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A fast finite difference method for three-dimensional time-dependent space-fractional diffusion equations and its efficient implementation

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ABSTRACT

Fractional diffusion equations model phenomena exhibiting anomalous diffusion that cannot be modeled accurately by second-order diffusion equations. Because of the non-local property of fractional differential operators, numerical methods for space-fractional diffusion equations generate dense or even full coefficient matrices with complicated structures. Traditionally, these methods were solved with Gaussian elimination, which requires computational work of $O(N^3)$ per time step and $O(N^2)$ of memory to store where N is the number of spatial grid points in the discretization. The significant computational work and memory requirement of these methods makes a numerical simulation of three-dimensional space-fractional diffusion equations computationally prohibitively expensive.
In this paper we develop an efficient and faithful solution method for the implicit finite difference discretization of time-dependent space-fractional diffusion equations in three space dimensions, by carefully analyzing the structure of the coefficient matrix of the finite difference method and delicately decomposing the coefficient matrix into a combination of sparse and structured dense matrices. The fast method has a computational work count of $O(N \log N)$ per iteration and a memory requirement of $O(N)$, while retaining the same accuracy as the underlying finite difference method solved with Gaussian elimination. Numerical experiments of a three-dimensional space-fractional diffusion equation show the utility of the fast method.

1. Introduction

Diffusion processes occur in nature, science, engineering, and other applications. The underlying assumption in the derivation of the classical second-order diffusion equation is the existence of a mean free path and a mean free time taken for a particle to perform a jump. That is, a particle's motion has virtually no spatial correlation and long walks in the same direction are rare, so the variance of a particle excursion distance is finite. The central limit theorem concludes that the probability of finding a particle somewhere in space satisfies a Gaussian distribution, which gives a probabilistic description of a diffusion process. In last few decades more and more diffusion processes were found to be non-Fickian. In these processes the overall motion of a particle is better described by steps that are not independent and that can take vastly different times to perform. A particle's long walk may have long correlation length so the processes can have large deviations from the stochastic process of Brownian motion.

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Recent studies 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 [3,30]. Subsequently, fractional diffusion equations have been applied in increasingly more applications. These applications range from the design of photocopiers and laser printers [30], the signaling of biological cells [27], anomalous electrodiffusion in nerve cells [10], foraging behavior of animals [26], electrochemistry [23], to physics [21], finance [25], fluid and continuum mechanics [17], viscoelastic and viscoplastic flow [24], and solute transport in groundwater [3].

Since the last decade or so, extensive research has been conducted on the development of numerical methods for fractional diffusion equations, including finite difference methods, finite element methods, and finite volume methods [4,6,14,18,22,15,28,31,37]. However, because of the non-local nature of fractional differential operators, numerical methods for fractional diffusion equations raise additional numerical difficulties that were not encountered in the numerical methods for second-order diffusion equations. In the context of space-fractional diffusion equations, the corresponding numerical methods often generate dense or even full coefficient matrices with complicated structures [6,18,28,36–38,40]. Traditionally, these methods were solved via Gaussian elimination, which requires $O(N^3)$ of operations per time step and $O(N^2)$ of memory to store where N is the number of spatial grid points in the discretization. This results in severe computational issues. For instance, each time we refine the spatial mesh size h by half, the number of spatial grids is octupled and the computational work increases 512 times while the memory requirement increases 64 times. If the time step size Δt is refined by half too, then the overall computational work of the numerical method increases 1024 times. Hence, the numerical simulation of space-fractional diffusion equations in three space dimensions is computationally prohibitively intensive. This is probably the reason why no numerical methods have been developed and implemented for space-fractional diffusion equations in three space dimensions in the literature, even though theoretical error estimates have been proved for some of the numerical methods [6,18]. Therefore, development of fast and faithful numerical methods with efficient storage for three-dimensional space-fractional diffusion equations is crucial for the applications of fractional diffusion equations.

In this paper we develop an efficient and faithful solution method for the implicit finite difference discretization of time-dependent space-fractional diffusion equations in three space dimensions, by carefully analyzing the structure of the coefficient matrix of the finite difference method and delicately decomposing the coefficient matrix into a combination of sparse and structured dense matrices. The fast method has a computational work count of $O(N\log N)$ per iteration and a memory requirement of $O(N)$ per time step, while retaining the same accuracy as the regular finite difference method. The rest of the paper is organized as follows. In Section 2 we outline the space-fractional diffusion equation we attempt to solve and present the corresponding finite difference method. In Section 3 we recall the conjugate gradient squared method and identify the bottleneck issues in the application of the method to time-dependent space-fractional diffusion equations. In Section 4 we develop an efficient $O(N)$ storage scheme for the dense stiffness matrix of the fractional diffusion equation. In Section 5 we develop a fast $O(N\log N)$ algorithm for evaluating the product of the stiffness matrix with any vector. In Section 6 we derive an efficient implementation algorithm for the fast method developed in Section 5. In Section 7 we carry out numerical experiments to study the performance of the fast conjugate gradient squared method with the efficient implementation developed in Sections 5–6.

2. Time-dependent space-fractional diffusion equations and its finite difference approximation

We consider the initial–boundary value problem of a class of time-dependent space-fractional diffusion equations in three space dimensions

$$\begin{aligned}
&\frac{\partial u(x,y,z,t)}{\partial t} - a_+(x,y,z,t)\frac{\partial^\alpha u(x,y,z,t)}{\partial_+ x^\alpha} - a_-(x,y,z,t)\frac{\partial^\alpha u(x,y,z,t)}{\partial_- x^\alpha}\\
&\quad - b_+(x,y,z,t)\frac{\partial^\beta u(x,y,z,t)}{\partial_+ y^\beta} - b_-(x,y,z,t)\frac{\partial^\beta u(x,y,z,t)}{\partial_- y^\beta}\\
&\quad - c_+(x,y,z,t)\frac{\partial^\gamma u(x,y,z,t)}{\partial_+ z^\gamma} - c_-(x,y,z,t)\frac{\partial^\gamma u(x,y,z,t)}{\partial_- z^\gamma} = f(x,y,z,t),\\
&(x,y,z)\in\Omega, \quad t\in(0,T],\\
&u(x,y,z,t)=0, \quad (x,y,z)\in\partial\Omega,\ t\in[0,T],\\
&u(x,y,z,0)=u_o(x,y,z), \quad (x,y,z)\in\overline{\Omega}.
\end{aligned} \tag{1}$$

Here $\Omega := (x_L,x_R)\times(y_L,y_R)\times(z_L,z_R)$ is a cuboid domain. The left-sided and the right-sided fractional derivatives $\frac{\partial^\alpha u(x,y,z,t)}{\partial_+ x^\alpha}$, $\frac{\partial^\alpha u(x,y,z,t)}{\partial_- x^\alpha}$, $\frac{\partial^\beta u(x,y,z,t)}{\partial_+ y^\beta}$, $\frac{\partial^\beta u(x,y,z,t)}{\partial_- y^\beta}$, $\frac{\partial^\gamma u(x,y,z,t)}{\partial_+ z^\gamma}$ and $\frac{\partial^\gamma u(x,y,z,t)}{\partial_- z^\gamma}$ are defined as [24,29]

$$\frac{\partial^\alpha u(x,y,z,t)}{\partial_+ x^\alpha} := \lim_{h\to 0^+}\frac{1}{h^\alpha}\sum_{l=0}^{\lfloor (x-x_L)/h\rfloor} g_l^{(\alpha)} u(x-lh,y,z,t),$$