = \beta \int_{\hat{t}_p}^1 \hat{s}^{-\beta-1}(1-\hat{s})^{-\alpha}\,d\hat{s} = \hat{t}_p^{-\beta}(1-\hat{t}_p)^\beta \le \hat{t}_p^{-\beta}(1 - \beta\hat{t}_p).$$

Now, using $t^{-1}\hat{t}_p^{-\beta} = t_p^{-\beta}t^{-\alpha}$, one concludes for $t > t_p$ that

(A.1) $$\Gamma(1-\alpha)\,D_t^\alpha B(t) \ge t_p^{-\beta}t^{-\alpha}\,(\beta t_p/t) = \beta t_p^\alpha t^{-\alpha-1} = \beta p^\alpha\,(\tau^\alpha t^{-\alpha-1}).$$

So, to complete the proof, it remains to show that $\frac{1}{2}D_t^\alpha B(t_m) \ge |\delta_t^\alpha B^m - D_t^\alpha B(t_m)|$ for any $m > p$. For the latter, with the notation $F(s) := \beta^{-1}(t_m - s)^\beta$, note that $\delta_t^\alpha B^m$ involves $\sum_{j=1}^m$ of the terms

$$\delta_t B^j \int_{t_{j-1}}^{t_j} \underbrace{(t_m - s)^{-\alpha}}_{=F'(s)}\,ds = \delta_t F^j \int_{t_{j-1}}^{t_j} B'(s)ds.$$

Note also that the component $\sum_{j=1}^p$ is identical in $\delta_t^\alpha B^m$ and $D_t^\alpha B(t_m)$. Now, subtracting one of the above representations from the corresponding components $\int_{t_{j-1}}^{t_j} B'(s)F'(s)\,ds$ of $D_t^\alpha B(t_m)$ yields

$$|\delta_t^\alpha B^m - D_t^\alpha B(t_m)| \lesssim \tau \int_{t_p}^{t_n} s^{-\beta-1}(t_{m-1}-s)^{-\alpha-1}\,ds + \tau \int_{t_n}^{t_m}(s-\tau)^{-\beta-2}(t_m-s)^{-\alpha}ds,$$

where $n := \max\{p, \lfloor m/2 \rfloor\}$, and $n \le m-2$ whenever $n > p$. Here, when dealing with $s \in (t_{j-1}, t_j)$, we also used $|\delta_t F^j - F'(s)| \le \tau|F''(t_j)| \lesssim \tau(t_{m-1}-s)^{-\alpha-1}$ for $j \le n$, and $|\delta_t B^j - B'(s)| \le \tau|B''(t_{j-1})| \lesssim \tau(s-\tau)^{-\beta-2}$ for $j > n$. Estimating the above integrals $\int_{t_p}^{t_n}$ and $\int_{t_n}^{t_m}$ similarly to I and, respectively, using $(t_{m-1}-s)^{-1} \le 2(t_m-s)^{-1}$ and $(s-\tau)^{-1} \le 2s^{-1}$, one finally gets

$$|\delta_t^\alpha B^m - D_t^\alpha B(t_m)| \lesssim \tau t_m^{-2}(t_p/t_m)^{-\beta} \simeq p^{-\beta}\,(\tau^\alpha t_m^{-\alpha-1}).$$

Combining this with (A.1) and choosing p sufficiently large yields the desired assertion $\delta_t^\alpha B^m \gtrsim \tau^\alpha t_m^{-\alpha-1}$.

(ii) It remains to consider $\gamma \in (0, \alpha)$. Set $p_m := 2^m p$ and $c_m := 2^{-m\gamma}$. Now, set $B_m(s) := \min\{st_{p_m}^{-\beta-1}, s^{-\beta}\}$ (i.e., $B_0(s) = B(s)$), and $B_m^j := B_m(t_j)$, and then

$\bar{B}^j := \sum_{m=0}^{\infty} c_m B_m^j$. Here p is from part (i), and, when using the notation of type $\lesssim$, the dependence on γ and m, but not on p, will be shown explicitly.

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

Appendix B. 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 $\rho(\cdot, t) = \mathcal{R}_h u - u$, defined by $\langle \nabla \hat{\rho}_h, \nabla v_h \rangle = \langle \mathring{\mathcal{L}} u, v_h \rangle_h - \langle \mathring{\mathcal{L}} u, v_h \rangle \ \forall v_h \in S_h$. We claim that

$$(B.1) \qquad \|\hat{\rho}_h\|_{L_\infty(\Omega)} \lesssim h^{2-q} |\ln h| \, \|\mathring{\mathcal{L}} u(\cdot, t)\|_{W_{d/2}^{2-q}(\Omega)} \qquad \text{for } q = 0, 1.$$

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

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

$$|\langle \nabla \hat{\rho}_h, \nabla v_h \rangle| \lesssim h^{2-q} \Big\{ \|\mathring{\mathcal{L}} u\|_{W_{d/2}^{2-q}(\Omega)} \|v_h\|_{L_{d/(d-2)}(\Omega)} + \|\mathring{\mathcal{L}} u\|_{W_d^{1-q}(\Omega)} \|\nabla v_h\|_{L_{d/(d-1)}(\Omega)} \Big\}.$$

In view of the Sobolev embedding $\|\mathring{\mathcal{L}} u\|_{W_d^{1-q}(\Omega)} \lesssim \|\mathring{\mathcal{L}} u\|_{W_{d/2}^{2-q}(\Omega)}$, one arrives at

$$(B.2) \quad |\langle \nabla \hat{\rho}_h, \nabla v_h \rangle| \lesssim h^{2-q} \Big\{ \|v_h\|_{L_{d/(d-2)}(\Omega)} + \|\nabla v_h\|_{L_{d/(d-1)}(\Omega)} \Big\} \|\mathring{\mathcal{L}} u\|_{W_{d/2}^{2-q}(\Omega)}.$$

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 (B.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 $\|\nabla \hat{\rho}_h\|_{L_2(\Omega)} \lesssim h^{2-q} |\ln h|^{1/2} \|\mathring{\mathcal{L}} u\|_{W_{d/2}^{2-q}(\Omega)}$, so (B.1) follows.

For $d = 3$, with $\|\hat{\rho}_h\|_{L_\infty(\Omega)} = |\hat{\rho}_h(x^*)|$ for some interior node $x^* \in \mathcal{N}$, let $g_h \in S_h$ be a discrete version of the Green's function $g_h \in S_h$ associated with x^* and defined by $\langle \nabla g_h, \nabla v_h \rangle = v_h(x^*) \ \forall v_h \in S_h$. Now set $v_h := g_h$ in (B.2), so

$$\|\hat{\rho}_h\|_{L_\infty(\Omega)} = |\langle \nabla \hat{\rho}_h, \nabla g_h \rangle| \lesssim h^{2-q} \Big\{ \underbrace{\|g_h\|_{L_3(\Omega)}}_{\lesssim |\ln h|^{1/3}} + \underbrace{\|\nabla g_h\|_{L_{3/2}(\Omega)}}_{\lesssim |\ln h|^{2/3}} \Big\} \|\mathring{\mathcal{L}} u\|_{W_{d/2}^{2-q}(\Omega)},$$

where we employed the bounds on $\|g_h\|_{L_3(\Omega)}$ and $\|\nabla g_h\|_{L_{3/2}(\Omega)}$ from [14, see (3.10), (3.11), and the final formula in §3]. So we again get (B.1).

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