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A fast algorithm for solving the space–time fractional diffusion equation[☆]

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ABSTRACT

In this paper, we propose a fast algorithm for efficient and accurate solution of the space–time fractional diffusion equations defined in a rectangular domain. The spatial discretization is done by using the central finite difference scheme and matrix transfer technique. Due to its nonlocality, numerical discretization of the spectral fractional Laplacian $(-\Delta)_s^{\alpha/2}$ results in a large dense matrix. This causes considerable challenges not only for storing the matrix but also for computing matrix–vector products in practice. By utilizing the compact structure of the discrete system and the discrete sine transform, our algorithm avoids to store the large matrix from discretizing the nonlocal operator and also significantly reduces the computational costs. We then use the Laplace transform method for time integration of the semi-discretized system and a weighted trapezoidal method to numerically compute the convolutions needed in the resulting scheme. Various experiments are presented to demonstrate the efficiency and accuracy of our method.

1. Introduction

The space–time fractional diffusion equation, obtained from the standard diffusion equation by replacing the integer-order spatial and temporal derivatives with their fractional counterparts, has received great attention in the literature [1–9]. It has been widely applied to study the anomalous diffusive processes associated with sub-diffusion (fractional in time) and super-diffusion (fractional in space) in many fields [10–12]. However, the nonlocality of the fractional derivatives introduces considerable challenges in both analysis and simulations of the fractional diffusion equation. In this paper, we present an efficient and accurate numerical method to solve the space–time fractional diffusion equation, which has significantly less computational complexity and memory than the existing methods in the literature.

Let $\Omega \subset \mathbb{R}^d$ (for $d = 1, 2$ or 3) denote an open and bounded domain. We consider a space–time fractional diffusion equation of the following form [7,2,13,9]:

$$\partial_t^\gamma u(\mathbf{x},t) = -\kappa_\alpha(-\Delta)_s^{\alpha/2} u(\mathbf{x},t) + f(\mathbf{x},t), \quad \mathbf{x}\in\Omega,\ t>0, \tag{1.1}$$

$$u(\mathbf{x},t) = 0, \quad \mathbf{x}\in\partial\Omega,\ t\ge 0, \tag{1.2}$$

$$u(\mathbf{x},0) = u_0(\mathbf{x}), \quad \mathbf{x}\in\overline{\Omega}, \tag{1.3}$$

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for $0 < \gamma < 1$ and $\alpha > 0$, where κ_α is the diffusion coefficient, and f denotes a source term. The operator ∂_t^γ is defined as the Caputo fractional derivative of order γ, i.e.,

$$\partial_t^\gamma u(\mathbf{x}, t) = \frac{1}{\Gamma(1-\gamma)} \int_0^t \frac{1}{(t-\tau)^\gamma} \partial_\tau u(\mathbf{x}, \tau)\, d\tau, \quad 0 < \gamma < 1, \tag{1.4}$$

where $\Gamma(\cdot)$ represents the Gamma function. As $\gamma \to 1$, the Caputo derivative in (1.4) gives the first-order temporal derivative ∂_t. The *spectral fractional Laplacian* (also known as the *fractional power of the Dirichlet Laplacian*) is defined via the spectral decomposition [14,13,9,15,7,16,17], i.e.,

$$(-\Delta)_s^{\alpha/2} u(\mathbf{x}) = \sum_{k\in\mathbb{N}^d} c_k\, \lambda_k^{\alpha/2} \varphi_k(\mathbf{x}), \quad \alpha > 0, \tag{1.5}$$

where λ_k and φ_k are the eigenvalues and eigenfunctions of the Laplace operator $-\Delta$ on the bounded domain $\Omega \subset \mathbb{R}^d$ with homogeneous Dirichlet boundary conditions. We would like to specially remark that the operator in (1.5) is different from the fractional Laplacian with extended homogeneous Dirichlet boundary condition (i.e., $u \equiv 0$, for $\mathbf{x} \in \mathbb{R}^d \setminus \Omega$), although these two operators are freely interchanged in some literature. The *fractional Laplacian* $(-\Delta)^{\alpha/2}$ is defined via a pseudo-differential operator with the symbol $-|\xi|^\alpha$ [18,19]:

$$(-\Delta)^{\alpha/2} u(\mathbf{x}) = \mathcal{F}^{-1}[|\xi|^\alpha \mathcal{F}[u](\xi)], \quad \alpha > 0, \tag{1.6}$$

where $\mathcal{F}$ represents the Fourier transform, and $\mathcal{F}^{-1}$ denotes its inverse transform. For $\alpha \in (0, 2)$, the fractional Laplacian can be also defined as the following integral form [19,20,18]:

$$(-\Delta)^{\alpha/2} u(\mathbf{x}) = c_{d,\alpha}\, \text{P.V.} \int_{\mathbb{R}^d} \frac{u(\mathbf{x}) - u(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^{d+\alpha}}\, d\mathbf{y}, \quad \alpha \in (0, 2), \tag{1.7}$$

where P.V. stands for the principal value integral, and $c_{d,\alpha}$ denotes a normalization constant. From a probabilistic point of view, the fractional Laplacian $(-\Delta)^{\alpha/2}$ with extended homogeneous Dirichlet boundary condition represents an infinitesimal generator of a symmetric α-stable Lévy process that particles are killed upon leaving the domain Ω, while the spectral fractional Laplacian $(-\Delta)_s^{\alpha/2}$ represents an infinitesimal generator of the process that first kills Brownian motion in a bounded domain Ω and then subordinates the killed Brownian motion via a $\frac{\alpha}{2}$-stable subordinator; see [21] for more discussion and comparison of these two operators. To distinguish them, we will include the subscript '*s*' in the operator $(-\Delta)_s^{\alpha/2}$ to indicate that it is defined via the spectral decomposition.

The nonlocal nature of the spectral fractional Laplacian $(-\Delta)_s^{\alpha/2}$ introduces considerable challenges in solving the space–time fractional diffusion equations (1.1)–(1.3), especially in high spatial dimensions. To the best of our knowledge, numerical studies of (1.1)–(1.3) in the literature are still limited to one- and two-dimensional problems [13,1,7,9,4,5]. To localize the problem, a Dirichlet-to-Neumann mapping approach is proposed in [22,7], where $(-\Delta)_s^{\alpha/2}$ is realized by an operator mapping the Dirichlet boundary condition to a Neumann type condition, and different numerical methods are proposed to solve the extended problems [7,1]. In these methods, one solves a local problem instead of the nonlocal one, however, this comes at the cost of introducing one more spatial dimension to the problem and raises questions about computational efficiency [7,1]. In [4,9], another approach is proposed to first discretize $-\Delta$ by using the finite difference/element methods and obtain its matrix representation A, and then the matrix representation of the spectral fractional Laplacian $(-\Delta)_s^{\alpha/2}$ can be given by $\mathrm{A}^{\alpha/2}$. Usually, $\mathrm{A}^{\alpha/2}$ is a dense matrix, and it is costly to directly compute this exponent. In [9], to avoid directly evaluating $\mathrm{A}^{\alpha/2}$, they rewrite the scheme in terms of the matrix function vector product, $g(\mathrm{A})\mathbf{b}$, for a suitable vector $\mathbf{b}$, and then approximate this product by preconditioned Lanczos methods. Later, various methods are proposed in [23] to improve the efficiency in computing $g(\mathrm{A})\mathbf{b}$. In addition, quadrature approximation methods for discretizing Dunford Taylor integral representation of the inverse operator $(-\Delta)_s^{-\alpha/2}$ can be found in [14,24], which can be applied to solve the fractional diffusion problem.

In this paper, we propose an efficient and accurate numerical method to solve the space–time fractional diffusion equations (1.1)–(1.3) in a rectangular domain. It is based on the matrix transfer technique proposed in [4]. The main merits of our algorithm include that it requires less computational cost and memory, and thus it is more efficient in solving higher dimensional problems. Moreover, our method can be easily implemented in computer codes. The rest of the paper is organized as follows. In Section 2, we present the spatial discretization of (1.1) and propose a fast algorithm for its efficient computation. In Section 3, we introduce the Laplace transform for time integration and obtain the full discretization of the space–time fractional diffusion equation by using the weighted trapezoidal rule. In Section 4, we test the accuracy and efficiency of the proposed algorithm by studying both time-independent and time-dependent problems. Some conclusions and remarks are provided in Section 5.

2. Semi-discretization in space

In this section, we introduce a finite difference method for discretizing the spatial operator $(-\Delta)_s^{\alpha/2}$ and propose a fast algorithm based on the discrete sine transform for its efficient computation. We will start introducing our method for the one-dimensional ($d = 1$) case and then generalize it to the higher dimensions ($d > 1$).