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1. Introduction

Numbers of very interesting and novel applications of fractional differential equations in physics, chemistry, engineering, finance, hydrology, and other sciences that have been developed in the last few decades [1–8], have led to an intensive effort recently to find accurate and stable numerical methods that are also straightforward to implement. The one-dimensional fractional sub-diffusion equation (FSDE) has the following form

$$\frac{\partial u(x,t)}{\partial t} = {}_0\mathcal{D}_t^{1-\alpha}\frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t),$$

where ${}_{0}\mathcal{D}_{t}^{1-\alpha}$ is the fractional derivative defined by the Riemann–Liouville operator

$$_{0}\mathcal{D}_{t}^{1-\alpha}y(t)=\frac{1}{\Gamma(\alpha)}\frac{\mathrm{d}}{\mathrm{d}t}\int_{0}^{t}\frac{y(\tau)}{\left(t-\tau\right)^{1-\alpha}}\mathrm{d}\tau,$$

and $0 < \alpha < 1$ is the anomalous diffusion exponent.

Eq. (1.1) is the evolution equation for the probability density function that describes particles diffusing with mean square displacement [9]

 $\langle x^2(t) \rangle \sim t^{\alpha}.$

When $0 < \alpha < 1$, the diffusion is anomalously slow (sub-diffusion) compared to the normal diffusion behavior with $\alpha = 1$.

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ABSTRACT

Combining order reduction approach and *L*1 discretization, a box-type scheme is presented for solving a class of fractional sub-diffusion equation with Neumann boundary conditions. A new inner product and corresponding norm with a Sobolev embedding inequality are introduced. A novel technique is applied in the proof of both stability and convergence. The global convergence order in maximum norm is $O(\tau^{2-\alpha} + h^2)$. The accuracy and efficiency of the scheme are checked by two numerical tests.

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Much previous attention has been paid to this equation. The analytical solution to FSDE on a fixed domain can be evaluated using separation of variables in terms of the Mittag-Leffler function [10]. While there are also various numerical methods, Yuste and Acedo [11] combined the forward time centered space method and the Grünwald-Letnikov discretization of the Riemann-Liouville derivative to obtain an explicit scheme, where the stability analysis of this scheme was carried out by means of von Neumann method. Furthermore, weighted average method presented by Yuste [12] indicated that its stability depends strongly on the value of the weighted parameter. Chen et al. [13] constructed an implicit difference approximation scheme, and analyzed the stability and convergence of the scheme using Fourier method. In [14], Murio developed an implicit finite difference method, and used Fourier method to show the stability. Cui [15] constructed a fourth order compact difference scheme for the spatial discretization. Chen et al. were also interested in high accuracy numerical method for the variable-order anomalous differential equation [16]. Some related equations of importance are the fractional reactionsubdiffusion equation (FR-subDE) [17] with sources and sinks, the fractional Fokker-Planck equation, and the fractional diffusion-wave equation. Chen et al. [17] presented two methods for the FR-subDE using the relationship between the Riemann-Liouville and Grünwald-Letnikov definitions of fractional derivative. The stability and convergence of the two numerical schemes were investigated by Fourier analysis, besides, a high-accuracy algorithm was structured using Richardson extrapolation. As for works on numerical algorithm for the Fokker–Planck equation, one can refer to [18–20]. Cuesta et al. [21] focused on solving fractional diffusion-wave equation. Zhuang and Liu [22] and Brunner et al. [23] investigated algorithms for two-dimensional fractional diffusion equation. In addition, Zhuang et al. [24] introduced a new way for solving sub-diffusion equation by integration of the original equation on the both sides to obtain an implicit numerical method. The stability and convergence of the scheme were proved by energy method. Later, the new method and supporting theoretical results were also applied to non-linear fractional reaction-subdiffusion process [25], anomalous subdiffusion equation with a nonlinear source term [26]. Several studies on this equation related to L1 discretization, which is derived by Oldham and Spanier [27], have proposed finite difference schemes with higher accuracy in time direction. In [28], Sun and Wu gave a fully discrete difference scheme for the fractional diffusion-wave equation, and proved that the scheme was uniquely solvable, unconditionally stable and convergent in maximum norm, then they constructed the implicit difference scheme for the sub-diffusion equation with the convergence order of $O(\tau^{2-\alpha} + h^2)$. Du et al. [29] proposed a compact difference scheme for the fractional diffusion-wave equation. Gao and Sun [30] transformed the original subdiffusion problem, then they presented the compact difference scheme. The stability and convergence of the scheme were proved by energy method with the help of a new inner product.

The works mentioned above for Eq. (1.1) are dealing with the Dirichlet boundary conditions, where no boundary discretization errors are involved. However, with the flux boundary conditions

$$u_{x}(0,t) = 0, \quad u_{x}(L,t) = 0, \quad t \in (0,T],$$
(1.2)

Langlands and Henry [31] considered this case by means of fictitious points and *L*1 discretization with respect to Riemann–Liouville derivative, as a result, a difference scheme with second order convergence in spatial direction was achieved, even though there was no proof of convergence of the numerical discretization.

In recent years, the method of order reduction for one-dimensional parabolic differential equation with the mixed initialboundary value problem, which was originally proposed by Keller [32], has been extended to many classical integer order partial differential equations by Sun [33–35]. Many important PDEs such as heat equations with nonlinear boundary conditions, wave equations with heat conduction, Timoshenko beam equations with boundary feedback, superthermal electron transport equations, the Cahn–Hilliard equation as well as some coupled systems of parabolic and elliptic equations, can be solved by introducing the new variable such that there are no derivatives in the boundary conditions. The main purpose of introducing a new variable is for the theoretical analysis of the resulting scheme, which is usually called box scheme and has second order global accuracy.

In this paper we consider FSDE (1.1) with flux boundary conditions (1.2). Based on the methodology of order reduction approach, we transform the original problem by introducing a new variable into an equivalent system of lower order differential equations, and then construct a box-type scheme for the equivalent system. In what follows, the discrete variables are separated to obtain the difference scheme only containing the original variable for the convenience of computation. Due to that the fractional derivative operator is nonlocal, we name the scheme as box-type scheme, which is different from standard box scheme for integer order differential equations.

The structure of this article is arranged in the following way. We construct a difference scheme for (1.1) and (1.2) by combining the order reduction method with L1 discretization of the fractional derivative in Section 2. Then, in Section 3, the stability and convergence of the scheme are proved with the help of a new Sobolev embedding inequality. Numerical examples are provided to demonstrate the theoretical results and some comparisons are made with LH scheme [31] in Section 4. Finally, we complete the paper by some conclusions.

2. Derivation of the box-type scheme

We consider the fractional sub-diffusion equation (1.1) with (1.2) and the initial condition

$$u(\mathbf{x},\mathbf{0})=\varphi(\mathbf{x}), \quad \mathbf{x}\in[\mathbf{0},L],$$

where $\varphi(x)$ and f(x,t) are known smooth functions.

(2.1)

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