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A second-order difference scheme for the time fractional substantial diffusion equation

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A B S T R A C T

In this work, a second-order approximation of the fractional substantial derivative is presented by considering a modified shifted substantial Grünwald formula and its asymptotic expansion. Moreover, the proposed approximation is applied to a fractional diffusion equation with fractional substantial derivative in time. With the use of the fourth-order compact scheme in space, we give a fully discrete Grünwald–Letnikov-formula-based compact difference scheme and prove its stability and convergence by the energy method under smooth assumptions. In addition, the problem with nonsmooth solution is also discussed, and an improved algorithm is proposed to deal with the singularity of the fractional substantial derivative. Numerical examples show the reliability and efficiency of the scheme.

1. Introduction

Anomalous sub-diffusion process, commonly described by the continuous time random walks (CTRWs), and also known as non-Brownian sub-diffusion, arises in numerous physical, chemical and biological systems; see [1–4]. The Feynman–Kac formula named after Richard Feynman and Mark Kac, establishes a link between parabolic partial differential equations (PDEs) and Brownian functionals. To figure out the probability density function (PDF) of some non-Brownian functionals, the fractional Feynman–Kac equation has been derived in [5–9]. The non-Brownian functionals can be defined by $A = \int_0^t U(x(\tau))\mathrm{d}\tau$, where $x(t)$ is the trajectory of a non-Brownian particle and different choices of $U(x)$ can depict diverse systems. In particular, if taking $U(x) \equiv 0$, the fractional Feynman–Kac equation reduces to the well-known fractional Fokker–Planck equation; see [5,6,10] for details. Lévy walks give a proper dynamical description in the superdiffusive domain, where the temporal and spatial variables of Lévy walks are strongly correlated and the PDFs of waiting time and jump length are spatiotemporal coupling [8]. Thus, an important operator, fractional substantial derivative has been proposed to describe the CTRW models with coupling PDFs. This spatiotemporal coupling operator was also presented in [7], where the CTRW model with position-velocity coupling PDF was discussed. Recently, Carmi and Barkai [5] also used the substantial derivative to derive the forward and backward fractional Feynman–Kac equations. Due to its potential properties

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and wide application, the fractional substantial derivative has attracted many scholars' attention; see [11,12] and references therein.

The fractional substantial derivative operator of order α $(n-1<\alpha<n)$ is defined by [12]

$$ {}_aD_t^{\alpha,\lambda}f(t) = {}_aD_t^{n,\lambda}[{}_aI_t^{n-\alpha,\lambda}f](t), \qquad {}_aI_t^{\alpha,\lambda}f(t) = \frac{1}{\Gamma(\alpha)}\int_a^t \frac{f(\xi)}{(t-\xi)^{1-\alpha}e^{\lambda(t-\xi)}}d\xi; \tag{1.1}$$

where $\alpha>0$, λ is a constant or a function independent of variable t, ${}_aI_t^{\alpha,\lambda}$ denotes the fractional substantial operator, and

$$ {}_aD_t^{n,\lambda} = \left(\frac{d}{dt}+\lambda\right)^n = \left(\frac{d}{dt}+\lambda\right)\left(\frac{d}{dt}+\lambda\right)\cdots\left(\frac{d}{dt}+\lambda\right).$$

It is noted that if λ is a nonnegative constant, then the fractional substantial derivative is equivalent to the Riemann–Liouville tempered derivative defined in [13–15], and taking $\lambda=0$ in (1.1) leads to the left Riemann–Liouville derivative. Meanwhile, to obtain the non-Brownian functionals, whose path integrals are over Lévy trajectories, the space-fractional Fokker–Planck equation and the tempered space fractional diffusion equations have been widely used; see [16–18].

The current work is devoted to proposing a second-order Grünwald–Letnikov-formula-based approximation for the fractional substantial derivative (1.1), and applying it to derive a high-order fully discrete scheme for the time fractional substantial diffusion equation (TFSDE)

$$ {}_0D_t^{\alpha,\lambda}u(\mathbf{x},t) = \Delta u(\mathbf{x},t) + F(\mathbf{x},t), \quad \mathbf{x}\in\Omega,\ t\in(0,T], \tag{1.2}$$

$$ u(\mathbf{x},0) = u_0(\mathbf{x}), \quad \mathbf{x}\in\Omega, \tag{1.3}$$

$$ u(\mathbf{x},t)|_{\mathbf{x}\in\partial\Omega} = \phi(\mathbf{x},t), \quad t\in(0,T], \tag{1.4}$$

where Δ is the Laplacian operator, $\mathbf{x}$ denotes the one-dimensional or two-dimensional space variable, $\partial\Omega$ is the boundary of domain Ω, $F(\mathbf{x},t)$, $u_0(\mathbf{x})$ and $\phi(\mathbf{x},t)$ are given functions; ${}_0D_t^{\alpha,\lambda}$ is the substantial derivative defined by (1.1), and $0<\alpha\le 1$.

The main novelty of our paper is the derivation of a second-order operator, which is based on the modified definition of the Grünwald derivative (see Section 3.4, [19]), for the approximation of the fractional substantial derivative. The modified Grünwald derivative is defined by [19]

$$ {}_0^{GL}D_t^{\alpha}f(t) \equiv \lim_{\tau\to 0}\frac{1}{\tau^\alpha}\sum_{k=0}^{[t/\tau]} g_k^\alpha f\left(t-k\tau+\frac{\alpha}{2}\tau\right), \quad g_k^\alpha = (-1)^k\binom{\alpha}{k}. \tag{1.5}$$

Actually, if dropping the term $\frac{\alpha}{2}\tau$ off in the right side of above definition, one gets the original definition of the Grünwald derivative. The advantage of the modified Grünwald derivative is that it permits the design of more efficient algorithms to approximate the Riemann–Liouville fractional derivatives than using the shifted Grünwald–Letnikov formula directly. In this paper, by developing the modified Grünwald derivative and the shifted Grünwald–Letnikov formula to the fractional substantial derivative, a modified shifted substantial Grünwald formula and its asymptotic expansion are presented. Based upon the asymptotic expansion, a second-order approximation of the fractional substantial derivative is derived.

There are also some other approaches for the approximation of fractional derivatives, such as the $L1$ approximation [20,21], the fractional linear multi-step methods (FLMMs) developed by Lubich [22], the $L2$ approximation with using superior convergence [23,24], etc. However, to the best of authors' knowledge, very limited work has been presented for the fractional substantial derivative. Chen and Deng [12] extended the p-th order FLMMs [25] to approximate the fractional substantial derivative, and applied it to solve the fractional Feynman–kac equation [26] lately. Very recently, Chen and Deng [27] proposed some algorithms for the equation with the fractional substantial derivative in time and the tempered fractional derivatives in space, in which the numerical stability and error estimate have been given for a scheme with the first-order accuracy in time and the second-order accuracy in space.

The main goal of our paper is to construct a second-order approximation for the time fractional substantial derivative, and subsequently to solve the TFSDE (1.2)–(1.4) by combining the existed fourth-order compact approximation for the space derivatives [28], and establish the numerical stability and error estimate of the derived fully discretized scheme.

In this work, we assume that the solution to the underlying equation satisfies suitable regularity requirements. The assumption can be satisfied in certain conditions, while it may not hold for many time-fractional differential equations; see related discussion for the case $\lambda=0$ in [29–32]. To circumvent the requirement of high regularity of the solution, we apply starting quadrature to add correction terms in the proposed scheme. The starting quadrature was first developed in [25], and has been used to deal with problems with nonsmooth solution; see [26,22]. The validity of the proposed algorithm is illustrated in Example 6.3 by solving a two-dimensional time fractional substantial diffusion equation.

The remainder of this paper is organized as follows. In Section 2, a second-order operator for the approximation of the fractional substantial derivative is derived. In Section 3, the proposed approximation is applied to TFSDE (1.2)–(1.4), and a fully discretized scheme is derived by combining the fourth-order compact formula in space. In Section 4, we give a discrete prior estimate for the numerical solution, and then prove the convergence and stability of the proposed scheme. The behavior of our proposed scheme when applied to solve problems with non-smooth solution is further discussed and the improved algorithm is proposed in Section 5. Numerical results are presented in Section 6. Some concluding remarks are included in the final section.