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Research Article

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Space-Time Petrov–Galerkin FEM for Fractional Diffusion Problems

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Abstract: We present and analyze a space-time Petrov–Galerkin finite element method for a time-fractional diffusion equation involving a Riemann–Liouville fractional derivative of order $\alpha \in (0, 1)$ in time and zero initial data. We derive a proper weak formulation involving different solution and test spaces and show the inf-sup condition for the bilinear form and thus its well-posedness. Further, we develop a novel finite element formulation, show the well-posedness of the discrete problem, and derive error bounds in both energy and L^2 norms for the finite element solution. In the proof of the discrete inf-sup condition, a certain nonstandard L^2 stability property of the L^2 projection operator plays a key role. We provide extensive numerical examples to verify the convergence analysis.

Keywords: Space-Time Finite Element Method, Petrov–Galerkin Method, Fractional Diffusion, Error Estimates

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1 Introduction

In this work, we develop and analyze a novel space-time Petrov–Galerkin formulation for time-fractional diffusion. Let $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$) be a convex polyhedral domain with a boundary $\partial\Omega$. Consider the following initial boundary value problem for the function $u(x, t)$:

$$\begin{cases} {}_0\partial_t^\alpha u - \Delta u = f & \text{in } Q_T := \Omega \times (0, T], \\ u(x, t) = 0 & \text{on } \partial\Omega \times (0, T], \\ u(x, 0) = 0 & \text{in } \Omega, \end{cases} \tag{1.1}$$

where f is a given source and $T > 0$ is the final time. Here ${}_0\partial_t^\alpha u$ denotes the left-sided Riemann–Liouville derivative of order $\alpha \in (0, 1)$ in t (cf. (2.1)).

The interest in (1.1) is motivated by its numerous applications related to anomalously slow diffusion (also known as subdiffusion), e.g., underground flow, thermal diffusion in fractal domains, and dynamics of protein molecules, to name just a few. At a microscopic level, subdiffusion processes can be described by

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continuous time random walk with a heavy-tailed waiting time distribution, and the corresponding macroscopic model is a diffusion equation with a fractional derivative in time; cf. (1.1). We refer readers to [22] for an overview of physical backgrounds and an extensive list of applications in physics, engineering, and biology.

For parabolic problems, it is customary to apply time-stepping schemes [29]. Space-time discretizations have gained some popularity in the last decade. These studies are mostly motivated by the goal to obtain efficient and convergent numerical methods without any regularity assumptions [4, 6] or to design efficient space-time adaptive algorithms [1, 5, 26, 27] and high-order schemes [2]. In the past decades, time stepping methods have also been very popular for problems involving fractional derivatives in time (see, e.g., [14, 15, 21, 25] and the references therein). However, due to the non-locality of the fractional derivative ${}_0\partial_t^\alpha u$, at each time step one has to use the numerical solutions at all preceding time levels. Thus the advantages of time stepping schemes, compared to space-time schemes, are not as pronounced as in the case of standard parabolic problems, and it is natural to consider time-space discretization.

In this work, we present a space-time variational (weak) formulation for problem (1.1) and show an inf-sup condition in Lemma 2.4. Starting from the weak form we develop a novel discretization that is based on tensor product meshes in time and space. The spatial domain Ω is discretized by a quasi-uniform triangulation with a mesh size h, while in time by a uniform mesh with step-size τ. The approximation $u_{h\tau}$ is sought in the tensor product space $\mathbb{X}_h \otimes \mathbb{U}_\tau$, where $\mathbb{X}_h$ is the space of continuous piecewise linear functions in space x and $\mathbb{U}_\tau$ is the space of fractionalized piecewise constant functions in time t. The test space is a tensor product space $\mathbb{X}_h \otimes \mathbb{W}_\tau$, where $\mathbb{W}_\tau$ is the space of piecewise constant functions in time. We establish an inf-sup condition for the discrete problem, using the L^2-projection from $\mathbb{U}_\tau$ to $\mathbb{W}_\tau$; cf. Lemma 3.2. It is worth noting that the constant in the L^2-stability of this projection depends on α and deteriorates as $\alpha \to 1$; cf. Table 1 in Section 3.2. Thus, for standard parabolic problems ($\alpha = 1$), it depends on the time step size τ, leading to an CFL-condition, a fact proved in [17]. A distinct algorithmic feature of our approach is that it leads to a time-stepping like scheme, and thus admits an efficient implementation.

Optimal-order error estimates in both energy and $L^2(Q_T)$ norms are provided under suitable temporal regularity of the source f in Theorems 5.2 and 5.3. The error analysis is carried out in two steps. First, we introduce a space semidiscrete approximation u_h and derive sharp error bounds, using the inf-sup condition for the semidiscrete problem and an approximation result from [11]. Second, we bound the difference $u_h - u_{h\tau}$, by carefully studying the fractional ODE ${}_0\partial_t^\alpha u + \lambda u = f$, $\lambda > 0$. The uniform (with respect to λ) stability of the ODE and its optimal approximation in the space $\mathbb{U}_\tau$ play a key role in the analysis. This and the expansion of $u_h(t)$ and $u_{h\tau}$ in eigenfunctions of the discrete Laplacian yields the desired error estimates for $f \in \widetilde{H}_L^s(0, T; L^2(\Omega))$, $0 \le s \le 1$, in Theorem 5.3. In particular, for $f \in L^2(Q_T)$, we have

$$\|u - u_{h\tau}\|_{L^2(Q_T)} \le c(\tau^\alpha + h^2)\|f\|_{L^2(Q_T)}.$$

The rest of the paper is organized as follows. In Section 2, we recall preliminaries from fractional calculus, derive the space-time variational formulation, and analyze its well-posedness and solution regularity. In Section 3, we develop a Petrov–Galerkin FEM based on the variational formulation and a tensor product mesh, establish a discrete inf-sup condition and discuss the resulting linear system. The error analysis is given in Sections 4 and 5 for fractional ODEs and PDEs, respectively. Some illustrative numerical results are presented in Section 6.

Throughout, the notation c, with or without a subscript, denotes a generic constant, which may differ at each occurrence but which is always independent of h and τ. We will use the following convention: for a function space S (dependent of t or/and x), the notations $\mathbb{S}_\tau$ and $\mathbb{S}_h$ denote the time- and space-discrete counterpart, respectively, and $\mathbb{S}_{h\tau}$ denotes the space-time discrete counterpart.

2 Time-Space Formulation

In this section, we develop a space-time variational formulation.

2.1 Notation and Preliminaries

First, we recall some preliminary facts from fractional calculus. For any $\gamma > 0$ and $u \in L^2(0,T)$, we define the left-sided and right-sided Riemann–Liouville fractional integral operators, i.e., ${}_0I_t^\gamma$ and ${}_tI_T^\gamma$, of order γ respectively by

$$({}_0I_t^\gamma u)(t) = \frac{1}{\Gamma(\gamma)}\int_0^t (t-s)^{\gamma-1}u(s)\,ds, \quad ({}_tI_T^\gamma u)(t) = \frac{1}{\Gamma(\gamma)}\int_t^T (s-t)^{\gamma-1}u(s)\,ds,$$

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

For any $\beta > 0$ with $k-1 < \beta < k$, $k \in \mathbb{N}^+$, the (formal) left-sided and right-sided Riemann–Liouville derivative of order β are respectively defined by

$${}_0\partial_t^\beta u = \frac{d^k}{dt^k}({}_0I_t^{k-\beta}u) \quad \text{and} \quad {}_t\partial_T^\beta u = (-1)^k\frac{d^k}{dt^k}({}_tI_T^{k-\beta}u). \tag{2.1}$$

These fractional derivatives are well defined for sufficiently smooth functions.

Next, we introduce the space $\widetilde{H}_L^s(0,T)$ (respectively $\widetilde{H}_R^s(0,T)$), which consists of functions whose extension by zero belong to $H^s(-\infty,T)$ (respectively $H^s(0,\infty)$); cf. [8]. We have the following useful identity [16, p. 76, Lemma 2.7]:

$$\int_0^T ({}_0\partial_t^\alpha u(t))v(t)\,dt = \int_0^T u(t)({}_t\partial_T^\alpha v(t))\,dt \quad \text{for all } u \in \widetilde{H}_L^\alpha(0,T),\ v \in \widetilde{H}_R^\alpha(0,T). \tag{2.2}$$

On the cylinder $Q_T = \Omega \times (0,T)$, we define the $L^2(Q_T)$-norm by

$$\langle u, v\rangle_{L^2(Q_T)} = \int_0^T\int_\Omega uv\,dx\,dt \quad \text{for all } u, v \in L^2(Q_T).$$

The notation $(\cdot,\cdot)_{L^2(\Omega)}$ denotes the duality pairing between $H_0^1(\Omega)$ and its dual $H^{-1}(\Omega)$, also the inner product in $L^2(\Omega)$. For $u, v \in L^2(Q_T)$, further for each $t \in (0,T)$, $u(t), v(t) \in H_0^1(\Omega)$, we use the standard definition of Dirichlet form

$$D(u,v) = \langle \nabla u, \nabla v\rangle_{L^2(Q_T)}.$$

Further, on Q_T, we introduce the following Bochner spaces:

$$\begin{aligned}
L^2 &:= L^2(Q_T) = L^2(0,T;L^2(\Omega)) && \text{with norm} && \|v\|_{L^2(Q_T)}^2 = \int_{Q_T} v^2\,dx\,dt,\\
V &:= V(Q_T) = L^2(0,T;H_0^1(\Omega)) && \text{with norm} && \|v\|_V^2 = D(v,v),\\
V^* &:= V(Q_T)^* = L^2(0,T;H^{-1}(\Omega)) && \text{with norm} && \|v\|_{V^*} = \sup_{\phi\in V}\frac{\langle v,\phi\rangle_{L^2(Q_T)}}{\|\phi\|_V}.
\end{aligned}$$

We will use an equivalent shorthand notation $L^2(0,T;X(\Omega))$ for these norms:

$$\|v\|_{L^2(0,T;X(\Omega))}^2 := \int_0^T \|v(t,\cdot)\|_{X(\Omega)}^2\,dt.$$

Below we will also use $\langle\cdot,\cdot\rangle_{L^2(Q_T)}$ for the duality pairing between V and V^*. For any $0 < s < 1$, we define the function space $B^s(Q_T)$ by

$$B^s(Q_T) = \widetilde{H}^s_L(0,T;H^{-1}(\Omega)) \cap L^2(0,T;H^1_0(\Omega)).$$

The space is endowed with the norm

$$\|v\|^2_{B^s(Q_T)} = \|{}_0\partial^s_t v\|^2_{V^*} + D(v,v).$$

Lemma 2.1. *For any $v \in B^\alpha(Q_T)$, $\alpha \in (0,1)$,*

$$\|v\|_{\widetilde{H}^\alpha_L(0,T;H^{-1}(\Omega))} \sim \|{}_0\partial^\alpha_t u\|_{V^*}.$$

Proof. By either [7, Theorem 3.1] or [10, Theorem 3.1], the norm equivalence

$$\|v(t,\cdot)\|_{\widetilde{H}^\alpha_L(0,T)} \sim \|{}_0\partial^\alpha_t v(t,\cdot)\|_{L^2(0,T)}$$

holds. Then the desired assertion follows from the definition of the norms. □

The following two results give the non-negativity of the fractional operators.

Lemma 2.2. *For any $v \in V$, we have $D({}_0I^\alpha_t v, v) \geq 0$.*

Proof. Let $\tilde{v}$ be the extension of v to $\Omega \times \mathbb{R}$ by zero. Then we have

$${}_0I^\alpha_t v(t) = \frac{1}{\Gamma(\alpha)} \int_{-\infty}^{t} (t-s)^{\alpha-1}\tilde{v}(s)\,ds := {}_{-\infty}I^\alpha_t \tilde{v}(t).$$

With $\hat{}$ being the Fourier transform in time, by Parseval's identity, we have

$$\begin{aligned} D({}_0I^\alpha_t v, v) &= \int_0^T \int_\Omega (\nabla {}_0I^\alpha_t v)\cdot(\nabla v)\,dx\,dt = \int_0^T \int_\Omega ({}_0I^\alpha_t \nabla v)\cdot(\nabla v)\,dx\,dt \\ &= \int_{-\infty}^{\infty} \int_\Omega ({}_{-\infty}I^\alpha_t \nabla\tilde{v})\cdot(\nabla\tilde{v})\,dx\,dt = \int_\Omega \int_{-\infty}^{\infty} ({}_{-\infty}I^\alpha_t \nabla\tilde{v})\cdot(\nabla\tilde{v})\,dt\,dx \\ &= \int_\Omega \int_{-\infty}^{\infty} \widehat{{}_{-\infty}I^\alpha_t \nabla\tilde{v}}(\xi)\cdot\widehat{\nabla\tilde{v}}(\xi)\,dt\,dx = c_\alpha \int_\Omega \int_0^{\infty} |\xi|^{-\alpha}|\nabla\tilde{v}|^2\,d\xi\,dx \geq 0, \end{aligned}$$

where the last identity follows from $\widehat{{}_{-\infty}I^\alpha_t f}(\xi) = (-\mathrm{i}\xi)^{-\alpha}\hat{f}(\xi)$; cf. [16, p. 90]. □

Lemma 2.3. *For $v \in B^\alpha(Q_T)$, we have $\langle {}_0\partial^\alpha_t v, v\rangle_{L^2(Q_T)} \geq 0$.*

Proof. For $v(\cdot,t) \in \widetilde{H}^\alpha_L(0,T)$, let $v_\alpha = {}_0\partial^\alpha_t v$. Since ${}_0I^\alpha_t$ is the left inverse of ${}_0\partial^\alpha_t$ on the space $\widetilde{H}^\alpha_L(0,T)$ (cf. [16, p. 75, Lemma 2.6]), we have $v = {}_0I^\alpha_t v_\alpha$ and

$$\langle {}_0\partial^\alpha_t v, v\rangle_{L^2(Q_T)} = \langle v_\alpha, {}_0I^\alpha_t v_\alpha\rangle_{L^2(Q_T)}.$$

This and Parseval's identity conclude the proof. □

2.2 Weak Space-Time Formulation

Inspired by the recent works [24, 28] on space-time formulations for standard parabolic problems, we develop such a formulation for problem (1.1). First, we define a bilinear form $a(\cdot,\cdot) : B^\alpha(Q_T) \times V \to \mathbb{R}$ by

$$a(v,\phi) := \langle {}_0\partial^\alpha_t v, \phi\rangle_{L^2(Q_T)} + D(v,\phi).$$

Then the weak form of problem (1.1) is: find $u \in B^\alpha(Q_T)$ such that

$$a(u, \phi) = \langle f, \phi \rangle_{L^2(Q_T)} \quad \text{for all } \phi \in V. \tag{2.3}$$

By Lemma 2.1, $a(\cdot, \cdot)$ is continuous on the product space $B^\alpha(Q_T) \times V$:

$$|a(v, \phi)| \le |\langle {}_0\partial_t^\alpha v, \phi \rangle_{L^2(Q_T)}| + |D(v, \phi)| \le \|v\|_{B^\alpha(Q_T)} \|\phi\|_V.$$

Next, we show the inf-sup condition of the bilinear form $a(\cdot, \cdot)$.

Lemma 2.4 (Inf-sup Condition). *For all $v \in B^\alpha(Q_T)$, there holds*

$$\sup_{\phi \in V} \frac{a(v, \phi)}{\|\phi\|_V} \ge \|v\|_{B^\alpha(Q_T)}. \tag{2.4}$$

Moreover, for any $\phi \in V$ with $\phi \ne 0$ the following compatibility condition holds:

$$\sup_{v \in B^\alpha(Q_T)} a(v, \phi) > 0.$$

Proof. First, following [28], we introduce a Newton potential operator $N : V^* \to V$ as $N\psi = w$, where $w \in V$ satisfies $D(w, \phi) = \langle \psi, \phi \rangle_{L^2(Q_T)}$ for all $\phi \in V$. By Lax–Milgram theorem, it has a unique solution $w = N\psi \in V$, and

$$\|w\|_V = \|N\psi\|_V = \|\psi\|_{V^*}. \tag{2.5}$$

For any given $v \in B^\alpha(Q_T)$, let $\phi_v = v + N_0\partial_t^\alpha v$. Obviously, $\phi_v \in V$ and by (2.5),

$$\|\phi_v\|_V = \|v + N_0\partial_t^\alpha v\|_V \le \|v\|_V + \|N_0\partial_t^\alpha v\|_V = \|v\|_V + \|{}_0\partial_t^\alpha v\|_{V^*} = \|v\|_{B^\alpha(Q_T)}.$$

Using the function ϕ_v, we have

$$\begin{aligned} a(v, \phi_v) &= \langle {}_0\partial_t^\alpha v, \phi_v \rangle_{L^2(Q_T)} + D(v, \phi_v) \\ &= \langle {}_0\partial_t^\alpha v, v \rangle_{L^2(Q_T)} + D(v, v) + \langle {}_0\partial_t^\alpha v, N_0\partial_t^\alpha v \rangle_{L^2(Q_T)} + D(v, N_0\partial_t^\alpha v). \end{aligned}$$

By the definition of N, we have $\langle {}_0\partial_t^\alpha v, N_0\partial_t^\alpha v \rangle_{L^2(Q_T)} = D(N_0\partial_t^\alpha v, N_0\partial_t^\alpha v)$ and $D(v, N_0\partial_t^\alpha v) = \langle {}_0\partial_t^\alpha v, v \rangle_{L^2(Q_T)}$, and consequently

$$a(v, \phi_v) = 2\langle {}_0\partial_t^\alpha v, v \rangle_{L^2(Q_T)} + D(v, v) + D(N_0\partial_t^\alpha v, N_0\partial_t^\alpha v).$$

Then Lemmas 2.1 and 2.3 and (2.5) yield

$$a(v, \phi_v) \ge \|v\|_V^2 + \|{}_0\partial_t^\alpha v\|_{V^*}^2 = \|v\|_{B^\alpha(Q_T)}^2.$$

This completes the proof of the inf-sup condition.

Next, we prove the compatibility condition. For a given $0 \ne \phi \in V$, let $v_\phi = {}_0I_t^\alpha \phi$. Then

$${}_0\partial_t^\alpha v_\phi = {}_0\partial_t^\alpha ({}_0I_t^\alpha \phi) = \phi.$$

Thus, $\|{}_0\partial_t^\alpha v_\phi\|_{L^2(Q_T)} = \|\phi\|_{L^2(Q_T)} \le \|\phi\|_V$, and as a result $v_\phi \in B^\alpha(Q_T)$ and

$$\langle {}_0\partial_t^\alpha v_\phi, \phi \rangle_{L^2(Q_T)} = \langle \phi, \phi \rangle_{L^2(Q_T)} = \|\phi\|_{L^2(Q_T)}^2 > 0.$$

The required bound $\sup_{v \in B^\alpha} a(v, \phi) > 0$ follows easily from the inequality $D({}_0I_t^\alpha \phi, \phi) \ge 0$ (cf. Lemma 2.2), which completes the proof of the lemma. □

Theorem 2.5. *For any $f \in V^*(Q_T)$, problem (2.3) has a unique solution $u \in B^\alpha(Q_T)$, and it satisfies*

$$\|u\|_{B^\alpha(Q_T)} \le c\|f\|_{V^*(Q_T)}.$$

Proof. The existence, uniqueness and stability follow directly from Lemma 2.4, and the continuity of the bilinear form $a(\cdot, \cdot)$. □

Remark 2.6. Li and Xu [19] proposed the following Galerkin weak formulation: find

$$u \in \tilde{B}^{\frac{\alpha}{2}}(Q_T) := H^{\frac{\alpha}{2}}(0, T; L^2(\Omega)) \cap L^2(0, T; H_0^1(\Omega))$$

such that $a(u, v) = \langle f, v\rangle_{L^2(Q_T)}$ for all $v \in \tilde{B}^{\alpha/2}(Q_T)$, with the bilinear form $a(\cdot\,,\cdot)$ defined by

$$a(u, v) = \langle {}_0\partial_t^{\frac{\alpha}{2}} u, {}_t\partial_T^{\frac{\alpha}{2}} v\rangle_{L^2(Q_T)} + D(u, v).$$

The bilinear form $a(\cdot\,,\cdot)$ is continuous and coercive on $\tilde{B}^{\alpha/2}(Q_T)$ (cf. [19]), and thus the variational problem is well-posed. Further, they studied a spectral approximation. For other interesting extensions of space-time fractional models, see [20, 30].

Remark 2.7. Note that for $f \in L^2(0, T; L^2(\Omega))$ the initial condition $u(0) = 0$ in (1.1) makes sense only if $\alpha > \frac{1}{2}$. For $\alpha \le \frac{1}{2}$, one should not impose any initial condition, unless f has extra temporal regularity [7].

2.3 Regularity of the Solution

If the source f has higher spatial and/or temporal regularity, then accordingly the solution u is more regular than that in Theorem 2.5. Now we study the solution regularity, which is useful for the error analysis in Section 5.

Let $\{\varphi_n\}_{n=1}^{\infty} \in H^2(\Omega) \cap H_0^1(\Omega)$ and $\{\lambda_n\}_{n=1}^{\infty}$ denote respectively the $L^2(\Omega)$-orthonormal eigenfunctions of the operator $-\Delta$ (with a zero Dirichlet boundary condition) and the corresponding eigenvalues (ordered nondecreasingly with multiplicity counted). Then the solution u of problem (1.1) can be expressed by

$$u(t) = \int_0^t E(t-s)f(s)\,ds = \int_0^t E(s)f(t-s)\,ds. \tag{2.6}$$

Here the operator $E(t)$ is defined by $E(t)v = t^{\alpha-1}E_{\alpha,\alpha}(t^{\alpha}\Delta)v$, where for any $\alpha > 0$ and $\beta \in \mathbb{R}$ (see [16, p. 42]),

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k\alpha + \beta)}.$$

The next result gives the solution stability and regularity pickup.

Theorem 2.8. *For $f \in \widetilde{H}_L^s(0, T; L^2(\Omega))$, $s \in [0, 1]$, the solution u to problem* (1.1) *belongs to*

$$\widetilde{H}_L^{\alpha+s}(0, T; L^2(\Omega)) \cap \widetilde{H}_L^s(0, T; H_0^1(\Omega) \cap H^2(\Omega)),$$

and

$$\|u\|_{\widetilde{H}_L^{\alpha+s}(0,T;L^2(\Omega))} + \|u\|_{\widetilde{H}_L^s(0,T;H^2(\Omega))} \le c\|f\|_{\widetilde{H}_L^s(0,T;L^2(\Omega))}.$$

Furthermore, if $f \in \widetilde{H}_L^s(0, T; H_0^1(\Omega))$, then $u \in \widetilde{H}_L^{\alpha+s}(0, T; H_0^1(\Omega))$.

Proof. By [7, Theorem 4.1], the assertion holds for $s = 0$. Now we turn to the case $s = 1$, i.e., $f \in \widetilde{H}_L^1(0, T; L^2(\Omega))$. Then $f(0) = 0$, and by (2.6) we have

$$u'(t) = E(t)f(0) + \int_0^t E(t-s)f'(s)\,ds = \int_0^t E(t-s)f'(s)\,ds.$$

By the preceding estimate, the term $v = \int_0^t E(t-s)f'(s)\,ds$ satisfies

$$\|{}_0\partial_t^{\alpha} v\|_{L^2(Q_T)} + \|\Delta v\|_{L^2(Q_T)} \le c\|f'\|_{L^2(Q_T)}.$$

By [11, Lemma 2.2], since $L^{\infty}(0, T; L^2(\Omega)) \subset \widetilde{H}_L^1(0, T; L^2(\Omega))$, for $s = 1$ we get

$$\|u(t)\|_{L^2(\Omega)} \le c\int_0^t (t-s)^{\alpha-1}\|f(s)\|_{L^2(\Omega)}\,ds \le ct^{\alpha}\|f\|_{L^{\infty}(0,T;L^2(\Omega))} \to 0 \quad \text{as } t \to 0,$$

and hence $u(0) = 0$. Consequently, we have

$$ {}_0\partial_t^\alpha v(t) = \partial_t({}_0I_t^{1-\alpha}(\partial_t u))(t) = \partial_t^2({}_0I_t^{1-\alpha}u)(t) = {}_0\partial_t^{\alpha+1}u(t). $$

Thus, the assertion holds for $s = 1$. Since only temporal regularity index is concerned, an interpolation argument shows the case $0 < s < 1$ (see [23, Lemma 2.8] or [9, Theorem 2.35]). The case $f \in \widetilde{H}_L^s(0, T; H_0^1(\Omega))$ follows similarly. □

3 Petrov–Galerkin FEM

Based on the space-time variational formulation in Section 2, we now develop a novel Petrov–Galerkin finite element method (FEM), establish the discrete inf-sup condition and describe its linear algebraic formulation.

3.1 Finite Element Method

First, we introduce a quasi-uniform shape regular partition of the domain Ω into simplicial elements of maximal diameter h, denoted by $\mathcal{T}_h$. We consider the space of continuous piecewise linear functions on $\mathcal{T}_h$ with $N \in \mathbb{N}$ being the number of degrees of freedom. Let $\{\varphi_i\}_{i=1}^N \subset H_0^1(\Omega)$ be the nodal basis functions and

$$ \mathbb{X}_h := \operatorname{span}(\{\varphi_i\}_{i=1}^N). $$

On the space $\mathbb{X}_h$, we recall the L^2-projection $P_h : L^2(\Omega) \to \mathbb{X}_h$ defined by

$$ (\phi - P_h\phi, \chi)_{L^2(\Omega)} = 0 \quad \text{for all } \chi \in \mathbb{X}_h. $$

It satisfies the following error estimate [29]: for $q = 1, 2$,

$$ \|P_h\phi - \phi\|_{L^2(\Omega)} + h\|P_h\phi - \phi\|_{H^1(\Omega)} \le ch^q\|\phi\|_{H^q(\Omega)} \quad \text{for all } \phi \in H_0^1(\Omega) \cap H^q(\Omega), $$

and the following negative norm estimate [29, p. 69]:

$$ \|P_h\phi - \phi\|_{H^{-1}(\Omega)} \le ch\|\phi\|_{L^2(\Omega)}. \tag{3.1} $$

Next, we uniformly partition the time interval $(0, T)$ with grid points $t_k = k\tau$, $k = 0, \dots, K$, $K \in \mathbb{N}$, and a time step size $\tau = \frac{T}{K}$. Following [13], we define a set of "fractionalized" piecewise constant basis functions $\phi_k(t)$, $k = 1, \dots, K$, by

$$ \phi_k(t) = \begin{cases} 0 & \text{if } 0 \le t \le t_{k-1} \\ (t - t_{k-1})^\alpha & \text{if } t_{k-1} \le t \le T \end{cases} := (t - t_{k-1})^\alpha \chi_{[t_{k-1},T]}(t), $$

where χ_S denotes the characteristic function of the set S. Then for $k = 1, \dots, K$,

$$ \phi_k(t) = \Gamma(\alpha + 1)\,{}_0I_t^\alpha \chi_{[t_{k-1},T]}(t) \quad \text{and} \quad {}_0\partial_t^\alpha \phi_k(t) = \Gamma(\alpha + 1)\chi_{[t_{k-1},T]}(t). $$

Clearly, $\phi_k \in \widetilde{H}_L^{\alpha+s}(0, T)$ for any $s \in [0, \frac{1}{2})$. Further, we denote

$$ \mathbb{U}_\tau = \operatorname{span}\{\phi_k(t)\}_{k=1}^K \quad \text{and} \quad \mathbb{W}_\tau := \operatorname{span}\{\chi_{[t_{k-1},T]}(t)\}_{k=1}^K. \tag{3.2} $$

With the tensor product notation $\otimes$, the solution space $\mathbb{B}_{h\tau}^\alpha \subset B^\alpha(Q_T)$ and test space $\mathbb{V}_{h\tau} \subset V(Q_T)$ are respectively defined by

$$ \mathbb{B}_{h\tau}^\alpha := \mathbb{X}_h \otimes \mathbb{U}_\tau \quad \text{and} \quad \mathbb{V}_{h\tau} := \mathbb{X}_h \otimes \mathbb{W}_\tau. $$

The FEM problem of (2.3) reads: given $f \in V^*$, find $u_{h\tau} \in \mathbb{B}_{h\tau}^\alpha$ such that

$$ a(u_{h\tau}, \phi) \equiv \langle {}_0\partial_t^\alpha u_{h\tau}, \phi\rangle_{L^2(Q_T)} + D(u_{h\tau}, \phi) = \langle f, \phi\rangle_{L^2(Q_T)} \quad \text{for all } \phi \in \mathbb{V}_{h\tau}. \tag{3.3} $$

The bilinear form $a(\cdot\,,\cdot)$ is non-symmetric, and to show the existence and stability of the solution $u_{h\tau}$ we need a discrete analogue of (2.4). To prove this, we first introduce and study the L^2-projection onto the space $\mathbb{W}_\tau$.

3.2 The Projection Π_τ and its Properties

For $v \in L^2(0,T)$, we introduce the L^2-projection $\Pi_\tau : L^2(0,T) \to \mathbb{W}_\tau$ by

$$(\Pi_\tau v, \phi)_{L^2(0,T)} = (v, \phi)_{L^2(0,T)} \quad \text{for all } \phi \in \mathbb{W}_\tau,$$

where $(\cdot,\cdot)_{L^2(0,T)}$ denotes the inner product on the space $L^2(0,T)$, i.e.,

$$(\Pi_\tau v)(t) = \tau^{-1} \int_{t_n}^{t_{n+1}} v(t)\,dt \quad \text{for } t \in [t_n, t_{n+1}) := [t_n, t_n + \tau).$$

Then it satisfies

$$\|v - \Pi_\tau v\|_{L^2(0,T)} \le c\tau^s \|v\|_{H^s(0,T)}, \quad s \in [0,1]. \tag{3.4}$$

Below, we study the L^2-stability of the operator Π_τ when restricted to the space $\mathbb{U}_\tau$. This is given in Lemma 3.2 below, whose proof will require the following result.

Lemma 3.1. *For $u \in H^{\alpha/2}(0,T)$ and $v \in \widetilde{H}^\alpha_L(0,T)$,*

$$(u, {}_0\partial_t^\alpha v)_{L^2(0,T)} = ({}_t\partial_T^{\frac{\alpha}{2}} u, {}_0\partial_t^{\frac{\alpha}{2}} v)_{L^2(0,T)}.$$

Proof. Given u and v as in the lemma, let $\tilde{u}$ be the zero extension of u to $\mathbb{R}$ and

$$\widetilde{v}(t) = \begin{cases} 0 & \text{if } t \notin [0, 2T], \\ v(t) & \text{if } t \in [0, T], \\ v(2T - t) & \text{if } t \in (T, 2T]. \end{cases}$$

Then there holds

$$(u, {}_0\partial_t^\alpha v)_{L^2(0,T)} = (\tilde{u}, {}_{-\infty}\partial_t^\alpha \widetilde{v})_{L^2(\mathbb{R})} = ({}_t\partial_\infty^{\frac{\alpha}{2}} \tilde{u}, {}_{-\infty}\partial_t^{\frac{\alpha}{2}} \widetilde{v})_{L^2(\mathbb{R})} = ({}_t\partial_T^{\frac{\alpha}{2}} u, {}_0\partial_t^{\frac{\alpha}{2}} v)_{L^2(0,T)},$$

where the middle equality follows by examining the expressions after applying the Fourier transform as in the proof of Lemma 2.2. □

By using an argument similar to the proof of Lemma 2.3 (cf. also [16, p. 90]), we conclude that there is a constant c_α satisfying

$$c_\alpha^{-1} \|v\|^2_{H^{\frac{\alpha}{2}}(0,T)} \le (v, {}_0\partial_t^\alpha v)_{L^2(0,T)} \le c_\alpha \|v\|^2_{H^{\frac{\alpha}{2}}(0,T)} \quad \text{for all } v \in \widetilde{H}^\alpha_L(0,T). \tag{3.5}$$

Lemma 3.2. *There is a constant $c(\alpha) > 0$ such that*

$$c(\alpha)\|v\|^2_{L^2(0,T)} \le \|\Pi_\tau v\|^2_{L^2(0,T)} \le \|v\|^2_{L^2(0,T)} \quad \textit{for all } v \in \mathbb{U}_\tau.$$

Proof. The second assertion follows directly from the definition of Π_τ. For the first, note

$$\|v\|^2_{L^2(0,T)} = \|\Pi_\tau v\|^2_{L^2(0,T)} + \|(I - \Pi_\tau)v\|^2_{L^2(0,T)}. \tag{3.6}$$

The approximation property (3.4) implies that for any $v \in \mathbb{U}_\tau$,

$$\|(I - \Pi_\tau)v\|_{L^2(0,T)} \le c\tau^{\frac{\alpha}{2}} \|v\|_{H^{\frac{\alpha}{2}}(0,T)}. \tag{3.7}$$

Since ${}_0\partial_t^\alpha v$ belongs to $\mathbb{W}_\tau$ for any $v \in \mathbb{U}_\tau$, Lemma 3.1 and (3.5) imply

$$\begin{aligned} c^{-1}\|v\|^2_{H^{\frac{\alpha}{2}}(0,T)} &\le (v, {}_0\partial_t^\alpha v)_{L^2(0,T)} = (\Pi_\tau v, {}_0\partial_t^\alpha v)_{L^2(0,T)} \\ &= ({}_t\partial_T^{\frac{\alpha}{2}}(\Pi_\tau v), {}_0\partial_t^{\frac{\alpha}{2}} v)_{L^2(0,T)} \le c\|\Pi_\tau v\|_{H^{\frac{\alpha}{2}}(0,T)} \|v\|_{H^{\frac{\alpha}{2}}(0,T)}. \end{aligned} \tag{3.8}$$

$\alpha \setminus K$	20	40	80	160	320	640
0.3	0.7711	0.7697	0.7693	0.7693	0.7693	0.7692
0.5	0.4754	0.4714	0.4703	0.4700	0.4700	0.4699
0.7	0.1982	0.1911	0.1891	0.1886	0.1884	0.1884
0.9	0.0326	0.0251	0.0228	0.0221	0.0220	0.0219
0.98	0.0076	0.0030	0.0015	0.0011	0.0010	0.0010

Table 1. The lower bound $c(\alpha)$ for the L^2-norm of Π_τ for various α.

Note that $\mathbb{W}_\tau$ satisfies inverse inequalities, i.e., for $s \in (0, \frac{1}{2})$,

$$\|\Pi_\tau v\|_{H^s(0,T)} \le c_s \tau^{-s} \|\Pi_\tau v\|_{L^2(0,T)}.$$

Using this with $s = \frac{\alpha}{2}$ in (3.8) implies

$$\|v\|_{H^{\frac{\alpha}{2}}(0,T)} \le c\tau^{-\frac{\alpha}{2}} \|\Pi_\tau v\|_{L^2(0,T)}. \tag{3.9}$$

Substituting (3.9) into (3.7) and combining it with (3.6) give

$$\|v\|_{L^2(0,T)} \le c\|\Pi_\tau v\|_{L^2(0,T)},$$

which completes the proof of the lemma. □

In Table 1, we give the best constant $c(\alpha) \equiv c(\alpha, K)$ (recall that $\tau K = T$) as a function of the mesh parameter $K = \frac{T}{\tau}$ when $T = 1$. The results clearly show the convergence to a lower bound as K becomes large. Further, we note that it is a consequence of the work of Larsson and Monteli [17] that $c(\alpha) \to 0$ when $\alpha \to 1$, for which our discretization coincides with that in [17].

3.3 Stability of the Petrov–Galerkin FEM

Now we prove a discrete inf-sup condition. In this part, we consider K, N, τ, and h as fixed, although the estimates are independent of them.

Let $\{\psi_j\}_{j=1}^N \subset \mathbb{X}_h$ denote an $L^2(\Omega)$-orthonormal basis for $\mathbb{X}_h$ of generalized eigenfunctions (of the negative discrete Laplacian), i.e., $(\nabla\psi_j, \nabla\chi)_{L^2(\Omega)} = \lambda_{j,h}(\psi_j, \chi)_{L^2(\Omega)}$ for all $\chi \in \mathbb{X}_h$. It follows that for any $\phi \in \mathbb{X}_h$, there hold

$$\phi = \sum_{j=1}^N (\phi, \psi_j)_{L^2(\Omega)}\psi_j, \quad \|\phi\|_{L^2(\Omega)}^2 = \sum_{j=1}^N (\phi, \psi_j)_{L^2(\Omega)}^2, \quad \|\nabla\phi\|_{L^2(\Omega)}^2 = \sum_{j=1}^N \lambda_{j,h}(\phi, \psi_j)_{L^2(\Omega)}^2.$$

We also define

$$N_h\phi = \sum_{j=1}^N \lambda_{j,h}^{-1}(\phi, \psi_j)_{L^2(\Omega)}\psi_j \quad \text{and} \quad \|\phi\|_{H_h^{-1}(\Omega)}^2 = \sum_{j=1}^N \lambda_{j,h}^{-1}(\phi, \psi_j)_{L^2(\Omega)}^2.$$

The operator N_h is a discrete Riesz map, i.e., the inverse of the discrete Laplacian on the space $\mathbb{X}_h$. It is known that there is a constant c independent of h satisfying

$$\|\phi\|_{H^{-1}(\Omega)} \le c\|\phi\|_{H_h^{-1}(\Omega)} \quad \text{for all } \phi \in \mathbb{X}_h. \tag{3.10}$$

Further, due to the tensor construction of $\mathbb{B}_{h\tau}^\alpha$ and $\mathbb{V}_{h\tau}$, functions $v \in \mathbb{B}_{h\tau}^\alpha$ and $\phi \in \mathbb{V}_{h\tau}$ can be expanded as

$$v(x,t) = \sum_{i,j} c_{ij}\phi_i(t)\psi_j(x) \quad \text{and} \quad \phi(x,t) = \sum_{i,j} d_{ij}\chi_i(t)\psi_j(x),$$

where the summation over i, j denotes the sum over $i = 1, \dots, K$ and $j = 1, \dots, N$. This discussion extends to Q_T as well. For example, for $v \in \mathbb{B}^\alpha_{h\tau}$, we have the following expansion (with $v_j(t) = (v(\cdot, t), \psi_j)_{L^2(\Omega)}$):

$$D(v, v) = \sum_{j=1}^{N} \lambda_{j,h} \|v_j(t)\|^2_{L^2(0,T)}, \quad \|{}_0\partial_t^\alpha v\|^2_{L^2(Q_T)} = \sum_{j=1}^{N} \|{}_0\partial_t^\alpha v_j(t)\|^2_{L^2(0,T)},$$

$$\|{}_0\partial_t^\alpha v\|^2_{L^2(0,T;H^{-1}(\Omega))} \le c\|{}_0\partial_t^\alpha v\|^2_{L^2(0,T;H_h^{-1}(\Omega))} = c\sum_{j=1}^{N} \lambda_{j,h}^{-1} \|{}_0\partial_t^\alpha v_j(t)\|^2_{L^2(0,T)}.$$

For $\phi \in \mathbb{V}_{h\tau}$, we have

$$\|\phi\|_V^2 = \sum_{j=1}^{N} \lambda_{j,h} \|\phi_j(t)\|^2_{L^2(0,T)} \quad \text{with} \quad \phi_j(t) = (\phi(\cdot, t), \psi_j)_{L^2(\Omega)}.$$

Now we give a discrete inf-sup condition. It yields the well-posedness of (3.3).

Lemma 3.3. *There is a constant $c_\alpha > 0$, independent of h and τ, such that*

$$\sup_{\phi \in \mathbb{V}_{h\tau}} \frac{a(v, \phi)}{\|\phi\|_V} \ge c_\alpha \|v\|_{B^\alpha(Q_T)} \quad \textit{for all } v \in \mathbb{B}^\alpha_{h\tau}. \tag{3.11}$$

Proof. For any $v \in \mathbb{B}^\alpha_{h\tau}$, we define a norm

$$|||v|||^2 = \|{}_0\partial_t^\alpha v\|^2_{L^2(0,T;H_h^{-1}(\Omega))} + D(\Pi_\tau v, \Pi_\tau v).$$

Meanwhile, we set $\phi \in \mathbb{V}_{h\tau}$ by

$$\phi = \begin{cases} N_h {}_0\partial_t^\alpha v & \text{if } \|{}_0\partial_t^\alpha v\|^2_{L^2(0,T;H_h^{-1}(\Omega))} \ge D(\Pi_\tau v, \Pi_\tau v) \text{ (case 1)}, \\ \phi = \Pi_h v & \text{otherwise (case 2)}. \end{cases}$$

For ϕ given by case 1, we have

$$\begin{aligned} a(v, \phi) &= \|{}_0\partial_t^\alpha v\|^2_{L^2(0,T;H_h^{-1}(\Omega))} + (v, {}_0\partial_t^\alpha v)_{L^2(Q_T)} \\ &\ge \|{}_0\partial_t^\alpha v\|^2_{L^2(0,T;H_h^{-1}(\Omega))} \ge \tfrac{1}{2}|||v|||^2. \end{aligned}$$

By the definition of the operator N_h,

$$\begin{aligned} \|\phi\|_V^2 = D(\phi, \phi) &= D(N_h {}_0\partial_t^\alpha v, N_h {}_0\partial_t^\alpha v) \\ &= ({}_0\partial_t^\alpha v, N_h {}_0\partial_t^\alpha v)_{L^2(Q_T)} \\ &= \|{}_0\partial_t^\alpha v\|^2_{L^2(0,T;H_h^{-1}(\Omega))} \le |||v|||^2. \end{aligned}$$

Alternatively, if ϕ is given by case 2, since ${}_0\partial_t^\alpha v \in \mathbb{V}_{h\tau}$ for $v \in \mathbb{B}^\alpha_{h\tau}$, we derive

$$\begin{aligned} a(v, \phi) &= ({}_0\partial_t^\alpha v, \Pi_\tau v)_{L^2(Q_T)} + D(v, \Pi_\tau v) \\ &= ({}_0\partial_t^\alpha v, v)_{L^2(Q_T)} + D(\Pi_\tau v, \Pi_\tau v) \\ &\ge D(\Pi_\tau v, \Pi_\tau v) \ge \tfrac{1}{2}|||v|||^2. \end{aligned}$$

By Lemma 3.2, we have $c_\alpha \|\phi\|_V^2 \le D(\Pi_\tau v, \Pi_\tau v) \le |||v|||^2$. Thus, for any $v \in \mathbb{B}^\alpha_{h\tau}$,

$$\tfrac{1}{2}|||v||| \le \frac{a(v, \phi)}{|||v|||} \le c\frac{a(v, \phi)}{\|\phi\|_V} \le c \sup_{\phi \in \mathbb{V}_{h\tau}} \frac{a(v, \phi)}{\|\phi\|_V}.$$

Then applying (3.10) yields

$$\big(\|{}_0\partial_t^\alpha v\|^2_{L^2(0,T;H^{-1}(\Omega))} + D(v, v)\big)^{\frac{1}{2}} \le c|||v|||$$

for all $v \in \mathbb{B}^\alpha_{h\tau}$, from which the desired inf-sup condition (3.11) follows. □

3.4 Linear Algebraic Problem

Now we discuss the solution of the resulting linear system. Let

$$\chi_\ell(t) = \chi_{[t_{\ell-1},t_\ell]}(t) \quad \text{and} \quad \phi_k(t) = (t-t_{k-1})^\alpha \chi_{[t_{k-1},T]}(t).$$

Then we define two matrices by

$$M_\tau = \{(\phi_k, \chi_\ell)_{L^2(0,T)}\}_{k,\ell=1}^K \quad \text{and} \quad M_\tau^\alpha = \{({}_0\partial_t^\alpha \phi_k, \chi_\ell)_{L^2(0,T)}\}_{k,\ell=1}^K.$$

The temporal mass matrix M_τ is lower triangular Toeplitz, with its first column given by

$$\frac{\tau^{\alpha+1}}{\alpha+1}[d_1 \cdots d_K]^t, \quad d_k = k^{\alpha+1} - (k-1)^{\alpha+1},\ k = 1, 2, \dots, K,$$

and the temporal stiffness matrix M_τ^α is lower triangular Toeplitz, with its first column being $\tau\Gamma(\alpha+1)[1 \cdots 1]^t$. Likewise, we define the spatial "mass" and "stiffness" matrices

$$M_h = \{(\varphi_i, \varphi_j)_{L^2(\Omega)}\}_{i,j=1}^N \quad \text{and} \quad A_h = \{(\nabla\varphi_i, \nabla\varphi_j)_{L^2(\Omega)}\}_{i,j=1}^N,$$

where $\varphi_i(x)$, $i = 1, \dots, N$, are the nodal basis functions of the space $\mathbb{X}_h$.

We denote by U the coefficient vector in the representation of the solution $u_{h,\tau} \in \mathbb{B}_{h\tau}^\alpha$, and by F the vector of the projection of the source f onto $\mathbb{V}_{h\tau}$. Then problem (3.3) can be written as an algebraic system

$$AU = F, \quad \text{with} \quad A = M_\tau^\alpha \otimes M_h + M_\tau \otimes A_h.$$

Due to the block triangular structure of the matrix A, the solution process is essentially time stepping, i.e., solving first for the unknowns at $t_1 = \tau$, and then recursively for t_k, $k = 2, \dots, K$.

Alternatively, one may take

$$\chi_\ell(t) = \chi_{[t_{\ell-1},t_\ell]}(t) \quad \text{and} \quad \phi_k(t) = (t-t_{k-1})^\alpha \chi_{[t_{k-1},T]}(t) - (t-t_k)^\alpha \chi_{[t_k,T]}(t).$$

Then, with the identity

$${}_0\partial_t^\alpha \phi_k(t) = \Gamma(\alpha+1)\chi_{[t_{k-1},t_k]}(t),$$

the matrix M_τ is lower triangular Toeplitz with its first column given by

$$\frac{\tau^{\alpha+1}}{\alpha+1}[e_1 \cdots e_K]^t, \quad e_k = d_{k+1} - d_k = (k+1)^{\alpha+1} + (k-1)^{\alpha+1} - 2k^{\alpha+1},$$

and $M_\tau^\alpha = \tau\Gamma(\alpha+1)I$. This formulation has been used in our implementation.

4 Error Estimate for Fractional ODEs

To give the idea of error analysis, we first derive error estimates for ODEs.

4.1 Fractional ODE

Consider the following fractional-order ODE for $\lambda \geq 0$: find $u(t)$ such that

$${}_0\partial_t^\alpha u + \lambda u = f \quad \text{for all } t \in (0,T),\ \text{with } u(0) = 0. \tag{4.1}$$

The weak form reads: given $f \in L^2(0,T)$, find $u \in \widetilde{H}_L^\alpha(0,T)$ such that

$$a_\lambda(u,\phi) \equiv ({}_0\partial_t^\alpha u, \phi)_{L^2(0,T)} + \lambda(u,\phi)_{L^2(0,T)} = (f,\phi)_{L^2(0,T)} \quad \text{for all } \phi \in L^2(0,T) \tag{4.2}$$

By choosing $\phi = {}_0\partial_t^\alpha v + \lambda v$ in $a_\lambda(\cdot,\cdot)$, since $({}_0\partial_t^\alpha v, v)_{L^2(0,T)} \geq 0$ for $v \in \widetilde{H}_L^\alpha(0,T)$, we deduce

$$\begin{aligned} a_\lambda(v,\phi) &= \|{}_0\partial_t^\alpha v\|_{L^2(0,T)}^2 + 2\lambda({}_0\partial_t^\alpha v, v)_{L^2(0,T)} + \lambda^2\|v\|_{L^2(0,T)}^2 \\ &\geq \tfrac{1}{2}\big(\|{}_0\partial_t^\alpha v\|_{L^2(0,T)} + \lambda\|v\|_{L^2(0,T)}\big)^2. \end{aligned}$$

Since $\|\phi\|_{L^2(0,T)} \leq \|{}_0\partial_t^\alpha v\|_{L^2(0,T)} + \lambda\|v\|_{L^2(0,T)}$, we obtain the inf-sup condition

$$\|{}_0\partial_t^\alpha v\|_{L^2(0,T)} + \lambda\|v\|_{L^2(0,T)} \leq 2 \sup_{\phi\in L^2(0,T)} \frac{a_\lambda(v,\phi)}{\|\phi\|_{L^2(0,T)}}.$$

For $\phi \in L^2(0,T)$, $\phi \neq 0$, let $v = {}_0I_t^\alpha \phi$. By Lemma 2.2, $a_\lambda(v,\phi) = (\phi,\phi)_{L^2(0,T)} + \lambda(\phi, v)_{L^2(0,T)} > 0$. Thus $a_\lambda(\cdot,\cdot)$ satisfies also a compatibility condition and problem (4.2) is well-posed.

Further, for $f \in \widetilde{H}_L^s(0,T)$, problem (4.1) has a unique solution $u \in \widetilde{H}_L^{\alpha+s}(0,T)$ and

$$\|u\|_{\widetilde{H}_L^{\alpha+s}(0,T)} + \lambda\|u\|_{\widetilde{H}_L^s(0,T)} \leq c\|f\|_{\widetilde{H}_L^s(0,T)}, \tag{4.3}$$

where the constant c is independent of λ. This estimate follows directly from Theorem 2.8 by identifying the operator $-\Delta$ with the scalar λ.

Remark 4.1. For the adjoint problem, to find $w \in \widetilde{H}_R^\alpha(0,T)$ such that $a_\lambda(\phi, w) = (\phi, f)_{L^2(0,T)}$ for all $\phi \in L^2(0,T)$, a similar inf-sup condition and regularity pickup hold.

With the spaces $\mathbb{U}_\tau$ and $\mathbb{W}_\tau$ defined in (3.2), the Petrov–Galerkin FEM for problem (4.1) reads: given $f \in L^2(0,T)$, find $u_\tau \in \mathbb{U}_\tau$ such that

$$a_\lambda(u_\tau, \phi) = (f,\phi)_{L^2(0,T)} \quad \text{for all } \phi \in \mathbb{W}_\tau. \tag{4.4}$$

For any $v \in \mathbb{U}_\tau$, by letting $\phi = \phi_v = {}_0\partial_t^\alpha v + \lambda\Pi_\tau v$ and Lemma 2.3, and repeating the preceding argument, we derive the following discrete inf-sup condition:

$$\|v\|_{\widetilde{H}_L^\alpha(0,T)} + \lambda\|\Pi_\tau v\|_{L^2(0,T)} \leq c \sup_{\phi\in\mathbb{W}_\tau} \frac{a_\lambda(v,\phi)}{\|\phi\|_{L^2(0,T)}},$$

where c is independent of λ. Thus (4.4) is well-posed and stable in the $\widetilde{H}_L^\alpha(0,T)$-norm.

4.2 Fractional Ritz and L^2-Projections

Now we define a fractional Ritz projection $R_\tau^\alpha : \widetilde{H}_L^\alpha(0,T) \to \mathbb{U}_\tau$ by

$$({}_0\partial_t^\alpha R_\tau^\alpha v, \phi)_{L^2(0,T)} = ({}_0\partial_t^\alpha v, \phi)_{L^2(0,T)} \quad \text{for all } \phi \in \mathbb{W}_\tau.$$

The operator R_τ^α has optimal approximation property in both $\widetilde{H}_L^\alpha$- and L^2-norms.

Lemma 4.2. *For the fractional Ritz projection R_τ^α, for $0 \leq s \leq 1$ there holds*

$$\tau^\alpha\|{}_0\partial_t^\alpha(v - R_\tau^\alpha v)\|_{L^2(0,T)} + \|v - R_\tau^\alpha v\|_{L^2(0,T)} \leq c\tau^{\alpha+s}\|v\|_{\widetilde{H}_L^{\alpha+s}(0,T)}.$$

Proof. Let $e = v - R_\tau^\alpha v$. Clearly, for any $v_\tau \in \mathbb{U}_\tau$,

$$({}_0\partial_t^\alpha(R_\tau^\alpha v - v_\tau), \phi)_{L^2(0,T)} = ({}_0\partial_t^\alpha(v - v_\tau), \phi)_{L^2(0,T)} \quad \text{for all } \phi \in \mathbb{W}_\tau.$$

Upon taking $\phi = {}_0\partial_t^\alpha(R_\tau^\alpha v - v_\tau)$ and by the Cauchy–Schwarz inequality, we have

$$\|{}_0\partial_t^\alpha e\|_{L^2(0,T)} \leq 2 \inf_{v_\tau\in\mathbb{U}_\tau} \|{}_0\partial_t^\alpha(v - v_\tau)\|_{L^2(0,T)}.$$

By repeating the arguments of [13, Lemma 4.2], for $0 \leq s \leq 1$ we obtain

$$\|{}_0\partial_t^\alpha e\|_{L^2(0,T)} \leq c\tau^s\|v\|_{\widetilde{H}_L^{\alpha+s}(0,T)}. \tag{4.5}$$

Now we prove the L^2-error bound. Let $w \in \widetilde{H}_R^\alpha(0,T)$ be the solution to $(\phi, {}_t\partial_T^\alpha w)_{L^2(0,T)} = (\phi, e)_{L^2(0,T)}$ for all $\phi \in L^2(0,T)$. By Remark 4.1, w satisfies

$$\|w\|_{\widetilde{H}_R^\alpha(0,T)} \le c\|e\|_{L^2(0,T)}.$$

Then by (2.2) and Galerkin orthogonality,

$$\begin{aligned}\|e\|_{L^2(0,T)}^2 &= (e, {}_t\partial_T^\alpha w)_{L^2(0,T)} = ({}_0\partial_t^\alpha e, w - w_\tau)_{L^2(0,T)}\\ &\le \|{}_0\partial_t^\alpha e\|_{L^2(0,T)} \inf_{w_\tau \in \mathbb{W}_\tau} \|w - w_\tau\|_{L^2(0,T)}\\ &\le c\tau^\alpha \|{}_0\partial_t^\alpha e\|_{L^2(0,T)} \|w\|_{\widetilde{H}_R^\alpha(0,T)} \le c\tau^\alpha \|{}_0\partial_t^\alpha e\|_{L^2(0,T)} \|e\|_{L^2(0,T)}.\end{aligned}$$

This together with (4.5) yields the desired error estimate. □

Next, we introduce a fractionalized L^2-projection $P_\tau : L^2(0,T) \to \mathbb{U}_\tau$, defined by

$$(P_\tau v, \phi)_{L^2(0,T)} = (v, \phi)_{L^2(0,T)} \quad \text{for all } \phi \in \mathbb{W}_\tau.$$

Let $b(\cdot,\cdot) : \mathbb{U}_\tau \times \mathbb{W}_\tau \to \mathbb{R}$ by $b(v,\phi) = (v,\phi)_{L^2(0,T)}$. For any $v \in \mathbb{U}_\tau$, choosing $\phi = \Pi_\tau v$ yields

$$b(v,\phi) = (v, \Pi_\tau v)_{L^2(0,T)} = \|\Pi_\tau v\|_{L^2(0,T)}^2.$$

This and Lemma 3.2 yield the following inf-sup condition:

$$\sup_{\phi \in \mathbb{W}_\tau} \frac{b(v,\phi)}{\|\phi\|_{L^2(0,T)}} \ge c\|v\|_{L^2(0,T)}.$$

Thus the operator P_τ is well defined. Next, we study its approximation property.

Lemma 4.3. *For the fractionalized L^2-projection P_τ, there holds*

$$\begin{aligned}\|v - P_\tau v\|_{L^2(0,T)} &\le c\tau^s \|v\|_{\widetilde{H}_L^s(0,T)}, \qquad 0 \le s \le \alpha + 1,\\ \|v - P_\tau v\|_{\widetilde{H}_L^\alpha(0,T)} &\le c\tau^s \|v\|_{\widetilde{H}_L^{\alpha+s}(0,T)}, \qquad 0 \le s \le 1.\end{aligned}$$

Proof. By Lemma 3.2, it is stable in $L^2(0,T)$, i.e., $\|P_\tau v\|_{L^2(0,T)} \le c\|v\|_{L^2(0,T)}$. By the inf-sup condition,

$$\|v - P_\tau v\|_{L^2(0,T)} \le c \inf_{v_\tau \in \mathbb{U}_\tau} \|v - v_\tau\|_{L^2(0,T)}.$$

In particular, if $v \in \widetilde{H}_L^s(0,T)$ with $s \ge \alpha$, we may take $v_\tau = R_\tau^\alpha v$ to deduce

$$\|v - P_\tau v\|_{L^2(0,T)} \le c\tau^s \|v\|_{\widetilde{H}_L^s(0,T)}, \quad \alpha \le s \le \alpha + 1.$$

This estimate, the L^2-stability, and interpolation yield the first estimate. Next, by the triangle inequality, we derive the $\widetilde{H}_L^\alpha$-estimate:

$$\begin{aligned}\|v - P_\tau v\|_{\widetilde{H}_L^\alpha(0,T)} &\le \|v - R_\tau^\alpha v\|_{\widetilde{H}_L^\alpha(0,T)} + \|R_\tau^\alpha v - P_\tau v\|_{\widetilde{H}_L^\alpha(0,T)}\\ &\le (1 + \|P_\tau\|_{\widetilde{H}_L^\alpha(0,T) \to \widetilde{H}_L^\alpha(0,T)}) \|v - R_\tau^\alpha v\|_{\widetilde{H}_L^\alpha(0,T)}\\ &\le c\tau^s \|v\|_{\widetilde{H}_L^{\alpha+s}(0,T)},\end{aligned}$$

where the last line follows by the $\widetilde{H}_L^\alpha$-stability of P_τ in Lemma 4.4 below. □

The next result gives the $\widetilde{H}_L^\alpha$-stability of P_τ, which is needed in the proof of Lemma 4.3.

Lemma 4.4. *The fractionalized L^2-projection P_τ is stable on $\widetilde{H}_L^\alpha(0,T)$.*

Proof. First, we show the inverse estimate

$$\|v\|_{\widetilde{H}^{\alpha}_L(0,T)} \le c\tau^{-\alpha}\|v\|_{L^2(0,T)} \quad \text{for all } v \in \mathbb{U}_\tau. \tag{4.6}$$

For any $v \in \mathbb{U}_\tau$, there exists $\phi \in \mathbb{W}_\tau$ such that $v = {}_0I_t^\alpha \phi$. Thus it is equivalent to $\|\phi\|_{L^2(0,T)} \le c\tau^{-\alpha}\|{}_0I_t^\alpha\phi\|_{L^2(0,T)}$ for all $\phi \in \mathbb{W}_\tau$. Further, by (2.2) and norm equivalence, we have

$$\|\phi\|_{H^{-\alpha}(0,T)} \equiv \sup_{\psi\in\widetilde{H}^\alpha_L(0,T)} \frac{(\phi,\psi)_{L^2(0,T)}}{\|\psi\|_{\widetilde{H}^\alpha_L(0,T)}} = \sup_{\psi\in\widetilde{H}^\alpha_T(0,T)} \frac{({}_0I_t^\alpha\phi, {}_t\partial_T^\alpha\psi)_{L^2(0,T)}}{\|\psi\|_{\widetilde{H}^\alpha_T(0,T)}} \le c\|{}_0I_t^\alpha\phi\|_{L^2(0,T)}.$$

Recall the following inverse estimate [3, Theorem 4.6] (see also Remark 4.5 below):

$$\|\phi\|_{L^2(0,T)} \le c\tau^{-\alpha}\|\phi\|_{H^{-\alpha}(0,T)} \quad \text{for all } \phi \in \mathbb{W}_\tau, \tag{4.7}$$

which directly yields (4.6). Now it follows from (4.6) that for any $v \in \widetilde{H}^\alpha_L(0,T)$,

$$\begin{aligned}\|P_\tau v\|_{\widetilde{H}^\alpha_L(0,T)} &\le \|R^\alpha_\tau v\|_{\widetilde{H}^\alpha_L(0,T)} + \|R^\alpha_\tau v - P_\tau v\|_{\widetilde{H}^\alpha_L(0,T)}\\ &\le c\|v\|_{\widetilde{H}^\alpha_L(0,T)} + c\tau^{-\alpha}\|R^\alpha_\tau v - P_\tau v\|_{L^2(0,T)}\\ &\le c\|v\|_{\widetilde{H}^\alpha_L(0,T)},\end{aligned}$$

where the last step follows from Lemmas 4.2 and 4.3. □

Remark 4.5. The inverse inequality (4.7) is a special case of a general result in [3]. In our case, it follows from a duality argument. For a given $\phi \in \mathbb{W}_\tau$, find $v_\phi \in \widetilde{H}^1_L(0,T)$ such that $(v'_\phi, \varphi')_{L^2(0,T)} = (\phi,\varphi)_{L^2(0,T)}$ for all $\varphi \in \widetilde{H}^1_L(0,T)$. Then

$$\|v'_\phi\|_{L^2(0,T)} \le c\|\phi\|_{H^{-1}(0,T)} \quad \text{and} \quad \|v''_\phi\|_{L^2(0,T)} = \|\phi\|_{L^2(0,T)}.$$

Since $\phi \in \mathbb{W}_\tau$, the function v'_ϕ is conforming piecewise linear and the inverse inequality

$$\|v''_\phi\|_{L^2(0,T)} \le c\tau^{-1}\|v'_\phi\|_{L^2(0,T)}$$

holds. Thus, $\|\phi\|_{L^2(0,T)} \le c\tau^{-1}\|v'_\phi\|_{L^2(0,T)} \le c\tau^{-1}\|\phi\|_{H^{-1}(0,T)}$, and by interpolation, inequality (4.7) holds for $\alpha \in (0,1)$.

4.3 Error Estimates for Fractional ODEs

Now we derive error estimates for the scheme (4.4).

Theorem 4.6. *Let $f \in \widetilde{H}^s_L(0,T)$. Then the solution $u_\tau \in \mathbb{U}_\tau$ of (4.4) satisfies*

$$\begin{aligned}\|{}_0\partial_t^\alpha(u-u_\tau)\|_{L^2(0,T)} + \lambda\|u-u_\tau\|_{L^2(0,T)} &\le c\tau^s\|f\|_{\widetilde{H}^s_L(0,T)},\\ \|u-u_\tau\|_{L^2(0,T)} &\le c\tau^{\alpha+s}\|f\|_{\widetilde{H}^s_L(0,T)}.\end{aligned}$$

Proof. Repeating the arguments in Section 4.2 yields

$$\|{}_0\partial_t^\alpha(u-u_\tau)\|_{L^2(0,T)} + \lambda\|u-u_\tau\|_{L^2(0,T)} \le 2\inf_{v\in\mathbb{U}_\tau}\big(\|{}_0\partial_t^\alpha(u-v)\|_{L^2(0,T)} + \lambda\|u-v\|_{L^2(0,T)}\big).$$

Taking $v = P_\tau u$ and Lemma 4.3 and (4.3) yield the first estimate. Next, we apply a duality argument. Let $z \in \widetilde{H}^\alpha_R(0,T)$ solve (with $e = u - u_\tau$)

$$(\phi, {}_t\partial_T^\alpha z)_{L^2(0,T)} + \lambda(\phi, z)_{L^2(0,T)} = (\phi, e)_{L^2(0,T)} \quad \text{for all } \phi \in L^2(0,T).$$

Then, by Remark 4.5, there holds $\|z\|_{\widetilde{H}^\alpha_R(0,T)} + \lambda\|z\|_{L^2(0,T)} \le c\|e\|_{L^2(0,T)}$. By (2.2) and Galerkin orthogonality, we deduce for any $z_\tau \in \mathbb{W}_\tau$,

$$\begin{aligned}\|e\|^2_{L^2(0,T)} = a(e, z - z_\tau) &\le \big(\|{}_0\partial_t^\alpha e\|_{L^2(0,T)} + \lambda\|e\|_{L^2(0,T)}\big)\inf_{z_\tau\in\mathbb{W}_\tau}\|z-z_\tau\|_{L^2(0,T)}\\ &\le c\tau^\alpha\|z\|_{\widetilde{H}^\alpha_R(0,T)}\big(\|{}_0\partial_t^\alpha e\|_{L^2(0,T)} + \lambda\|e\|_{L^2(0,T)}\big).\end{aligned}$$

Now using the bound on z and Theorem 4.6 complete the proof. □

4.4 Enhanced Error Estimates for $f \in H^s(0,T)$, $\frac{1}{2} < s \le 1$

The trial space $\mathbb{U}_\tau$ allows improving the error estimates. First, we consider the special case of a source term $f \equiv 1$. Clearly, $f \in \widetilde{H}_L^\beta(0,T)$ for any $\beta < \frac{1}{2}$, and thus $u \in \widetilde{H}_L^{\alpha+\beta}(0,T)$. Theorem 4.6 gives an L^2-error with the rate $O(\tau^{\alpha+\beta})$. By Laplace transform, we derive $u(t) = t^\alpha E_{\alpha,\alpha+1}(-\lambda t^\alpha)$. In the splitting

$$u = \frac{t^\alpha}{\Gamma(\alpha+1)} + \tilde{u},$$

since $\tilde{u} \in \widetilde{H}_L^{2\alpha+\beta}(0,T)$ and $t^\alpha \in \mathbb{U}_\tau$, we obtain

$$\inf_{v\in\mathbb{V}_\tau} \|u - v\|_{\widetilde{H}_L^\alpha(0,T)} = \inf_{v\in\mathbb{V}_\tau} \|\tilde{u} - v\|_{\widetilde{H}_L^\alpha(0,T)} \le c\tau^{\min(\alpha+\beta,1)} \quad \text{for all } \beta \in [0, \tfrac{1}{2}).$$

Then by a duality argument we have

$$\|u - u_\tau\|_{L^2(0,T)} \le c\tau^{\alpha+\min(\alpha+\beta,1)} \quad \text{for all } \beta \in [0, \tfrac{1}{2}).$$

Generally, for $f \in H^s(0,T)$, $\frac{1}{2} < s \le 1$, one may split $f = f(0) + \tilde{f}$, with $\tilde{f} = f - f(0) \in \widetilde{H}_L^s(0,T)$, and accordingly $u = \hat{u} + \tilde{u}$, where ${}_0\partial_t^\alpha \hat{u} + \lambda\hat{u} = f(0)$ and ${}_0\partial_t^\alpha \tilde{u} + \lambda\tilde{u} = \tilde{f}(t)$, with $\hat{u}(0) = \tilde{u}(0) = 0$. By (4.3), $\tilde{u} \in \widetilde{H}_L^{\alpha+s}(0,T)$ and it can be approximated with an L^2-error $O(\tau^{\alpha+s})$. Hence we have

$$\|u - u_\tau\|_{L^2(0,T)} + \tau^\alpha \|u - u_\tau\|_{\widetilde{H}_L^\alpha(0,T)} \le c\tau^{\alpha+\min(\alpha+\beta,s)} \quad \text{for all } \beta \in [0, \tfrac{1}{2}).$$

5 Error Estimates for Fractional PDE

Now we derive error estimates for the scheme (3.3). Recall the semidiscrete Galerkin problem for problem (1.1): for $t \in (0,T]$, find $u_h(t) \in \mathbb{X}_h$ such that

$$({}_0\partial_t^\alpha u_h(t), \phi)_{L^2(\Omega)} + (\nabla u_h(t), \nabla\phi)_{L^2(\Omega)} = (f(t), \phi)_{L^2(\Omega)} \quad \text{for all } \phi \in \mathbb{X}_h, \tag{5.1}$$

with $u_h(0) = 0$. Next, we recast it into a space semidiscrete space-time formulation by defining a trial space $\mathbb{B}_h^\alpha := \widetilde{H}_L^\alpha(0,T) \otimes \mathbb{X}_h \subset B^\alpha(Q_T)$ and a test space $\mathbb{V}_h := L^2(0,T) \otimes \mathbb{X}_h \subset V(Q_T)$, with the associated norms on $B^\alpha(Q_T)$ and $V(Q_T)$, respectively. Then (5.1) is equivalent to: find $u_h \in \mathbb{B}_h^\alpha$ such that

$$a(u_h, \phi) = \langle f, \phi\rangle_{L^2(Q_T)} \quad \text{for all } \phi \in \mathbb{V}_h.$$

The argument of Lemma 2.4 similarly yields an inf-sup condition for the semidiscrete problem: there holds, for some c independent of h,

$$\sup_{\phi\in\mathbb{V}_h} \frac{a(v,\phi)}{\|\phi\|_V} \ge c\|v\|_{B^\alpha(Q_T)} \quad \text{for all } v \in \mathbb{B}_h^\alpha. \tag{5.2}$$

Using the basis $\{\psi_j\}_{j=1}^N$ (cf. Section 3.3), we expand u_h and $u_{h\tau}$ into

$$u_h(t) = \sum_{j=1}^N u_{j,h}(t)\psi_j \quad \text{and} \quad u_{h\tau}(t) = \sum_{j=1}^N u_{j,h\tau}(t)\psi_j, \tag{5.3}$$

where

$$u_{j,h}(t) = (u_h(t), \psi_j)_{L^2(\Omega)} \quad \text{and} \quad u_{j,h\tau}(t) = (u_{h\tau}(t), \psi_j)_{L^2(\Omega)}.$$

Further, the function $u_{j,h}(t)$ satisfies $u_{j,h}(0) = 0$ and

$${}_0\partial_t^\alpha u_{j,h} + \lambda_{j,h} u_{j,h} = f_{j,h}, \quad 0 < t \le T,$$

where

$$f_{j,h}(t) = (P_h f(\cdot,t), \psi_j)_{L^2(\Omega)} \in \widetilde{H}_L^s(0,T) \quad \text{if } f \in \widetilde{H}_L^s(0,T; L^2(\Omega)).$$

Similarly, the function $u_{j,h\tau} \in \mathbb{U}_\tau$ satisfies

$$({}_0\partial_t^\alpha u_{j,h\tau} + \lambda_{j,h} u_{j,h\tau}, \phi)_{L^2(0,T)} = (f_{j,h}, \phi)_{L^2(0,T)} \quad \text{for all } \phi \in \mathbb{W}_\tau.$$

That is, $u_{j,h\tau}$ is the Petrov–Galerkin approximation of $u_{j,h}$, and thus Theorem 4.6 gives the following error estimates on $e_{j,h} := u_{j,h} - u_{j,h\tau}$:

$$\|{}_0\partial_t^\alpha e_{j,h}\|_{L^2(0,T)} + \lambda_{j,h}\|e_{j,h}\|_{L^2(0,T)} \le c\tau^s \|f_{j,h}\|_{\widetilde{H}_L^s(0,T)}, \tag{5.4}$$

$$\|e_{j,h}\|_{L^2(0,T)} \le c\tau^{\alpha+s}\|f_{j,h}\|_{\widetilde{H}_L^s(0,T)}. \tag{5.5}$$

Next, we give an energy error estimate for u_h.

Lemma 5.1. *For $f \in L^2(Q_T)$, the semidiscrete solution u_h satisfies*

$$\|u_h - u\|_{B^\alpha(Q_T)} \le ch\|f\|_{L^2(Q_T)}.$$

Proof. By (3.1) and Theorem 2.8, for $\varrho := P_h u - u$ we have

$$\|\varrho\|_{B_L^\alpha(Q_T)} \le ch(\|u\|_{\widetilde{H}_L^\alpha(0,T;L^2(\Omega))} + \|u\|_{L^2(0,T;H^2(\Omega))}) \le ch\|f\|_{L^2(Q_T)}.$$

The function $\vartheta := u_h - P_h u$ satisfies $\vartheta(0) = 0$ and

$${}_0\partial_t^\alpha \vartheta - \Delta_h \vartheta = \Delta_h(P_h u - R_h u) = \Delta_h R_h \varrho,$$

where R_h is the Ritz projection [12, (3.22)]. By (5.2) and (3.10),

$$\|\vartheta\|_{B_L^\alpha(Q_T)} \le c\|\Delta_h R_h \varrho\|_{L^2(0,T;H^{-1}(\Omega))} \le c\|R_h\varrho\|_{L^2(0,T;H^1(\Omega))} \le ch\|f\|_{L^2(Q_T)}.$$

These two estimates and the triangle inequality complete the proof. □

Then we can derive an energy norm estimate for the scheme (3.3).

Theorem 5.2. *Let $f \in \widetilde{H}_L^s(0,T;L^2(\Omega))$ with $0 \le s \le 1$, and let u and $u_{h\tau}$ be the solutions of (2.3) and (3.3), respectively. Then there holds*

$$\|u - u_{h\tau}\|_{B^\alpha(Q_T)} \le c(\tau^s + h)\|f\|_{\widetilde{H}_L^s(0,T;L^2(\Omega))}.$$

Proof. By the expansions (5.3) and (5.4), we bound the error $e_h := u_h - u_{h\tau}$ by

$$\begin{aligned}\|e_h\|_{B^\alpha(Q_T)}^2 &= \sum_{j=1}^N \lambda_{j,h}^{-1}\|{}_0\partial_t^\alpha e_{j,h}\|_{L^2(0,T)}^2 + \sum_{j=1}^N \lambda_{j,h}\|e_{j,h}\|_{L^2(0,T)}^2 \\ &\le c\tau^{2s}\sum_{j=1}^N \lambda_{j,h}^{-1}\|f_{j,h}\|_{\widetilde{H}_L^s(0,T)}^2 \le c\tau^{2s}\|f\|_{\widetilde{H}_L^s(0,T;H^{-1}(\Omega))}^2.\end{aligned}$$

This, Lemma 5.1 and the triangle inequality give the desired assertion. □

Finally, we present the $L^2(Q_T)$ error estimate.

Theorem 5.3. *For $f \in \widetilde{H}_L^s(0,T;L^2(\Omega))$, let u and $u_{h\tau}$ be the solutions of (2.3) and (3.3), respectively. Then there holds*

$$\|u - u_{h\tau}\|_{L^2(Q_T)} \le c(\tau^{\alpha+s} + h^2)\|f\|_{\widetilde{H}_L^s(0,T;L^2(\Omega))}.$$

Proof. By (5.5) and the $L^2(\Omega)$-stability of P_h, we bound $e_h := u_h - u_{h\tau}$ by

$$\|e_h\|_{L^2(Q_T)}^2 = \sum_{j=1}^N \|e_{j,h}\|_{L^2(0,T)}^2 \le c\tau^{2(\alpha+s)}\sum_{j=1}^N \|f_{j,h}\|_{\widetilde{H}_L^s(0,T)}^2 \le c\tau^{2(\alpha+s)}\|f\|_{\widetilde{H}_L^s(0,T;L^2(\Omega))}^2.$$

Then the estimate $\|u_h - u\|_{L^2(Q_T)} \le ch^2\|f\|_{L^2(Q_T)}$ (see [11, Theorem 3.4]) completes the proof. □

α	K	10	20	40	80	160	320	Rate
0.3	L^2	8.49e-3	3.96e-3	1.92e-3	9.57e-4	4.68e-4	2.36e-4	1.03(1.10)
	H^α	3.15e-2	1.78e-2	1.04e-2	6.18e-3	3.75e-3	2.33e-3	0.75(0.80)
0.5	L^2	3.88e-3	1.51e-3	5.89e-4	2.29e-4	8.74e-5	3.37e-5	1.36(1.50)
	H^α	3.20e-2	1.74e-2	9.48e-3	5.12e-3	2.78e-3	1.54e-3	0.87(1.00)
0.7	L^2	1.66e-3	5.15e-4	1.59e-4	4.94e-5	1.52e-5	4.73e-6	1.69(1.70)
	H^α	2.98e-2	1.53e-2	7.81e-3	3.96e-3	2.01e-3	1.04e-3	0.96(1.00)
0.9	L^2	8.51e-4	2.21e-4	5.74e-5	1.49e-5	3.91e-6	1.03e-6	1.93(1.90)
	H^α	2.84e-2	1.42e-2	7.12e-3	3.56e-3	1.78e-3	9.10e-4	0.99(1.00)

Table 2. The errors $\|u - u_\tau\|_{L^2(0,T)}/\|u\|_{L^2(0,T)}$ and $\|u - u_\tau\|_{H^\alpha(0,T)}/\|u\|_{L^2(0,T)}$ for the fractional ODE with $\alpha = 0.3, 0.5, 0.7$, and 0.9.

Remark 5.4. In practice, the Caputo derivative is preferred, since it allows specifying initial conditions as usual [16, pp. 353–358]; see [18] for a thorough discussion. Our approach can be extended to the case of smooth initial data:

$$\begin{cases} \partial_t^\alpha u - \Delta u = f & \text{in } \Omega \times (0, T), \\ u = 0 & \text{on } \partial\Omega \times (0, T), \\ u(0) = u_0 & \text{in } \Omega, \end{cases}$$

where $u_0 \in H_0^1(\Omega) \cap H^2(\Omega)$ and $\partial_t^\alpha u := {}_0I_t^{1-\alpha} u'$ denotes the Caputo derivative of order $\alpha \in (0, 1)$. The function $w := u - u_0$ satisfies (1.1) with a source $F = f + \Delta u_0$, to which our approach applies.

6 Numerical Examples

Now we numerically illustrate our theoretical findings. Since the semidiscrete problem has been verified [11], we focus on the temporal discretization error below. In all tables the computed rates are given in the last column, whereas the numbers in brackets denote the theoretical rates.

6.1 Fractional ODEs

First, we examine the convergence of the method for fractional ODEs. We consider the initial value problem ${}_0\partial_t^\alpha u(t) + u(t) = e^t$ in $(0, T)$, with $u(0) = 0$. The source term $f(t) = e^t$ belongs to the space $H^1(0, T)$, and also in $\widetilde{H}_L^s(0, T)$ for $s < \frac{1}{2}$. Thus, Theorem 4.6 gives a convergence rate $O(\tau^s)$ in the $H^\alpha(0, T)$-norm, and $O(\tau^{\alpha+s})$ in the $L^2(0, T)$-norm, respectively. By the discussion in Section 4.4, we have an improved convergence rate $O(\tau^{\min(1,\alpha+s)})$ in the $\widetilde{H}_L^\alpha(0, T)$-norm and $O(\tau^{\alpha+\min(1,\alpha+s)})$ in the $L^2(0, T)$-norm, $s \in (0, \frac{1}{2})$. These improved rates are numerically confirmed by Table 2 for $T = 1$, where the reference solution is computed on a finer mesh with a time step size $\tau = \frac{1}{2000}$.

6.2 1-D Fractional PDEs

Now we consider examples on the unit interval $\Omega = (0, 1)$ with $T = 1$, and perform numerical tests on the following four sets of problem data:

(a) $f(x, t) = x(1 - x)(e^t - 1)$, with $e^t - 1 \in \widetilde{H}_L^1(0, T)$.
(b) $f(x, t) = x(1 - x)e^t$, with $e^t \in \widetilde{H}_L^s(0, T) \cap H^1(0, T)$, $s < \frac{1}{2}$.
(c) $f(x, t) = t^{-0.3} x(1 - x)$, with $t^{-0.3} \in \widetilde{H}_L^s(0, T)$, $s < 0.2$.
(d) $f(x, t) = t^{-0.3}$, with $t^{-0.3} \in \widetilde{H}_L^s(0, T)$, $s < 0.2$.

In cases (a)–(c), the source f is compatible with the zero initial data, but not in case (d). In our computation, we fix the spatial mesh size h at $h = \frac{1}{2000}$. The reference solutions are computed on a finer temporal

Case	$\alpha \setminus K$	10	20	40	80	160	320	Rate
(a)	0.3	1.85e-2	7.50e-3	3.07e-3	1.27e-3	5.17e-4	2.12e-4	1.28(1.30)
	0.5	8.95e-3	3.16e-3	1.12e-3	4.03e-4	1.42e-4	5.05e-5	1.49(1.50)
	0.7	4.71e-3	1.45e-3	4.44e-4	1.36e-4	4.12e-5	1.26e-5	1.70(1.70)
	0.9	2.84e-3	7.60e-4	2.00e-4	5.27e-5	1.38e-5	3.65e-6	1.92(1.90)
(b)	0.3	2.66e-2	1.76e-2	1.14e-2	7.33e-3	4.48e-3	2.77e-3	0.65(0.80)
	0.5	2.87e-2	1.58e-2	8.17e-3	3.99e-3	1.81e-3	8.20e-4	1.02(1.00)
	0.7	2.21e-2	8.94e-3	3.28e-3	1.12e-3	3.67e-4	1.18e-4	1.50(1.20)
	0.9	1.23e-2	3.53e-3	9.64e-4	2.57e-4	6.76e-5	1.77e-5	1.88(1.40)
(c)	0.3	2.90e-1	2.36e-1	1.90e-1	1.52e-1	1.18e-1	9.08e-2	0.33(0.50)
	0.5	2.44e-1	1.73e-1	1.18e-1	7.90e-2	5.10e-2	3.27e-2	0.58(0.70)
	0.7	1.80e-1	1.01e-1	5.48e-2	2.89e-2	1.51e-2	8.01e-3	0.89(0.90)
	0.9	1.10e-1	4.92e-2	2.15e-2	9.55e-3	4.29e-3	1.95e-3	1.16(1.10)
(d)	0.3	2.90e-1	2.36e-1	1.90e-1	1.52e-1	1.18e-1	9.10e-2	0.33(0.50)
	0.5	2.45e-1	1.73e-1	1.19e-1	7.96e-2	5.16e-2	3.34e-2	0.57(0.70)
	0.7	1.81e-1	1.02e-1	5.59e-2	2.99e-2	1.60e-2	8.66e-3	0.87(0.90)
	0.9	1.12e-1	5.11e-2	2.31e-2	1.05e-2	4.81e-3	2.21e-3	1.13(1.10)

Table 3. The relative error $\|u - u_{h\tau}\|_{L^2(Q_T)}/\|u\|_{L^2(Q_T)}$ for examples (a)–(d) with $\alpha = 0.3, 0.5, 0.7, 0.9$, and $h = \frac{1}{2000}$.

Case	$\alpha \setminus K$	10	20	40	80	160	320	Rate
(c)	0.3	6.20e-3	2.46e-3	9.83e-4	3.92e-4	1.54e-4	5.91e-5	1.34(–)
	0.5	2.26e-3	7.82e-4	2.71e-4	9.39e-5	3.23e-5	1.08e-5	1.54(–)
	0.7	4.37e-4	1.36e-4	4.16e-5	1.26e-5	3.82e-6	1.13e-6	1.71(–)
	0.9	3.13e-4	6.68e-5	1.57e-5	3.63e-6	7.96e-7	1.60e-7	2.18(–)
(d)	0.3	6.20e-3	2.46e-3	9.83e-4	3.92e-4	1.54e-4	5.91e-5	1.34(–)
	0.5	2.26e-3	7.82e-4	2.70e-4	9.38e-5	3.23e-5	1.08e-5	1.54(–)
	0.7	4.54e-4	1.36e-4	4.16e-5	1.26e-5	3.81e-6	1.13e-6	1.73(–)
	0.9	2.46e-3	1.19e-4	1.58e-5	3.63e-6	7.98e-7	1.60e-7	2.78(–)

Table 4. The relative error $\|u(\cdot, T) - u_{h\tau}(\cdot, T)\|_{L^2(\Omega)}/\|u(\cdot, T)\|_{L^2(\Omega)}$ at the time $T = 1$ for examples (c)–(d) with $\alpha = 0.3, 0.5, 0.7$, and 0.9, and $h = \frac{1}{2000}$.

mesh with a time step size $\tau = \frac{1}{2000}$. The numerical results are given in Table 3. The empirical $L^2(Q_T)$ convergence rate agrees well with the theoretical one $O(\tau^{s+\alpha})$; cf. Theorem 5.3. The (temporal) convergence improves steadily with the temporal regularity of the source f and for a fixed f, with the fractional order α, reflecting the improved temporal solution regularity. It is also worth noting that the spatial regularity of the source f does not influence the temporal convergence, which concurs with Theorem 5.3. Further, for case (b) with large fractional order α, e.g., $\alpha = 0.7$ or 0.9, we observe an empirical convergence rate higher than the theoretical one $O(\tau^{s+\alpha})$. This phenomenon is analogous to that for fractional ODEs in Section 4.4, due to the special construction of the trial space $\mathbb{B}^{\alpha}_{h\tau}$, and might be analyzed as in the ODE case, which, however, is beyond the scope of this work.

In Table 4, we present the $L^2(\Omega)$-error at the final time T for examples (c) and (d), by viewing (3.3) as a time-stepping scheme. Numerically one observes an $O(\tau^{\alpha+1})$ rate, irrespective of the spatial regularity of f. The precise mechanism for the high convergence rate in the case of nonsmooth data is to be studied.

6.3 2-D Fractional PDEs

Last, we consider two examples in two space dimension, with the domain $\Omega = (0, 1)^2$ and $T = 1$, and perform a numerical test on the following data:

(e) $f(x, y, t) = x(1 - x)y(1 - y)\sin t$, with $\sin t \in \widetilde{H}^1_L(0, T)$.

(f) $f(x, y, t) = x(1 - x)y(1 - y)t^{-0.3}$, with $t^{-0.3} \in \widetilde{H}^s_L(0, T)$, $s < 0.2$.

Case	$\alpha \setminus K$	10	20	40	80	160	320	Rate
(e)	0.3	1.50e-2	6.15e-3	2.52e-3	1.05e-3	4.26e-4	1.75e-4	1.28(1.30)
	0.5	8.38e-3	3.06e-3	1.10e-3	4.02e-4	1.41e-4	5.05e-5	1.47(1.50)
	0.7	5.65e-3	1.88e-3	6.00e-4	1.85e-4	5.54e-5	1.67e-5	1.68(1.70)
	0.9	4.46e-3	1.30e-3	3.52e-4	9.28e-5	2.41e-5	6.31e-6	1.89(1.90)
(f)	0.3	3.31e-1	2.78e-1	2.31e-1	1.91e-1	1.54e-1	1.22e-1	0.28(0.50)
	0.5	3.15e-1	2.39e-1	1.77e-1	1.27e-1	8.74e-2	5.90e-2	0.48(0.70)
	0.7	2.76e-1	1.73e-1	1.01e-1	5.60e-2	2.98e-2	1.58e-2	0.82(0.90)
	0.9	2.06e-1	9.81e-2	4.37e-2	1.92e-2	8.50e-3	3.81e-3	1.15(1.10)

Table 5. The relative error $\|u - u_{h\tau}\|_{L^2(Q_T)}/\|u\|_{L^2(Q_T)}$ for examples (e) and (f) with $\alpha = 0.3, 0.5, 0.7$, and 0.9, and $h = \frac{1}{100}$.

In either case, the source term is compatible with the zero initial data. In the computation, we first divide the unit interval $(0, 1)$ into M equally spaced subintervals with a mesh size $h = \frac{1}{M}$, which partitions the domain Ω into M^2 small squares. Then we obtain a regular partition of the domain by connecting the diagonals. The results for cases (e) and (f) are given in Table 5, where the mesh size h is fixed at $h = \frac{1}{100}$ and the reference solution is computed with $\tau = \frac{1}{2000}$. In case (e), the source f is smooth in time, and the empirical convergence agrees well with the theoretical prediction. In case (f), f is nonsmooth in time, and the convergence rate for a small fractional order α suffers some loss, similar to the one-dimensional case.

7 Concluding Remarks

In this paper, we have explored the viability of space-time discretizations for numerically solving time-dependent fractional-order differential equations, and proposed a novel Petrov–Galerkin finite element method on the pair of spaces $\mathbb{X}_h \times \mathbb{U}_\tau$ as the trial space and $\mathbb{X}_h \times \mathbb{W}_\tau$ as the test space, where the space $\mathbb{U}_\tau$ consists of fractionalized piecewise constant functions. One distinct feature of our approach is that it leads to an unconditionally stable time stepping scheme. It may have interesting applications to other types of fractional-order differential equations.

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