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Fast Evaluation of the Caputo Fractional Derivative and its Applications to Fractional Diffusion Equations

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Abstract. The computational work and storage of numerically solving the time fractional PDEs are generally huge for the traditional direct methods since they require total $\mathcal{O}(N_S N_T)$ memory and $\mathcal{O}(N_S N_T^2)$ work, where N_T and N_S represent the total number of time steps and grid points in space, respectively. To overcome this difficulty, we present an efficient algorithm for the evaluation of the Caputo fractional derivative ${}_0^C D_t^\alpha f(t)$ of order $\alpha \in (0,1)$. The algorithm is based on an efficient sum-of-exponentials (SOE) approximation for the kernel $t^{-1-\alpha}$ on the interval $[\Delta t, T]$ with a uniform absolute error ε. We give the theoretical analysis to show that the number of exponentials N_{exp} needed is of order $\mathcal{O}(\log N_T)$ for $T \gg 1$ or $\mathcal{O}(\log^2 N_T)$ for $T \approx 1$ for fixed accuracy ε. The resulting algorithm requires only $\mathcal{O}(N_S N_{\text{exp}})$ storage and $\mathcal{O}(N_S N_T N_{\text{exp}})$ work when numerically solving the time fractional PDEs. Furthermore, we also give the stability and error analysis of the new scheme, and present several numerical examples to demonstrate the performance of our scheme.

AMS subject classifications: 33C10, 33F05, 35Q40, 35Q55, 34A08, 35R11, 26A33

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

1 Introduction

Over the last few decades the fractional calculus has received much attention of both physical scientists and mathematicians since they can faithfully capture the dynamics of

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physical process in many applied sciences including biology, ecology, and control system. The anomalous diffusion, also referred to as the non-Gaussian process, has been observed and validated in many phenomena with accurate physical measurement [19,28,29,46,48, 51]. The mathematical and numerical analysis of the factional calculus became a subject of intensive investigations.

In this paper, we consider a fast evaluation of the following fractional partial differential equation:

$$ {}_0^C D_t^\alpha u(x,t) = \Delta u(x,t) + F(u,x,t), \quad 0<\alpha<1, \tag{1.1} $$

where the Caputo fractional derivative ${}_0^C D_t^\alpha u(x,t)$ is defined by the formula

$$ {}_0^C D_t^\alpha u(x,t) = \frac{1}{\Gamma(m-\alpha)} \int_0^t \frac{u^{(m)}(x,\tau)}{(t-\tau)^{\alpha+1-m}} d\tau, \quad m-1<\alpha<m, \quad m\in\mathbb{Z}. \tag{1.2} $$

The existing schemes for solving (1.1) require the storage of the solution at all previous time steps and the computational complexity of these schemes is $\mathcal{O}(N_T^2 N_S)$ with N_T the total number of time steps and N_S the number of grid points in space. This is in dark contrast with the usual diffusion equations where one only needs to store the solution at a fixed number of time steps and the computational complexity is linear with respect to N_T.

It is easy to see that the difficulty is caused by the Caputo factional derivative appeared in (1.1). Indeed, one of the popular schemes of discretizing the Caputo fractional derivative is the so-called $L1$ approximation [15,16,23,30,32,36,39–41,52], which is simply based on the piecewise linear interpolation of u on each subinterval. For $0<\alpha<1$, the order of accuracy of the $L1$ approximation is $2-\alpha$. There are also high-order discretization schemes by using piecewise high-order polynomial interpolation of u [10,17,33,47] and [9,34,37]. For each spatial point x, these methods require the storage of all previous function values $u(0),u(t_1),\cdots,u(t_n)$ and $\mathcal{O}(n)$ flops at the nth step. Thus it requires on average $\mathcal{O}(N_T)$ storage and the total computational cost is $\mathcal{O}(N_T^2)$, which forms a bottleneck for long time simulations, especially when one tries to solve the time fractional partial differential equations (PDEs).

Here we present an efficient scheme for solving the fractional PDEs (1.1). Our key observation is that the Caputo derivative can be evaluated almost as efficient as the usually derivatives (besides some logarithmic factors). We first split the convolution integral in (1.2) into two parts - a local part containing the integral from $t-\Delta t$ to t, and a history part containing the integral from 0 to $t-\Delta t$. The local part is approximated using the standard $L1$ approximation. For the history part, integration by parts leads to a convolution integral of u with the kernel $t^{-1-\alpha}$. We show that $t^{-1-\alpha}$ $(0<\alpha<1)$ admits an efficient sum-of-exponentials (SOE) approximation on the interval $[\delta,T]$ with $\delta=\Delta t$, a uniform absolute error ε and the number of exponentials needed is of the order

$$ N_{\text{exp}} = \mathcal{O}\left(\log\frac{1}{\varepsilon}\left(\log\log\frac{1}{\varepsilon}+\log\frac{T}{\delta}\right)+\log\frac{1}{\delta}\left(\log\log\frac{1}{\varepsilon}+\log\frac{1}{\delta}\right)\right). \tag{1.3} $$