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A FAST SECOND-ORDER FINITE DIFFERENCE METHOD FOR SPACE-FRACTIONAL DIFFUSION EQUATIONS

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Abstract. Fractional diffusion equations provide an adequate and accurate description of transport processes that exhibit anomalous diffusion that cannot be modeled accurately by classical second-order diffusion equations. However, numerical discretizations of fractional diffusion equations yield full coefficient matrices, which require a computational operation of $O(N^3)$ per time step and a memory of $O(N^2)$ for a problem of size N. In this paper we develop a fast second-order finite difference method for space-fractional diffusion equations, which only requires memory of $O(N)$ and computational work of $O(N \log^2 N)$. Numerical experiments show the utility of the method.

Key Words. circulant and Toeplitz matrix, fast direct solver, fast finite difference methods, fractional diffusion equations

1. Introduction

Fractional diffusion equations model phenomena exhibiting anomalous diffusion that cannot be modeled accurately by classical second-order diffusion equations. For instance, in contaminant transport in groundwater flow the solutes moving through aquifers do not generally follow a Fickian, second-order partial differential equation because of large deviations from the stochastic process of Brownian motion. Instead, a governing equation with a fractional-order anomalous diffusion provides a more adequate and accurate description of the movement of the solutes [4].

Compared to the classical second-order diffusion equations, the fractional diffusion equations have salient features which introduce new difficulties. From a computational point of view, fractional differential operators are nonlocal and so raise subtle stability issues on the corresponding numerical approximations. Numerical methods for space-fractional diffusion equations yield full coefficient matrices, which require a computational operation of $O(N^3)$ per time step and a memory of $O(N^2)$ for a problem of size N. This is in contrast to numerical methods for second-order diffusion equations which usually generate banded coefficient matrices of $O(N)$ nonzero entries and can be solved by fast solution methods such as multigrid methods, domain decomposition methods, and wavelet methods in $O(N)$ (or $O(N \log N)$) operations per time step with $O(N)$ memory requirement.

Meerschaert and Tadjeran [7, 8] showed that a direct truncation of the Grünwald-Letnikov form of fractional derivative, even though discretized implicitly in time, leads to unstable discretizations. They proposed a shifted Grünwald discretization to approximate the fractional diffusion equation and proved the unconditional stability and convergence of the corresponding finite difference scheme. Numerical experiments showed that these methods generate satisfactory numerical results.

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However, the shifted Grünwald discretization is only first-order accurate in space. Tadjeran et al [11] developed a Crank-Nicolson scheme which is second-order accurate in time. They recovered second-order spatial accuracy by a Richardson extrapolation. However, these methods still generate full coefficient matrices and so require storage of $O(N^2)$ and computational work of $O(N^3)$ per time step.

In this paper we develop a fast second-order finite difference method for two-sided space-fractional diffusion equations. The method has a significantly reduced memory requirement of $O(N)$ and computational work of $O(N \log^2 N)$ per time step. The method is an extension of the fast solution method developed in [13] and can also viewed as an extension of the superfast method [1, 2, 3], which was a direct solution method of $O(N \log^2 N)$ operations for a symmetric positive-definite Toeplitz system. The rest of the paper is organized as follows. In Section 2 we present the fractional diffusion equation and its Crank-Nicolson finite difference approximation. In Section 3 we develop the fast second-order finite difference method. In Section 4 we carry out numerical experiments to compare the performance of the fast finite difference method with the Crank-Nicolson finite difference method developed and analyzed in [11].

2. Fractional diffusion equations and its finite difference approximation

We consider the following initial-boundary value problem of a two-sided space-fractional diffusion equation with an anomalous diffusion of order $1 < \alpha < 2$

$$
\begin{gathered}
\frac{\partial u(x,t)}{\partial t} - d_+(x,t)\frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha} - d_-(x,t)\frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha} = f(x,t), \\
x_L < x < x_R,\ 0 < t \le T, \\
u(x_L,t) = 0, \quad u(x_R,t) = 0, \qquad 0 \le t \le T, \\
u(x,0) = u_0(x), \qquad x_L \le x \le x_R.
\end{gathered}
\tag{1}
$$

The left-sided (+) and the right-sided (−) fractional derivatives $\frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha}$ and $\frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha}$ of equation (1) are defined in the Grünwald-Letnikov form

$$
\begin{aligned}
\frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha} &= \lim_{h\to 0^+} \frac{1}{h^\alpha} \sum_{k=0}^{\lfloor (x-x_L)/h \rfloor} g_k^{(\alpha)} u(x-kh,t), \\
\frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha} &= \lim_{h\to 0^+} \frac{1}{h^\alpha} \sum_{k=0}^{\lfloor (x_R-x)/h \rfloor} g_k^{(\alpha)} u(x+kh,t)
\end{aligned}
\tag{2}
$$

where $\lfloor x \rfloor$ represents the floor of x and the Grünwald weights $g_k^{(\alpha)}$ are defined as $g_k^{(\alpha)} = (-1)^k \binom{\alpha}{k}$ where $\binom{\alpha}{k}$ represents fractional binomial coefficients. We note that the Grünwald weights $g_k^{(\alpha)}$ have the recursive relation

$$
g_0^{(\alpha)} = 1, \qquad g_k^{(\alpha)} = \left(1 - \frac{\alpha+1}{k}\right) g_{k-1}^{(\alpha)} \quad \text{for} \quad k \ge 1.
\tag{3}
$$

Moreover, for $1 < \alpha < 2$ the coefficients $g_k^{(\alpha)}$ satisfy the following properties:

$$
\begin{cases}
g_0^{(\alpha)} = 1, \qquad g_1^{(\alpha)} = -\alpha < 0, \qquad 1 \ge g_2^{(\alpha)} \ge g_3^{(\alpha)} \ge \cdots \ge 0, \\
\displaystyle\sum_{k=0}^{\infty} g_k^{(\alpha)} = 0, \qquad \sum_{k=0}^{m} g_k^{(\alpha)} < 0 \quad (m \ge 1).
\end{cases}
\tag{4}
$$