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FINITE ELEMENT APPROXIMATION OF A TIME-FRACTIONAL DIFFUSION PROBLEM FOR A DOMAIN WITH A RE-ENTRANT CORNER

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Abstract

An initial-boundary value problem for a time-fractional diffusion equation is discretized in space, using continuous piecewise-linear finite elements on a domain with a re-entrant corner. Known error bounds for the case of a convex domain break down, because the associated Poisson equation is no longer H^2-regular. In particular, the method is no longer second-order accurate if quasi-uniform triangulations are used. We prove that a suitable local mesh refinement about the re-entrant corner restores second-order convergence. In this way, we generalize known results for the classical heat equation.

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1. Introduction

In a standard model of subdiffusion [10], each particle undergoes a continuous-time random walk with a common waiting-time distribution that obeys a power law. Consequently, the expected waiting time is infinite and the mean-square displacement of a particle is proportional to t^α, with $0 < \alpha < 1$. Such behaviour has been observed in many settings. For example, Drazer and Zanette [5] measured $\alpha = 0.63$ in tracer-dispersion experiments in a medium made of activated carbon porous grains, and Weiss et al. [17, Table 1] observed values of α ranging from 0.59 to 0.84 in fluorescence correlation spectroscopy experiments with inert tracer particles in the cytoplasm of living cells.

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The macroscopic concentration $u(x,t)$ of the particles satisfies the time-fractional (sub)diffusion equation [10, equation (6.8)],

$$\partial_t u - \partial_t^{1-\alpha} K\nabla^2 u = f(x,t). \tag{1.1}$$

Here, $\partial_t = \partial/\partial t$ and ∇^2 denotes the spatial Laplacian. The fractional time derivative is of Riemann–Liouville type [14]:

$$\partial_t^{1-\alpha} v(x,t) = \frac{\partial}{\partial t}\int_0^t \omega_\alpha(t-s)v(x,s)\,ds, \quad \omega_\alpha(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)} \quad \text{for } t>0.$$

If no sources or sinks are present, then the inhomogeneous term f is identically zero. We assume for simplicity that the generalized diffusivity K is a positive constant, and that the fractional partial differential equation (PDE) (1.1) holds for x in a polygonal domain, $\Omega \subseteq \mathbb{R}^2$, subject to homogeneous Dirichlet boundary conditions, with the initial condition

$$u(x,0) = u_0(x) \quad \text{for } x \in \Omega.$$

In the limiting case, when $\alpha \to 1$, the fractional PDE (1.1) reduces to the classical heat equation that arises when the diffusing particles instead undergo Brownian motion.

Consider a spatial discretization of the preceding initial-boundary value problem using continuous piecewise-linear finite elements to obtain a semidiscrete solution u_h, and suppose that $f \equiv 0$. The behaviour of u_h is well understood if Ω is convex [9, 12]; in this case, for general initial data $u_0 \in L_2(\Omega)$ and an appropriate choice of $u_h(0)$, we have

$$\|u_h(t) - u(t)\| \le Ct^{-\alpha}h^2\|u_0\|, \quad 0 < t \le T,$$

whereas for smoother initial data $u_0 \in H^2(\Omega)$,

$$\|u_h(t) - u(t)\| \le Ch^2\|u_0\|_{H^2(\Omega)}, \quad 0 \le t \le T,$$

where $\|\cdot\| = \|\cdot\|_{L_2(\Omega)}$. Throughout the paper, C denotes a generic constant, independent of t, h and u. The error analysis establishing these bounds relies on the H^2-regularity property of the associated elliptic equation in Ω, namely, that if

$$-K\nabla^2 u = f \text{ in } \Omega, \quad \text{with } u = 0 \text{ on } \partial\Omega, \tag{1.2}$$

then $u \in H^2(\Omega)$ with $\|u\|_{H^2(\Omega)} \le C\|f\|$.

In the present work, our aim is to study u_h in the case where Ω has a re-entrant corner, and, therefore, is not convex. Since the above H^2-regularity breaks down, we can no longer expect $O(h^2)$ convergence if the finite element mesh is quasi-uniform. Our results generalize those of Chatzipantelidis et al. [3] for the heat equation (the limiting case $\alpha = 1$) to the fractional-order case ($0 < \alpha < 1$). Our method of analysis relies on the Laplace transformation, extending the approach of McLean and Thomee [12] for the fractional-order problem on a convex domain.

To focus on the essential difficulty, we assume that Ω has only a single re-entrant corner with angle π/β for $1/2 < \beta < 1$. Without loss of generality, we assume that this

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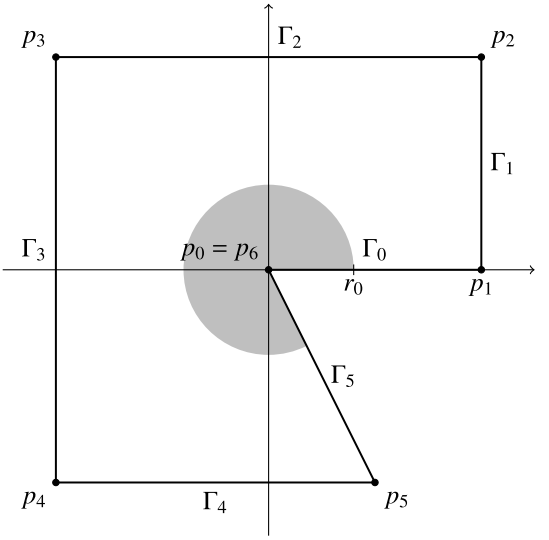

FIGURE 1. A polygonal domain with a re-entrant corner; the region (1.3) is shaded.

corner is located at the origin and that, for some $r_0 > 0$, the intersection of Ω with the open disk $|x| < r_0$ is described in polar coordinates by

$$0 < r < r_0 \quad \text{and} \quad 0 < \theta < \pi/\beta, \tag{1.3}$$

as illustrated in Figure 1. We denote the vertices of Ω by $p_0 = (0,0), p_1, p_2, \ldots, p_J = p_0$, and the jth side by

$$\Gamma_j = (p_j, p_{j+1}) = \{\, (1-\sigma)p_j + \sigma p_{j+1} : 0 < \sigma < 1 \,\} \quad \text{for } 0 \le j \le J-1.$$

Section 2 summarizes some key facts about the singular behaviour of the solution to the elliptic problem (1.2). In Section 3, we describe a family of shape-regular triangulations $\mathcal{T}_h$ (indexed by the mesh parameter h) that depend on a local refinement parameter $\gamma \ge 1$. The elements near the origin have sizes of order h^γ, so the $\mathcal{T}_h$ are quasi-uniform if $\gamma = 1$, but become more highly refined with increasing γ. Our error bounds will be stated in terms of the quantity

$$\epsilon(h,\gamma) = \begin{cases} h^{\gamma\beta}/\sqrt{\gamma^{-1}-\beta}, & 1 \le \gamma < 1/\beta, \\ h\sqrt{\log(1+h^{-1})}, & \gamma = 1/\beta, \\ h/\sqrt{\beta-\gamma^{-1}}, & \gamma > 1/\beta, \end{cases} \tag{1.4}$$

which ranges in size from $O(h^\beta)$ when $\gamma = 1$ (the quasi-uniform case) down to $O(h)$ when $\gamma > 1/\beta$. We briefly review results for the finite element approximation of the elliptic problem, needed for our subsequent analysis: the error in $H^1(\Omega)$ is of order $\epsilon(h,\gamma)$, and the error in $L_2(\Omega)$ is of order $\epsilon(h,\gamma)^2$, assuming $f \in L_2(\Omega)$.

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Section 4 gathers together some pertinent facts about the solution of the time-dependent problem (1.1) and its Laplace transform. Next, in Section 5, we introduce the semidiscrete finite element solution $u_h(t)$ of the time-dependent problem, and see that its stability properties mimic those of $u(t)$. In Section 6 we study first the homogeneous equation (that is, the case $f \equiv 0$), showing that the error in $L_2(\Omega)$ is of order $t^{-\alpha}\epsilon(h,\gamma)^2$ when $u_0 \in L_2(\Omega)$. For smoother initial data, the L_2-error is of order $\epsilon(h,\gamma)^2$ uniformly for $0 \le t \le T$. We also prove that for the inhomogeneous equation ($f \not\equiv 0$) with vanishing initial data ($u_0 \equiv 0$), the error in $L_2(\Omega)$ is of order $t^{1-\alpha}\epsilon(h,\gamma)^2$. Thus, by choosing the mesh refinement parameter $\gamma > 1/\beta$ we can restore second-order convergence in $L_2(\Omega)$. Section 7 outlines briefly how these results are affected by different choices of the boundary conditions, and Section 8 discusses two numerical examples that illustrate our theoretical error bounds. Finally, we offer some concluding remarks in Section 9.

2. Singular behaviour in the elliptic problem

In the weak formulation of the elliptic boundary-value problem (1.2) we introduce the Sobolev space

$$V = \widetilde{H}^1(\Omega) = H^1_0(\Omega),$$

and seek $u \in V$ such that

$$a(u,v) = \langle f, v\rangle \quad \text{for all } v \in V,$$

where

$$a(u,v) = K\int_\Omega \nabla u \cdot \nabla v\, dx \quad \text{and} \quad \langle f, v\rangle = \int_\Omega f v\, dx. \tag{2.1}$$

Here, f may belong to the dual space $V^* = H^{-1}(\Omega)$, if $\langle f, v\rangle$ is interpreted as the duality pairing on $V^* \times V$. Since $a(u,v)$ is bounded and coercive on $\widetilde{H}^1(\Omega)$, the Lax–Milgram theorem [4, Theorem 1.1.3] ensures the existence of a unique weak solution u satisfying

$$\|u\|_{\widetilde{H}^1(\Omega)} \le C\|f\|_{H^{-1}(\Omega)}. \tag{2.2}$$

To understand the difficulty created by the re-entrant corner, we separate variables in polar coordinates and construct the functions

$$u_n^\pm(x) = r^{\pm n\beta}\sin(n\beta\theta) \quad \text{for } x = (r\cos\theta, r\sin\theta) \text{ and } n = 1, 2, 3, \ldots,$$

which satisfy

$$\nabla^2 u_n^\pm = 0 \quad \text{for } 0 < r < \infty \text{ and } 0 < \theta < \pi/\beta \tag{2.3}$$

with $u_n^\pm = 0$, if $\theta = 0$ or $\theta = \pi/\beta$. Introducing a C^∞ cutoff function η with

$$\eta(x) = 1 \quad \text{for } |x| \le r_0/2 \quad \text{and} \quad \eta(x) = 0 \quad \text{for } |x| \ge r_0,$$

we find that

$$\eta u_n^+ \in \widetilde{H}^1(\Omega), \quad \text{but} \quad \eta u_n^- \notin \widetilde{H}^1(\Omega) \quad \text{for all } n \ge 1,$$

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and that

$$\eta u_n^+ \in H^2(\Omega) \quad \text{for all } n \geq 2, \quad \text{but} \quad \eta u_1^+ \notin H^2(\Omega).$$

Now consider the function $f = -K\nabla^2(\eta u_1^+)$. The choice of η means that $f(x) = 0$ for $|x| \leq r_0/2$, and consequently f is C^∞ on $\overline{\Omega}$. Nevertheless, the (unique weak) solution of (1.2), namely $u = \eta u_1^+$, fails to belong to $H^2(\Omega)$.

Let $A = -K\nabla^2$ and

$$V^2 = H^2(\Omega) \cap \widetilde{H}^1(\Omega) = \{\, v \in H^2(\Omega) \mid v = 0 \text{ on } \partial\Omega \,\}. \tag{2.4}$$

THEOREM 2.1. *The bounded linear operator defined by the restriction*

$$A|_{V^2} : V^2 \to L_2(\Omega),$$

is one-to-one and has a closed range.

PROOF. See Grisvard [8, Section 2.3]. □

Our task now is to identify the orthogonal complement in $L_2(\Omega)$ of the range

$$\mathcal{R} = \{\, f \in L_2(\Omega) \mid f = Au \text{ for some } u \in V^2 \,\}.$$

To this end, we define in the usual way the Hilbert space

$$L_2(\Omega, A) = \{\, \phi \in L_2(\Omega) \mid A\phi \in L_2(\Omega) \,\}$$

with the graph norm $\|\phi\|^2_{L_2(\Omega,A)} = \|\phi\|^2 + \|A\phi\|^2$. Let ∂_n denote the outward normal derivative operator. It can be shown [8, Theorems 1.4.2 and 1.5.2] that the trace map $\phi \mapsto (\phi|_{\Gamma_j}, \partial_n\phi|_{\Gamma_j})$ has unique extensions from $C^1(\overline{\Omega})$ to bounded linear operators

$$H^2(\Omega) \to H^{3/2}(\Gamma_j) \times H^{1/2}(\Gamma_j) \quad \text{and} \quad L_2(\Omega, A) \to \widetilde{H}^{-1/2}(\Gamma_j) \times \widetilde{H}^{-3/2}(\Gamma_j),$$

and that the second Green identity holds in the form [8, Theorem 1.5.3]

$$\int_\Omega [(Au)v - u(Av)]\, dx = \sum_{j=0}^{J-1} K[\langle u, \partial_n v\rangle_{\Gamma_j} - \langle \partial_n u, v\rangle_{\Gamma_j}]$$

for $u \in H^2(\Omega)$ and $v \in L_2(\Omega, A)$. Hence,

$$\langle Au, \phi\rangle = \langle u, A\phi\rangle \quad \text{if } u \in V^2,\ \phi \in L_2(\Omega, A) \text{ and } \phi|_{\Gamma_j} = 0 \text{ for all } j,$$

implying that $\mathcal{R}$ is orthogonal in $L_2(\Omega)$ to the closed subspace

$$\mathcal{N} = \{\phi \in L_2(\Omega, A) \mid A\phi = 0 \text{ in } \Omega, \text{ and } \phi|_{\Gamma_j} = 0 \text{ for every } j\}.$$

Notice that $\mathcal{N} \cap \widetilde{H}^1(\Omega) = \{0\}$, because if $f = 0$, then the unique weak solution of (1.2) in $\widetilde{H}^1(\Omega)$ is $u = 0$.

THEOREM 2.2. *The Hilbert space $L_2(\Omega)$ is the orthogonal direct sum of $\mathcal{R}$ and $\mathcal{N}$, and* $\dim \mathcal{N} = 1$ *(assuming that Ω has only a single re-entrant corner).*

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Proof. See Grisvard [8, Theorem 2.3.7]. □

Thus, given any $f \in L_2(\Omega)$, the solution $u \in \widetilde{H}^1(\Omega)$ of (1.2) belongs to $H^2(\Omega)$ if and only if $f \perp \mathcal{N}$. Consequently, the following holds for f in general.

Theorem 2.3. *There exists $q \in \mathcal{N}$ (depending only on Ω and η) such that if $f \in L_2(\Omega)$ then the weak solution u of (1.2) satisfies $u - \langle f, q\rangle \eta u_1^+ \in V^2$ with*

$$\|u - \langle f, q\rangle \eta u_1^+\|_{H^2(\Omega)} \le C\|f\|.$$

Proof. Choose any nonzero $\phi \in \mathcal{N}$. Since $\eta u_1^+ \in L_2(\Omega, A)$ but $\eta u_1^+ \notin V^2$, we have $\langle A(\eta u_1^+), \phi\rangle \ne 0$ and may therefore define $q = c\phi \in \mathcal{N}$ by letting $c = 1/\langle A(\eta u_1^+), \phi\rangle$, so that $\langle A(\eta u_1^+), q\rangle = 1$. Define

$$u_1 = u - \langle f, q\rangle \eta u_1^+ \in \widetilde{H}^1(\Omega),$$

and observe that u_1 satisfies $Au_1 = f_1$ where $f_1 = f - \langle f, q\rangle A(\eta u_1^+)$. We deduce that $u_1 \in H^2(\Omega)$ because $\langle f_1, q\rangle = 0$, with

$$\|u_1\|_{H^2(\Omega)} \le C\|f_1\| \le C\|f\| + C|\langle f, q\rangle| \le C\|f\|,$$

since $A(\eta u_1^+) \in C^\infty(\overline{\Omega})$ and $q \in L_2(\Omega)$. □

3. Finite element approximation

Consider a family $\mathcal{T}_h$ of shape-regular triangulations of Ω, indexed by the maximum element diameter h. For each element $\triangle \in \mathcal{T}_h$, let

$$h_\triangle = \operatorname{diam}(\triangle) \quad \text{and} \quad r_\triangle = \operatorname{dist}(0, \triangle),$$

and suppose that for some $\gamma \ge 1$,

$$chr_\triangle^{1-1/\gamma} \le h_\triangle \le Chr_\triangle^{1-1/\gamma}, \quad \text{whenever } h^\gamma \le r_\triangle \le 1, \tag{3.1}$$

with

$$ch^\gamma \le h_\triangle \le Ch^\gamma, \quad \text{whenever } r_\triangle \le h^\gamma. \tag{3.2}$$

Thus, if $\gamma = 1$ then the mesh is globally quasi-uniform, but for $\gamma > 1$ the element diameter decreases from order h, when $r_\triangle \ge 1$, to order h^γ, when $r_\triangle \le h^\gamma$. Such triangulations are widely used for elliptic problems on domains with re-entrant corners (see, for instance, Apel et al. [1, Section 3]).

For each triangulation $\mathcal{T}_h$, we let V_h denote the corresponding space of continuous piecewise-linear functions that vanish on $\partial\Omega$, so that $V_h \subseteq V = \widetilde{H}^1(\Omega)$. Since the bilinear form (2.1) is bounded and coercive on V, there exists a unique finite element solution $u_h \in V_h$ defined by

$$a(u_h, v) = \langle f, v\rangle \quad \text{for all } v \in V_h. \tag{3.3}$$

This solution is stable in $\widetilde{H}^1(\Omega)$,

$$\|u_h\|_{\widetilde{H}^1(\Omega)} \le C\|f\|_{H^{-1}(\Omega)}, \tag{3.4}$$

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and Céa's lemma [4, Theorem 2.4.1] gives the quasi-optimal error bound

$$\|u_h - u\|_{\widetilde{H}^1(\Omega)} \le C \min_{v\in V_h} \|v - u\|_{\widetilde{H}^1(\Omega)}. \tag{3.5}$$

Let $\Pi_h : C(\overline{\Omega}) \to V_h$ denote the nodal interpolation operator, define the seminorm

$$|v|_{m,\Omega} = \Big(\sum_{j_1+j_2=m} \int_\Omega |\partial^j v(x)|^2 \, dx \Big)^{1/2},$$

where $\partial^j = \partial_{x_1}^{j_1} \partial_{x_2}^{j_2}$, and recall the standard interpolation error bounds [4]

$$|v - \Pi_h v|_{m,\triangle} \le C h_\triangle^{2-m} |v|_{2,\triangle}, \quad m \in \{0, 1\}. \tag{3.6}$$

The next theorem reflects the influence of the singular behaviour of u and the local mesh refinement parameter γ on the accuracy of the approximation $u \approx \Pi_h u$.

THEOREM 3.1. *If $f \in L_2(\Omega)$, then the solution $u \in V$ of the elliptic problem (1.2) satisfies*

$$\|u - \Pi_h u\| \le Ch\epsilon(\gamma, h)\|f\| \quad \textit{and} \quad \|u - \Pi_h u\|_{\widetilde{H}^1(\Omega)} \le C\epsilon(\gamma, h)\|f\|,$$

where $\epsilon(h, \gamma)$ is given by (1.4).

PROOF. We use Theorem 2.3 to split u into singular and regular parts:

$$u = u_{\rm s} + u_{\rm r}, \quad u_{\rm s} = \langle f, q\rangle \eta u_1^+, \quad u_{\rm r} \in H^2(\Omega),$$

with $\|u_{\rm r}\|_{H^2(\Omega)} \le C\|f\|$, leading to a corresponding decomposition of the interpolation error,

$$u - \Pi_h u = (u_{\rm s} - \Pi_h u_{\rm s}) + (u_{\rm r} - \Pi_h u_{\rm r}).$$

We see from (3.6) that

$$\|u_{\rm r} - \Pi_h u_{\rm r}\| \le Ch^2 |u_{\rm r}|_{2,\Omega} \le Ch^2\|f\| \le Ch\epsilon(h, \gamma)\|f\|$$

and

$$|u_{\rm r} - \Pi_h u_{\rm r}|_{1,\Omega} \le Ch|u_{\rm r}|_{2,\Omega} \le Ch\|f\| \le C\epsilon(h, \gamma)\|f\|,$$

so it suffices to consider $u_{\rm s} - \Pi_h u_{\rm s}$. Note that $|\partial^j u_{\rm s}(x)| \le C\|f\| \, |x|^{\beta-|j|}$ for any multi-index j, because u_1^+ is homogeneous of degree β.

We partition the triangulation into three subsets,

$$\mathcal{T}_h^1 = \{ \triangle \in \mathcal{T}_h \mid r_\triangle < h^\gamma\}, \quad \mathcal{T}_h^2 = \{ \triangle \in \mathcal{T}_h \mid h^\gamma \le r_\triangle < 1\}, \quad \mathcal{T}_h^3 = \{ \triangle \in \mathcal{T}_h \mid r_\triangle \ge 1\},$$

and write

$$|u_{\rm s} - \Pi_h u_{\rm s}|_{1,\Omega}^2 = S_1 + S_2 + S_3 \quad \text{where } S_p = \sum_{\triangle\in\mathcal{T}_h^p} |u_{\rm s} - \Pi_h u_{\rm s}|_{1,\triangle}^2 \text{ for } p = 1, 2, 3.$$

If $r_\triangle < h^\gamma$, then $|u_{\rm s} - \Pi_h u_{\rm s}|_{1,\triangle} \le |u_{\rm s}|_{1,\triangle} + |\Pi_h u_{\rm s}|_{1,\triangle}$, and we estimate separately

$$|u_{\rm s}|_{1,\triangle}^2 \le C\|f\|^2 \int_\triangle |x|^{2(\beta-1)} dx$$

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and, using (3.2),

$$|\Pi_h u_s|^2_{1,\triangle} \le Ch_\triangle^{-2}|\Pi_h u_s|^2_{0,\triangle} \le Ch^{-2\gamma}\|f\|^2 \int_\triangle |x|^{2\beta}\,dx.$$

Since $|x| \le r_\triangle + h_\triangle \le Ch^\gamma$ for $x \in \triangle$, we have

$$S_1 \le C\|f\|^2 \int_{|x|\le Ch^\gamma} |x|^{2(\beta-1)}\,dx + Ch^{-2\gamma}\|f\|^2 \int_{|x|\le Ch^\gamma} |x|^{2\beta}\,dx \le Ch^{2\gamma\beta}\|f\|^2. \tag{3.7}$$

If $h^\gamma \le r_\triangle < 1$, then (3.6) gives

$$|u_s - \Pi_h u_s|^2_{1,\triangle} \le Ch_\triangle^2\|f\|^2 \int_\triangle |x|^{2(\beta-2)}\,dx,$$

and our assumption (3.1) on the mesh implies that for $x \in \triangle$,

$$h_\triangle|x|^{\beta-2} \le Chr_\triangle^{1-1/\gamma}|x|^{\beta-2} = Ch\left(\frac{r_\triangle}{|x|}\right)^{1-1/\gamma}|x|^{\beta-1-1/\gamma} \le Ch|x|^{\beta-1-1/\gamma},$$

so

$$\begin{aligned} S_2 &\le Ch^2\|f\|^2 \int_{h^\gamma\le|x|\le 1+h} |x|^{2(\beta-1-1/\gamma)}\,dx \\ &\le Ch^2\|f\|^2 \int_{h^\gamma}^{1+h} r^{2(\beta-1/\gamma)-1}\,dr \le C\epsilon(h,\gamma)^2\|f\|^2. \end{aligned} \tag{3.8}$$

In the remaining case, $r_\triangle \ge 1$, putting $R = \sup\{|x| \mid x \in \Omega\}$, we have $1 \le |x| \le R$ for $x \in \triangle$, and thus,

$$S_3 \le \sum_{\triangle\in\mathcal{T}_h^3} Ch_\triangle^2\|f\|^2 \int_\triangle dx \le Ch^2\|f\|^2 \int_{1\le|x|\le R} dx \le Ch^2\|f\|^2. \tag{3.9}$$

Together, (3.7)–(3.9) show that $|u_s - \Pi_h u_s|_{1,\Omega} \le C\epsilon(h,\gamma)\|f\|$.

A similar argument shows that

$$\sum_{\triangle\in\mathcal{T}_h^1} |u_s - I_h u_s|^2_{0,\triangle} \le C\|f\|^2 \int_0^{Ch^\gamma} h^{2\gamma\beta} r\,dr \le Ch^{2\gamma(\beta+1)}\|f\|^2$$

and

$$\begin{aligned} \sum_{\triangle\in\mathcal{T}_h^2\cup\mathcal{T}_h^3} |u_s - I_h u_s|^2_{0,\triangle} &\le Ch^4\|f\|^2 \int_{h^\gamma}^R r^{2(\beta-1/\gamma)-1} r^{2(1-1/\gamma)}\,dr \\ &\le Ch^2\epsilon(h,\gamma)^2\|f\|^2. \end{aligned}$$

Hence, $\|u_s - \Pi_h u_s\| \le Ch\epsilon(h,\gamma)\,\|f\|$ and the desired bounds follow. □

We are now able to estimate the finite element error.

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THEOREM 3.2. *If $f \in L_2(\Omega)$, then the finite element solution $u_h \in V_h$ of the elliptic problem (1.2) satisfies*

$$\|u_h - u\| \le C\epsilon(\gamma, h)^2\|f\| \quad \text{and} \quad \|u_h - u\|_{\widetilde{H}^1(\Omega)} \le C\epsilon(\gamma, h)\|f\|,$$

where $\epsilon(h, \gamma)$ is given by (1.4).

PROOF. The bound in $\widetilde{H}^1(\Omega)$ follows at once from (3.5) and Theorem 3.1. The error bound in $L_2(\Omega)$ is proved via the usual Aubin–Nitsche method [4, Theorem 3.2.4]. In fact, given any $\phi \in L_2(\Omega)$, the dual variational problem

$$a(w, \psi) = \langle w, \phi\rangle \quad \text{for all } w \in \widetilde{H}^1(\Omega)$$

has a unique solution $\psi \in \widetilde{H}^1(\Omega)$. Since the bilinear form a is symmetric, the preceding estimate for $u - \Pi_h u$ carries over, with ϕ playing the role of f to yield $\|\psi - \Pi_h\psi\|_{\widetilde{H}^1(\Omega)} \le C\epsilon(h, \gamma)\|\phi\|$. Thus,

$$\begin{aligned}|\langle u_h - u, \phi\rangle| &= |a(u_h - u, \psi)| = |a(u_h - u, \psi - \Pi_h\psi)| \\ &\le C\|u_h - u\|_{\widetilde{H}^1(\Omega)}\|\psi - \Pi_h\psi\|_{\widetilde{H}^1(\Omega)} \\ &\le C\epsilon(h, \gamma)^2\|f\|\,\|\phi\|,\end{aligned}$$

implying that $\|u_h - u\| \le C\epsilon(h, \gamma)^2\|f\|$. □

4. The time-dependent problem

We may view $A = -K\nabla^2$ as an unbounded operator on $L_2(\Omega)$ with domain V^2 given by (2.4). Since the associated bilinear form (2.1) is symmetric and coercive, and since the inclusion $\widetilde{H}^1(\Omega) \subseteq L_2(\Omega)$ is compact, there exists a complete orthonormal sequence of eigenfunctions $\phi_1, \phi_2, \phi_3, \ldots$ and corresponding real eigenvalues $\lambda_1, \lambda_2, \lambda_3, \ldots$ with $\lambda_j \to \infty$ as $j \to \infty$. Thus,

$$A\phi_n = \lambda_n\phi_n \quad \text{and} \quad \langle\phi_m, \phi_n\rangle = \delta_{mn} \quad \text{for all } m, n \in \{1, 2, 3, \ldots\}, \tag{4.1}$$

and we may assume that $0 < \lambda_1 \le \lambda_2 \le \lambda_3 \le \cdots$. Moreover,

$$(zI - A)^{-1} : L_2(\Omega) \to L_2(\Omega)$$

is a bounded linear operator for each complex number z not in the spectrum, $\mathrm{spec}(A) = \{\lambda_1, \lambda_2, \lambda_3, \ldots\}$, and, given any $\theta_0 \in (0, \pi)$, we have a resolvent estimate in the induced operator norm [7, Lemma 1],

$$\|(zI - A)^{-1}\| \le \frac{1 + 2/\lambda_1}{\sin\theta_0}\,\frac{1}{1 + |z|} \quad \text{for } |\arg z| > \theta_0. \tag{4.2}$$

Define the Laplace transform $\hat{f} = \mathcal{L}f$ of a suitable $f : [0, \infty) \to L_2(\Omega)$ by

$$\hat{f}(z) = (\mathcal{L}f)(z) = \mathcal{L}\{f(t)\}_{t\to z} = \int_0^\infty e^{-zt}f(t)\,dt,$$

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for $\Re z$ sufficiently large. Since $\mathcal{L}\{\partial_t^{1-\alpha} f\}_{t\to z} = z^{1-\alpha}\hat{f}(z)$, a formal calculation implies that the fractional diffusion equation (1.1) transforms into an elliptic problem (with complex coefficients) for $\hat{u}(z)$,

$$z\hat{u}(z) + z^{1-\alpha}A\hat{u}(z) = u_0 + \hat{f}(z),$$

and so

$$\hat{u}(z) = z^{\alpha-1}(z^\alpha I + A)^{-1}(u_0 + \hat{f}(z)). \tag{4.3}$$

The boundary condition $u(t) = 0$ on $\partial\Omega$ transforms to give $\hat{u}(z) = 0$ on $\partial\Omega$. Using $\mathcal{L}\{t^{p\alpha}/\Gamma(1+p\alpha)\}_{t\to z} = z^{-1-p\alpha}$, we find that for $\lambda > 0$ and $|z| > \lambda^{1/\alpha}$,

$$\begin{aligned} z^{\alpha-1}(z^\alpha + \lambda)^{-1} &= z^{-1}\sum_{p=0}^{\infty}(-\lambda z^{-\alpha})^p \\ &= \mathcal{L}\Big\{\sum_{p=0}^{\infty}\frac{(-\lambda t^\alpha)^p}{\Gamma(1+p\alpha)}\Big\}_{t\to z} = \mathcal{L}\{E_\alpha(-\lambda t^\alpha)\}, \end{aligned}$$

where $E_\alpha(y) = \sum_{p=0}^{\infty} y^p/\Gamma(1+p\alpha)$ denotes the Mittag–Leffler function. The inequalities $0 \le E_\alpha(-t) \le 1$, for $0 \le t < \infty$ [11, (2.8)], imply that the sum

$$\mathcal{E}(t)v = \sum_{n=1}^{\infty} E_\alpha(-\lambda_n t^\alpha)\langle v, \phi_n\rangle\phi_n \tag{4.4}$$

defines a bounded linear operator $\mathcal{E}(t) : L_2(\Omega) \to L_2(\Omega)$, satisfying

$$\|\mathcal{E}(t)v\| \le \|v\| \quad \text{for } 0 \le t < \infty. \tag{4.5}$$

Thus, for each eigenfunction ϕ_n,

$$z^{\alpha-1}(z^\alpha I + A)^{-1}\phi_n = z^{\alpha-1}(z^\alpha + \lambda_n)^{-1}\phi_n = \mathcal{L}\{E_\alpha(-\lambda_n t^\alpha)\phi_n\}_{t\to z},$$

and we conclude that

$$\widehat{\mathcal{E}}(z) = z^{\alpha-1}(z^\alpha I + A)^{-1}.$$

Writing (4.3) as $\hat{u}(z) = \widehat{\mathcal{E}}(z)u_0 + \widehat{\mathcal{E}}(z)\hat{f}(z)$ yields the Duhamel formula,

$$u(t) = \mathcal{E}(t)u_0 + \int_0^t \mathcal{E}(t-s)f(s)\,ds \quad \text{for } t > 0 \tag{4.6}$$

that serves to define the *mild solution* of the initial-boundary value problem for (1.1). In particular, $\mathcal{E}(t)$ is the solution operator for the homogeneous problem ($f \equiv 0$) with initial data $u_0 \in L_2(\Omega)$. Also, the bound (4.5) immediately implies a stability estimate in $L_2(\Omega)$ for a general, locally integrable $f : [0,\infty) \to L_2(\Omega)$, namely

$$\|u(t)\| \le \|u_0\| + \int_0^t \|f(s)\|\,ds \quad \text{for } t > 0.$$

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5. The semidiscrete finite element solution

Let P_h denote the orthoprojector $L_2(\Omega) \to V_h$, that is, $P_h v \in V_h$ satisfies

$$\langle P_h v, w\rangle = \langle v, w\rangle \quad \text{for all } v \in L_2(\Omega) \text{ and } w \in V_h.$$

There exists a unique linear operator $A_h : V_h \to V_h$ such that

$$\langle A_h v, w\rangle = a(v, w) \quad \text{for all } v, w \in V_h,$$

and the operator equation $A_h u_h = P_h f$ is equivalent to the variational equation (3.3) used to define the finite element solution $u_h \in V_h$ of the elliptic problem (1.2). Denote the number of degrees of freedom by $N = \dim V_h$, and equip V_h with the norm induced from $L_2(\Omega)$. The finite element space V_h has an orthonormal basis of eigenfunctions $\Phi_1, \Phi_2, \ldots, \Phi_N$ with corresponding real eigenvalues $\Lambda_1, \Lambda_2, \ldots, \Lambda_N$. Thus,

$$A_h \Phi_n = \Lambda_n \Phi_n \quad \text{and} \quad \langle \Phi_m, \Phi_n\rangle = \delta_{mn} \quad \text{for } m, n \in \{1, 2, \ldots, N\},$$

and we assume that $0 < \Lambda_1 \le \Lambda_2 \le \cdots \le \Lambda_N$. Moreover, the resolvent

$$(zI - A_h)^{-1} : V_h \to V_h$$

exists for every $z \notin \operatorname{spec}(A_h) = \{\Lambda_1, \Lambda_2, \ldots, \Lambda_N\}$, and we have the following estimate corresponding to (4.2):

$$\|(zI - A_h)^{-1}\| \le \frac{1 + 2/\Lambda_1}{\sin\theta_0} \frac{1}{1 + |z|} \quad \text{for } |\arg z| > \theta_0. \tag{5.1}$$

Note that $\lambda_1 \le \Lambda_1$, so this bound is uniform in h.

The first Green identity [4, equation (1.2.5)] yields the variational formulation for (1.1),

$$\langle \partial_t u, v\rangle + a(\partial_t^{1-\alpha} u, v) = \langle f(t), v\rangle \quad \text{for all } v \in \widetilde{H}^1(\Omega) \text{ and } t > 0, \tag{5.2}$$

so we define the finite element solution $u_h : [0, \infty) \to V_h$ by

$$\langle \partial_t u_h, v\rangle + a(\partial_t^{1-\alpha} u_h, v) = \langle f(t), v\rangle \quad \text{for all } v \in V_h \text{ and } t > 0, \tag{5.3}$$

with $u_h(0) = u_{0h}$, where $u_{0h} \in V_h$ is a suitable approximation to the initial data u_0. Thus, the vector of nodal values $\mathbf{U}(t)$ satisfies a system of fractional ordinary differential equations (ODEs) in $\mathbb{R}^N$,

$$\mathbf{M}\partial_t \mathbf{U} + \mathbf{S}\partial_t^{1-\alpha}\mathbf{U} = \mathbf{F}(t), \tag{5.4}$$

where $\mathbf{M}$ and $\mathbf{S}$ denote the $N \times N$ mass and stiffness matrices, respectively, and $\mathbf{F}(t)$ denotes the load vector. In the limiting case as $\alpha \to 1$, when (1.1) becomes the heat equation, we see that equation (5.4) reduces to the usual system of (stiff) ODEs arising in the method of lines.

The variational equation (5.3) is equivalent to

$$\partial_t u_h + \partial_t^{1-\alpha} A_h u_h = P_h f(t) \quad \text{for } t > 0.$$

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Taking Laplace transforms as in Section 4, we find that

$$\hat{u}_h(z) = z^{\alpha-1}(z^\alpha I + A_h)^{-1}(u_{0h} + P_h\hat{f}(z)),$$

and thus,

$$u_h(t) = \mathcal{E}_h(t)u_{0h} + \int_0^t \mathcal{E}_h(t-s)P_h f(s)\,ds \quad \text{for } t > 0,$$

where

$$\mathcal{E}_h(t)v = \sum_{n=1}^{N} E_\alpha(-\Lambda_n t^\alpha)\langle v, \Phi_n\rangle\Phi_n.$$

In the same way as (4.5) we have

$$\|\mathcal{E}_h(t)v\| \le \|v\| \quad \text{for } t > 0 \text{ and } v \in V_h, \tag{5.5}$$

implying that the finite element solution is stable in $L_2(\Omega)$, that is,

$$\|u_h(t)\| \le \|u_{0h}\| + \int_0^t \|f(s)\|\,ds. \tag{5.6}$$

For convenience, we put

$$B(z) = (z^\alpha I + A)^{-1} \quad \text{and} \quad B_h(z) = (z^\alpha I + A_h)^{-1},$$

which satisfy the following bounds.

Lemma 5.1. *If* $|\arg z^\alpha| < \pi - \theta_0$, *then:*

(i) $\|B(z)v\| \le C\|v\|/(1+|z|^\alpha)$ *and* $\|B(z)v\|_{\widetilde{H}^1(\Omega)} \le C\|v\|$ *for* $v \in L_2(\Omega)$;
(ii) $\|B_h(z)v\| \le C\|v\|/(1+|z|^\alpha)$ *and* $\|B_h(z)v\|_{\widetilde{H}^1(\Omega)} \le C\|v\|$ *for* $v \in V_h$.

Proof. First, let $v \in L_2(\Omega)$. The resolvent estimate (4.2) immediately implies the desired bounds for $w(z) = B(z)v$ in $L_2(\Omega)$. To estimate the norm of $w(z)$ in $\widetilde{H}^1(\Omega)$, observe that $Aw(z) = v - z^\alpha w(z)$ so by (2.2),

$$\|w(z)\|_{\widetilde{H}^1(\Omega)} \le C\|v - z^\alpha w(z)\|_{H^{-1}(\Omega)} \le C\|v - z^\alpha B(z)v\| \le C\|v\|.$$

When $v \in V_h$, the estimates for $B_h(z)v$ follow in the same way from (5.1) and (3.4). □

Since $\mathcal{L}\{\mathcal{E}(t)\phi_n\}_{t\to z} = z^{\alpha-1}(z^\alpha + \lambda_n)^{-1}\phi_n = z^{\alpha-1}B(z)\phi_n$, the Laplace inversion formula implies that

$$\begin{aligned}\mathcal{E}(t)\phi_n &= \lim_{M\to\infty}\Big(\frac{1}{2\pi i}\int_{1-iM}^{1+iM} e^{zt}z^{\alpha-1}(z^\alpha+\lambda_n)^{-1}\,dz\Big)\phi_n \\ &= \frac{1}{2\pi i}\int_\Gamma e^{zt}z^{\alpha-1}B(z)\phi_n\,dz,\end{aligned}$$

for $t > 0$ and for a Hankel contour Γ that encircles the negative real axis counterclockwise. The factor e^{zt} is exponentially small as $\Re z \to -\infty$, so (4.5) and Lemma 5.1 ensure that

$$\mathcal{E}(t)v = \frac{1}{2\pi i}\int_\Gamma e^{zt}z^{\alpha-1}B(z)v\,dz \quad \text{for } t > 0 \text{ and } v \in L_2(\Omega), \tag{5.7}$$

where the integral over Γ is absolutely convergent in $L_2(\Omega)$.

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Likewise, $\mathcal{L}\{\mathcal{E}_h(t)\Phi_n\}_{t\to z} = z^{\alpha-1}(z^\alpha + \Lambda_n)^{-1}\Phi_n = z^{\alpha-1}B_h(z)\Phi_n$ so we have a corresponding integral representation

$$\mathcal{E}_h(t)v = \frac{1}{2\pi i}\int_\Gamma e^{zt}z^{\alpha-1}B_h(z)v\,dz \quad \text{for } t>0 \text{ and } v\in V_h. \tag{5.8}$$

6. Error bounds

Since the continuous and semidiscrete problems are both linear, for our error analysis it suffices to consider separately the cases $f\equiv 0$ and $u_0 = u_{0h} = 0$.

6.1. The homogeneous equation To find the error bound for $u_h(t) - u(t)$ in the case $f\equiv 0$, the main difficulty is to estimate the difference

$$\mathcal{E}_h(t)P_hu_0 - \mathcal{E}(t)u_0 = \frac{1}{2\pi i}\int_\Gamma e^{zt}z^{\alpha-1}G_h(z)u_0\,dz, \tag{6.1}$$

where, by equations (5.7) and (5.8), $G_h(z) = B_h(z)P_h - B(z)$. We begin by estimating $G_h(z)v$.

LEMMA 6.1. *If $v\in L_2(\Omega)$ and $|\arg z^\alpha| < \pi - \theta_0$, then*

$$\|G_h(z)v\| \le C\epsilon(h,\gamma)^2\|v\| \quad \textit{and} \quad \|G_h(z)v\|_{\widetilde{H}^1(\Omega)} \le C(1+|z|^\alpha)\epsilon(h,\gamma)\|v\|.$$

PROOF. Given $v\in L_2(\Omega)$, let $w(z) = B(z)v\in V$, so that $Aw(z) = v - z^\alpha w(z)$, and let $w_h(z)\in V_h$ be the solution of

$$A_hw_h(z) = P_h[v - z^\alpha w(z)].$$

In this way, $P_hv = z^\alpha P_hw(z) + A_hw_h(z) = (z^\alpha I + A_h)w_h(z) - z^\alpha[w_h(z) - P_hw(z)]$, and thus $B_h(z)P_hv = w_h(z) - z^\alpha B_h(z)[w_h(z) - P_hw(z)]$, implying that

$$G_h(z)v = w_h(z) - w(z) - z^\alpha B_h(z)P_h[w_h(z) - w(z)]. \tag{6.2}$$

Lemma 5.1 shows that $\|w(z)\| \le C\|v\|/(1+|z|^\alpha)$ so $\|v - z^\alpha w(z)\| \le C\|v\|$. By applying Theorem 3.2, with $w(z)$ and $v - z^\alpha w(z)$ playing the roles of u and f, respectively, we deduce that

$$\|w_h(z) - w(z)\| \le C\epsilon(h,\gamma)^2\|v\| \quad \text{and} \quad \|w_h(z) - w(z)\|_{\widetilde{H}^1(\Omega)} \le C\epsilon(h,\gamma)\|v\|.$$

The result now follows from (6.2) after another application of Lemma 5.1. □

THEOREM 6.2. *Assume that $f\equiv 0$. If $u_0\in L_2(\Omega)$, then the mild solution $u(t) = \mathcal{E}(t)u_0$ and its finite element approximation $u_h(t) = \mathcal{E}_h(t)u_{0h}$ satisfy*

$$\|u_h(t) - u(t)\| \le \|u_{0h} - P_hu_0\| + Ct^{-\alpha}\epsilon(h,\gamma)^2\|u_0\|$$

and

$$\|u_h(t) - u(t)\|_{\widetilde{H}^1(\Omega)} \le Ct^{-\alpha}\|u_{0h} - P_hu_0\| + C(t^{-2\alpha} + t^{-\alpha})\epsilon(h,\gamma)\|u_0\|$$

for $t>0$.

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PROOF. We split the error into two terms,

$$u_h(t) - u(t) = [\mathcal{E}_h(t)(u_{0h} - P_h u_0)] + [\mathcal{E}_h(t)P_h u_0 - \mathcal{E}(t)u_0]. \tag{6.3}$$

It follows from (5.5) that $\|\mathcal{E}_h(t)(u_{0h} - P_h u_0)\| \le \|u_{0h} - P_h u_0\|$. To estimate the second term in equation (6.3), we use the integral representation (6.1) with $\Gamma = \Gamma_+ - \Gamma_-$, where $\Gamma_\pm$ is the contour $z = se^{\pm i3\pi/4}$ for $0 < s < \infty$. Applying Lemma 6.1 and then making the substitution $y = st$, we find that

$$\begin{aligned}\|\mathcal{E}_h(t)P_h u_0 - \mathcal{E}(t)u_0\| &\le C\epsilon(h,\gamma)^2\|u_0\| \int_0^\infty e^{-st/\sqrt{2}} s^\alpha \frac{ds}{s} \\ &= C\epsilon(h,\gamma)^2\|u_0\| t^{-\alpha} \int_0^\infty e^{-y/\sqrt{2}} y^\alpha \frac{dy}{y},\end{aligned}$$

which proves the first error bound of the theorem.

Choosing $\Gamma = \Gamma_+ - \Gamma_-$ in the integral representation (5.8) of $\mathcal{E}_h(t)v$, and using Lemma 5.1, we have for $v \in V_h$,

$$\|\mathcal{E}_h(t)v\|_{\widetilde{H}^1(\Omega)} \le C \int_0^\infty e^{-st/\sqrt{2}} s^\alpha \|v\| \frac{ds}{s} = Ct^{-\alpha}\|v\| \int_0^\infty e^{-s/\sqrt{2}} s^\alpha \frac{ds}{s} \le Ct^{-\alpha}\|v\|,$$

so in particular, when $v = u_{0h} - P_h u_0$,

$$\|\mathcal{E}_h(t)(u_{0h} - P_h u_0)\|_{\widetilde{H}^1(\Omega)} \le Ct^{-\alpha}\|u_{0h} - P_h u_0\|.$$

Finally, using (6.1) and Lemma 6.1 again,

$$\begin{aligned}\|\mathcal{E}_h(t)P_h u_0 - \mathcal{E}(t)u_0\|_{\widetilde{H}^1(\Omega)} &\le C\epsilon(h,\gamma)\|u_0\| \int_0^\infty e^{-st/\sqrt{2}} s^\alpha (1 + s^\alpha) \frac{ds}{s} \\ &= C\epsilon(h,\gamma)\|u_0\| t^{-2\alpha} \int_0^\infty e^{-s/\sqrt{2}} s^\alpha (t^\alpha + s^\alpha) \frac{ds}{s} \\ &\le C\epsilon(h,\gamma)(t^{-\alpha} + t^{-2\alpha})\|u_0\|,\end{aligned}$$

proving the second error estimate of the theorem. □

When u_0 is sufficiently regular we obtain an error bound that is uniform in t. The proof uses the Ritz projector $R_h : \widetilde{H}^1(\Omega) \to V_h$, defined by

$$a(R_h u, v) = a(u, v) \quad \text{for all } v \in V_h, \tag{6.4}$$

and relies on the following decay property of $G_h(z)$, as $|z| \to \infty$.

LEMMA 6.3. *If $Av \in L_2(\Omega)$ and $|\arg z^\alpha| < \pi - \theta_0$, then*

$$\|G_h(z)v\| \le C\epsilon(h,\gamma)^2\|B(z)Av\| \le C|z|^{-\alpha}\epsilon(h,\gamma)^2\|Av\|.$$

PROOF. First note that by Theorem 3.2,

$$\|v - P_h v\| \le \|v - R_h v\| \le C\epsilon(h,\gamma)^2\|Av\|.$$

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We use the splitting $G_h(z) = B_h(z)P_h - B(z) = G_h^1(z) + G_h^2(z)$, where

$$G_h^1(z) = (P_h - I)B(z) \quad \text{and} \quad G_h^2(z) = B_h(z)P_h - P_hB(z).$$

Since A commutes with $B(z)$, it follows at once that

$$\|G_h^1(z)v\| \le C\epsilon(h,\gamma)^2\|AB(z)v\| = C\epsilon(h,\gamma)^2\|B(z)Av\|.$$

The definitions of P_h, A_h and R_h imply that $P_hA = A_hR_h$ (see Thomée [15, page 10]), so

$$\begin{aligned} G_h^2(z) &= B_h(z)[P_h(z^\alpha I + A) - (z^\alpha I + A_h)P_h]B(z) = B_h(z)[P_hA - A_hP_h]B(z) \\ &= B_h(z)[A_hR_h - A_hP_h]B(z) = -B_h(z)A_hP_h(I - R_h)B(z), \end{aligned}$$

and therefore, because $B_h(z)A_h = I - z^\alpha B_h(z)$, it follows that

$$\|G_h^2(z)v\| \le C\|(I - R_h)B(z)v\| \le C\epsilon(h,\gamma)^2\|AB(z)v\| = C\epsilon(h,\gamma)^2\|B(z)Av\|,$$

as required. Finally, $\|B(z)Av\| \le C\|Av\|/(1 + |z|^\alpha) \le C|z|^{-\alpha}\|Av\|$ by Lemma 5.1. □

Notice that since $B(z)A = I - z^\alpha B(z)$, Lemma 6.3 provides an alternative proof of the first conclusion of Lemma 6.1.

THEOREM 6.4. *Assume that $f \equiv 0$. If $Au_0 \in L_2(\Omega)$, then*

$$\|u_h(t) - u(t)\| \le \|u_{0h} - P_hu_0\| + C\epsilon(h,\gamma)^2\|Au_0\| \quad \textit{for } t \ge 0.$$

PROOF. In view of equation (6.3), it is again sufficient to estimate the contour integral (6.1). This time, we choose $\Gamma = \Gamma_+^t + \Gamma_0^t - \Gamma_-^t$ where $\Gamma_\pm^t$ is parameterized by $z = se^{\pm i3\pi/4}$ for $t^{-1} < s < \infty$ and where Γ_0^t is parameterized by $z = t^{-1}e^{i\theta}$ for $-3\pi/4 \le \theta \le 3\pi/4$. Lemma 6.3 implies that $\|z^{\alpha-1}G_h(z)u_0\| \le C|z|^{-1}\epsilon(h,\gamma)^2\|Au_0\|$ so

$$\|\mathcal{E}_h(t)P_hu_0 - \mathcal{E}(t)u_0\| \le C\epsilon(h,\gamma)^2\|Au_0\| \int_\Gamma |e^{zt}|\,\frac{|dz|}{|z|},$$

and it suffices to note that the integrals

$$\int_{\Gamma_\pm^t} |e^{zt}|\,\frac{|dz|}{|z|} = \int_{t^{-1}}^\infty e^{-st/\sqrt{2}}\,\frac{ds}{s} = \int_1^\infty e^{-s/\sqrt{2}}\,\frac{ds}{s}$$

and

$$\int_{\Gamma_0^t} |e^{zt}|\,\frac{|dz|}{|z|} = \int_{-3\pi/4}^{3\pi/4} e^{-\cos\theta}\,d\theta$$

are bounded independently of t. □

For intermediate regularity of u_0, we have the following error bound in which the fractional power of A is defined via the eigensystem (4.1):

$$A^\theta v = \sum_{j=1}^\infty \lambda_j^\theta \langle v, \phi_j\rangle \phi_j.$$

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Corollary 6.5. *Assume that $f \equiv 0$ and $0 < \theta < 1$. If $A^\theta u_0 \in L_2(\Omega)$ and $u_{0h} = P_h u_0$, then*

$$\|u_h(t) - u(t)\| \le Ct^{-\alpha(1-\theta)}\epsilon(h,\gamma)^2\|A^\theta u_0\| \quad \text{for } t > 0.$$

Proof. The choice of u_{0h} means that the error bounds of Theorems 6.2 and 6.4 simplify to

$$\|u_h(t) - u(t)\| \le Ct^{-\alpha}\epsilon(h,\gamma)^2\|u_0\| \quad \text{and} \quad \|u_h(t) - u(t)\| \le C\epsilon(h,\gamma)^2\|Au_0\|.$$

Hence, by interpolation, $\|u_h(t) - u(t)\| \le C(t^{-\alpha}\epsilon(h,\gamma)^2)^{1-\theta}(\epsilon(h,\gamma)^2)^\theta\|A^\theta u_0\|$. □

6.2. The inhomogeneous equation When $u_0 \equiv 0$ and $f \not\equiv 0$, we use a different approach [12, Lemma 4.1] that relies on the regularity result [11, Theorem 4.1]

$$\|A\mathcal{E}(t)v\| \le Ct^{-\alpha}\|v\| \quad \text{for } t > 0. \tag{6.5}$$

The error bound requires no spatial regularity of the source term; it suffices that $f(0) \in L_2(\Omega)$ and $\|\partial_t f\|$ is integrable in time.

Theorem 6.6. *If $u_0 = u_{0h} = 0$, then*

$$\|u_h(t) - u(t)\| \le Ct^{1-\alpha}\epsilon(h,\gamma)^2\Big(\|f(0)\| + \int_0^t \|\partial_t f(s)\|\,ds\Big) \quad \text{for } t > 0.$$

Proof. In the usual way, decompose the error as $u_h(t) - u(t) = \vartheta(t) + \varrho(t)$, where

$$\vartheta(t) = u_h(t) - R_h u(t) \in V_h \quad \text{and} \quad \varrho(t) = R_h u(t) - u(t).$$

Notice that $\vartheta(0) = \varrho(0) = 0$ and, since $\varrho(t) = \int_0^t \partial_t\varrho(s)\,ds$,

$$\|\varrho(t)\| \le \int_0^t \|\partial_t\varrho(s)\|\,ds.$$

By (5.3), if $v \in V_h$ then

$$\langle\partial_t\vartheta, v\rangle + a(\partial_t^{1-\alpha}\vartheta, v) = \langle f, v\rangle - \langle\partial_t R_h u, v\rangle - a(\partial_t^{1-\alpha}R_h u, v),$$

and using the definition of the Ritz projector (6.4) followed by (5.2),

$$a(\partial_t^{1-\alpha}R_h u, v) = a(\partial_t^{1-\alpha}u, v) = \langle f, v\rangle - \langle\partial_t u, v\rangle.$$

Thus,

$$\langle\partial_t\vartheta, v\rangle + a(\partial_t^{1-\alpha}\vartheta, v) = -\langle\partial_t\varrho, v\rangle,$$

which means that $\vartheta : [0,\infty) \to V_h$ is the finite element solution of the fractional diffusion problem with source term $-\partial_t\varrho(t)$ and zero initial data. The stability estimate (5.6) gives

$$\|\vartheta(t)\| \le \int_0^t \|\partial_t\varrho(s)\|\,ds,$$

and Theorem 3.2 implies that $\|\partial_t\rho(t)\| = \|(R_h - I)\partial_t u(t)\| \le C\epsilon(h,\gamma)^2\|A\partial_t u(t)\|$, so

$$\|u_h(t) - u(t)\| \le 2\int_0^t \|\partial_t\varrho(s)\|\,ds \le C\epsilon(h,\gamma)^2\int_0^t \|A\partial_t u(s)\|\,ds.$$

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Since

$$Au(s) = A\int_0^s \mathcal{E}(s-\tau)f(\tau)\,d\tau = \int_0^s A\mathcal{E}(\tau)f(s-\tau)\,d\tau,$$

we have

$$A\partial_t u(s) = A\mathcal{E}(s)f(0) + \int_0^s A\mathcal{E}(\tau)\partial_t f(s-\tau)\,d\tau,$$

and therefore, using (6.5),

$$\|A\partial_t u(s)\| \le Cs^{-\alpha}\|f(0)\| + \int_0^s \tau^{-\alpha}\|\partial_t f(s-\tau)\|\,d\tau.$$

Thus,

$$\int_0^t \|A\partial_t u(s)\|\,ds \le Ct^{1-\alpha}\|f(0)\| + \int_0^t\int_0^s \tau^{-\alpha}\|\partial_t f(s-\tau)\|\,d\tau\,ds,$$

and the double integral equals

$$\int_0^t\int_0^s (s-\tau)^{-\alpha}\|\partial_t f(\tau)\|\,d\tau\,ds = \int_0^t \|\partial_t f(\tau)\|(t-\tau)^{1-\alpha}\,d\tau,$$

yielding the desired estimate. □

7. Alternative boundary conditions

7.1. Neumann boundary conditions Separation of variables in polar coordinates yields the functions

$$u_n^{\pm} = r^{\pm n\beta}\cos(n\beta\theta) \quad \text{for } n = 1, 2, 3, \ldots,$$

satisfying (2.3) with $\partial_\theta u_n^{\pm} = 0$, if $\theta = 0$ or $\theta = \pi/\beta$. In addition, for $n = 0$ we find $u_0^+ = 1$ and $u_0^- = \log r$, and can readily check that

$$\eta u_n^+ \in H^1(\Omega) \quad \text{but} \quad \eta u_n^- \notin H^1(\Omega) \quad \text{for all } n \ge 0 \tag{7.1}$$

with $\eta u_n^+ \in H^2(\Omega)$ if and only if $n \ne 1$. If we impose a homogeneous Neumann boundary condition $\partial_n u = 0$ on $\partial\Omega$, then our results are essentially unchanged, but the fact that $A = -K\nabla^2$ now possesses a zero eigenvalue complicates the analysis [13, Section 4].

7.2. Mixed boundary conditions For $n = 1, 2, 3, \ldots$, the functions

$$u_n^{\pm} = r^{(n-1/2)\beta}\sin(n - \tfrac{1}{2})\beta\theta$$

satisfy (2.3) with $u_n^{\pm} = 0$ if $\theta = 0$ and $\partial_\theta u_n^{\pm} = 0$ if $\theta = \pi/\beta$. Once again, (7.1) holds for all $n \ge 1$; however, we now have

$$\eta u_n^+ \in H^2(\Omega) \quad \text{for all } n \ge 3, \quad \text{but} \quad \eta u_1^+, \eta u_2^+ \notin H^2(\Omega),$$

assuming $1/2 < \beta < 1$. Moreover, a new feature is that $\eta u_1^+ \notin H^2(\Omega)$ when $1 \le \beta < 2$, that is, for an interior angle between $\pi/2$ and π, in which case Ω is in fact convex.

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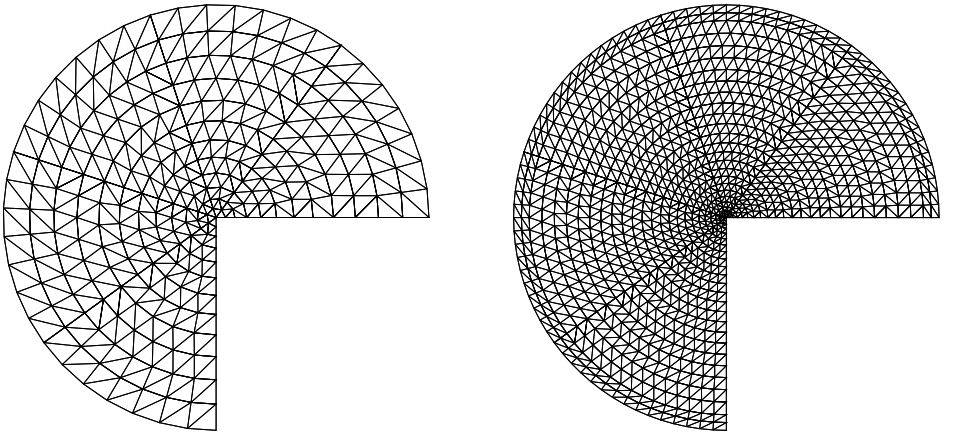

FIGURE 2. Meshes with $h_* = 2^{-3}$ (left) and $h_* = 2^{-4}$ (right) from a sequence satisfying (3.1) and (3.2) for $\gamma = 3/2$.

The proof of Theorem 3.1 must be modified by replacing β with $\beta/2$, and replacing $\epsilon(h, \gamma)$ with

$$\epsilon_{\text{mix}}(h,\gamma) = \begin{cases} h^{\gamma\beta/2}/\sqrt{\gamma^{-1} - \beta/2}, & 1 \le \gamma < 2/\beta, \\ h\sqrt{\log(1+h^{-1})}, & \gamma = 2/\beta, \\ h/\sqrt{\beta/2 - \gamma^{-1}}, & \gamma > 2/\beta, \end{cases} \tag{7.2}$$

provided the interior angles at the other vertices $p_1, p_2, \ldots, p_{J-1}$ are all less than or equal to $\pi/2$. We may then proceed as for Dirichlet boundary conditions (since all the eigenvalues of A are strictly positive), with $\epsilon(h, \gamma)$ replaced by $\epsilon_{\text{mix}}(h, \gamma)$ in our error estimates.

8. Numerical experiments

We consider two problems posed on a domain of the form

$$\Omega = \{(r\cos\theta, r\sin\theta) \mid 0 < r < 1 \text{ and } 0 < \theta < \pi/\beta\}$$

with $\beta = 2/3$. Although Ω is not a polygon, the additional error in u_h due to approximation of the curved part of $\partial\Omega$ is of order h^2 in $L_2(\Omega)$, and hence our error bounds should remain unchanged. To fix the time scale for the solutions of the fractional diffusion equation (1.1), the generalized diffusitivity K was chosen so that the smallest eigenvalue of $A = -K\nabla^2$ equals one. Figure 2 shows two successive meshes out of a sequence satisfying our assumptions (3.1) and (3.2) for $\gamma = 1/\beta = 3/2$; notice that these meshes are not nested. The mesh generation code takes a specified h_* and γ and produces a triangulation with maximum element diameter h equivalent to h_*. All source files were written in Julia 0.5 [2] with some calls to Gmsh 2.12.0 [6], and all computations performed on a desktop PC with 8 GB of RAM and an AMD A10-7850K CPU.

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For the time integration, we use a technique [12, 16] based on a quadrature approximation to the Laplace inversion formula

$$u_h(t) = \frac{1}{2\pi i}\int_\Gamma e^{zt}\hat{u}_h(z)\,dz = \frac{1}{2\pi i}\int_{-\infty}^{\infty} e^{z(\xi)t}\hat{u}(z(\xi))z'(\xi)\,d\xi,$$

where the contour Γ has the parametric representation

$$z(\xi) = \mu(1 - \sin(\delta - i\xi)) \quad \text{for } -\infty < \xi < \infty,$$

with $\delta = 1.172\,104\,23$ and $\mu = 4.492\,075\,28\,M/t$ for given $t > 0$ and a chosen positive integer M. Therefore, the contour Γ is the left branch of a hyperbola with asymptotes $y = \pm(x - \mu)\cot\delta$ for $z = x + iy$. Putting

$$z_j = z(\xi_j), \quad z'_j = z'(\xi_j), \quad \xi_j = j\,\Delta\xi, \quad \Delta\xi = \frac{1.081\,792\,14}{M},$$

we define

$$U_{M,h}(t) = \frac{\Delta\xi}{2\pi i}\sum_{j=-M}^{M} e^{z_j t}\hat{u}_h(z_j)z'_j \approx u_h(t).$$

To compute $\hat{u}_h(z_j)$ we solve the (complex) finite element equations

$$z_j^\alpha\langle\hat{u}_h(z_j),\chi\rangle + a(\hat{u}_h(z_j),\chi) = z_j^{\alpha-1}\langle u_{0h} + \hat{f}(z_j),\chi\rangle, \quad \chi \in V_h,$$

and since we choose real u_{0h} and f, it follows that $\hat{u}_h(z_{-j}) = \hat{u}_h(\bar{z}_j) = \overline{\hat{u}_h(z_j)}$. Thus, the number of elliptic solutions needed to evaluate $U_{M,h}(t)$ is only $M + 1$ rather than $2M + 1$. An error bound for the quadrature error $\|U_{M,h}(t) - u_h(t)\|$ includes a decay factor 10.1315^{-M}, and we observe that the overall error $\|U_{M,h}(t) - u(t)\|$ is dominated by the finite element error $\|u_h(t) - u(t)\|$ for some modest values of M. In the computations reported below, we used $M = 8$ to compute $U_{M,h}(t) \approx u_h(t)$, and chose $u_{0h} = P_h u_0$ for the discrete initial data.

Example 8.1. In our first example, $\alpha = 1/2$ and we chose u_0 and f so that the solution of the initial-boundary value problem for (1.1) was

$$u(x, y, t) = (1 + \omega_{\alpha+1}(t))r^\beta(1 - r)\sin(\beta\theta).$$

In view of (4.4) and (4.6), the singular behaviour of u as $r \to 0$ or $t \to 0$ is typical for such problems. Figure 3 compares the L_2-error at $t = 1$ for quasi-uniform ($\gamma = 1$) and locally refined ($\gamma = 1/\beta = 3/2$) triangulations. From Theorems 6.2 and 6.6, we expect errors of order $\epsilon(h, 1)^2 = h^{2\gamma\beta} = h^{4/3}$ and $\epsilon(h, 3/2)^2 = h^2\log^2(1 + h^{-1})$, respectively. The number of degrees of freedom is of order h^{-2} in both cases, so in Figure 3 we expect the corresponding error curves to be straight lines with gradients $-2/3$ and -1, which are in fact close to the observed values -0.7249 and -0.9707, respectively, as determined by simple, linear least-squares fits.

Example 8.2. In our second example, we imposed *mixed* boundary conditions: a homogeneous Dirichlet condition where $\theta = 0$ or $r = 1$, and a homogeneous Neumann condition where $n\theta = \pi/\beta$. As the initial data we chose the first eigenfunction of the linear operator $A = -K\nabla^2$,

$$u_0(x, y) = J_{\beta/2}(\omega r)\sin(\tfrac{1}{2}\beta\theta),$$

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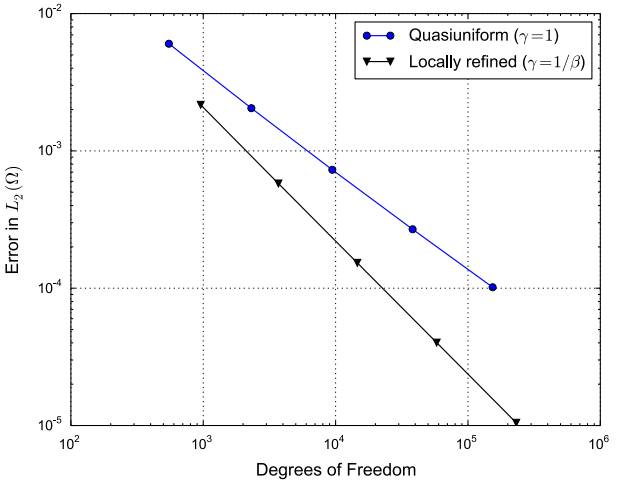

FIGURE 3. Behaviour of the L_2-error $\|u_h(t) - u(t)\|$ for Example 8.1 when $t = 1$; quasi-uniform versus locally refined triangulations.

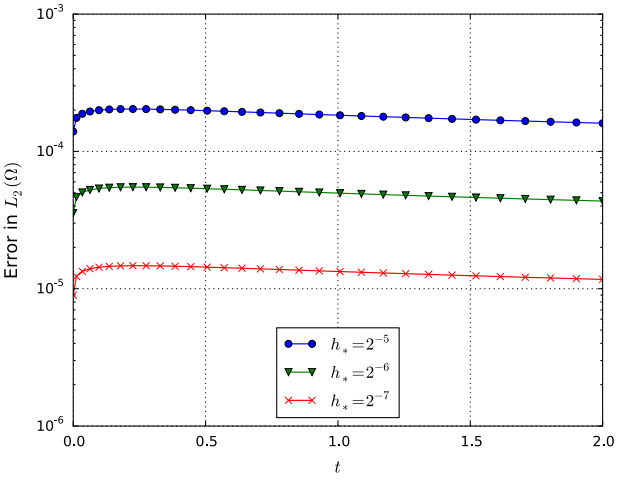

FIGURE 4. The L_2-error as a function of t for Example 8.2 with $\alpha = 1/2$ and $\gamma = 2/\beta$.

where ω is the first positive zero of the Bessel function $J_{\beta/2}$. We put $f = 0$ so (recalling that our choice of K means that the corresponding eigenvalue equals one) the solution is $u(x, y, t) = \mathcal{E}(t)u_0 = E_\alpha(-t^\alpha)u_0(x, y)$, and chose $\gamma = 2/\beta = 3$, giving $\epsilon_{\text{mix}}(h, \gamma)$ of order $h \log(1 + h^{-1})$; see (7.2). Since $A^r u_0 \propto u_0 \in L_2(\Omega)$ for all $r > 0$, we conclude from Theorem 6.4 that the L_2-error $\|u_h(t) - u(t)\|$ is of order $h^2 \log^2(1 + h^{-1})$ uniformly for $0 \le t \le T$. Figure 4 confirms this behaviour in the case $\alpha = 1/2$. Finally, Table 1 shows that at a fixed positive time $t = 1$ the L_2-error does not vary much with α.

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TABLE 1. L_2-Errors and empirical convergence rates (powers of h) for Example 8.2 when $t = 1$, with $\gamma = 2/\beta$ and different choices of α. (Recall that N denotes the number of degrees of freedom in the finite element triangulation.)

		$\alpha = 1/4$		$\alpha = 1/2$		$\alpha = 3/4$	
h_*	N	error	rate	error	rate	error	rate
2^{-4}	1957	1.465e-03		1.485e-03		1.452e-03	
2^{-5}	7593	3.673e-04	1.996	3.723e-04	1.996	3.640e-04	1.997
2^{-6}	29771	9.471e-05	1.955	9.597e-05	1.956	9.380e-05	1.956
2^{-7}	117039	2.420e-05	1.969	2.451e-05	1.970	2.391e-05	1.972
2^{-8}	466089	6.059e-06	1.998	6.119e-06	2.002	5.931e-06	2.011

9. Concluding remarks

A characteristic feature of two-dimensional elliptic boundary-value problems is that the solution is typically singular in the neighbourhood of a re-entrant corner. This behaviour carries over to the solution of the time-dependent diffusion and *fractional* diffusion equations. Our analysis shows how the accuracy of finite element approximations is compromised, unless a suitable local mesh refinement is employed to handle the large gradients around a re-entrant corner. The overall approach could be extended to treat three-dimensional problems, but it would depend on the more complicated results for the possible singularities of the elliptic problem [1]. We expect that a more promising direction for further research is to design adaptive mesh refinement schemes based on suitable *a posteriori* error indicators.

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