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Fast finite difference methods for space-fractional diffusion equations with fractional derivative boundary conditions

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ABSTRACT

Numerical methods for space-fractional diffusion equations often generate dense or even full stiffness matrices. Traditionally, these methods were solved via Gaussian type direct solvers, which requires $O(N^3)$ of computational work per time step and $O(N^2)$ of memory to store where N is the number of spatial grid points in the discretization.
In this paper we develop a preconditioned fast Krylov subspace iterative method for the efficient and faithful solution of finite difference methods (both steady-state and time-dependent) space-fractional diffusion equations with fractional derivative boundary conditions in one space dimension. The method requires $O(N)$ of memory and $O(N \log N)$ of operations per iteration. Due to the application of effective preconditioners, significantly reduced numbers of iterations were achieved that further reduces the computational cost of the fast method. Numerical results are presented to show the utility of the method.

1. Introduction

Fractional diffusion equations provide an adequate and accurate description of transport processes that exhibit anomalous diffusive behavior, which cannot be modeled properly by canonical second-order diffusion equations [3,16]. Because of the nonlocal nature of fractional differential operators, numerical methods for space-fractional diffusion equations often generate dense or even full coefficient matrices. Traditionally, these methods were solved via Gaussian elimination, which requires $O(N^3)$ of computational work per time step and $O(N^2)$ of memory to store where N is the number of spatial grid points in the discretization. Consequently, the numerical simulation of space-fractional diffusion equations can be very expensive, especially in multiple space dimensions.

In [22] we proved that the stiffness matrix of the Meerschaert–Tadjeran finite difference method for the homogeneous Dirichlet boundary-value problem of the one-dimensional space-fractional diffusion equations can be decomposed as a sum of diagonal-multiply-Toeplitz matrices. We based on the decomposition to develop a fast operator-splitting finite difference method, which has a computational work account of $O(N \log^2 N)$ per time step and has a memory requirement of $O(N \log N)$ while retaining the accuracy of the Meerschaert–Tadjeran method. This was extended to multidimensional problems subsequently.

In this paper we consider the fractional derivative boundary-value problems of both steady-state and time-dependent space-fractional diffusion equations in one space dimension. Again, because of the nonlocal nature of the fractional Neumann and Robin boundary operator, the resulting discretization couples the unknowns in the entire domain and destroys

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the structure of the stiffness matrix. We carefully investigate the properties of the stiffness matrix, and develop a preconditioned fast Krylov subspace iterative method for the efficient and faithful solution of the finite difference methods for the problem. The method requires $O(N)$ of memory and $O(N\log N)$ of operations per iteration. Due to the application of effective preconditioners, significantly reduced numbers of iterations were achieved that further reduces the computational cost of the fast method. Numerical results are presented to show the utility of the method. The rest of the paper is organized as follows: in Section 2 we present the Meerschaert–Tadjeran method for the Neumann boundary-value problem of steady-state space-fractional diffusion equations. In Section 3 we study the properties and structure of the stiffness matrix and prove the efficient storage and fast matrix–vector multiplication. In Section 4 we develop preconditioned fast conjugate gradient squared methods for the finite difference method in Section 2. In Section 5 we outline the extension of the preconditioned fast iterative methods for the Neumann-boundary value problem of time-dependent space-fractional diffusion equations. In Section 5 we present numerical experiments to investigate the performance of the method developed.

2. Finite difference approximation for the fractional diffusion equations

2.1. A steady-state space-fractional diffusion equation

We consider the steady-state space-fractional diffusion equation with an anomalous diffusion of order $1<\alpha<2$ [3,15]

$$\begin{aligned}
&-d_+(x)\frac{\partial^\alpha u}{\partial_+ x^\alpha}-d_-(x)\frac{\partial^\alpha u}{\partial_- x^\alpha}+q(x)u=f(x),\quad 0<x<1,\\
&u(0)=0,\qquad \beta u(1)+\left(d_+(x)\frac{\partial^{\alpha-1} u}{\partial_+ x^{\alpha-1}}+d_-(x)\frac{\partial^{\alpha-1} u}{\partial_- x^{\alpha-1}}\right)\Bigg|_{x=1}=b.
\end{aligned}\tag{1}$$

Here $d_-(x)$ and $d_+(x)$ are the left-sided and right-sided diffusivity coefficients, $f(x)$ is the source and sink term, $q\geq 0$ is the reaction coefficient. $\beta=0$ corresponds to a fractional Neumann boundary condition and $\beta>0$ corresponds to a fractional Robin boundary condition. The left-sided (+) and right-sided (−) fractional derivatives $\frac{\partial^\alpha u}{\partial_- x^\alpha}$ and $\frac{\partial^\alpha u}{\partial_+ x^\alpha}$ are the Grünwald–Letnikov fractional derivatives [17]

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

where $\lfloor x\rfloor$ represents the floor of x and $g_k^{(\alpha)}=(-1)^k\binom{\alpha}{k}$ with $\binom{\alpha}{k}$ being the fractional binomial coefficients. Let N be a positive integer and $h=1/N$. We define $x_i=ih$, $u_i=u(x_i)$, $d_{+,i}=d_+(x_i)$, $d_{-,i}=d_-(x_i)$, $q_i=q(x_i)$, and $f_i=f(x_i)$ for $i=0,1,\ldots,N$. The Meerschaert–Tadjeran finite difference method is of the form [15]

$$-d_{+,i}\sum_{k=0}^{i} g_k^{(\alpha)}u_{i-k+1}-d_{-,i}\sum_{k=0}^{N-i+1} g_k^{(\alpha)}u_{i+k-1}+h^\alpha q_i u_i=h^\alpha f_i,\quad 1\leq i\leq N-1.\tag{3}$$

To close the system, we need to use the fractional derivative boundary condition at $x=1$ to set up an equation at $i=N$. We use the Grünwald–Letnikov fractional derivative (i.e. (2) with α being replaced by $\alpha-1$) to get

$$\begin{aligned}
d_+(x)\frac{\partial^{\alpha-1} u}{\partial_+ x^{\alpha-1}}\Bigg|_{x=1}&\approx\frac{d_{+,N}}{h^{\alpha-1}}\sum_{k=0}^{N} g_k^{(\alpha-1)}u_{N-k},\\
d_-(x)\frac{\partial^{\alpha-1} u}{\partial_- x^{\alpha-1}}\Bigg|_{x=1}&\approx\frac{d_{-,N}}{h^{\alpha-1}}g_0^{(\alpha-1)}u_N.
\end{aligned}$$

We incorporate these approximations to the fractional derivative boundary condition at $x=1$ in (1) to obtain the following equation at $i=N$

$$\beta h^{\alpha-1}u_N+d_{+,N}\sum_{k=0}^{N} g_k^{(\alpha-1)}u_{N-k}+d_{-,N}g_0^{(\alpha-1)}u_N=h^{\alpha-1}b.\tag{4}$$

Let $u=[u_1,u_2,\cdots,u_N]$. Then the finite difference method (3)–(4) can be expressed in the following matrix form

$$Au=f.\tag{5}$$

Here the stiffness matrix $A=[a_{i,j}]_{i,j=1}^N$ has the form