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A divide-and-conquer fast finite difference method for space–time fractional partial differential equation

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ABSTRACT

Fractional partial differential equations (FPDEs) provide better modeling capabilities for challenging phenomena with long-range time memory and spatial interaction than integer-order PDEs do. A conventional numerical discretization of space–time FPDEs requires $\mathcal{O}(N^2 + MN)$ memory and $\mathcal{O}(MN^3 + M^2N)$ computational work, where N is the number of spatial freedoms per time step and M is the number of time steps.

We develop a fast finite difference method (FDM) for space–time FPDE: (i) We utilize the Toeplitz-like structure of the coefficient matrix to develop a matrix-free preconditioned fast Krylov subspace iterative solver to invert the coefficient matrix at each time step. (ii) We utilize a divide-and-conquer strategy, a recursive direct solver, to handle the temporal coupling of the numerical scheme. The fast method has an optimal memory requirement of $O(MN)$ and an approximately linear computational complexity of $\mathcal{O}(NM(\log N + \log^2 M))$, without resorting to any lossy compression. Numerical experiments show the utility of the method.

1. Introduction

FPDEs provide better modeling capabilities for challenging phenomena with long-range time memory and spatial interactions than integer-order PDEs do [1–6]. However, due to the nonlocal nature of fractional differential operators, the numerical schemes of FPDEs give rise to dense stiffness matrices and/or long tails in time or a combination of both. Traditionally, a time-marching solution method with direct solvers has been used to solve these schemes that require $\mathcal{O}(N^2 + MN)$ memory and $\mathcal{O}(MN^3 + M^2N)$ overall computational work, where N is the number of spatial unknowns at each time step and M is the number of time steps. This is deemed computationally very expensive in terms of computational complexity and memory requirement, especially for problems in multiple space dimensions [7,8]. The significantly increased computational complexity and memory requirements is one of the main reasons why FPDE models have not been used widely.

In this paper we develop a divide-and-conquer fast FDM for space–time FPDE: (i) We utilize the Toeplitz-like structure of the coefficient matrix to develop a matrix-free preconditioned fast Krylov subspace iterative method to invert the coefficient matrix at each time step. (ii) We utilize a divide-and-conquer strategy, a recursive direct solver, to handle the temporal coupling of the numerical scheme. The fast method has an optimal memory requirement of $O(MN)$ and an approximately linear computational complexity of $\mathcal{O}(NM(\log N + \log^2 M))$, without resorting to any lossy compression. Numerical experiments show the utility of the method.

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The rest of the paper is organized as follows. In Section 2 we present the model space–time FPDE and its finite difference discretization. In Section 3 we develop a matrix-free preconditioned fast Krylov subspace iterative method to invert the coefficient matrix of the FDM, without resorting to any lossy compression, but rather, by exploring the structure of the coefficient matrix. In Section 4 we present a divide-and-conquer fast FDM for the space–time FPDE. In Section 5 we carry out numerical experiments to investigate the performance of the divide-and-conquer fast FDM.

2. A space–time FPDE and its finite difference discretization

We consider the space–time FPDE in one space dimension [9,4,5]

$$\begin{aligned} &{}_0^C D_t^\beta u(x,t) - d_+(x,t)\,{}_aD_x^\alpha u(x,t) - d_-(x,t)\,{}_xD_b^\alpha u(x,t) = f(x,t),\\ &\quad a < x < b,\ 0 < t \le T,\ 1 < \alpha < 2,\ 0 < \beta < 1,\\ &u(a,t) = u(b,t) = 0, \quad 0 \le t \le T, \qquad u(x,0) = 0, \quad a \le x \le b. \end{aligned} \tag{2.1}$$

Here ${}_0^C D_t^\beta u$ is the Caputo fractional derivative of order β defined by

$${}_0^C D_t^\beta u(x,t) := \frac{1}{\Gamma(1-\beta)} \int_0^t \frac{\partial u(x,s)}{\partial s} (t-s)^{-\beta} ds. \tag{2.2}$$

$d_+(x,t)$ and $d_-(x,t)$ are the left-sided and right-sided diffusivity coefficients, and $f(x,t)$ is the source and sink term. ${}_aD_x^\alpha u$ and ${}_xD_b^\alpha u$ are the left-sided and right-sided Grünwald–Letnikov fractional derivatives of order α [6]

$$\begin{aligned} {}_aD_x^\alpha u(x,t) &:= \lim_{\varepsilon\to 0^+} \frac{1}{\varepsilon^\alpha} \sum_{k=0}^{\lfloor (x-a)/\varepsilon \rfloor} g_k^{(\alpha)} u(x-k\varepsilon, t),\\ {}_xD_b^\alpha u(x,t) &:= \lim_{\varepsilon\to 0^+} \frac{1}{\varepsilon^\alpha} \sum_{k=0}^{\lfloor (b-x)/\varepsilon \rfloor} g_k^{(\alpha)} u(x+k\varepsilon, t) \end{aligned} \tag{2.3}$$

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.

For the homogeneous initial condition, the Caputo time-fractional derivative ${}_0^C D_t^\beta u$ and the Grünwald–Letnikov time-fractional derivative ${}_0D_t^\beta u$ coincide [6,10]. Hence, we can replace the Caputo time-fractional derivative ${}_0^C D_t^\beta u$ in (2.1) by the following Grünwald–Letnikov time-fractional derivative

$${}_0D_t^\beta u(x,t) := \lim_{\varepsilon\to 0^+} \frac{1}{\varepsilon^\beta} \sum_{k=0}^{\lfloor t/\varepsilon \rfloor} g_k^{(\beta)} u(x, t-k\varepsilon) \tag{2.4}$$

in the development of numerical schemes.

Let N and M be two positive integers. Let $h := (b-a)/(N+1)$ be a spatial mesh size and $\tau := T/M$ be a time step size. We define a uniform spatial partition $x_i := a + ih$ for $i = 0, 1, \ldots, N+1$ and a uniform temporal partition $t^m := m\tau$ for $m = 0, 1, \ldots, M$. Let u_i^m be the finite difference approximations to $u(x_i, t^m)$, $d_{+,i}^m := d_+(x_i, t^m)$, $d_{-,i}^m := d_-(x_i, t^m)$, and $f_i^m := f(x_i, t^m)$. A shifted Grünwald approximation to the space-fractional derivatives gives rise to the implicit FDM for problem (2.1)

$$\frac{1}{\tau^\beta} \sum_{k=0}^{m-1} g_k^{(\beta)} u_i^{m-k} - \frac{d_{+,i}^m}{h^\alpha} \sum_{k=0}^{i} g_k^{(\alpha)} u_{i-k+1}^m - \frac{d_{-,i}^m}{h^\alpha} \sum_{k=0}^{N-i+1} g_k^{(\alpha)} u_{i+k-1}^m = f_i^m, \quad 1 \le i \le N,\ 1 \le m \le M. \tag{2.5}$$

Traditionally, the FDM (2.5) is solved in a time-marching fashion

$$A^m u^m = \hat{f}^m := \tau^\beta f^m - \sum_{k=1}^{m-1} g_k^{(\beta)} u^{m-k}, \quad 1 \le m \le M. \tag{2.6}$$

Here u^m and f^m are vectors of size N defined by

$$u^m = [u_1^m, u_2^m, \ldots, u_N^m]^{\mathrm{T}}, \qquad f^m = [f_1^m, f_2^m, \ldots, f_N^m]^{\mathrm{T}}, \tag{2.7}$$

and the coefficient matrix A^m is defined by

$$A^m := I_N + S^m, \tag{2.8}$$

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