



# Numerical simulation for conservative fractional diffusion equations by an expanded mixed formulation<sup>☆</sup>

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## HIGHLIGHTS

- A locally-conservative expanded mixed finite element scheme is developed based on the saddle-point variational formulation.
- The well-posedness of the saddle-point variational formulation and the expanded mixed formulation is established.
- The equivalence of the negative fractional spaces and the negative Sobolev spaces is established.
- Optimal order error estimates are derived for sufficiently smooth solution and non-smooth solution.

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## ABSTRACT

In this article we adopt the saddle-point theoretical framework to analyze the conservative fractional diffusion equations. By introducing a fractional-order flux as auxiliary variable, we establish the well-posedness of the saddle-point variational formulation. Based on the formulation we propose a locally-conservative expanded mixed finite element procedure to approximate the unknown, its derivative and the fractional flux directly, and prove the existence and uniqueness of the mixed finite element solution. By proving that the negative fractional derivative spaces are equivalent to the negative fractional-order Sobolev spaces we derive the approximation capability of the standard projection operator in fractional Sobolev spaces for non-smooth functions. This leads an optimal-order error estimates in terms of the right-hand side both for sufficiently smooth solution and non-smooth solution. Numerical experiments are included to confirm our theoretical findings.

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## 1. Introduction

We consider the boundary value problem of the conservative fractional diffusion equation of order  $2 - \beta$  with  $0 < \beta < 1$

$$\begin{aligned} -D\{K {}_0I_x^\beta Du\}(x) &= f(x), \quad x \in \Omega = (0, 1), \\ u(0) &= u(1) = 0. \end{aligned} \quad (1.1)$$

Here  $K$  is the diffusivity coefficient and  $f \in L^2(\Omega)$  is the source or sink term.  $D = \frac{d}{dx}$  is the first-order derivative operator and  ${}_0I_x^\beta$  represents the left Riemann–Liouville fractional integral operator of order  $\beta$  defined below by (2.3).

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The fractional diffusion equation (1.1) describes phenomena such as anomalous or non-Fickian diffusion processes that arise from turbulent flow [1,2], chaotic dynamics [3], viscoelasticity [1] and contaminant transport in groundwater flow [4]. Numerous experiments show that fractional diffusion equations provide an adequate and accurate description of transport processes that exhibit anomalous diffusion, which cannot be modeled properly by second-order diffusion equations [4–6], and thus have attracted considerable attention in practical applications.

Since the closed-form solutions to general fractional partial differential equations, given by analytic methods such as the Fourier and Laplace transform method, are available only in a few limited cases, one has to resort to numerical means in general. In the last decade different numerical methods have been developed for space-fractional partial differential equations. Liu, Anh, and Turner [7] and Meerschaert and Tadjeran [8] were the first in the development of numerical methods for fractional partial differential equations. Since then, the difference method, the spectral method, the multi-grid method, the fast difference method and the finite volume method are consecutively developed for space-fractional partial differential equations, see [9–14] and the references therein.

As another important numerical approach, Galerkin finite element analysis on space-fractional partial differential equations like problem (1.1) remains open until Ervin and Roop [15–17] presented a first rigorous analysis of the well-posedness of the weak formulation in  $H^{1-\frac{\beta}{2}}(\Omega)$  for the stationary space-fractional partial differential equations with two-sided Riemann–Liouville fractional derivatives via their relation to fractional-order Sobolev spaces. The paper [16] also provided an optimal error estimate for the Galerkin finite element method under the assumption that the solution has full regularity. Subsequently, many researchers extended the analysis to other methods such as the discontinuous Galerkin method and the spectral method [18,10]. Unfortunately, such regularity is not justified in general. Recently, Wang and Yang [19] generalized the analysis to the case of fractional-order derivatives involving a variable coefficient, analyzed the regularity of the solution in Hölder spaces  $C^{2-\beta,\alpha}(\Omega)$ , and established the well-posedness of a Petrov–Galerkin formulation when  $0 < \beta < \frac{1}{2}$ . However, the discrete inf-sup condition was not established and hence an error estimate of the discrete approximations was not provided. Jin, Lazarov and Pasciak [20] establish the variational stability in  $H^{1-\beta+\gamma}(\Omega)$  with  $\gamma \in (0, \frac{1}{2})$  for (1.1), and develop relevant finite element analysis and derive error estimates of the discrete approximations expressed in terms of the smoothness of the right-hand side only.

From the point of view of numerical issue, an ideal numerical procedure should recognize both the unknown function and its flux to comply with engineering needs, and obey the conservation law to reflect the physical character of the diffusion model (1.1). Hence we should involve the diffusion equation (1.1) and the fractional-order flux  $p = -K_0 I_x^\beta Du$  to form a saddle-point formulation, then design a locally conservative numerical procedure.

A natural way should be to involve the unknown concentration  $u$  and the flux  $p = -K_0 I_x^\beta Du$  in a saddle-point formulation and to design the standard mixed finite element method. Unfortunately, since the operators  $D$  and  ${}_0 I_x^\beta Du$  are not symmetric it seems to be impossible to find an appropriate bilinear form  $b(\cdot, \cdot)$  satisfying the *inf-sup* constraint. We have to add  $q = Du$  as the second intermediate variable and turn to the expanded mixed formulation.

The goals of the paper are to: (1) establish the well-posedness of the saddle-point variational formulation for (1.1) by introducing two intermediate variables,  $q = Du$  and the flux  $p = -K_0 I_x^\beta Du$ , and develop a locally-conservative expanded mixed finite element method; (2) define the negative fractional derivative spaces to fit in with the low regularity of  $q$ , prove that the defined negative fractional spaces are equal to the negative Sobolev spaces  $H^{-s}(\Omega)$ , and thus are dual pairs of  $H^s(\Omega)$ . This facilitates handling the singularity contained in the exact solution and eases the derivation of the approximation properties of the standard projection operators in  $H^{1-\beta+\gamma}(\Omega)$ ; and (3) prove an optimal-order error estimate for sufficiently smooth solution, as well as prove the  $\mathcal{O}(h^{\gamma-\frac{\beta}{2}})$ -order convergence for the solution only in  $H^{1-\beta+\gamma}(\Omega)$  for  $0 < \beta < 1$ .

The rest of the paper is organized as follows. In Section 2, we revisit the fractional integral and derivative operators, and present their well-established properties. We also define some negative fractional derivative spaces and prove them to be the standard Sobolev spaces  $H^{-s}(\Omega)$ . In Section 3, by introducing the flux function  $p = -K_0 I_x^\beta Du$  and rewriting (1.1) we formulate the corresponding saddle-point formulation, prove its well-posedness and the equivalence. In Section 4, we are devoted to designing a locally-conservative expanded mixed finite element procedure to approximate the unknown  $u$ , its derivative  $q = Du$  and the fractional-order flux  $p$  based on the saddle-point formulation, prove the existence and uniqueness of the mixed finite element solution. We also prove the approximation capability of  $L^2$ -projector in fractional-order Sobolev spaces through the standard real interpolation methods and the dual argument, especially in low regularity spaces  $H^{1-\beta+\gamma}(\Omega)$ . In Section 5, we conduct an optimal-order error analysis both for fully regular solution and for low regular solution. In Section 6, we perform numerical experiments to verify our theoretical findings presented in this paper. In the last section we are devoted to some concluding remarks.

## 2. Revisit fractional operators and fractional Sobolev spaces

We first briefly recall the left-sided and right-sided Riemann–Liouville fractional derivatives. For any positive real number  $\mu$  with  $n - 1 < \mu < n$ , the left-sided Riemann–Liouville fractional derivative of order  $\mu$  is defined by [21–23]:

$${}_0 D_x^\mu u = \frac{d^n}{dx^n} ({}_0 I_x^{n-\mu} u). \quad (2.2)$$

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