FEM FOR TIME-FRACTIONAL DIFFUSION EQUATIONS, NOVEL OPTIMAL ERROR ANALYSES

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ABSTRACT. A semidiscrete Galerkin finite element method applied to time-fractional diffusion equations with time-space dependent diffusivity on bounded convex spatial domains will be studied. The main focus is on achieving optimal error results with respect to both the convergence order of the approximate solution and the regularity of the initial data. By using novel energy arguments, for each fixed time t, optimal error bounds in the spatial L^2 - and H^1 -norms are derived for both cases: smooth and nonsmooth initial data. Some numerical results will be provided at the end.

1. Introduction

In this work, we consider the spatial discretisation via Galerkin finite elements of the following time-fractional diffusion problem: find u = u(x, t) so that

(1.1a)
$${}^{C}\partial_{t}^{\alpha}u(x,t) - \operatorname{div}(\kappa_{\alpha}(x,t)\nabla u(x,t)) = 0 \quad \text{in } \Omega \times (0,T],$$

(1.1b)
$$u(x,t) = 0 \qquad \text{on } \partial\Omega \times (0,T],$$

$$(1.1c) u(x,0) = u_0(x) in \Omega,$$

where Ω is a bounded, convex polygonal domain in \mathbb{R}^d $(d \geq 1)$ with boundary $\partial\Omega$, κ_{α} and u_0 are given functions defined on their respective domains. Here, ${}^C\!\partial_t^{\alpha}$ is the Caputo time-fractional derivative defined by: for $0 < \alpha < 1$,

$$(1.2) \quad {}^{C}\partial_{t}^{\alpha}\varphi(t) := \mathcal{I}^{1-\alpha}\varphi'(t) := \int_{0}^{t} \omega_{1-\alpha}(t-s)\varphi'(s) \, ds, \text{ with } \omega_{1-\alpha}(t) := \frac{t^{-\alpha}}{\Gamma(1-\alpha)},$$

where φ' denotes the (partial) time derivative of φ and for $\nu > 0$, \mathcal{I}^{ν} is the Riemann–Liouville time-fractional integral operator of order ν which reduces to the classical definite integral when ν is a positive integer. The diffusivity coefficient κ_{α} satisfies the positivity property:

(1.3)
$$0 < \kappa_{\min} \le \kappa_{\alpha}(x, t) \le \kappa_{\max} < \infty \quad \text{for } (x, t) \in \overline{\Omega} \times [0, T].$$

Numerical solutions for time fractional diffusion problem (1.1) with constant or space dependent diffusion parameter κ_{α} have been studied by various authors over the last decade. For finite difference (including alternating direction implicit schemes) and finite element (conforming and nonconforming) schemes, we refer to [2–6, 10, 13, 19, 21, 22, 24, 25] and related references therein. Discontinuous Galerkin (DG) methods (including local DG and hybridizable DG schemes) were investigated

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in [14,16,20], and in [9,23] the spectral method was studied. The convergence analyses in most of these studies required the solution u of problem (1.1) to be sufficiently regular including at t=0 which is not practically the case.

Having time dependent variable diffusivity κ_{α} in the fractional diffusion problem (1.1) is indeed very interesting and also practically important. The numerical solutions of (1.1) were considered by a few authors only. For one-dimensional spatial domain Ω , a finite difference scheme was proposed and analyzed by Alikhanov [1]. In the error analysis, the continuous solution u was assumed to be smooth including at t = 0. In [17], a piecewise linear time-stepping DG method combined with the standard Galerkin finite element scheme in space was investigated. The convergence of the scheme had been proven assuming that u is sufficiently regular. Consequently, the convergence results in these papers are not valid if the initial data u_0 is not sufficiently regular where some compatibility conditions are also required.

For constant diffusivity κ_{α} , Jin et al. [5] studied the error analysis of the spatial semidiscrete piecewise linear Galerkin finite element scheme for problem (1.1). Over a quasi-uniform spatial mesh, quasi-optimal convergence order results (but optimal with respect to the regularity of the initial data u_0) were proved. The used error analysis (based on semigroup) approach can be extended for the case of space dependent parameter κ_{α} , however is not feasible when κ_{α} is a time or a time-space dependent function. Therefore, the optimality of the finite element error estimates with respect to the convergence order and to the solution smoothness expressed through the problem data u_0 is indeed missing, even for constant κ_{α} . So, obtaining optimal finite element error bounds for the case of time-space dependent diffusivity κ_{α} is definitely challenging.

The aim of this work is to show optimal error estimates with respect to both the convergence order and the regularity of the initial data u_0 of the semidiscrete Galerkin method for problem (1.1) allowing both smooth and nonsmooth u_0 . For each $t \in (0,T]$, by using a novel energy arguments approach, we show optimal convergence results in the spatial $L^2(\Omega)$ - and $H^1(\Omega)$ -norms over a (conforming) regular triangulation mesh (need not be quasi-uniform). It is straightforward to extend our error analysis approach to allow for an inhomogenous source term or homogenous Neumann boundary conditions in problem (1.1).

Note, for time independent diffusivity κ_{α} , problem (1.1) can be rewritten as:

(1.4)
$$u'(x,t) - {}^{R}D^{1-\alpha}\operatorname{div}(\kappa_{\alpha}(x)\nabla u(x,t)) = 0 \quad \text{for } (x,t) \in \Omega \times (0,T],$$

where ${}^R D^{1-\alpha} u := \frac{\partial}{\partial t}(\mathcal{I}^\alpha u)$ is the Riemann–Liouville fractional derivative. Recently, Karaa et al. [7] investigated the error analysis of the Galerkin finite element scheme applied to problem (1.4). Using a delicate energy argument, optimal error bounds in $L^2(\Omega)$ - and $H^1(\Omega)$ -norms, and quasi-optimal in $L^\infty(\Omega)$ -norm were derived for cases of smooth and nonsmooth initial data. Unfortunately, extending the considered approach for the case of time dependent diffusivity is not feasible.

Outline of the paper. In Section 2, the required regularity assumptions on the solution u of problem (1.1) will be given. We also state and derive some technical results that will be used in our error analysis. In Section 3, we introduce our semidiscrete Galerkin scheme for problem (1.1) and recall some error projection results from the existing literature. In Section 4, optimal error estimates (with respect to both the convergence order and the regularity of u_0) in the $L^2(\Omega)$ -norm will be proved using novel energy arguments; see Theorem 4.3. For $t \in (0,T]$ and when $u_0 \in \dot{H}^{\delta}(\Omega)$

(this Sobolev space will be defined in the next section), an $O(t^{-\alpha(2-\delta)/2}h^2)$ error estimate is proved for $0 \le \delta \le 2$ (that is, allowing both smooth and nonsmooth initial data), h denoting the maximum diameter of the spatial mesh elements. Furthermore, in the $H^1(\Omega)$ -norm, we show an optimal error bounded by $Ch \, t^{\alpha(\delta-2)/2} \|u_0\|_{\delta}$ for $0 \le \delta \le 1$, and by $Ch \, \max\{h \, t^{-\alpha/2}, 1\}t^{\alpha(\delta-2)/2}\|u_0\|_{\delta}$ for $1 < \delta \le 2$, where C is a generic constant that may depend on α , T, and the norms of κ_{α} , κ'_{α} and κ''_{α} , but is independent of the spatial mesh size element h. The derived optimal bounds in both $L^2(\Omega)$ - and $H^1(\Omega)$ -norms provide remarkable improvements of results obtained by Jin et al. in [5, Theorem 3.7]. Therein, for a quasi-uniform mesh and assuming that the parameter κ_{α} is constant, an $O(t^{-\alpha(2-\delta)/2}h^{2-m}|\log h|)$ error bound was derived in the $H^m(\Omega)$ -norm (m=0,1) when $u_0 \in \dot{H}^{\delta}(\Omega)$ with $\delta=0,1,2$. Finally, for the numerical illustration of these achievements for the case of constant and space dependent diffusivity coefficient κ_{α} , various tests were carried out in [5]. For the case of time-space dependent κ_{α} , one numerical example will be provided in Section 5.

2. Regularity and technical results

It is known that the solution u of problem (1.1) has singularity near t = 0, even for smooth given data. In our error analysis, we assume that for $0 \le p \le q \le 2$,

$$(2.1) ||u(t)||_q + t||u'(t)||_q \le Ct^{\alpha(p-q)/2}||u_0||_p,$$

where $\|\cdot\|_r$ denotes the norm on the Hilbert space $\dot{H}^r(\Omega) \subset L^2(\Omega)$ defined by

$$||v||_r^2 = ||\mathcal{L}^{r/2}v||^2 = \sum_{j=1}^{\infty} \lambda_j^r(v, \phi_j)^2$$
, with $\mathcal{L}v := -\text{div}(\kappa_{\alpha} \nabla v)$,

where for each fixed t, $\{\lambda_j\}_{j=1}^{\infty}$ (with $0 < \lambda_1 \le \lambda_2 \le \ldots$) are the eigenvalues of the operator \mathcal{L} (subject to homogeneous Dirichlet boundary conditions) and $\{\phi_j\}_{j=1}^{\infty}$ are the associated orthonormal eigenfunctions. In the above definition, (\cdot,\cdot) denotes the $L^2(\Omega)$ -norm and $\|\cdot\| := \|\cdot\|_0$ is the associated norm. Note, $\dot{H}^r(\Omega) = H^r(\Omega)$ for $0 \le r < 1/2$, however, for a convex polygonal domain Ω , $\dot{H}^r(\Omega) = \{w \in H^r(\Omega) : w = 0 \text{ on } \partial\Omega\}$ when $1/2 < r \le 2$, where $H^r(\Omega)$ (with $H^0(\Omega) = L^2(\Omega)$) is the standard Sobolev space.

Indeed, for the time independent function κ_{α} , the above regularity assumption holds assuming that the domain Ω is convex; see Theorems 4.1 and 4.2 in [12]. We conjecture that the same is true for a sufficiently regular time dependent κ_{α} .

Next, we state some properties of the fractional integral operators \mathcal{I}^{α} , and derive some technical results that will be used later. By [15, Lemma 3.1(ii)], it follows that for piecewise time continuous functions $\varphi : [0, T] \to L^2(\Omega)$,

$$(2.2) \qquad \int_0^T (\mathcal{I}^\alpha \varphi, \varphi) \, dt \geq \cos(\alpha \pi/2) \int_0^T \|\mathcal{I}^{\alpha/2} \varphi\|^2 \, dt \geq 0 \text{ for } 0 < \alpha < 1 \, .$$

Furthermore, by [15, Lemma 3.1(iii)] and the inequality $\cos(\alpha\pi/2) \geq 1 - \alpha$, we obtain the following continuity property of \mathcal{I}^{α} : for φ , $\psi \in L^{2}((0,T); L^{2}(\Omega))$,

$$\int_0^t (\mathcal{I}^{1-\alpha}\varphi, \psi) ds \le \epsilon \int_0^t (\mathcal{I}^{1-\alpha}\varphi, \varphi) ds + \frac{1}{4\epsilon(1-\alpha)^2} \int_0^t (\mathcal{I}^{1-\alpha}\psi, \psi) ds \quad \text{for } \epsilon > 0.$$

In our convergence analysis, we also make use of the inequality below, where the proof follows from [8, Lemma 2.1] and the positivity property of $\mathcal{I}^{1-\alpha}$ (by (2.2)). If $\varphi': [0,T] \to L^2(\Omega)$ is a piecewise time continuous function, then we have

(2.4)
$$\|\varphi(t)\|^2 \le Ct^{\alpha} \int_0^t (\mathcal{I}^{1-\alpha}\varphi', \varphi') \, ds, \quad \text{for } t > 0.$$

Based on the generalized Leibniz formula and the relation between Riemann–Liouville and Caputo fractional derivatives, we show the identity in the next lemma. For convenience, we use the notations:

$$v_i(t) := t^i v(t)$$
 for $i = 1, 2$.

Lemma 2.1. Let $0 < \alpha < 1$. The following holds: for $0 \le t \le T$,

$$t^2\mathcal{I}^\alpha v'(t) = \mathcal{I}^\alpha(v_2)'(t) + 2(\alpha-1)\mathcal{I}^\alpha v_1(t) + \alpha(\alpha-1)\mathcal{I}^{1+\alpha}v(t) - t^2\omega_\alpha(t)v(0) \,.$$

Proof. Since $\mathcal{I}^{\alpha}v'(t) = (\mathcal{I}^{\alpha}v(t))' - \omega_{\alpha}(t)v(0)$, the use of the fractional Leibniz formula $t(\mathcal{I}^{\alpha}v(t))' = (\mathcal{I}^{\alpha}v_1(t))' + (\alpha - 1)\mathcal{I}^{\alpha}v(t)$ (see [18]) and the equality $(\mathcal{I}^{\alpha}v_1(t))' = \mathcal{I}^{\alpha}(v_1)'(t)$ yield the following identity:

(2.5)
$$t\mathcal{I}^{\alpha}v'(t) = \mathcal{I}^{\alpha}(v_1)'(t) + (\alpha - 1)\mathcal{I}^{\alpha}v(t) - t\omega_{\alpha}(t)v(0).$$

Now, multiplying both sides of the above identity by t and applying the identity $t\mathcal{I}^{\alpha}\phi(t) = \mathcal{I}^{\alpha}\phi_1(t) + \alpha\mathcal{I}^{1+\alpha}\phi(t)$ (see [7, Lemma 4.1 (b)] for the proof) twice,

$$t^{2}\mathcal{I}^{\alpha}v'(t) = t\mathcal{I}^{\alpha}(v_{1})'(t) + (\alpha - 1)t\mathcal{I}^{\alpha}v(t) - t^{2}\omega_{\alpha}(t)v(0)$$

= $[\mathcal{I}^{\alpha}((v_{1})')_{1}(t) + \alpha\mathcal{I}^{1+\alpha}(v_{1})'(t)] + (\alpha - 1)[\mathcal{I}^{\alpha}v_{1}(t) + \alpha\mathcal{I}^{1+\alpha}v(t)] - t^{2}\omega_{\alpha}(t)v(0)$.

Since $((v_1)')_1(t) = t(v_1)'(t) = (v_2)'(t) - v_1(t)$ and $\mathcal{I}^{1+\alpha}(v_1)'(t) = \mathcal{I}^{\alpha}v_1(t)$, the desired identity follows after simple simplifications.

Lemma 2.2. Let $g \ge 0$ be a nondecreasing function of t. (i) If

(2.6)
$$\int_0^t (\mathcal{I}^{1-\alpha}v, v) \, ds + 2 \int_0^t (\mathcal{I}(\kappa_{\alpha}w), w) \, ds \le g(t) \quad \text{for } t > 0,$$

for suitable functions v and w, then for $\kappa'_{\alpha} \in L^{\infty}((0,T);L^{\infty}(\Omega))$, we have

$$\int_0^t (\mathcal{I}^{1-\alpha}v, v) \, ds + \|\mathcal{I}w(t)\|^2 \le Cg(t).$$

(ii) If

(2.7)
$$\int_0^t (\mathcal{I}^{2-\alpha}v, \mathcal{I}v) \, ds + 2 \int_0^t (\mathcal{I}^2(\kappa_{\alpha}w), \mathcal{I}w) \, ds \le g(t) \quad \text{for } t > 0,$$

for suitable functions v and w, then for $\kappa'_{\alpha}, \kappa''_{\alpha} \in L^{\infty}((0,T); L^{\infty}(\Omega))$, we have

$$\int_0^t (\mathcal{I}^{2-\alpha}v, \mathcal{I}v) \, ds + \|\mathcal{I}^2w(t)\|^2 \le Cg(t).$$

Proof. Let $w_I(t) := \mathcal{I}w(t) = \int_0^t w(s) ds$. Since $\mathcal{I}(\kappa_{\alpha} w) = \kappa_{\alpha} w_I - \mathcal{I}(\kappa'_{\alpha} w_I)$, an integration by parts yields

$$\begin{split} 2\int_0^t \left(\mathcal{I}(\kappa_\alpha w), w\right) ds &= \int_0^t \left(\kappa_\alpha, (w_I^2)'\right) ds - 2\int_0^t \left(\mathcal{I}(\kappa_\alpha' w_I), w_I'\right) ds \\ &= \left(\kappa_\alpha(t), w_I^2(t)\right) - \int_0^t \left(\kappa_\alpha', w_I^2\right) ds - 2\left(\mathcal{I}(\kappa_\alpha' w_I)(t), w_I(t)\right) + 2\int_0^t \left(\kappa_\alpha', w_I^2\right) ds \\ &= \left(\kappa_\alpha(t), w_I^2(t)\right) - 2\left(\mathcal{I}(\kappa_\alpha' w_I)(t), w_I(t)\right) + \int_0^t \left(\kappa_\alpha', w_I^2\right) ds \,. \end{split}$$

Therefore, by inserting this in (2.6), then using the positivity assumption on the diffusion coefficient κ_{α} , (1.3), and the Cauchy-Schwarz inequality, we conclude that

$$\int_0^t (\mathcal{I}^{1-\alpha}v, v) \, ds + \|w_I(t)\|^2 \le Cg(t) + C \int_0^t \|w_I\| ds \|w_I(t)\| + C \int_0^t \|w_I\|^2 \, ds$$

$$\le Cg(t) + \frac{1}{2} \|w_I(t)\|^2 + C \int_0^t \|w_I\|^2 \, ds.$$

Thus,

$$\int_0^t (\mathcal{I}^{1-\alpha}v, v) \, ds + \|w_I(t)\|^2 \le Cg(t) + C \int_0^t \|w_I\|^2 ds.$$

Since $\int_0^t (\mathcal{I}^{1-\alpha}v, v) ds \ge 0$ by the positivity property in (2.2), an application of the continuous version of Gronwalls inequality yields the first desired result.

To show (ii), we let $w_{II} := \mathcal{I}^2 w$. Since $\mathcal{I}(\kappa_{\alpha} w''_{II}) = \kappa_{\alpha} w'_{II} - \mathcal{I}(\kappa'_{\alpha} w'_{II})$,

$$\mathcal{I}^{2}(\kappa_{\alpha}w_{II}'')(s) = \mathcal{I}(\kappa_{\alpha}w_{II}')(s) - \mathcal{I}^{2}(\kappa_{\alpha}'w_{II}')(s)$$

$$= \kappa_{\alpha}(s)w_{II}(s) - \mathcal{I}(\kappa_{\alpha}'w_{II})(s) - \mathcal{I}^{2}(\kappa_{\alpha}'w_{II}')(s)$$

$$= \kappa_{\alpha}(s)w_{II}(s) - 2\mathcal{I}(\kappa_{\alpha}'w_{II})(s) + \mathcal{I}^{2}(\kappa_{\alpha}'w_{II})(s).$$

Thus, an integration by parts yields

$$\begin{split} &2\int_{0}^{t} \left(\mathcal{I}^{2}(\kappa_{\alpha}w), \mathcal{I}w\right) ds = 2\int_{0}^{t} \left(\mathcal{I}^{2}(\kappa_{\alpha}w_{II}''), w_{II}'\right) ds \\ &= \int_{0}^{t} \left(\kappa_{\alpha}, \left(w_{II}^{2}\right)'\right) ds - 2\int_{0}^{t} \left(2\mathcal{I}(\kappa_{\alpha}'w_{II}) - \mathcal{I}^{2}(\kappa_{\alpha}''w_{II}), w_{II}'\right) ds \\ &= \left(\kappa_{\alpha}(t), w_{II}^{2}(t)\right) - \int_{0}^{t} \left(\kappa_{\alpha}', w_{II}^{2}\right) ds \\ &- 2\left(2\mathcal{I}(\kappa_{\alpha}'w_{II})(t) - \mathcal{I}^{2}(\kappa_{\alpha}''w_{II})(t), w_{II}(t)\right) + 2\int_{0}^{t} \left(2\kappa_{\alpha}'w_{II} - \mathcal{I}(\kappa_{\alpha}''w_{II}), w_{II}\right) ds \\ &= \left(\kappa_{\alpha}(t), w_{II}^{2}(t)\right) + 3\int_{0}^{t} \left(\kappa_{\alpha}', w_{II}^{2}\right) ds \\ &- 2\left(2\mathcal{I}(\kappa_{\alpha}'w_{II})(t) - \mathcal{I}^{2}(\kappa_{\alpha}''w_{II})(t), w_{II}(t)\right) - 2\int_{0}^{t} \left(\mathcal{I}(\kappa_{\alpha}''w_{II}), w_{II}\right) ds \,. \end{split}$$

Now, by proceeding as in the proof of (i), we obtain the second desired result. \Box

3. Finite element discretization

This section focuses on the spatial semidiscrete Galerkin finite element scheme for the time fractional diffusion problem (1.1). Let \mathcal{T}_h be a family of shape-regular triangulations (made of simplexes K) of the domain $\overline{\Omega}$ and let $h = \max_{K \in \mathcal{T}_h} (\operatorname{diam} K)$, where h_K denotes the diameter of the element K. Let $S_h \in H_0^1(\Omega)$ denote the usual space of continuous, piecewise-linear functions on \mathcal{T}_h that vanish on $\partial\Omega$.

The weak formulation for problem (1.1) is to find $u:(0,T]\longrightarrow H^1_0(\Omega)$ such that

(3.1)
$$({}^{C}\partial_{t}^{\alpha}u, v) + A(u, v) = 0 \quad \forall v \in H_{0}^{1}(\Omega)$$

with given $u(0) = u_0$. Here $A(\cdot, \cdot)$ is the bilinear form associated with the elliptic operator \mathcal{L} , i.e., $A(v, w) = (\kappa_{\alpha} \nabla v, \nabla w)$, which is symmetric positive definite on the Sobolev space $H_0^1(\Omega)$ for each fixed $t \in [0, T]$.

Now, the semidiscrete scheme for (1.1) is to seek $u_h:(0,T]\longrightarrow S_h$ such that

(3.2)
$$({}^{C}\partial_{t}^{\alpha}u_{h},\chi) + A(u_{h},\chi) = 0 \quad \forall \chi \in S_{h},$$

with given $u_h(0) := u_{h0} = P_h u_0$, where $P_h : L^2(\Omega) \to S_h$ denotes the L^2 -projection defined by $(P_h v - v, \chi) = 0$ for all $\chi \in S_h$. Indeed, for initial data $u_0 \in \dot{H}^1(\Omega)$, one may choose instead $u_h(0) = R_h u_0$, where $R_h : H_0^1(\Omega) \to S_h$ is the Ritz projection defined by the following relation: $A(R_h v - v, \chi) = 0$ for all $\chi \in S_h$.

For the error analysis, we use the following decomposition:

$$(3.3) u - u_h = (u - R_h u) - (u_h - R_h u) =: \rho - \theta.$$

For $t \in (0,T]$, from the projection error estimates [11, (3.2) and (3.3)] and the regularity assumption in (2.1), for $0 \le \delta \le m$ with m = 1, 2,

(3.4)
$$\|\rho(t)\| + h\|\rho(t)\|_1 \le Ch^m \|u(t)\|_m \le Ch^m t^{\alpha(\delta-m)/2} \|u_0\|_{\delta},$$

and

$$(3.5) \|\rho'(t)\| + h\|\rho'(t)\|_1 \le Ch^m \Big(\|u(t)\|_m + \|u'(t)\|_m \Big) \le Ch^m t^{\alpha(\delta - m)/2 - 1} \|u_0\|_{\delta}.$$

We need to assume that $\kappa_{\alpha} \in L^{\infty}((0,T);W^{1,\infty}(\Omega))$ in (3.4), and in addition to this, $\kappa'_{\alpha} \in L^{\infty}((0,T);W^{1,\infty}(\Omega))$ in (3.5). Noting that, when m=1, for the H^1 -norm projection error estimates, $W^{1,\infty}(\Omega)$ can be replaced with $L^{\infty}(\Omega)$ in these assumptions.

Therefore, for later use, we have

(3.6)
$$\|\mathcal{I}^{1-\alpha}\rho(t)\| + \|\mathcal{I}^{1-\alpha}\rho_1'(t)\| \le C \int_0^t (t-s)^{-\alpha} [\|\rho(s)\| + s\|\rho'(s)\|] ds$$

$$\le Ch^m \int_0^t (t-s)^{-\alpha} s^{\alpha(\delta-m)/2} ds \|u_0\|_{\delta}$$

$$= Ch^m t^{1-\alpha+\alpha(\delta-m)/2} \|u_0\|_{\delta}, \text{ for } 0 \le \delta \le m, \text{ with } m = 1, 2.$$

In a similar fashion, for $t \in (0,T]$, we have

Via an energy argument approach, we estimate θ (and consequently the finite element error) in the next section.

4. Error estimates

This section is devoted to derive optimal error bounds from the Galerkin approximation in both $L^2(\Omega)$ - and $H^1(\Omega)$ -norms, for the case of smooth and nonsmooth initial data u_0 . More precisely, for $t \in (0,T]$ and for $u_0 \in \dot{H}^{\delta}(\Omega)$, we show

$$\|(u-u_h)(t)\| + h\|\nabla(u-u_h)(t)\| \le Ch^2t^{\alpha(\delta-2)/2}\|u_0\|_{\delta}$$
 for $0 \le \delta \le 2$;

see Theorem 4.3 and the estimates in (4.11) and (4.13). Noting that, for the $H^1(\Omega)$ -norm error, the spatial mesh is assumed to be quasi-uniform when $1 < \delta \le 2$.

The estimate of θ_1 in the next lemma plays a crucial role in achieving our error bounds.

Lemma 4.1. Assume that κ'_{α} , $\kappa''_{\alpha} \in L^{\infty}((0,T); L^{\infty}(\Omega))$. For $0 \le t \le T$, we have

$$\int_0^t (\mathcal{I}^{1-\alpha}\theta_1,\theta_1)ds + \|\mathcal{I}(\nabla\theta_1)(t)\|^2 \le C \int_0^t [|(\mathcal{I}^{1-\alpha}\rho_1,\rho_1)| + |(\mathcal{I}^{2-\alpha}\rho,\mathcal{I}\rho)|]ds.$$

Proof. From (3.1) and (3.2), the error decomposition $u - u_h = \rho - \theta$ in (3.3), and the property of the Ritz projection, we obtain

$$(\mathcal{I}^{1-\alpha}\theta',\chi) + A(\theta,\chi) = (\mathcal{I}^{1-\alpha}\rho',\chi) \quad \forall \ \chi \in S_h.$$

Multiplying both sides of (4.1) by t, gives

$$(t\mathcal{I}^{1-\alpha}\theta',\chi) + A(\theta_1,\chi) = (t\mathcal{I}^{1-\alpha}\rho',\chi).$$

Hence, by the identity in (2.5) and the equality $(u_0 - u_{h0}, \chi) = 0$, we obtain

$$(4.2) \qquad (\mathcal{I}^{1-\alpha}\theta_1' - \alpha \mathcal{I}^{1-\alpha}\theta, \chi) + A(\theta_1, \chi) = (\mathcal{I}^{1-\alpha}\rho_1' - \alpha \mathcal{I}^{1-\alpha}\rho, \chi).$$

Integrating (4.2) in time and rearranging the terms to get

$$(\mathcal{I}^{1-\alpha}\theta_1,\chi) + (\mathcal{I}(\kappa_{\alpha}\nabla\theta_1),\nabla\chi) = (\mathcal{I}^{1-\alpha}\rho_1 - \alpha\mathcal{I}^{1-\alpha}(\mathcal{I}\rho) + \alpha\mathcal{I}^{1-\alpha}(\mathcal{I}\theta),\chi)$$

for all $\chi \in S_h$. Choosing $\chi = \theta_1(s) \in S_h$, and then integrating again in time and using the continuity property in (2.3) (with $\epsilon = \frac{1}{4}$) for the three terms on the right-hand side, we observe that

$$(4.3) \qquad \int_0^t [(\mathcal{I}^{1-\alpha}\theta_1, \theta_1) + (\mathcal{I}(\kappa_{\alpha}\nabla\theta_1), \nabla\theta_1)]ds$$

$$\leq C \int_0^t [(\mathcal{I}^{1-\alpha}\rho_1, \rho_1) + (\mathcal{I}^{1-\alpha}(\mathcal{I}\rho), \mathcal{I}\rho) + (\mathcal{I}^{1-\alpha}(\mathcal{I}\theta), \mathcal{I}\theta)]ds.$$

To estimate the last term on the right-hand side of (4.3), we first integrate both sides of (4.1) in time and use the identity $\mathcal{I}^{2-\alpha}v'(t) = \mathcal{I}^{1-\alpha}v(t) - \omega_{2-\alpha}(t)v(0)$,

$$(\mathcal{I}^{1-\alpha}\theta,\chi)+(\mathcal{I}(\kappa_{\alpha}\nabla\theta),\nabla\chi)=(\mathcal{I}^{1-\alpha}\rho-\omega_{2-\alpha}(t)[u_{0}-u_{h0}],\chi)\quad\forall\ \chi\in S_{h}.$$

Since $(u_0 - u_{h0}, \chi) = (u_0 - P_h u_0, \chi) = 0$,

$$(4.4) (\mathcal{I}^{1-\alpha}\theta, \chi) + (\mathcal{I}(\kappa_{\alpha}\nabla\theta), \nabla\chi) = (\mathcal{I}^{1-\alpha}\rho, \chi) \quad \forall \ \chi \in S_h.$$

Integrating both sides of (4.4) yields

$$(4.5) (\mathcal{I}^{1-\alpha}(\mathcal{I}\theta), \chi) + (\mathcal{I}^{2}(\kappa_{\alpha}\nabla\theta), \nabla\chi) = (\mathcal{I}^{1-\alpha}(\mathcal{I}\rho), \chi) \quad \forall \ \chi \in S_{h}.$$

Setting $\chi = \mathcal{I}\theta(s) \in S_h$ and then, integrating over the time variable and applying the continuity property of $\mathcal{I}^{1-\alpha}$ (with $\epsilon = \frac{1}{2}$), we find that

$$\begin{split} \int_0^t (\mathcal{I}^{1-\alpha}(\mathcal{I}\theta), \mathcal{I}\theta) \, ds + \int_0^t (\mathcal{I}^2(\kappa_\alpha \nabla \theta), \mathcal{I}(\nabla \theta)) \, ds &= \int_0^t (\mathcal{I}^{1-\alpha}(\mathcal{I}\rho), \mathcal{I}\theta) ds \\ &\leq \frac{1}{2} \int_0^t (\mathcal{I}^{1-\alpha}(\mathcal{I}\theta), \mathcal{I}\theta) \, ds + C \int_0^t (\mathcal{I}^{1-\alpha}(\mathcal{I}\rho), \mathcal{I}\rho) ds \, . \end{split}$$

After simplification, an application of Lemma 2.2 (ii) gives

(4.6)
$$\int_0^t (\mathcal{I}^{2-\alpha}\theta, \mathcal{I}\theta) \, ds \le C \int_0^t |(\mathcal{I}^{2-\alpha}\rho, \mathcal{I}\rho)| ds.$$

Inserting this bound in (4.3) gives

$$\int_0^t [(\mathcal{I}^{1-\alpha}\theta_1,\theta_1) + (\mathcal{I}(\kappa_{\alpha}\nabla\theta_1),\nabla\theta_1)]ds \leq C \int_0^t \Big[|(\mathcal{I}^{1-\alpha}\rho_1,\rho_1)| + |(\mathcal{I}^{2-\alpha}\rho,\mathcal{I}\rho)| \Big] ds.$$

Finally, an application of Lemma 2.2 (i) yields the desired bound.

Now, we are ready to derive an estimate of θ that will be used later to derive optimal finite element error bounds for the case of smooth and nonsmooth initial data.

Lemma 4.2. Assume that $\kappa'_{\alpha}, \kappa''_{\alpha} \in L^{\infty}((0,T); L^{\infty}(\Omega))$. For $0 < t \leq T$, the following estimate holds:

$$\begin{aligned} \|\theta(t)\|^2 + t^{\alpha} \|\nabla \theta(t)\|^2 \\ &\leq C t^{\alpha - 4} \int_0^t \left(\|\mathcal{I}^{1 - \alpha} \rho_2'\| + \|\mathcal{I}^{1 - \alpha} \rho_1\| + \|\mathcal{I}^{2 - \alpha} \rho\| \right) \left(\|\rho_2'\| + \|\rho_1\| + \|\mathcal{I}\rho\| \right) ds \,. \end{aligned}$$

Proof. Multiplying both sides of (4.1) by t^2 gives

$$(t^2 \mathcal{I}^{1-\alpha} \theta', \chi) + A(\theta_2, \chi) = (t^2 \mathcal{I}^{1-\alpha} \rho', \chi) \quad \forall \ \chi \in S_h.$$

Using the identity in Lemma 2.1 and the fact that $(u_0 - u_{h0}, \chi) = 0$ yields

(4.7)
$$(\mathcal{I}^{1-\alpha}[\theta'_2 - 2\alpha\theta_1 - \alpha(1-\alpha)\mathcal{I}\theta], \chi) + A(\theta_2, \chi) = (\mathcal{I}^{1-\alpha}\eta, \chi) \quad \forall \ \chi \in S_h,$$
 where

(4.8)
$$\eta = \rho_2' - 2\alpha\rho_1 - \alpha(1-\alpha)\mathcal{I}\rho.$$

Rearranging the terms, we get

$$(\mathcal{I}^{1-\alpha}\theta_2',\chi) + A(\theta_2,\chi) = (\mathcal{I}^{1-\alpha}\eta,\chi) + 2\alpha(\mathcal{I}^{1-\alpha}\theta_1,\chi) + \alpha(1-\alpha)(\mathcal{I}^{1-\alpha}(\mathcal{I}\theta),\chi).$$

Setting $\chi = \theta_2'(s) \in S_h$, integrating over the time interval (0,t), and using the continuity property of $\mathcal{I}^{1-\alpha}$ in (2.3) (for an appropriate choice of ϵ) for each term on the right-hand side, we reach

$$\begin{split} & \int_0^t [(\mathcal{I}^{1-\alpha}\theta_2',\theta_2') + A(\theta_2,\theta_2')] \, ds \\ & \leq \frac{1}{2} \int_0^t (\mathcal{I}^{1-\alpha}\theta_2',\theta_2') \, ds + C \int_0^t [(\mathcal{I}^{1-\alpha}\eta,\eta) + (\mathcal{I}^{1-\alpha}\theta_1,\theta_1) + (\mathcal{I}^{2-\alpha}\theta,\mathcal{I}\theta)] ds. \end{split}$$

Integration by parts follows by using the positivity assumption of κ_{α} in (1.3), gives

$$2\int_0^t A(\theta_2, \theta_2') ds = \int_0^t \left(\kappa_\alpha, ((\nabla \theta_2)^2)'\right) ds$$
$$= (\kappa_\alpha(t), (\nabla \theta_2)^2(t)) - \int_0^t \left(\kappa_\alpha', (\nabla \theta_2)^2\right) ds$$
$$\geq \kappa_{\min} \|\nabla \theta_2(t)\|^2 - \int_0^t \left(\kappa_\alpha', (\nabla \theta_2)^2\right) ds,$$

and hence,

$$\int_{0}^{t} (\mathcal{I}^{1-\alpha}\theta'_{2}, \theta'_{2}) ds + \frac{\kappa_{\min}}{2} \|\nabla\theta_{2}(t)\|^{2} \leq C \int_{0}^{t} \|\nabla\theta_{2}\|^{2} ds + \frac{1}{2} \int_{0}^{t} (\mathcal{I}^{1-\alpha}\theta'_{2}, \theta'_{2}) ds + C \int_{0}^{t} [(\mathcal{I}^{1-\alpha}\eta, \eta) + (\mathcal{I}^{1-\alpha}\theta_{1}, \theta_{1}) + (\mathcal{I}^{2-\alpha}\theta, \mathcal{I}\theta)] ds.$$

Simplifying, and then using (4.6) and Lemma 4.1, we obtain

$$\begin{split} & \int_0^t (\mathcal{I}^{1-\alpha}\theta_2', \theta_2') \, ds + \|\nabla \theta_2(t)\|^2 \\ & \leq C \int_0^t \left(|(\mathcal{I}^{1-\alpha}\eta, \eta)| + |(\mathcal{I}^{1-\alpha}\rho_1, \rho_1)| + |(\mathcal{I}^{2-\alpha}\rho, \mathcal{I}\rho)| \right) ds + C \int_0^t \|\nabla \theta_2\|^2 ds \, . \end{split}$$

Therefore, applications of the inequality in (2.4) and the continuous version of Gronwalls inequality yield

$$t^{-\alpha} \|\theta_2(t)\|^2 + \|\nabla \theta_2(t)\|^2 \le C \int_0^t \left(|(\mathcal{I}^{1-\alpha} \eta, \eta)| + |(\mathcal{I}^{1-\alpha} \rho_1, \rho_1)| + |(\mathcal{I}^{2-\alpha} \rho, \mathcal{I} \rho)| \right) ds.$$

The desired result follows immediately after using the fact that $\theta(t) = t^{-2}\theta_2(t)$, the definition of η in (4.8), and the Cauchy-Schwarz inequality.

In the next theorem, we show that the $L^2(\Omega)$ -norm error from the spatial discretization by the scheme (3.2) is bounded by $Ch^2t^{\alpha(\delta-2)/2}\|u_0\|_{\delta}$ for $0 \le \delta \le 2$.

Theorem 4.3. Let u be the solution of the time fractional diffusion problem (1.1) and let u_h be the finite element solution defined by (3.2), with $u_{h0} = P_h u_0$. Assume that κ_{α} , $\kappa'_{\alpha} \in L^{\infty}((0,T); W^{1,\infty}(\Omega))$ and $\kappa''_{\alpha} \in L^{\infty}((0,T); L^{\infty}(\Omega))$. Then, for $t \in (0,T]$, we have

$$||(u - u_h)(t)|| \le Ch^2 t^{\alpha(\delta - 2)/2} ||u_0||_{\delta} \text{ for } 0 \le \delta \le 2.$$

Proof. By using the estimate in (3.7) and the projection error bounds in (3.4)–(3.6) (with m=2) and (3.7), we find that for $t \in (0,T]$,

$$\int_{0}^{t} (\|\mathcal{I}^{1-\alpha}\rho_{2}'\| + \|\mathcal{I}^{1-\alpha}\rho_{1}\| + \|\mathcal{I}^{2-\alpha}\rho\|) (\|\rho_{2}'\| + \|\rho_{1}\| + \|\mathcal{I}\rho\|) ds$$

$$\leq C h^{4} \int_{0}^{t} s^{2-\alpha+\alpha(\delta-2)/2} s^{1+\alpha(\delta-2)/2} ds \|u_{0}\|_{\delta}^{2}$$

$$\leq C h^{4} t^{4-\alpha+\alpha(\delta-2)} \|u_{0}\|_{\delta}^{2}, \quad \text{for } 0 \leq \delta \leq 2.$$

Inserting this bound in the achieved estimate in Lemma 4.2 yields

On the other hand, from the error projection estimate of ρ in (3.4) for m=2,

Therefore, the desired error bounds follow from the decomposition $u-u_h=\rho-\theta$ and the above estimates.

The $H^1(\Omega)$ -norm convergence will be discussed next. By using (3.4), (3.5), and (3.6), but with m=1,

$$\int_{0}^{t} (\|\mathcal{I}^{1-\alpha}\rho_{2}'\| + \|\mathcal{I}^{1-\alpha}\rho_{1}\| + \|\mathcal{I}^{2-\alpha}\rho\|) (\|\rho_{2}'\| + \|\rho_{1}\| + \|\mathcal{I}\rho\|) ds$$

$$\leq C h^{2} \|u_{0}\|_{\delta}^{2} \int_{0}^{t} s^{3-\alpha+\alpha(\delta-1)} ds$$

$$\leq C h^{2} t^{4-2\alpha+\alpha\delta} \|u_{0}\|_{\delta}^{2}, \quad \text{for } 0 \leq \delta \leq 1.$$

Hence, by Lemma 4.2,

$$\|\nabla \theta(t)\|^2 \le C h^2 t^{\alpha(\delta-2)} \|u_0\|_{\delta}^2 \quad \text{for } 0 \le \delta \le 1.$$

Therefore, from the decomposition $u - u_h = \rho - \theta$, the above estimate, and (3.4) with m = 1, we reach the following optimal $H^1(\Omega)$ -norm error bound:

(4.11)
$$\|\nabla(u - u_h)(t)\| \le C h t^{\alpha(\delta - 2)/2} \|u_0\|_{\delta} \quad \text{for } 0 \le \delta \le 1.$$

However, for $u_0 \in \dot{H}^{\delta}(\Omega)$ with $1 < \delta \le 2$, once again, from the decomposition $u - u_h = \rho - \theta$ and the estimates in (4.9) and (4.10), we find that

$$\|\nabla(u - u_h)(t)\| \le C h t^{\alpha(\delta - 2)/2} \max\{h t^{-\alpha/2}, 1\} \|u_0\|_{\delta} \text{ for } 1 < \delta \le 2.$$

This error bound is optimal provided that $h^2 \leq t^{\alpha}$. Indeed, by assuming that the spatial mesh is quasi-uniform, this optimality can also be preserved even if $h^2 > t^{\alpha}$. To see this, we apply the inverse inequality and use the achieved estimate in (4.9),

$$(4.12) \|\nabla \theta(t)\| \le Ch^{-1} \|\theta(t)\| \le Ch t^{\alpha(\delta-2)/2} \|u_0\|_{\delta} for 1 < \delta \le 2.$$

Hence, for $t \in (0,T]$, we have

(4.13)
$$\|\nabla (u - u_h)(t)\| \le C h t^{\alpha(\delta - 2)/2} \|u_0\|_{\delta} \quad \text{for } 1 < \delta \le 2.$$

5. Numerical results

The aim of this section is to validate the achieved theoretical results numerically for the case of time-space dependent variable coefficient κ_{α} and nonsmooth initial data u_0 . For smooth u_0 , some numerical results were carried out in [17]. Furthermore, for time independent κ_{α} , extensive numerical tests were carried out in [5], where the empirical convergence rates in all numerical experiments confirm the theoretical findings for both smooth and nonsmooth initial data.

To compute the finite element solution, time discretization via a piecewise linear discontinuous Galerkin method will be considered [17]. For time levels $0=t_0 < t_1 < t_2 < \cdots < t_N = T$, we denote the *n*th step size by $\tau_n = t_n - t_{n-1}$ and the associated subinterval by $I_n = (t_{n-1}, t_n)$ for $1 \le n \le N$. The maximum time step size is denoted by τ . Let

$$W = \{ w \in L^2((0,T), S_h) : w|_{I_n} \in \mathcal{P}_1(S_h) \text{ for } 1 \le n \le N \},$$

where $\mathcal{P}_1(S_h)$ denotes the space of linear polynomials in the time variable t, with coefficients in S_h . Using the elementary identity ${}^C\!\partial_t^{\alpha}\varphi(t) = {}^R D^{\alpha}\varphi(t) - \omega_{1-\alpha}(t)\varphi(0)$

 $(^{R}\mathrm{D}^{1-\alpha})$ is the Riemann–Liouville fractional derivative), the finite element scheme (3.2) can be rewritten as: for 0 < t < T,

$$(^{R}D^{\alpha}u_{h}(t),\chi) + A(u_{h}(t),\chi) = \omega_{1-\alpha}(t)(u_{h0},\chi) \quad \forall \chi \in S_{h}.$$

We approximate $u_h(t_n)$ by $U^n := U(t_n^-)$ where $U \in \mathcal{P}_1(S_h)$ satisfying

$$\int_{I_n} \left[\left(^{\mathbf{R}} \mathbf{D}^{\alpha} U, X \right) + A \left(U, X \right) \right] dt = \int_{I_n} \left(\omega_{1-\alpha}(t) u_{h0}, X \right) dt \quad \forall X \in \mathcal{P}_1(S_h), \text{ with } t \in I_n$$

for $1 \leq n \leq N$. For a smooth initial data u_0 , by using a graded mesh of the form $t_n = (n/N)^{\gamma}T$ where the exponent $\gamma \geq 1$ chosen appropriately (depends on the regularity of the continuous solution), the numerical results in [17] showed that the above numerical scheme is second-order accurate in both time and space. However, the theoretical results there were slightly pessimistic, where an $O(h^2 + \tau^{2-\frac{\alpha}{2}})$ error bound was achieved.

In our test example, $\kappa_{\alpha}(x,t) = 2 + \sin(2\pi x) + t^{2+\alpha}$, T = 1 and $\Omega = (0,1)$, and discontinuous initial data given by $u_0(x) = 1$ for $x \in [1/4, 3/4]$ and $u_0(x) = 0$ elsewhere. Since $u_0 \in \dot{H}^{\delta}(\Omega)$ for $0 \le \delta < 1/2$, by applying Theorem 4.3 with $\delta = \frac{1}{2} - \epsilon$ and $\epsilon^{-1} = \log(e^2 + t^{-1})$ (so that $t^{-\epsilon} \le e$ and $0 < \epsilon < 1/2$), gives

(5.1)
$$||u(t) - u_h(t)|| \le Ct^{-3\alpha/4}h^2\sqrt{\log(e^2 + t^{-1})}$$
 for $0 < t \le 1$.

In our computations, a uniform spatial mesh with h=1/M was employed. In all cases, M was divisible by 4 so that the points 1/4 and 3/4 (where u_0 is discontinuous) coincided with two of the nodes. We first computed a reference solution $U_{\text{ref}}^n=U^n$ using a fine spatial mesh with M=1024 and a fine time graded mesh of the form $t_n=(n/N)^2$ with N=5,000. We then computed U^n for $M\in\{16,32,64,128,256\}$, again with N=5,000. The initial data was chosen as $u_{0h}=P_hu_0$ in each case. With such a small τ , for $1\leq n\leq N$, the $L^2(\Omega)$ -norm error $E_{h,0}^n:=\|U^n-U_{\text{ref}}^n\|$ and the $H^1(\Omega)$ -norm error $E_{h,1}^n:=\|U^n-U_{\text{ref}}^n\|_1$, were dominated by the influence of the spatial discretisation. We sought to estimate the L^2 convergence rates $\sigma_{h,0}$ and H^1 convergence rates $\sigma_{h,1}$ from the relation $\sigma_{h,\ell}=\log_2(E_{2h,\ell}^*/E_{h,\ell}^*)$, where the weighted error

(5.2)
$$E_{h,\ell}^* = \max_{1 \le n \le N} \frac{t_n^{3\alpha/4} E_{h,\ell}^n}{\sqrt{\log(e^2 + t_n^{-1})}} \quad \text{for } \ell = 0, 1.$$

Table 1. Weighted $L^2(\Omega)$ -norm errors and convergence rates.

M	$\alpha = 0.3$		$\alpha = 0.5$		$\alpha = 0.8$	
16	1.9861e-04		1.7497e-04		1.5665 e-04	
32	4.9618e-05	2.0010	4.3705 e-05	2.0012	3.9116e-05	2.0017
64	1.2376e-05	2.0034	1.0900e-05	2.0035	9.7531e-06	2.0038
128	3.0654 e-06	2.0134	2.6995e-06	2.0136	2.4135e-06	2.0147
256	7.3777e-07	2.0548	6.4937e-07	2.0556	5.7866e-07	2.0603

For three different values of α , Table 1 and Table 2 show the values of $E_{h,0}^*$ and $\sigma_{h,0}$, and of $E_{h,1}^*$ and $\sigma_{h,1}$, respectively. As expected from Theorem 4.3 and the

M	$\alpha = 0.3$		$\alpha = 0.50$		$\alpha = 0.8$	
16	1.1876e-02		1.0309e-02		8.2688e-03	
32	5.9376e-03	1.0001	5.1529e-03	1.0004	4.1321e-03	1.0008
64	2.9647e-03	1.0020	2.5727e-03	1.0021	2.0629e-03	1.0022
128	1.4736e-03	1.0085	1.2788e-03	1.0085	1.0253e-03	1.0086
256	7.1905e-04	1.0352	6.2398e-04	1.0352	5.0032e-04	1.0352

Table 2. Weighted $H^1(\Omega)$ -norm errors and convergence rates.

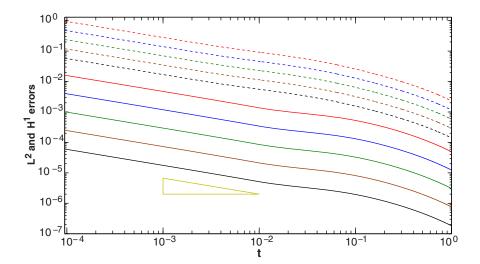


FIGURE 1. Plots of the errors $E_{h,0}^n$ (solid lines) and $E_{h,1}^n$ (dashed lines) as a function of t_n , for $\alpha = 0.7$ with M = 16, 32, 64, 128, and 256 (in order from top to bottom). The triangle indicates the gradient $-3\alpha/4$ for a function proportional to $t^{-3\alpha/4}$; cf. (5.1).

estimate in (4.11), the computed values of $\sigma_{h,0}$ and $\sigma_{h,1}$ are close to 2 and 1, respectively. Furthermore, Figure 1 shows how the L^2 error $E^n_{h,0}$ (solid lines) and H^1 error $E^n_{h,1}$ (dashed lines) vary with t_n for different mesh size h. Due to the log-log scale, the graph of a function proportional to $t^{-3\alpha/4}$ appears as a straight line with gradient $-3\alpha/4$, indicated by the small triangle, and we observe exactly this behavior of the error for t (relatively) close to zero.

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