Numer. Math. Theor. Meth. Appl.
doi: 10.4208/nmtma.OA-2022-0023

Vol. **15**, No. 3, pp. 679-714
August 2022

A Unified Fast Memory-Saving Time-Stepping Method for Fractional Operators and Its Applications

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Received 6 February 2022; Accepted (in revised version) 14 March 2022

Abstract. Time-dependent fractional partial differential equations typically require huge amounts of memory and computational time, especially for long-time integration, which taxes computational resources heavily for high-dimensional problems. Here, we first analyze existing numerical methods of sum-of-exponentials for approximating the kernel function in constant-order fractional operators, and identify the current pitfalls of such methods. In order to overcome the pitfalls, an improved sum-of-exponentials is developed and verified. We also present several sum-of-exponentials for the approximation of the kernel function in variable-order fractional operators. Subsequently, based on the sum-of-exponentials, we propose a unified framework for fast time-stepping methods for fractional integral and derivative operators of constant and variable orders. We test the fast method based on several benchmark problems, including fractional initial value problems, the time-fractional Allen-Cahn equation in two and three spatial dimensions, and the Schrödinger equation with nonreflecting boundary conditions, demonstrating the efficiency and robustness of the proposed method. The results show that the present fast method significantly reduces the storage and computational cost especially for long-time integration problems.

AMS subject classifications: 26A33, 65M06, 65M12, 65M15, 35R11

Key words: Sum-of-exponentials, contour quadrature, fractional integral and derivative operators, fast time-stepping methods, time-fractional Allen-Cahn equation, nonreflecting boundary conditions.

1. Introduction

Fractional calculus has been a powerful tool to model physical processes involving

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historical memory and global correlation and thus has led to successful applications in the fields of physics, mechanics, and biology [3, 5, 30, 31, 37, 44]. For example, the fractional integral and derivative of constant orders have been successfully applied to describe the dynamical process in complex systems [27, 28]. Apart from the constant-order fractional calculus, many studies have found that the memory and nonlocality of complex physical systems may change with time, space or other conditions and thus the fractional order is modelled by a function depending on time and/or space. Readers are referred to [16, 23, 32] and the comprehensive review papers [9, 29, 35] for works on variable-order fractional calculus and its applications.

Mathematical models using constant/variable-order fractional calculus are usually formulated as fractional differential equations (FDEs), including time, space, and time-space FDEs. It is difficult to obtain analytical solutions of complex FDEs, especially for nonlinear fractional partial differential equations (FPDEs). In this paper, we focus on numerical simulation of time-fractional equations, including both constant and variable-order fractional cases. One of challenges of numerically solving FDEs is rooted in long time integration, which leads to expensive computational cost and high memory requirements. To tackle this challenge, some fast memory-saving time-stepping methods have been developed for discretizing the following convolution:

$$k_\alpha * u(t) = \int_0^t k_\alpha(t-s)u(s)\mathrm{d}s, \quad k_\alpha(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)}. \tag{1.1}$$

For $\alpha \geq 0$, (1.1) is the Riemann-Liouville (RL) fractional integral of order α. For $\alpha < 0$, the integral (1.1) is interpreted in terms of the principal value, which is equivalent to the RL fractional derivative of order $-\alpha$ [33], see details in Appendix A.

The aim of this paper is to develop the unified memory-saving fast time-stepping methods for discretizing the fractional integral and derivative operators defined in terms of (1.1). One of the key steps of the current fast method is to look for a suitable sum-of-exponentials to approximate the kernel function $k_\alpha(t)$ with the desired accuracy.

A widely used approach is to express the kernel function by its inverse Laplace transform as a contour integral

$$k_\alpha(t) = \frac{1}{2\pi\mathrm{i}} \int_{\mathcal{C}} \mathcal{L}[k_\alpha](\lambda)e^{\lambda t}\mathrm{d}\lambda = \frac{1}{2\pi\mathrm{i}} \int_{\mathcal{C}} \lambda^{-\alpha}e^{\lambda t}\mathrm{d}\lambda, \quad \mathrm{i}^2 = -1. \tag{1.2}$$

By choosing a suitable contour $\mathcal{C}$, the integral (1.2) is discretized by the famous exponentially convergent trapezoidal/mid-point rule [39] that leads to the desired sum-of-exponentials as $\sum w_j e^{\lambda_j t}$. The popularly used contours include the Talbot contour, the parabolic contour, and the hyperbolic contour [10, 21, 22, 24, 40, 43, 46]. In [2, 3], the Laplace transform of the kernel function is approximated by a rational approximation, which leads to the desired sum-of-exponentials. By choosing a special contour, the contour integral (1.2) can be further transformed into an integral on the half line

$$k_\alpha(t) = \frac{\sin(\alpha\pi)}{\pi} \int_0^\infty \lambda^{-\alpha}e^{-t\lambda}\mathrm{d}\lambda, \quad \alpha < 1. \tag{1.3}$$