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A Petrov–Galerkin finite element method for variable-coefficient fractional diffusion equations

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Abstract

Fractional diffusion equations have found increasingly more applications in recent years but introduce new mathematical and numerical difficulties. Galerkin formulation, which was proved to be coercive and well-posed for fractional diffusion equations with a constant diffusivity coefficient, may lose its coercivity for variable-coefficient problems. The corresponding finite element method fails to converge.

We utilize the discontinuous Petrov–Galerkin (DPG) framework to develop a Petrov–Galerkin finite element method for variable-coefficient fractional diffusion equations. We prove the well-posedness and optimal-order convergence of the Petrov–Galerkin finite element method. Numerical examples are presented to verify the theoretical results.

Keywords: Discontinuous Petrov–Galerkin framework; Fractional diffusion equations; Petrov–Galerkin finite element method; Weak coercivity

1. Introduction

In the last few decades fractional differential equations (FDEs) have found increasingly more applications in fluid mechanics [1], anomalous diffusion and acceleration of steep fronts in reaction–diffusion processes [2,3], turbulence in geophysical flows or plasma physics [4–6], continuum mechanics [7], as they provide very effective alternatives for modeling complex systems characterized by nonlocal phenomena and long range interactions. However, FDEs present mathematical difficulties that have not been encountered in the context of second-order differential equations. In their pioneer work [8], Ervin and Roop proved coercivity of a Galerkin formulation and the well-posedness of the homogeneous Dirichlet boundary-value problem of a constant–coefficient conservative FDE. We showed that for variable-coefficient FDEs the Galerkin formulation loses its coercivity [9] and that the Galerkin finite element methods might fail to converge [10].

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To overcome these difficulties we proposed a Petrov–Galerkin formulation for the homogeneous Dirichlet boundary-value problem of FDEs, and proved its weak coercivity and well-posedness [9]. However, there is a sharp difference between a Galerkin formulation and a Petrov–Galerkin formulation: Coercivity of a Galerkin formulation on an infinite-dimensional admissible space ensures that of the formulation on any finite-dimensional subspace. Consequently, the unique solvability and stability of Galerkin finite element methods are guaranteed automatically. In contrast, weak coercivity of a Petrov–Galerkin formulation on a pair of infinite-dimensional product spaces cannot ensure that of the formulation on any pair of finite-dimensional subspaces. Therefore, one still has to analyze how to choose appropriate finite-dimensional trial space and test space to ensure the weak coercivity and so the unique solvability and stability of the corresponding Petrov–Galerkin finite element method.

In this paper we utilize the DPG (discontinuous Petrov–Galerkin) framework of Demkowicz and Gopalakrishnan [11–14] to develop a Petrov–Galerkin finite element method for a class of variable-coefficient conservative FDEs in one space dimension. We prove its error estimate in the energy norm and the L^2 norm. Numerical experiments are presented to verify the convergence rates of the method. The rest of the paper is organized as follows: In Section 2 we present the model problem and cite known results to be used subsequently. In Section 3 we apply the DPG framework to the model problem. In Section 4 we develop a Petrov–Galerkin finite element method with optimal test functions for fractional diffusion equations with a constant diffusivity coefficient. We then prove the corresponding error estimates. In Section 5 we develop a Petrov–Galerkin finite element method with approximately optimal test functions for fractional diffusion equations with a variable diffusivity coefficient and prove the corresponding error estimates in the energy norm and the L^2 norm. In Section 6 we conduct numerical experiments to investigate the performance of the Petrov–Galerkin method and to verify its convergence rate numerically. In Section 7 we draw concluding remarks and outline future work.

2. Problem formulation

Let $C_0^\infty(0,1)$ be the space of infinitely many times differentiable functions on $(0,1)$ that are compactly supported within $(0,1)$. Let $L^p(0,1)$, with $1 \le p \le +\infty$, be the standard normed spaces of pth power Lebesgue integrable functions on $(0,1)$. Let $W^{m,p}(0,1)$ be the Sobolev space of functions on $(0,1)$ whose weak derivatives up to order m are in $L^p(0,1)$. Let $H^\mu(0,1)$, with $\mu > 1/2$, be the fractional Sobolev space of order μ and $H_0^\mu(0,1)$ be the completion of $C_0^\infty(0,1)$ with respect to the Sobolev norm $\|\cdot\|_{H^\mu(0,1)}$. Let $H^{-\mu}(0,1)$ be the dual space of $H_0^\mu(0,1)$.

We consider the variable-coefficient conservative FDE in one space dimension

$$-D\big[K(x)\big(\theta\,{}_0^CD_x^{1-\beta}u-(1-\theta)\,{}_x^CD_1^{1-\beta}u\big)\big]=f(x),\quad x\in(0,1),\qquad u(0)=u(1)=0. \tag{1}$$

Here $Du(x) := u'(x)$ is the first-order differential operator, $2-\beta$ with $0<\beta<1$ represents the order of anomalous diffusion of the problem, K is the diffusivity coefficient with

$$0 < K_{\min} \le K(x) \le K_{\max} < \infty, \tag{2}$$

$0 \le \theta \le 1$ indicates the relative weight of forward versus backward transition probability, and f is the right-hand side. The left and right fractional integrals of order β are defined for any function $u \in L^p(0,1)$ by [15,16]

$${}_0D_x^{-\beta}u(x) := \frac{1}{\Gamma(\beta)}\int_0^x \frac{u(s)}{(x-s)^{1-\beta}}ds,\qquad {}_xD_1^{-\beta}u(x) := \frac{1}{\Gamma(\beta)}\int_x^1 \frac{u(s)}{(s-x)^{1-\beta}}ds,$$

where $\Gamma(\cdot)$ is the Gamma function. The left and right Caputo and Riemann–Liouville fractional derivatives of order β are defined by

$$\begin{aligned}
{}_0^CD_x^\beta u(x) &:= {}_0D_x^{-(1-\beta)}Du(x), &\qquad {}_x^CD_1^\beta u(x) &:= -{}_xD_1^{-(1-\beta)}Du(x),\\
{}_0^RD_x^\beta u(x) &:= D\,{}_0D_x^{-(1-\beta)}u(x), &\qquad {}_x^RD_1^\beta u(x) &:= -D\,{}_xD_1^{-(1-\beta)}u(x).
\end{aligned}$$

The mathematical model (1) arises in many physical and engineering applications. In groundwater hydrology, (1) represents the pressure equation for the flow, in which u is the water head, $K(x)$ is the intrinsic permeability of the porous medium, and f is the source and sink term [17]. Eq. (1) is obtained by incorporating a fractional Darcy's law, which accounts for the non-local interaction in the flow, into a mass balance law for the flow [18]. In the context of elasticity, Eq. (1) can be viewed as a generalized elasticity equation obtained by incorporating a fractional Hooke's law into a classical force balance equation to take into account of the nonlocal interaction [19–22], which provides a fractional analogue to an alternative nonlocal elasticity model, i.e., the peridynamic model [23]. In anomalous diffusive transport processes, u is the concentration of the solute, K is the diffusivity coefficient, Eq. (1) can be derived by incorporating a fractional Fickian law into a mass conservation equation for the solute [2,4]. The model captures a power-law leading edge which is super-diffusive spreading away from the plume center of mass [24]. Although it was originally obtained via a data fitting technique, this model was later derived rigorously using a continuous time random walk approach [25].

Ervin and Roop derived a Galerkin formulation for problem (1) with a constant K: Given $f \in H^{-(1-\beta/2)}$, find $u \in H_0^{1-\beta/2}$ such that

$$B(u, v) = \langle f, v\rangle \quad \forall v \in H_0^{1-\beta/2}. \tag{3}$$

Here the bilinear form $B : H_0^{1-\beta/2} \times H_0^{1-\beta/2} \to \mathbb{R}$ is defined by

$$B(w, v) := \theta\big\langle K\, {}_0^C D_x^{1-\beta} w, Dv\big\rangle - (1-\theta)\big\langle K\, {}_x^C D_1^{1-\beta} w, Dv\big\rangle,$$

where $\langle\cdot,\cdot\rangle$ denotes the duality pairing of $H^{-\mu}$ and H_0^{μ}, $\mu \geq 0$. They further proved the following theorem [8].

Theorem 1. *If K is a positive constant, then $B(\cdot,\cdot)$ is coercive and continuous on the product space $H_0^{1-\beta/2} \times H_0^{1-\beta/2}$. Hence, the Galerkin formulation (3) has a unique solution $u \in H_0^{1-\beta/2}$ with*

$$\|u\|_{H^{1-\beta/2}} \leq \frac{K}{\gamma}\|f\|_{H^{-(1-\beta/2)}}.$$

Moreover, the optimal-order error estimate holds for the corresponding finite element method that consists of piecewise polynomials of degree up to $m-1$

$$\|u_h - u\|_{H^{1-\beta/2}} \leq Ch^{r-1+\beta/2}\|u\|_{H^r}, \quad 1-\beta/2 \leq r \leq m$$

provided that the true solution u has the desired regularity. Furthermore, if the solution v to the adjoint problem

$$-D\big[K\big(-\theta\, {}_x^C D_1^{1-\beta} v + (1-\theta)\, {}_0^C D_x^{1-\beta} v\big)\big] = g(x), \quad x \in (0,1), \qquad v(0) = v(1) = 0 \tag{4}$$

*is in $H^{2-\beta} \cap H_0^{1-\beta/2}$ for **each** right-hand side $g \in L^2$ so that*

$$\|v\|_{H^{2-\beta}} \leq C\|g\|_{L^2},$$

then the following optimal-order L^2 error estimate holds

$$\|u_h - u\|_{L^2} \leq Ch^r\|u\|_{H^r}, \quad 1-\beta/2 \leq r \leq m.$$

We showed in [9] that for a variable diffusivity coefficient K with large variations, the bilinear form $B(\cdot,\cdot)$ in (3) may lose its coercivity. Numerical experiments showed that the corresponding Galerkin finite element method may fail to converge in general [10]. In [9] we studied a one-sided analogue of problem (1)

$$-D\big(K(x)\, {}_0^C D_x^{1-\beta} u\big) = f(x), \quad x \in (0,1), \qquad u(0) = u(1) = 0. \tag{5}$$

This model, which corresponds to (1) with $\theta = 1$, describes a super-diffusive leading edge of a plume with a positive skewness in the profile, which has been observed from the data in the Macrodispersion Experimental site (MADE) at the Columbus AFB in Mississippi [24]. It was also reported that retention of contaminant particles in river beds and eddy pools causes a power-law trailing edge in the concentration profile, which corresponds to (1) with $\theta = 0$ [26,27]. Hence, the model is of the same form as (5), with the left fractional derivative replaced by the right fractional derivative, and hence can be solved by the same method developed in this paper.

In [9] we introduced a Petrov–Galerkin formulation for (5): Given $f \in H^{-(1-\beta)}$, find $u \in H_0^{1-\beta}$ such that

$$A(u, v) := \big\langle K {}_0^C D_x^{1-\beta} u, Dv\big\rangle = \big\langle f, v\big\rangle \quad \forall v \in H_0^1 \tag{6}$$

and proved its weak coercivity and well-posedness.

Theorem 2. *If* $K \in L^\infty(0,1)$ *in* (5) *satisfies* (2), *then the bilinear form* $A(\cdot,\cdot)$ *is continuous and weakly coercive on* $H_0^{1-\beta} \times H_0^1$, *i.e.,*

$$\inf_{w \in H_0^{1-\beta}} \sup_{v \in H_0^1} \frac{|A(w,v)|}{\|w\|_{H^{1-\beta}} \|v\|_{H^1}} \geq \gamma, \qquad \sup_{w \in H_0^{1-\beta}} |A(w,v)| > 0 \quad \forall\, v \in H_0^1 \setminus \{0\}.$$

Consequently, (6) *has a unique solution* $u \in H_0^{1-\beta}$ *such that*

$$\|u\|_{H^{1-\beta}} \leq \frac{K_{\max}}{\gamma} \|f\|_{H^{-1}}.$$

3. The discontinuous Petrov–Galerkin (DPG) framework

The Petrov–Galerkin formulation (6) suggests a finite element discretization for problem (5): Let $S_h \subset H_0^{1-\beta}$ and $V_h \subset H_0^1$ be finite dimensional trial and test spaces, respectively, with $\dim(S_h) = \dim(V_h)$. Find $u_h \in S_h$ such that

$$A(u_h, v_h) = \langle f, v_h \rangle \quad \forall v_h \in V_h. \tag{7}$$

For Galerkin formulation (3), the coercivity of the bilinear form B on the space $H_0^{1-\beta/2}$ automatically guarantees the coercivity and so the unique solvability and stability of Galerkin finite element methods for any finite element subspace $S_h \subset H_0^{1-\beta/2}$. However, the weak coercivity of the bilinear form A on the product space $H_0^{1-\beta} \times H_0^1$ does not ensure that on a pair of finite dimensional subspaces $S_h \times V_h$, in general. Extra care has to be taken in choosing the trial space S_h and the test space V_h to ensure the weak coercivity of the bilinear form A on the product space $(S_h \times V_h) \subset (H_0^{1-\beta} \times H_0^1)$. The following theorem states a sufficient condition for the well-posedness and convergence of a Petrov–Galerkin finite element method [28,29].

Theorem 3. *Assume that the condition of* Theorem 2 *holds and that* $\dim(S_h) = \dim(V_h)$. *In addition, if there exists a positive constant* γ_h *such that*

$$\inf_{u_h \in S_h} \sup_{0 \neq v_h \in V_h} \frac{|A(u_h, v_h)|}{\|u_h\|_{H^{1-\beta}} \|v_h\|_{H^1}} \geq \gamma_h, \tag{8}$$

then the Petrov–Galerkin method (7) *has a unique solution* $u_h \in S_h$ *with the error estimate*

$$\|u - u_h\|_{H^{1-\beta}} \leq \frac{M}{\gamma_h} \inf_{w_h \in S_h} \|u - w_h\|_{H^{1-\beta}}. \tag{9}$$

While it presents a sufficient condition for the well-posedness and an optimal-order error estimate in the energy norm for the Petrov–Galerkin method (7), the theorem gives no clue on the choice of the trial and test spaces to ensure that the condition (8) holds. In this paper we follow the framework of [30,11–14] to construct an optimal test space to ensure the weak coercivity of the discrete bilinear form A, i.e., (8), so that the well-posedness and the optimal-order error estimate (9) for the resulting Petrov–Galerkin method (7) hold. Define the *trial-to-test* operator $T : H_0^{1-\beta} \to H_0^1$ by

$$(Tw, v)_{H^1} = A(w,v) \quad \forall v \in H_0^1. \tag{10}$$

The map T is well defined since for each given $w \in H_0^{1-\beta}$, the bilinear form $A(w,\cdot)$ defines a bounded linear functional on H_0^1 and so there exists a unique $Tw \in H_0^1$ such that (10) holds by Riesz representation theorem. We then introduce the energy norm

$$\|w\|_E := \sup_{0 \neq v \in H_0^1} \frac{|A(w,v)|}{\|v\|_{H^1}} \quad \forall w \in H_0^{1-\beta}. \tag{11}$$

The following lemma shows the equivalence between the norms $\|\cdot\|_E$ and $\|\cdot\|_{H^{1-\beta}}$ on the space $H_0^{1-\beta}$ and the relation between the norm $\|\cdot\|_E$ and the map T [11–14].

Lemma 4. *Under the conditions of Theorem 2, we have*

$$\gamma \|w\|_{H^{1-\beta}} \le \|w\|_E \le K_{\max}\|w\|_{H^{1-\beta}} \quad \forall w \in H_0^{1-\beta}. \tag{12}$$

In addition, the energy norm $\|\cdot\|_E$ can be generated by the inner product

$$\|w\|_E = (Tw, Tw)_{H^1}^{1/2} = \|Tw\|_{H^1}. \tag{13}$$

Proof. The continuity and weak coercivity of the bilinear form A yields the estimate (12). From the definition of T in (10) and Cauchy–Schwarz inequality, we get

$$\|w\|_E = \sup_{0\neq v\in H_0^1} \frac{|A(w,v)|}{\|v\|_{H^1}} = \sup_{0\neq v\in H_0^1} \frac{|(Tw,v)_{H^1}|}{\|v\|_{H^1}} \le \|Tw\|_{H^1}.$$

The supremum is reached at $\|Tw\|_{H^1}$ by choosing $v = Tw$ in (11). □

In the Petrov–Galerkin method (7), we let the trial space to be a finite dimensional subspace spanned by a set of basis functions $\{w_i\}_{i=1}^N$

$$S_h := \text{span}\{w_i\}_{i=1}^N.$$

We define the optimal test space to be the image of S_h under the map T

$$V_h := T(S_h) = \text{span}\{Tw_i\}_{i=1}^N.$$

The following theorem shows the optimal approximation property of the numerical solution u_h of the Petrov–Galerkin method in the energy norm $\|\cdot\|_E$.

Theorem 5. *Under the condition of Theorem 2, we have* $\dim(S_h) = \dim(V_h)$. *Moreover, let u and u_h be the solutions of the Petrov–Galerkin formulation (6) and the Petrov–Galerkin method (7), respectively. Then the following optimal approximation property holds*

$$\|u-u_h\|_E = \min_{\forall w_h\in S_h} \|u-w_h\|_E. \tag{14}$$

Proof. To prove $\dim(S_h) = \dim(V_h)$, we need only to prove that T is injective. That is, for any $w, w' \in H_0^{1-\beta}$, if $w \neq w'$, then $Tw \neq Tw'$. Suppose not, then there exists a $0 \neq w \in H_0^{1-\beta}$ such that $0 = Tw \in H_0^1$. By (13), $w = 0$ which contradicts to the assumption. Hence, T is injective from S_h onto V_h, and so $\dim(S_h) = \dim(V_h)$.

To prove the optimal approximation property (14), we subtract (6) with $v = v_h \in V_n$ from (7) to obtain

$$A(u-u_h, v_h) = A(u-u_h, Tw_h) = 0 \quad \forall v_h = Tw_h \in V_h \text{ or } \forall w_h \in S_h. \tag{15}$$

We use (10) and (11) to conclude that for any $w_h \in S_h$

$$\begin{aligned}
\|u-u_h\|_E^2 &= (T(u-u_h), T(u-u_h))_{H^1} \\
&= A(u-u_h, T(u-u_h)) \\
&= A(u-u_h, T(u-u_h)) + A(u-u_h, T(u_h-w_h)) \\
&= A(u-u_h, T(u-w_h)) \\
&= (T(u-u_h), T(u-w_h))_{H^1} \\
&\le \|T(u-u_h)\|_{H^1}\|T(u-w_h)\|_{H^1} \\
&= \|u-u_h\|_E\|u-w_h\|_E.
\end{aligned} \tag{16}$$

Here for the second term on the right-hand side of the third equal sign, we have used (15) with w_h be replaced by $u_h - w_h$. Canceling $\|u-u_h\|_E$ on both sides of (16), we have proved that for any $w_h \in S_h$

$$\|u-u_h\|_E \le \|u-w_h\|_E.$$

The equality is reached if we take $w_h = u_h$ in (14). Thus, we prove (14). □

4. A Petrov–Galerkin finite element method with optimal test functions

We base on the abstract framework in Section 3 to develop a Petrov–Galerkin finite element method with a piecewise-linear trial functions space. Define a uniform partition $x_i := ih$ for $i = 0, 1, \ldots, N$ with $h := 1/N$, so the interior nodes are x_i for $i = 1, 2, \ldots, N-1$. We choose the trial space S_h to be the piecewise-linear finite element space on the uniform partition. The basis functions w_i associated with the nodes x_i are given by

$$w_i = \begin{cases} 1 - \dfrac{|x - x_i|}{h}, & x_{i-1} \le x \le x_{i+1}, \\ 0, & \text{otherwise}. \end{cases} \tag{17}$$

The test functions $v_h := Tw_h \in V_h$ with $w_h \in S_h$ are given by (10) which in turn can be expressed in the following strong form

$$\begin{aligned} &-v_h''(x) = -D\big(K(x)\,{}_0^C D_x^{1-\beta} w_h(x)\big) \quad \forall x \in (0,1), \\ &v_h(0) = v_h(1) = 0. \end{aligned} \tag{18}$$

The corresponding weak form for this problem reads as follows: Find $v_h := Tw_h \in V_h$ with $w_h \in S_h$ such that for any $\psi_h := T\phi_h \in V_h$ with $\phi_h \in S_h$

$$\big(v_h', \psi_h'\big)_{L^2} = \big(K\,{}_0^C D_x^{1-\beta} w_h, \psi_h'\big)_{L^2} = A(w_h, \psi_h). \tag{19}$$

Despite that different trial and test spaces are used, the stiffness matrix is symmetric and positive-definite due to the use of the optimal test space [30,11–14]. In fact, choosing $v_h = v_j$ and $\psi_h = v_i$ in (19) for $1 \le i, j \le N-1$ yields

$$A(w_j, v_i) = \big(v_j', v_i'\big)_{L^2} = \big(v_i', v_j'\big)_{L^2} = A(w_i, v_j) \quad \forall 1 \le i, j \le N-1.$$

The positive definiteness is a consequence of the injectiveness of T as proved in Theorem 5.

Solving problem (18) yields a closed-form expression for the test functions v_i

$$v_i(x) = \Psi_i(x) - \Psi_i(1)x \tag{20}$$

with $\Psi_i(x) := \int_0^x K(s)\,{}_0^C D_s^{1-\beta} \phi_i(s)ds$. When K is a positive constant, Ψ_i (and so the test functions v_i) can be evaluated analytically as follows:

$$\Psi_i(x) = \frac{K}{\Gamma(2+\beta)h} \times \begin{cases} 0, & x < x_{i-1}, \\ (x - x_{i-1})^{1+\beta}, & x_{i-1} \le x \le x_i, \\ \big[(x - x_{i-1})^{1+\beta} - 2(x - x_i)^{1+\beta}\big], & x_i \le x \le x_{i+1}, \\ \big[(x - x_{i-1})^{1+\beta} - 2(x - x_i)^{1+\beta} + (x - x_{i+1})^{1+\beta}\big], & x \ge x_{i+1}. \end{cases}$$

Note that Ψ_i and so v_i are nonlocal, as in the case of second-order (advection-) diffusion equations where the nonlocal behavior of the test functions was considered to be a shortcoming of the Petrov–Galerkin finite element method with the optimal test functions. Nevertheless, the method has demonstrated its strength especially in the numerical solution of complicated and difficult problems, which was the major motivation for the authors to develop a Petrov–Galerkin finite element method with optimal test functions for fractional diffusion equations. Demkowicz and Gopalakrishnan developed a general framework of the discontinuous Petrov–Galerkin finite element method to facilitate an efficient numerical solution of the resulting discrete numerical scheme as the test functions can be computed locally on an element-by-element basis [11–14].

While the same ideas can be utilized in the context of a fractional diffusion equation, the nonlocal nature of a fractional differential operator makes the stiffness matrix of the resulting numerical method to be a dense or full matrix, in general. Hence, an efficient computation of the stiffness matrix is still an important issue, but is not necessarily a dominating factor in the numerical solution of the Petrov–Galerkin finite element method. Next we prove the error estimates for the method.

Theorem 6. *Assume that the condition of Theorem 2 holds and that the true solution u to problem (6) is in H^r for some $1 - \beta < r \le 2$. Let u_h be the solution to the Petrov–Galerkin method (7) with the trial and test functions given* *by (17) and (20), respectively. Then the following error estimates hold*

$$\begin{aligned} &\|u_h - u\|_{H^{1-\beta}} \le Ch^{r-1+\beta}\|u\|_{H^r}, \quad 1-\beta \le r \le 2, \\ &\|u_h - u\|_{H^1} \le Ch^{r-1}\|u\|_{H^r}, \quad 1-\beta \le r \le 2. \end{aligned} \tag{21}$$

If the true solution v to the adjoint problem of problem (6)

$${}_x^R D_1^{1-\beta}\big(K(x)\, Dv\big) = g(x), \quad x \in (0,1), \qquad v(0) = v(1) = 0 \tag{22}$$

is in $H_0^1 \cap H^{1+\delta}$ for some $\delta > 0$ for each right-hand side $g \in L^2$ such that

$$\|v\|_{H^{1+\delta}} \le C\|g\|_{L^2},$$

the following L^2 error estimate holds

$$\|u_h - u\|_{L^2} \le Ch^{r-1+\beta+\delta}\|u\|_{H^r}. \tag{23}$$

Proof. To prove the first error estimate in (21), we need only to verify the discrete inf–sup condition (8) in Theorem 3

$$\begin{aligned} \sup_{0\ne v_h\in V_h} \frac{|A(u_h,v_h)|}{\|v_h\|_{H^1}} &= \sup_{0\ne v_h\in V_h} \frac{|(Tu_h,v_h)_{H^1}|}{\|v_h\|_{H^1}} \\ &\ge \frac{|(Tu_h,Tu_h)_{H^1}|}{\|Tu_h\|_{H^1}} \\ &= \|Tu_h\|_{H^1} = \|u_h\|_E \\ &\ge \gamma\|u_h\|_{H^{1-\beta}}, \end{aligned}$$

where at the last step we have used the left half of the estimate (12). Then we choose $w_h := \Pi u$ to be the piecewise-linear interpolation of u and use the approximation estimate to obtain the error estimate (21). To prove the second error estimate in (21), we have

$$\begin{aligned} \|u_h - u\|_{H^1} &\le \|u_h - \Pi u\|_{H^1} + \|\Pi u - u\|_{H^1} \\ &\le Ch^{-\beta}\|u_h - \Pi u\|_{H^{1-\beta}} + \|\Pi u - u\|_{H^1} \\ &\le Ch^{-\beta}\big(\|u_h - u\|_{H^{1-\beta}} + \|u - \Pi u\|_{H^{1-\beta}}\big) + \|\Pi u - u\|_{H^1} \\ &\le Ch^{r-1}\|u\|_{H^r}. \end{aligned} \tag{24}$$

To prove the L^2 error estimate (23), we introduce $v \in H_0^1$ to be the weak solution to the adjoint problem (22) with right-hand side $u - u_h$

$$A(w,v) = (u-u_h, w) \quad \forall w \in H_0^{1-\beta}. \tag{25}$$

Substituting $w = u - u_h$ in (25), we have

$$\begin{aligned} \|u-u_h\|_{L^2}^2 &= A(u-u_h, v) \\ &= A(u-u_h, v - \Pi v) \\ &\le K_{\max}\|u-u_h\|_{H^{1-\beta}}\|v-\Pi v\|_{H^1} \\ &\le C\|u-u_h\|_{H^{1-\beta}} h^{\delta}\|v\|_{H^{1+\delta}} \\ &\le Ch^{r-1+\beta+\delta}\|u\|_{H^r}\|u-u_h\|_{L^2}. \end{aligned}$$

At the second equal sign we have used (15) with $v_h = \Pi v \in V_h$. Canceling the $\|u-u_h\|_{L^2}$ on both sides of the preceding estimate yields (23). □

We emphasize a significant difference between the regularity of the true solutions to fractional diffusion equations and that to canonical second-order diffusion equations. For the latter, the smoothness of coefficients and the right-hand side of the problem (plus the smoothness of the domain in multiple space dimensions) ensures the smoothness of the true solution to the problem [31]. However, it was recently shown that the solution to a fractional diffusion equation with a constant diffusivity coefficient and right-hand side is not in the Sobolev space $W^{1,1/\beta}$ for any $0 < \beta < 1$. In particular, $u \notin H^1$ for any $1/2 \le \beta < 1$ [32,10]!

This has profound consequences in the error estimates of Galerkin and Petrov–Galerkin finite element methods for fractional diffusion equations. For example, up to now there are no verifiable conditions in the literature that ensure the regularity of the true solutions to fractional diffusion equations, which were assumed in the error estimates for the corresponding Galerkin or Petrov–Galerkin finite element methods in the energy norm. Furthermore, this implies that Nitsche-lifting based optimal-order error estimates in the L^2 norm are invalid, as they require that the solution to the dual problem (4) has the desired regularity for **each** right-hand side $g \in L^2$.

Jin et al. studied the regularity of the solution to a constant–coefficient analogue of problem (5), when the solution can be obtained analytically in a closed form [32]. Their results indicate that in this particular case, the parameter δ in Theorem 6 may be chosen to be any positive number $0 < \delta < 1/2 - \beta$. This suggests that even in this very special case, the best possible convergence rate of the Petrov–Galerkin finite element method in the L^2 norm is at most up to the order of 3/2, and is definitely not of optimal order.

5. A Petrov–Galerkin finite element method with approximately optimal test functions

The optimal test functions in the Petrov–Galerkin finite element method in Section 4 can be obtained in a closed form if K is a constant (as we already did) or is of some other simple forms (say, a piecewise polynomial), but cannot be obtained analytically for a general variable diffusivity coefficient K. Hence, numerical means has to be used. Demkowicz and Gopalakrishnan developed a discontinuous Petrov–Galerkin framework in which problem (18) is numerically solved *locally* on each cell to obtain "approximately optimal" test functions.

We could follow their ideas to evaluate the approximately optimal test functions locally. Alternatively, we could approximate K by some piecewise polynomial approximations in (18) to solve the resulting equation to obtain approximately optimal test functions that are continuous and piecewise power functions. As we discussed earlier, in the context of fractional diffusion equations, the computational cost of assembling the stiffness matrix does not dominate the overall computational cost. Below we illustrate the latter approach, the former can be developed in parallel.

Let $K_h : [0, 1] \to \mathbb{R}$ be a piecewise quadratic spline approximation to or a piecewise cubic Hermite interpolation of K on the uniform partition on [0, 1]. That is, K_h is continuously differentiable provided that K is. Instead of the Riesz presentation operator T that cannot be solved in a closed form from the trial space S_h to the test space V_h in general, we introduce a mesh-dependent approximate Riesz representation operator $T_h : S_h \to \hat{V}_h$ as follows: Find $\hat{v}_h := T_h w_h \in \hat{V}_h$ with $w_h \in S_h$ such that for any $\hat{\psi}_h := T_h \phi_h \in \hat{V}_h$ with $\phi_h \in S_h$

$$\left(\hat{v}_h', \hat{\psi}_h'\right)_{L^2} = \left(K_h \, {}_0^C D_x^{1-\beta} w_h, \hat{\psi}_h'\right)_{L^2} =: A_h(w_h, \hat{\psi}_h).$$

The Petrov–Galerkin method with the approximately optimal test functions reads as follows: Find $\hat{u}_h \in S_h$ such that for any $\hat{v}_h = T_h w_h \in \hat{V}_h$ with $w_h \in S_h$

$$A_h(u_h, \hat{v}_h) = \langle f, \hat{v}_h \rangle. \tag{26}$$

Although the approximately optimal test functions are used, the stiffness matrix is still symmetric as

$$A_h(w_j, \hat{v}_i) = \left(\hat{v}_j', \hat{v}_i'\right)_{L^2} = \left(\hat{v}_i', \hat{v}_j'\right)_{L^2} = A_h(w_i, \hat{v}_j) \quad \forall 1 \le i, j \le N - 1.$$

Theorem 7. *Assume that the condition of Theorem 2 hold and that $K \in W^{2,\infty}$. Then the bilinear form $A_h(\cdot, \cdot)$ is continuous and weakly coercive on the product space $H_0^{1-\beta} \times H_0^1$ for sufficiently small $h > 0$. Consequently, the Petrov–Galerkin formulation of finding $\hat{u} \in H_0^{1-\beta}$ such that*

$$A_h(\hat{u}, v) = l(v), \quad \forall v \in H_0^1, \tag{27}$$

has a unique weak solution such that

$$\|\hat{u}\|_{H^{1-\beta}} \le \frac{K_{\max}}{\gamma} \|f\|_{H^{-1}}.$$

Proof. By the approximation property of K_h to K, we have

$$\|K - K_h\|_{L^\infty} \le Ch^2 \|K\|_{W^{2,\infty}}.$$

As K has a positive lower bound, there exists an $h_0 > 0$ such that

$$K_{\min}/2 \le K_h \le 2K_{\max}$$

provided that $0 < h \le h_0$. That is, K_h has uniformly positive lower and upper bounds for $0 < h \le h_0$. Hence, the conditions of Theorem 2 and Lemma 4 still hold, so their conclusions still hold (possibly with different constants). □

Theorem 8. *Assume that the conditions of Theorem 6 hold and that $K \in W^{2,\infty}$. Assume that the solution $\hat{u}$ to problem (27) satisfies similar conditions to the solution u to problem (6) in Theorem 6 with the bilinear form A being replaced by A_h. Let u_h and $\hat{u}_h$ be the solutions to the Petrov–Galerkin methods (7) and (26), respectively. Then the following optimal-order error estimates hold*

$$\begin{aligned} &\|\hat{u}_h - u\|_{H^{1-\beta}} \le Ch^{r-1+\beta}\|\hat{u}\|_{H^r}, \quad 1-\beta \le r \le 2, \\ &\|\hat{u}_h - u\|_{L^2} \le Ch^{r-1+\beta+\delta}\|\hat{u}\|_{H^r}, \quad 1-\beta \le r \le 2. \end{aligned} \tag{28}$$

Proof. To estimate the global truncation error $\hat{u}_h - u$, in which $\hat{u}_h$ and u are defined by different weak formulations as well as on different spaces, we decompose the error as

$$\hat{u}_h - u = \big(\hat{u}_h - \hat{u}\big) + \big(\hat{u} - u\big). \tag{29}$$

We apply Theorem 6 to $\hat{u}$ and $\hat{u}_h$ to obtain the following error estimates

$$\begin{aligned} &\|\hat{u}_h - \hat{u}\|_{H^{1-\beta}} \le Ch^{r-1+\beta}\|\hat{u}\|_{H^r}, \quad 1-\beta \le r \le 2, \\ &\|\hat{u}_h - \hat{u}\|_{L^2} \le Ch^{r-1+\beta+\delta}\|\hat{u}\|_{H^r}, \quad 1-\beta \le r \le 2. \end{aligned}$$

We now estimate the second term on the right-hand side of (29), which represents the approximation $\hat{u}$ to u in the continuous setting. We subtract (27) from (6) to obtain

$$A(u, v) - A_h(\hat{u}, v) = 0 \quad \forall v \in H_0^1.$$

We decompose this equation as

$$\big(A(u, v) - A_h(u, v)\big) + A_h(u - \hat{u}, v) = 0 \quad \forall v \in H_0^1.$$

We utilize the weak coercivity of A_h to obtain

$$\begin{aligned} \|u - \hat{u}\|_{H_0^{1-\beta}} &\le \frac{1}{\gamma} \sup_{0 \ne v \in H_0^1} \frac{\big|A_h(u - \hat{u}, v)\big|}{\|v\|_{H_0^1}} \\ &\le \frac{1}{\gamma} \sup_{0 \ne v \in H_0^1} \frac{\big|A(u, v) - A_h(u, v)\big|}{\|v\|_{H_0^1}} \\ &\le \frac{1}{\gamma} \sup_{0 \ne v \in H_0^1} \frac{\Big|\int_0^1 (K - K_h) {}_0^C D_x^{1-\beta} u \; Dv dx\Big|}{\|v\|_{H_0^1}} \\ &\le \frac{1}{\gamma} \|u\|_{H_0^{1-\beta}} \|K - K_h\|_{L^\infty} \\ &\le Ch^2 \|u\|_{H_0^{1-\beta}}. \end{aligned} \tag{30}$$

The combination of (29) through (30) yields the estimates in (28). □

Remark 5.1. In Theorem 8 we have assumed the regularity of the true solution u to problem (6) and the regularity of the solution to the adjoint problem (22) for each right-hand side $g \in L^2$ as in Theorem 6. We have also assumed the regularity of the true solution $\hat{u}$ to the perturbed continuous problem (27). This extra assumption is unusual and is again due to the unconventional regularity behavior of the boundary value problem of fractional differential equations.

Table 1
The L^2-errors $\|u - u_h\|_{L^2}$ in Section 6.1.

$1/h$	$\beta : 0.1$	κ	$\beta : 0.25$	κ	$\beta : 0.5$	κ	$\beta : 0.75$	κ	$\beta : 0.9$	κ
8	1.03e−3	–	1.12e−3	–	1.48e−3	–	2.01e−3	–	2.27e−3	–
16	2.58e−4	2.00	2.96e−4	1.92	3.96e−4	1.90	5.51e−4	1.87	6.36e−4	1.84
32	6.44e−5	2.00	7.58e−5	1.97	1.10e−4	1.85	1.41e−4	1.97	1.67e−4	1.93
64	1.61e−5	2.00	1.90e−5	2.00	2.44e−5	2.17	3.51e−5	2.01	4.30e−5	1.96
128	4.04e−6	1.99	4.67e−6	2.02	5.70e−6	2.10	8.35e−6	2.07	1.07e−5	2.01
256	1.01e−6	2.00	1.10e−6	2.09	1.17e−6	2.28	1.75e−6	2.25	2.55e−6	2.07

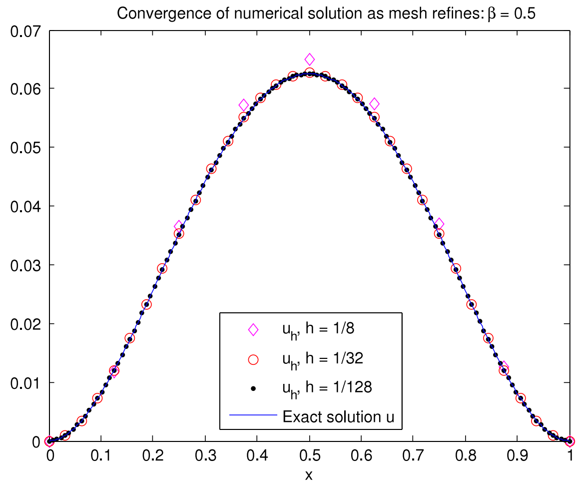

Fig. 1. The numerical solutions in Section 6.1 with $\beta = 0.5$.

6. Numerical examples

We carry out numerical experiments to investigate the performance of the Petrov–Galerkin finite element method for problem (5). We use a uniform space partition with a mesh size $h := 1/N$. We present the L^2 errors of the numerical solutions at successively refined meshes from $1/8$ to $1/256$ and report the convergence rate denoted by κ.

6.1. An example of a constant diffusivity coefficient

We consider problem (5) with a constant diffusivity coefficient $K \equiv 1$, and

$$f(x) = -2x^\beta \left(\frac{12}{\Gamma(3+\beta)} x^2 - \frac{6}{\Gamma(2+\beta)} x + \frac{1}{\Gamma(1+\beta)} \right).$$

The true solution is $u(x) = x^2(1-x)^2$. We present the numerical results for successively refined meshes in Table 1 and Fig. 1. We observe from Table 1 that the Petrov–Galerkin finite element method has a second-order convergence rate. We also find out that the numerical solutions retain the same behavior as the true solution.

6.2. An example of a variable diffusivity coefficient

We consider problem (5) with $K = \mathrm{e}^{\frac{1}{2}\sin(\pi x)}$, and

$$f(x) = \Gamma(4-\beta)\mathrm{e}^{\frac{1}{2}\sin(\pi x)} \left(\frac{\pi}{12} \cos(\pi x)\big((4-\beta)x^3 - 3x^2\big) + \frac{1}{2}\big((4-\beta)x^2 - 2x\big) \right).$$

The true solution is

$$u(x) = x^{3-\beta}(1-x).$$

Table 2
The L^2-errors $\|u - \hat{u}_h\|_{L^2}$ in the example in Section 6.2.

$1/h$	$\beta : 0.1$	κ	$\beta : 0.25$	κ	$\beta : 0.5$	κ	$\beta : 0.75$	κ	$\beta : 0.9$	κ
8	3.53e−3	–	3.29e−3	–	3.27e−3	–	2.95e−3	–	2.31e−3	–
16	8.59e−4	2.0	8.00e−4	2.04	8.25e−4	1.99	7.77e−4	1.92	5.90e−4	1.97
32	2.09e−4	2.0	1.95e−4	2.04	2.07e−4	1.99	2.03e−4	1.94	1.53e−4	1.95
64	5.15e−5	2.0	4.82e−5	2.02	5.20e−5	1.99	5.28e−5	1.94	4.03e−5	1.92
128	1.29e−5	2.0	1.20e−5	2.01	1.30e−5	2.00	1.35e−5	1.97	1.05e−5	1.94
256	3.32e−6	2.0	3.06e−6	1.97	3.27e−6	1.99	3.46e−6	1.96	2.76e−6	1.93

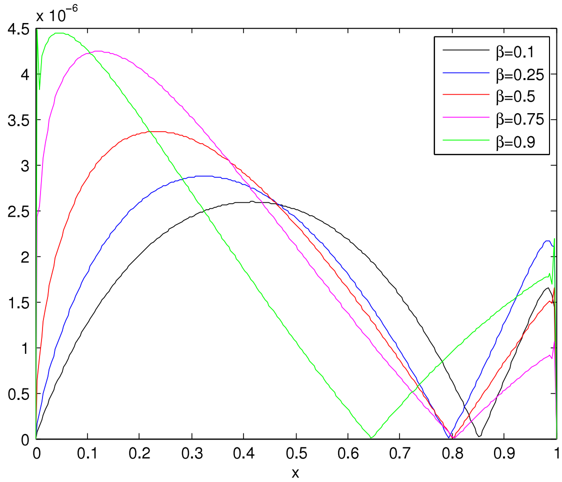

Fig. 2. The absolute errors $|u - \hat{u}_h|$ of the numerical solution in the example in Section 6.2 for different values of β, $h = 1/256$.

In the numerical experiments we use a cubic spline approximation K_h to approximate K, which allows us to construct the basis functions for the test space explicitly. We present the numerical results in Table 2 and Fig. 2. We observe from these results that the Petrov–Galerkin finite element method demonstrate a second-order convergence rate.

7. Concluding remarks

In this paper we utilize the DPG framework of Demkowicz and Gopalakrishnan [11–14] to develop a Petrov–Galerkin finite element method for one-dimensional variable-coefficient fractional diffusion equations, which arise in many physical and engineering applications. We note that the DPG framework applies to multidimensional space-fractional diffusion equations. Hence, in principle, we can apply the same idea in the current paper to develop Petrov–Galerkin finite element methods for multidimensional space-fractional diffusion equations. However, there exist major obstacles that need to be overcome in the development: (i) The proof of Theorem 2 in [9] relies heavily on the particular form of (5). (ii) Because of the weakly singular kernel and non-locality of fractional differential operators, the multidimensional trial to test operator can be expensive. (iii) The stiffness matrix of the Petrov–Galerkin finite element is full, for which traditional direct solver requires $O(N^3)$ computational complexity and $O(N^2)$ memory for a problem with N unknowns. A careful study needs to be carried out to investigate whether the stiffness matrix has certain Toeplitz-like structure as in the case of finite difference methods, so that a fast Fourier transform based fast Krylov subspace iterative method can be developed which has an almost linear computational complexity and memory requirement [33–35]. (iv) Efficient (usually full matrix) preconditioners need to be developed to significantly reduce the number of iterations in the Krylov subspace iterative method [36–38].

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