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Fast Evaluation of the Caputo Fractional Derivative and its Applications to Fractional Diffusion Equations: A Second-Order Scheme

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Abstract. The fractional derivatives include nonlocal information and thus their calculation requires huge storage and computational cost for long time simulations. We present an efficient and high-order accurate numerical formula to speed up the evaluation of the Caputo fractional derivative based on the $L2$-1_σ formula proposed in [A. Alikhanov, *J. Comput. Phys.*, 280 (2015), pp. 424-438], and employing the sum-of-exponentials approximation to the kernel function appeared in the Caputo fractional derivative. Both theoretically and numerically, we prove that while applied to solving time fractional diffusion equations, our scheme not only has unconditional stability and high accuracy but also reduces the storage and computational cost.

AMS subject classifications: 11T23, 26A33, 33F05, 34A08, 35R11, 65M06, 65M12

Key words: Caputo fractional derivative, fractional diffusion equation, stability analysis, sum-of-exponentials approximation, fast algorithm.

1 Introduction

Over the last few decades, fractional calculations have been wildly and effectively applied in various fields including physics, engineering, chemistry, biology, and even economics. The anomalous diffusion, also referred as non-Gaussian, has been observed and validated in various phenomena with accurate physical measurements [1–8]. In this paper we are concerned with the numerical computation of time fractional sub-diffusion equations in high dimensional spaces

$$ {}_0^C\mathcal{D}_t^\alpha u(x,t) = \Delta u(x,t) + f(x,t), \quad x\in\Omega, \quad t\in(0,T], \tag{1.1}$$

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$$u(x,t)=0, \quad x\in\partial\Omega, \quad t\in[0,T], \tag{1.2}$$

$$u(x,t)=u_0(x), \quad x\in\overline{\Omega}=\Omega\cup\partial\Omega. \tag{1.3}$$

where $x=(x^{(1)},x^{(2)},\cdots,x^{(d)})\in\mathbb{R}^d$, $\Omega=\prod_{k=1}^d(l^{(k)},r^{(k)})\subset\mathbb{R}^d,\partial\Omega$ is the boundary of Ω, $\Delta u=\sum_{k=1}^d\partial^2_{x^{(k)}}u$, $f(x,t)$ and $u_0(x)$ represent the given sufficiently smooth functions satisfying $u_0(x)=0$ when $x\in\partial\Omega$, the Caputo derivative ${}_0^C\mathcal{D}_t^\alpha u(x,t)$ with order of α is defined by

$${}_0^C\mathcal{D}_t^\alpha u(x,t)=\frac{1}{\Gamma(1-\alpha)}\int_0^t\frac{\partial u(x,s)}{\partial s}\frac{1}{(t-s)^\alpha}ds, \quad 0<\alpha<1. \tag{1.4}$$

Although there are some methods to analytically solve the fractional diffusion equations in some special cases [9–15], one may have to resort to the numerical methods to obtain their solutions in general. The time fractional derivative, unlike the classical case, requires all history information. For example, the widespread $\mathcal{L}1$ formula for (1.4) requires to store the solution at all previous time steps and its computational complexity is $\mathcal{O}(N^2)$ with N the total number of time steps. Applying the $\mathcal{L}1$ formula to solve fractional equations is rather time-consuming even for the case of $d=1$. This motivates us to enhance the research of numerical methods in two-folds:

1. construct stable and high-order accurate formulas for the Caputo derivative;
2. develop efficient algorithms to reduce the computational storage and cost.

In the literatures, there are many efforts to construct stable and high-order accurate approximations for the fractional calculation. Xu and Cao [16] developed a high order scheme for the fractional ordinary differential equations based on the block-by-block approach. Li [17] used higher order piecewise interpolation polynomial to approximate the fractional derivatives and used the Simpson method to design a high order algorithm for the fractional differential equations. Gao et al. [18] developed a high order formula called $\mathcal{L}1$-2 formula which had the temporal convergence order $\mathcal{O}(\tau^{3-\alpha})$ at time t_j $(j\geq 2)$ but $\mathcal{O}(\tau^{2-\alpha})$ at t_1. Alikhanov constructed a formula called $\mathcal{L}2$-1_σ formula which has temporal convergence order $\mathcal{O}(\tau^{3-\alpha})$ for time t_j $(j\geq 1)$ [19].

On the other hand, in the literatures, many efforts have also been made to develop efficient algorithms for the fractional calculation demanding less storage and computation. The implicit finite difference scheme with the shifted Grunwald formula for the space-fractional diffusion equations results in a Toeplitz-like system, which was calculated by the fourier transform and a circulant preconditioner in [20–22]. Multigrid method and interval clustering were also applied for the fractional calculation in [21]. To speed up the evaluation of weakly singular kernel, Lubich and Schädle [23] presented a fast convolution for non-reflecting boundary conditions. Jiang et al. [24] presented a fast evaluation of Caputo fractional derivative based on the $\mathcal{L}1$ formula and the sum-of-exponentials (SOE) approximation to the kernel function $t^{-1-\alpha}$. The resulting fast algorithm keeps the almost same accuracy of $\mathcal{O}(\tau^{2-\alpha})$ with the $\mathcal{L}1$ formula, at the same time, reduces