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Numerical Solution of the Time-Fractional Sub-Diffusion Equation on an Unbounded Domain in Two-Dimensional Space

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Abstract. The numerical solution of the time-fractional sub-diffusion equation on an unbounded domain in two-dimensional space is considered, where a circular artificial boundary is introduced to divide the unbounded domain into a bounded computational domain and an unbounded exterior domain. The local artificial boundary conditions for the fractional sub-diffusion equation are designed on the circular artificial boundary by a joint Laplace transform and Fourier series expansion, and some auxiliary variables are introduced to circumvent high-order derivatives in the artificial boundary conditions. The original problem defined on the unbounded domain is thus reduced to an initial boundary value problem on a bounded computational domain. A finite difference and L1 approximation are applied for the space variables and the Caputo time-fractional derivative, respectively. Two numerical examples demonstrate the performance of the proposed method.

AMS subject classifications: 65M06, 65M12, 65N06

Key words: Fractional sub-diffusion equation, unbounded domain, local artificial boundary conditions, finite difference method, Caputo time-fractional derivative.

1. Introduction

Time-fractional sub-diffusion equations describe anomalous diffusion in many complex systems such as porous materials, nuclear magnetic resonance, percolation clusters, and random and disordered media [1–6]. The time-fractional sub-diffusion equation also arises in continuous-time random walks with temporal memories, which is characterised by asymptotic behaviour of the mean-square displacement — i.e. $\langle r^2(t)\rangle \sim t^\alpha$ with an anomalous diffusion exponent $0 < \alpha < 1$ [3, 6].

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The increasing importance of time-fractional sub-diffusion equations in many practical applications has attracted immense interest in recent years, and their solution on bounded domains has been widely studied analytically and numerically. However, exact solutions of most fractional differential equations have only been obtained in specific cases associated with Fox, Wright and Mittag-Leffler special functions [7–9]. On the other hand, there are many numerical methods to solve related initial or boundary value problems on bounded domains in space. One numerical approach for the one-dimensional fractional sub-diffusion equation with Caputo time-fractional derivatives used the finite difference method [10], and another effective difference scheme was based on an L1 approximation for the Caputo time-fractional derivative [11]. An implicit meshless approach was proposed for the time-fractional sub-diffusion equation in two space dimensions [12], and the alternating direction implicit scheme has also been considered [13–15]. A semi-discrete method has been invoked for a class of time-fractional diffusion equations describing tracer solute transport in an aquifer [16], where the numerical predictions were compared with experimental data. A second-order finite difference method for two-dimensional fractional percolation equations has also been designed [17], and some other solution methods for fractional sub-diffusion equations can be found in Refs. [18–23] and references therein.

Numerical solution of time-fractional sub-diffusion equations on unbounded domains has also received some attention. The artificial boundary method (ABM), said to be very general and applicable, involves truncating the unbounded domain around the region of interest by using an artificial boundary and designing a suitable boundary condition on the artificial boundary. The original problem defined on the unbounded domain is thus reduced to an initial boundary value (IBV) problem on a bounded computational domain, which is a good approximation to the original problem with a suitably chosen boundary condition on the artificial boundary. Recently, Gao & Sun [24] designed exact artificial boundary conditions for the one-dimensional time-fractional sub-diffusion equation, and constructed some finite difference schemes to solve the reduced IBV problem. Brunner *et. al* [25] constructed exact artificial boundary conditions for a time-fractional diffusion-wave equation on a two-dimensional unbounded domain, and obtained a series of approximate artificial boundary conditions with high accuracy. Moreover, the order of convergence and stability estimates for two finite difference schemes were also analysed rigorously. For the time-fractional sub-diffusion equation on two-dimensional unbounded domains in space, Ghaffari & Hosseini [26] derived exact and approximate artificial boundary conditions on a circular artificial boundary using the Laplace transform and a Fourier series expansion. The classical Crank-Nicolson method for space variables and L1 approximation for the Caputo time-fractional derivative were used to solve the reduced problem. Other exact and local artificial boundary conditions have also been studied [27–31].

Here we consider high-order local artificial boundary conditions (LABCs) for the time-fractional sub-diffusion equation on two-dimensional unbounded domains. As it is difficult to design the suitable high-order artificial boundary conditions at the corners of a rectangular domain, in Section 2 a circular artificial boundary $\Gamma_R = \{(r,\theta)|r = R, 0 \le \theta < 2\pi\}$ with radius R is introduced to divide the unbounded domain into two parts — viz. the bounded computational domain $\Omega_R = \{(r,\theta)|r < R, 0 \le \theta < 2\pi\}$ and the unbounded exte-

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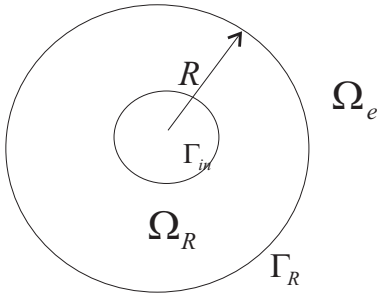


Figure 1: The unbounded domain divided into two parts by the artificial boundary Γ_R of radius R.

rior domain $\Omega_e = \{(r,\theta)|r > R, 0 \le \theta < 2\pi\}$ as shown in Fig. 1. The high-order LABCs are designed on the introduced artificial boundary for the time-fractional sub-diffusion equation, with some auxiliary variables introduced to circumvent the high-order derivatives involved in reducing the original problem to an IBV problem on a bounded computational domain. The Laplace transform and Fourier series expansion applied to the time-fractional sub-diffusion equation in the polar coordinate form on the exterior domain leads to the modified Bessel equation, which is solved by applying a rational function on introducing auxiliary variables to avoid high-order derivatives with respect to time t, before the high-order LABCs are obtained using the inverse Laplace transform.
The classical Crank-Nicolson scheme for space variables and the L1 approximation for the Caputo time-fractional derivative are constructed to numerically solve the reduced problem in Section 3. To demonstrate the efficiency and accuracy of the proposed method, numerical examples are presented in Section 4. Our conclusions and final brief remarks are in Section 5.

2. Local Artificial Boundary Conditions

We consider the following time-fractional sub-diffusion equation in $\mathbb{R}^2$:

$$ {}_0^C D_t^\alpha u(\mathbf{x},t) - \Delta u(\mathbf{x},t) = f(\mathbf{x},t), \qquad \mathbf{x} \in \mathbb{R}^2, 0 < t \le T, \tag{2.1} $$

$$ u(\mathbf{x},t)|_{\Gamma_{\text{in}}} = g(\mathbf{x},t), \qquad \mathbf{x} \in \mathbb{R}^2, 0 < t \le T, \tag{2.2} $$

$$ u(\mathbf{x},t)|_{t=0} = u_0(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^2 \setminus \bar{D}, \tag{2.3} $$

$$ u(\mathbf{x},t) \to 0, \qquad \text{as } \| \mathbf{x} \| \to \infty, t > 0, \tag{2.4} $$

where ${}_0^C D_t^\alpha u(\mathbf{x},t)$ denotes the Caputo time-fractional derivative with respect to t of order α $(0 < \alpha < 1)$ defined by

$$ {}_0^C D_t^\alpha u(\mathbf{x},t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(\mathbf{x},\varsigma)}{\partial \varsigma} (t-\varsigma)^{-\alpha} d\varsigma, $$

$\Gamma(\cdot)$ is the Gamma function, Δ is the two-dimensional Laplace operator, both $u_0(\mathbf{x})$ and the source term $f(\mathbf{x},t)$ are compactly supported functions, $\Gamma_{\text{in}} = \{\mathbf{x} \in \mathbb{R}^2 | \ ||\mathbf{x}|| = a\}$, and

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$D = \{\mathbf{x} \in \mathbb{R}^2 |\ ||\mathbf{x}|| < a\}$ is the bounded domain where $\mathbf{x} = (x_1, x_2)$ denotes the Cartesian coordinate in space, $||\mathbf{x}||^2 = x_1^2 + x_2^2$ and $a < R$.

The problem (2.1)-(2.4) can be rewritten in polar coordinates (r, θ) on the exterior domain:

$$
\begin{aligned}
&{}_0^C D_t^\alpha u(r,\theta,t) = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} \ \text{ in } \ \Omega_e \times (0,T], && (2.5)\\
&u(r,\theta,t)|_{\Gamma_R} = u(R,\theta,t), \quad t > 0, && (2.6)\\
&u(r,\theta,t)|_{t=0} = 0 \ \text{ in } \ \Omega_e, && (2.7)\\
&u(r,\theta,t) \to 0 \ \text{ as } \ r \to +\infty, \quad t > 0. && (2.8)
\end{aligned}
$$

We introduce the Laplace transform of $u(r, \theta, t)$ with respect to time

$$\hat{u}(r,\theta,s) = \int_0^{+\infty} u(r,\theta,t) e^{-st}\, dt,$$

so combining the initial condition (2.7) and the infinity condition (2.8) we obtain the Laplace transform of the Caputo fractional derivatives [32]

$$\mathscr{L}\left\{{}_0^C D_t^\alpha u(r,\theta,t)\right\}(s) = s^\alpha \mathscr{L}\left\{u(r,\theta,t)\right\}(s) - s^{\alpha-1} u(r,\theta,0),$$

and taking the Laplace transform of Eq. (2.5) we have

$$s^\alpha \hat{u} \ = \ \frac{\partial^2 \hat{u}}{\partial r^2} + \frac{1}{r}\frac{\partial \hat{u}}{\partial r} + \frac{1}{r^2}\frac{\partial^2 \hat{u}}{\partial \theta^2} \ \text{ in } \ \Omega_e. \tag{2.9}$$

On substituting the series expansion

$$\hat{u}(r,\theta,s) = \sum_{n=-\infty}^{\infty} C_n(r,s) e^{in\theta} \tag{2.10}$$

into Eq. (2.9) we obtain

$$s^\alpha \sum_{n=-\infty}^{\infty} C_n(r,s) e^{in\theta} = \sum_{n=-\infty}^{\infty} \frac{\partial^2 C_n(r,s)}{\partial r^2} e^{in\theta} + \frac{1}{r}\sum_{n=-\infty}^{\infty} \frac{\partial C_n(r,s)}{\partial r} e^{in\theta} - \frac{1}{r^2}\sum_{n=-\infty}^{\infty} n^2 C_n(r,s) e^{in\theta}$$

such that

$$\sum_{n=-\infty}^{\infty} \left\{ s^\alpha C_n(r,s) - \frac{\partial^2 C_n(r,s)}{\partial r^2} - \frac{1}{r}\frac{\partial C_n(r,s)}{\partial r} + \frac{n^2}{r^2} C_n(r,s) \right\} e^{in\theta} = 0,$$

so the coefficients $C_n(r,s)$ of the series satisfy

$$r^2 \frac{\partial^2 C_n(r,s)}{\partial r^2} + r\frac{\partial C_n(r,s)}{\partial r} - (n^2 + r^2 s^\alpha) C_n(r,s) = 0. \tag{2.11}$$

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Eq. (2.11) is the modified Bessel equation of order n with the general solution

$$C_n(r,s) = \alpha_n(s)K_n(rs^{\frac{\alpha}{2}}) + \beta_n(s)I_n(rs^{\frac{\alpha}{2}}),$$

where $\alpha_n(s)$ and $\beta_n(s)$ are arbitrary functions and $I_n(rs^{\frac{\alpha}{2}})$ and $K_n(rs^{\frac{\alpha}{2}})$ are the linearly independent modified Bessel functions of the first and second kind, respectively. From the decay at infinity condition (2.8) we have $\beta_n(s) = 0$ such that

$$C_n(r,s) = \alpha_n(s)K_n(rs^{\frac{\alpha}{2}}),$$

so Eq. (2.10) becomes

$$\begin{aligned}\hat{u}(r,\theta,s) &= \sum_{n=-\infty}^{\infty} C_n(r,s)e^{in\theta} = \sum_{n=-\infty}^{\infty} \alpha_n(s)K_n(rs^{\frac{\alpha}{2}})e^{in\theta} \\ &= \alpha_0(s)K_0(rs^{\frac{\alpha}{2}}) + \sum_{n=\pm1}^{\infty} \alpha_n(s)K_n(rs^{\frac{\alpha}{2}})e^{in\theta},\end{aligned}$$

and dividing by $K_0(rs^{\frac{\alpha}{2}}) \neq 0$ we have

$$\frac{\hat{u}(r,\theta,s)}{K_0(rs^{\frac{\alpha}{2}})} = \alpha_0(s) + \sum_{n=\pm1}^{\infty} \alpha_n(s)\frac{K_n(rs^{\frac{\alpha}{2}})}{K_0(rs^{\frac{\alpha}{2}})}e^{in\theta}. \tag{2.12}$$

Differentiating Eq. (2.12) with respect to r and θ respectively, we have

$$\frac{\partial}{\partial r}\left(\frac{\hat{u}(r,\theta,s)}{K_0(rs^{\frac{\alpha}{2}})}\right) = \sum_{n=\pm1}^{\infty} \alpha_n(s)\frac{\partial}{\partial r}\left[\frac{K_n(rs^{\frac{\alpha}{2}})}{K_0(rs^{\frac{\alpha}{2}})}\right]e^{in\theta}, \tag{2.13}$$

$$\frac{\partial^{2k}}{\partial\theta^{2k}}\left(\frac{\hat{u}(r,\theta,s)}{K_0(rs^{\frac{\alpha}{2}})}\right) = \sum_{n=\pm1}^{\infty} (in)^{2k}\alpha_n(s)\frac{K_n(rs^{\frac{\alpha}{2}})}{K_0(rs^{\frac{\alpha}{2}})}e^{in\theta}. \tag{2.14}$$

Following Refs. [33–35], we assume that Eq. (2.13) is equivalent to

$$\frac{\partial}{\partial r}\left(\frac{\hat{u}(r,\theta,s)}{K_0(rs^{\frac{\alpha}{2}})}\right) = \sum_{k=1}^{\infty} d_k\frac{\partial^{2k}}{\partial\theta^{2k}}\left(\frac{\hat{u}(r,\theta,s)}{K_0(rs^{\frac{\alpha}{2}})}\right), \tag{2.15}$$

so combining Eqs. (2.14) and (2.15) yields

$$\frac{\partial}{\partial r}\left(\frac{\hat{u}(r,\theta,s)}{K_0(rs^{\frac{\alpha}{2}})}\right) = \sum_{n=\pm1}^{\infty} \alpha_n(s)\frac{\partial}{\partial r}\left(\frac{K_n(rs^{\frac{\alpha}{2}})}{K_0(rs^{\frac{\alpha}{2}})}\right)e^{in\theta} = \sum_{n=\pm1}^{\infty} \alpha_n(s)\frac{K_n(rs^{\frac{\alpha}{2}})}{K_0(rs^{\frac{\alpha}{2}})}\sum_{k=1}^{\infty}(in)^{2k}d_k e^{in\theta}$$

such that

$$\begin{aligned}\frac{K_n(rs^{\frac{\alpha}{2}})}{K_0(rs^{\frac{\alpha}{2}})}\sum_{k=1}^{\infty}(in)^{2k}d_k &= \frac{s^{\frac{\alpha}{2}}[K_n'(rs^{\frac{\alpha}{2}})K_0(rs^{\frac{\alpha}{2}}) - K_n(rs^{\frac{\alpha}{2}})K_0'(rs^{\frac{\alpha}{2}})]}{K_0^2(rs^{\frac{\alpha}{2}})}, \\ \sum_{k=1}^{\infty}(in)^{2k}d_k &= s^{\frac{\alpha}{2}}\left(\frac{K_n'(rs^{\frac{\alpha}{2}})}{K_n(rs^{\frac{\alpha}{2}})} - \frac{K_0'(rs^{\frac{\alpha}{2}})}{K_0(rs^{\frac{\alpha}{2}})}\right), \quad n = 1,2,\cdots.\end{aligned} \tag{2.16}$$

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In the practical computation, we truncate the infinite series (2.16) to the first N terms,

$$\sum_{k=1}^{N}(in)^{2k}d_k = s^{\frac{\alpha}{2}}\left(\frac{K_n'(rs^{\frac{\alpha}{2}})}{K_n(rs^{\frac{\alpha}{2}})}-\frac{K_0'(rs^{\frac{\alpha}{2}})}{K_0(rs^{\frac{\alpha}{2}})}\right), \qquad n=1,2,\cdots,N\,, \tag{2.17}$$

a linear algebraic system in the coefficients d_k that has a unique solution for any N since the determinant of its Vandermonde coefficient matrix is nonzero. For example:

- $N=1$,
$$d_1 = \frac{s^{\frac{\alpha}{2}}K_0'(rs^{\frac{\alpha}{2}})}{K_0(rs^{\frac{\alpha}{2}})}-\frac{s^{\frac{\alpha}{2}}K_1'(rs^{\frac{\alpha}{2}})}{K_1(rs^{\frac{\alpha}{2}})}\,;$$
- $N=2$,
$$d_1 = \frac{5}{4}\frac{s^{\frac{\alpha}{2}}K_0^{'}(rs^{\frac{\alpha}{2}})}{K_0(rs^{\frac{\alpha}{2}})}-\frac{4}{3}\frac{s^{\frac{\alpha}{2}}K_1^{'}(rs^{\frac{\alpha}{2}})}{K_1(rs^{\frac{\alpha}{2}})}+\frac{1}{12}\frac{s^{\frac{\alpha}{2}}K_2^{'}(rs^{\frac{\alpha}{2}})}{K_2(rs^{\frac{\alpha}{2}})}\,,$$
$$d_2 = \frac{1}{4}\frac{s^{\frac{\alpha}{2}}K_0^{'}(rs^{\frac{\alpha}{2}})}{K_0(rs^{\frac{\alpha}{2}})}-\frac{1}{3}\frac{s^{\frac{\alpha}{2}}K_1^{'}(rs^{\frac{\alpha}{2}})}{K_1(rs^{\frac{\alpha}{2}})}+\frac{1}{12}\frac{s^{\frac{\alpha}{2}}K_2^{'}(rs^{\frac{\alpha}{2}})}{K_2(rs^{\frac{\alpha}{2}})}\,.$$

Consequently, Eq. (2.15) becomes

$$\frac{\partial\hat{u}(r,\theta,s)}{\partial r} = \sum_{k=0}^{N} d_k\frac{\partial^{2k}\hat{u}(r,\theta,s)}{\partial\theta^{2k}}\,, \tag{2.18}$$

where $d_0 = s^{\frac{\alpha}{2}}K_0'(rs^{\frac{\alpha}{2}})/K_0(rs^{\frac{\alpha}{2}})$ and d_k $(k=1,2,\cdots,N)$ are given by Eq. (2.17).

The inverse Laplace transform of Eq. (2.18) produces the exact boundary conditions represented by a series of special functions [26], but this is difficult to implement due to the complexity of the coefficients d_k. An alternative efficient method is to represent the coefficients d_k via rational approximations, producing a series of integer-order ordinary differential equations (ODEs). Thus assuming there exists a partition $s_e = s_0 \le s_1 \le \cdots \le s_{2L} = s_w$ of the interval $[s_e, s_w]$ and applying the rational approximation for a given $r = R$, we get

$$d_k(R,s) \approx \frac{P_L(s)}{Q_L(s)} = \frac{a_0+a_1s+\cdots+a_Ls^L}{1+b_1s+\cdots+b_Ls^L} = c_{k,0}+\sum_{l=1}^{L}\frac{f_{k,l}s}{s-s_{k,l}}\,, \tag{2.19}$$

where $s_{k,l}$ $(l=1,2,\cdots,L)$ are the roots of polynomial $Q_L(s) = 1+b_1s+\cdots+b_Ls^L$ and the constants $c_{k,0}$ and $f_{k,l}$ are obtained as fractions. To investigate the accuracy and effectiveness of our approach, we define the L_1^{e}-error by

$$L_1^e = \frac{1}{2L+1}\sum_{j=0}^{2L}\left|d_k^{ex}(R,s_j)-d_k^{nu}(R,s_j)\right|,$$

where d_k^{ex} and d_k^{nu} denote the respective exact and approximate solutions for the d_k. Tables 1 and 2 show this L_1^e—error for d_0 and d_1 for $N=1$, when $L=5$ and $L=7$ respectively. We

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Table 1: The L_1^e—error of the exact and approximate solutions for d_k $(k=0,1)$ for several α, $R=1$, $N=1$ and $L=5$ in the interval $[0.01,20]$.

α	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{2}{3}$	$\frac{4}{5}$
d_0	2.384e-005	3.353e-005	4.106e-005	4.540e-005
d_1	2.865e-006	4.058e-006	5.009e-006	5.571e-006

Table 2: The L_1^e—error of the exact and approximate solutions for d_k $(k=0,1)$ for several α, $R=1$, $N=1$ and $L=7$ in the interval $[0.01,20]$.

α	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{2}{3}$	$\frac{4}{5}$
d_0	5.135e-007	7.265e-007	8.942e-007	9.928e-007
d_1	6.379e-008	1.068e-007	1.057e-007	1.218e-007

observe that the accuracy of the approximation is very high. Figs. 2 and 3 show plots of the exact and approximate solutions for several α when $N=1$ and $L=5$ and 7 respectively, showing that the d_k $(k=0,1)$ are approximated very well.

Substituting equation Eq. (2.19) into Eq. (2.18) on the artificial boundary, we have

$$\frac{\partial \hat{u}(R,\theta,s)}{\partial r}=\sum_{k=0}^{N}\left(c_{k,0}+\sum_{l=1}^{L}\frac{f_{k,l}s}{s-s_{k,l}}\right)\frac{\partial^{2k}\hat{u}(R,\theta,s)}{\partial\theta^{2k}},$$

and taking the inverse Laplace transform we obtain LABCs that contain high-order derivatives with respect to time t, which prompts us to introduce some auxiliary variables — viz. $\hat{\psi}_k=\frac{\partial^{2k}\hat{u}(R,\theta,s)}{\partial\theta^{2k}}$ and $-\hat{\phi}_{k,l}=\frac{s}{s-s_{k,l}}\hat{\psi}_k\,(k=0,\cdots,N;\ l=1,\cdots,L)$. We then have the reduced IBV problem for the time-fractional sub-diffusion equation on a bounded domain:

$$ {}_0^C D_t^{\alpha}u=\Delta u+f \ \text{ in } \Omega_R\times(0,T], \tag{2.20}$$

$$u|_{\Gamma_{\text{in}}}=g(a,\theta,t),\quad t>0\,, \tag{2.21}$$

$$u|_{t=0}=u_0 \ \text{ in } \Omega_R\,, \tag{2.22}$$

$$\frac{\partial u}{\partial r}=\sum_{k=0}^{N}c_{k,0}\psi_k-\sum_{k=0}^{N}\sum_{l=1}^{L}f_{k,l}\phi_{k,l} \ \text{ on } \Gamma_R\,, \tag{2.23}$$

$$\psi_0=u \ \text{ on } \Gamma_R\,, \tag{2.24}$$

$$\psi_k=\frac{\partial^2\psi_{k-1}}{\partial\theta^2}\ (k=1,\cdots,N) \ \text{ on } \Gamma_R\,, \tag{2.25}$$

$$\partial_t\psi_k=-\partial_t\phi_{k,l}+s_{k,l}\phi_{k,l}\ (k=0,\cdots,N,\ l=1,\cdots,L) \ \text{ on } \Gamma_R\,. \tag{2.26}$$

3. Finite Difference Scheme

Our finite difference scheme for the reduced IBV problem involving the time-fractional sub-diffusion equation (2.20)-(2.26) on an bounded computational domain is detailed

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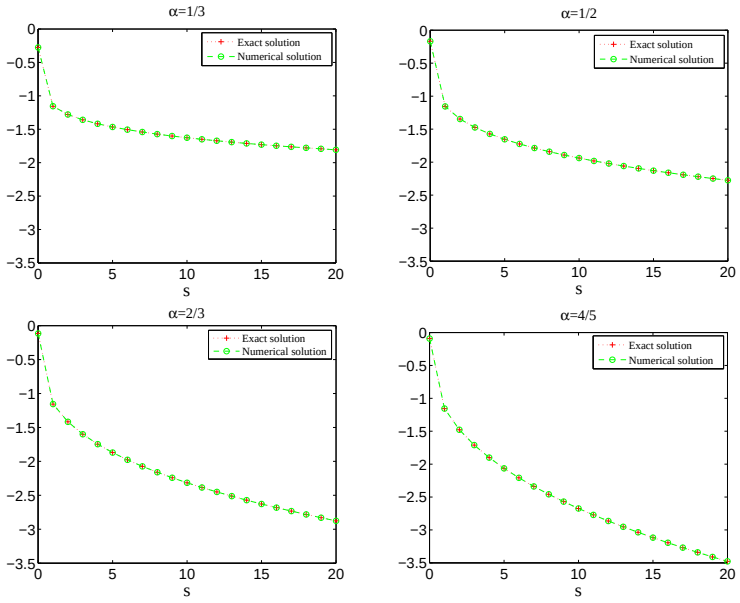


Figure 2: The numerical solution compared with the exact solution for d_0, $R=1$, $L=5$ and several α.

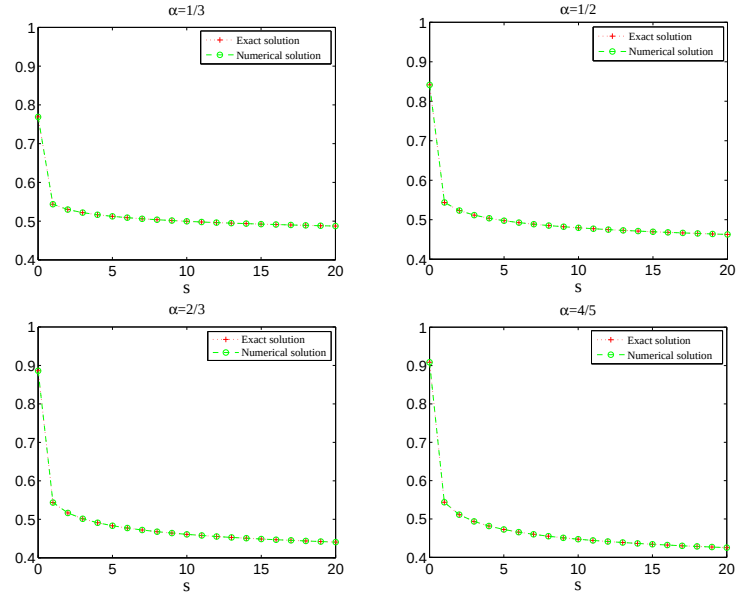


Figure 3: The numerical solution compared with the exact solution for d_1, $R=1$, $L=7$ and several α.

here. For positive integers I, J and M, we cover the truncated computational domain $[a,R]\times[0,2\pi]\times(0,T]$ by a uniform grid where the mesh sizes are $\Delta r=(R-a)/I$, $\Delta\theta=2\pi/J$ and $\tau=T/M$ such that the grid points are $r_i=i\Delta r$, $\theta_j=j\Delta\theta$ and $t_m=m\tau$.

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Let $u_{i,j}^m$ denote the approximation of $u(r_i,\theta_j,t_m)$, and introduce the finite differences

$$\delta_r u_{i-\frac{1}{2},j}^m = \frac{1}{\Delta r}(u_{i,j}^m - u_{i-1,j}^m),$$
$$\delta_r^2 u_{i,j}^m = \frac{1}{\Delta r}(\delta_r u_{i+\frac{1}{2},j}^m - \delta_r u_{i-\frac{1}{2},j}^m) = \frac{1}{\Delta r^2}(u_{i+1,j}^m - 2u_{i,j}^m + u_{i-1,j}^m),$$
$$\delta_t u_{i,j}^{m-\frac{1}{2}} = \frac{u_{i,j}^m - u_{i,j}^{m-1}}{\tau}, \qquad u_{i,j}^{m-\frac{1}{2}} = \frac{1}{2}(u_{i,j}^m + u_{i,j}^{m-1}), \qquad \delta_r^+ u_{i,j}^m = \frac{1}{2}(\delta_r u_{i-\frac{1}{2},j}^m + \delta_r u_{i+\frac{1}{2},j}^m),$$

and similarly the finite differences $\delta_\theta u_{i,j-\frac{1}{2}}^m$ and $\delta_\theta^2 u_{i,j}^m$. For the the Caputo time-fractional derivative, we adopt the L1 discrete operator (the L1 approximation)

$${}_0^C D_t^\alpha u_{i,j}^m = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}\left[a_0^{(\alpha)} u_{i,j}^m - \sum_{p=1}^{m-1}\left(a_{m-p-1}^{(\alpha)} - a_{m-p}^{(\alpha)}\right)u_{i,j}^p - a_{m-1}^{(\alpha)} u_{i,j}^0\right] + O(\tau^{2-\alpha}),$$

where $a_p^{(\alpha)} = (p+1)^{1-\alpha} - p^{1-\alpha}$, $p \ge 0$ and $0 < \alpha < 1$ — cf. Refs. [26, 36, 37].

Using the classical Crank-Nicolson finite difference scheme for the space variables and this L1 approximation for the fractional time derivative in the interior domain, we have

$${}_0^C D_t^\alpha u_{i,j}^m = \delta_r^2 u_{i,j}^{m-\frac{1}{2}} + \frac{1}{r_i}\delta_r^+ u_{i,j}^{m-\frac{1}{2}} + \frac{1}{r_i^2}\delta_\theta^2 u_{i,j}^{m-\frac{1}{2}} + f_{i,j}^{m-\frac{1}{2}}, \qquad 1 \le i \le I,\ 1 \le j \le J,\ 1 \le m \le M,$$
$$u_{i,0}^m = u_{i,J}^m, \qquad u_{i,-1}^m = u_{i,J-1}^m, \qquad 1 \le i \le I,\ 1 \le m \le M.$$

The discrete LABC schemes (2.23)-(2.26) are

$$\delta_r^+ u_{I-1,j}^{m-\frac{1}{2}} = \sum_{k=0}^{N} c_{k,0}\psi_{k,j}^{m-\frac{1}{2}} - \sum_{k=0}^{N}\sum_{l=1}^{L} f_{k,l}\phi_{k,l}^{m-\frac{1}{2}},$$
$$\psi_{k,j}^{m-\frac{1}{2}} = \delta_\theta^2 \psi_{k-1,j}^{m-\frac{1}{2}},$$
$$\delta_t \psi_{k,j}^{m-\frac{1}{2}} = -\delta_t \phi_{k,l}^{m-\frac{1}{2}} + s_{k,l}\phi_{k,l}^{m-\frac{1}{2}},$$

where

$$\psi_{0,j}^m = u_{I,j}^m, \quad u_{0,j}^m = u_{0,0}^m, \quad (j = 1,\cdots,J,\ \ m = 0,1,\cdots,M).$$

4. Numerical Examples

We considered two numerical examples to demonstrate the effectiveness and accuracy of the proposed high-order LABCs.

Example 4.1.

$${}_0^C D_t^\alpha u(r,\theta,t) = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} + f(r,\theta,t) \ \text{ in } \ \Omega_R \times (0,T],$$
$$u(r,\theta,t)\big|_{\Gamma_{\text{in}}} = u(a,\theta,t), \ \ t > 0,$$
$$u(r,\theta,t)\big|_{t=0} = u_0 \ \text{ in } \ \Omega_R,$$

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Table 3: The L_∞-error and convergence order for several α, time step $\tau = 5.0\text{e-}3$, $L = 5$ and $N = 0$ in Example 4.1.

α	$\frac{1}{3}$		$\frac{1}{2}$		$\frac{2}{3}$		$\frac{4}{5}$	
	error	order	error	order	error	order	error	order
4×4	2.452e-2	-	2.345e-2	-	2.237e-2	-	2.147e-2	-
8×8	3.834e-3	2.68	3.817e-3	2.62	3.964e-3	2.50	4.084e-3	2.39
16×16	7.261e-4	2.40	7.410e-4	2.36	8.747e-4	2.18	9.968e-4	2.03

Table 4: The L_∞-error and convergence order for several α, time step $\tau = 5.0\text{e-}3$, $L = 7$ and $N = 0$ in Example 4.1.

α	$\frac{1}{3}$		$\frac{1}{2}$		$\frac{2}{3}$		$\frac{4}{5}$	
	error	order	error	order	error	order	error	order
4×4	2.451e-2	-	2.357e-2	-	2.249e-2	-	2.156e-2	-
8×8	3.834e-3	2.68	3.851e-3	2.61	4.004e-3	2.49	4.122e-3	2.39
16×16	7.261e-4	2.40	7.410e-4	2.38	8.747e-4	2.19	9.968e-4	2.05

where $\Gamma_{\text{in}} = \{\mathbf{x}\in\mathbb{R}^2 |\ ||\mathbf{x}|| = a,\ 0 < a < R\}$. For the source term

$$f(r,\theta,t) = \begin{cases} (r-1)^2\exp(-r)t^3\big[(r-1)^2\frac{\Gamma(4+\alpha)}{6} + (-27+11r-r^2+\frac{5}{r})t^\alpha\big] \\ \qquad -4r^2(r-1)^2(16r^2-17r+4), \qquad (r,\theta,t)\in\Omega_R\times(0,T], \\ 0\,, \qquad \text{otherwise}\,, \end{cases}$$

the exact solution is

$$u(r,\theta,t) = \begin{cases} (r-1)^4\big[\exp(-r)t^{3+\alpha} + r^4\big], \quad (r,\theta,t)\in\Omega_R\times(0,T], \\ 0\,, \qquad \text{otherwise}\,, \end{cases}$$

which is radially symmetric so the θ-dependence can be dropped.

Let us adopt the circular artificial boundary of radius $R = 1.0$, $a = 0.1$ and the final time $T = 1.0$. We denote the L_∞-error by

$$L_\infty = \max_{i,j,k}\big|{}_{ex}u^k_{i,j} - {}_{nu}u^k_{i,j}\big|,$$

where ${}_{ex}u^k_{i,j}$ and ${}_{nu}u^k_{i,j}$ are the exact and numerical solution, respectively. Tables 3-6 list the L_∞-error and convergence order for several α and spatial sizes for the fixed time step $\tau =$ 5.0e-3, and we see that there is almost second order convergence in the spatial direction. Fig. 4 shows the L_∞-error for several α when $R = 1.0$ and $T = 1.0$.

Example 4.2.

$$\begin{aligned} &{}_0^C D_t^\alpha u(r,\theta,t) = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial\theta^2} + f(r,\theta,t) \ \text{ in } \ \Omega_R\times(0,T], \\ &u(r,\theta,t)\big|_{\Gamma_{\text{in}}} = u(a,\theta,t), \quad t>0\,, \\ &u(r,\theta,t)\big|_{t=0} = u_0 \ \text{ in } \ \Omega_R\,, \end{aligned}$$

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Table 5: The L_∞-error and convergence order for several α, time step $\tau = 5.0\text{e-}3$, $L = 5$ and $N = 1$ in Example 4.1.

α	$\frac{1}{3}$		$\frac{1}{2}$		$\frac{2}{3}$		$\frac{4}{5}$	
	error	order	error	order	error	order	error	order
4×4	2.452e-2	-	2.345e-2	-	2.237e-2	-	2.147e-2	-
8×8	3.834e-3	2.68	3.817e-3	2.62	3.964e-3	2.50	4.084e-3	2.39
16×16	7.261e-4	2.40	7.410e-4	2.36	8.747e-4	2.18	9.968e-4	2.03

Table 6: The L_∞-error and convergence order for several α, time step $\tau = 5.0\text{e-}3$, $L = 7$ and $N = 1$ in Example 4.1.

α	$\frac{1}{3}$		$\frac{1}{2}$		$\frac{2}{3}$		$\frac{4}{5}$	
	error	order	error	order	error	order	error	order
4×4	2.461e-2	-	2.357e-2	-	2.249e-2	-	2.156e-2	-
8×8	3.834e-3	2.68	3.851e-3	2.61	4.004e-3	2.49	4.122e-3	2.39
16×16	7.261e-4	2.40	7.410e-4	2.38	8.747e-4	2.19	9.968e-4	2.05

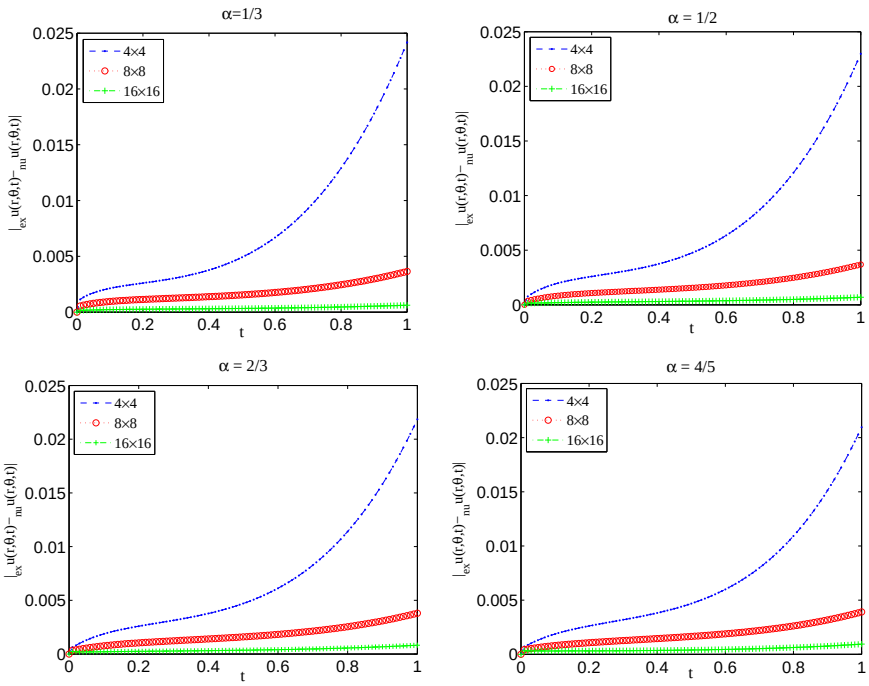


Figure 4: The L_∞-error for several spatial mesh sizes and several α in Example 4.1.

where $\Gamma_{\text{in}} = \{\mathbf{x} \in \mathbb{R}^2 | \ ||\mathbf{x}|| = a,\ 0 < a < R\}$, and

$$f(r,\theta,t) = \begin{cases} (r-1)^2\exp(-r)t^3\big[(r-1)^2\frac{\Gamma(4+\alpha)}{6} + (-27+11r-r^2+\frac{5}{r})t^\alpha\big] \\ \qquad -r^2(r-1)^2(63r^2-66r+15), \qquad (r,\theta,t) \in \Omega_R \times (0,T], \\ 0\,, \qquad \text{otherwise}\,. \end{cases}$$

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Table 7: The L_∞-error and convergence order for several α, time step $\tau = 5.0\text{e-}3$, $L = 5$ and $N = 0$ in Example 4.2.

α	$\frac{1}{3}$		$\frac{1}{2}$		$\frac{2}{3}$		$\frac{4}{5}$	
	error	order	error	order	error	order	error	order
4×4	2.388e-2	-	2.278e-2	-	2.168e-2	-	2.075e-2	-
8×8	3.395e-3	2.81	3.413e-3	2.74	3.546e-3	2.61	3.649e-3	2.51
16×16	8.630e-4	1.98	7.020e-4	2.28	7.774e-4	2.19	8.852e-4	2.04

Table 8: The L_∞-error and convergence order for several α, time step $\tau = 5.0\text{e-}3$, $L = 7$ and $N = 0$ in Example 4.2.

α	$\frac{1}{3}$		$\frac{1}{2}$		$\frac{2}{3}$		$\frac{4}{5}$	
	error	order	error	order	error	order	error	order
4×4	2.397e-2	-	2.290e-2	-	2.179e-2	-	2.085e-2	-
8×8	3.395e-3	2.82	3.448e-3	2.73	3.586e-3	2.60	3.686e-3	2.50
16×16	8.630e-4	1.98	7.020e-4	2.30	7.774e-4	2.21	8.852e-4	2.06

Table 9: The L_∞-error and convergence order for several α, time step $\tau = 5.0\text{e-}3$, $L = 5$ and $N = 1$ in Example 4.2.

α	$\frac{1}{3}$		$\frac{1}{2}$		$\frac{2}{3}$		$\frac{4}{5}$	
	error	order	error	order	error	order	error	order
4×4	2.317e-2	-	2.200e-2	-	2.084e-2	-	1.989e-2	-
8×8	3.104e-3	2.90	3.081e-3	2.84	3.194e-3	2.71	3.283e-3	2.60
16×16	8.531e-4	1.86	6.917e-4	2.16	7.112e-4	2.17	8.142e-4	2.01

The problem has the following exact solution that is not radially symmetric:

$$u(r,\theta,t) = \begin{cases} (r-1)^4\big[\exp(-r)t^{3+\alpha} + r^4\cos\theta\big], & (r,\theta,t)\in\Omega_R\times(0,T] \\ 0\,, \qquad \text{otherwise}\,. \end{cases}$$

Let us again adopt $R = 1.0$, $a = 0.1$ and the final time $T = 1.0$. The numerical results are listed in Tables 7-10 for several spatial sizes and several α at time $T = 1.0$. One can see that the spatial numerical accuracy of difference scheme is nearly the second order. Since the solution is radially non-symmetric, the error decreases as the parameter N increases. Overall, a good performance is obtained as $N = 1$ and $L = 5$, though certainly all parameter choices led to excellent accuracy at low cost. The error between the exact solution and the numerical solution is given for several α with $\theta = \pi/3$ and $t \in [0,T]$ in Fig. 5. One can see that the error is always very small in $t \in [0,T]$ as the spatial mesh size refines.

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Table 10: The L_∞-error and convergence order for several α, time step $\tau = 5.0\text{e-}3$, $L = 5$ and $N = 1$ in Example 4.2.

α	$\frac{1}{3}$		$\frac{1}{2}$		$\frac{2}{3}$		$\frac{4}{5}$	
	error	order	error	order	error	order	error	order
4×4	2.325e-2	-	2.210e-2	-	2.095e-2	-	1.998e-2	-
8×8	3.104e-3	2.90	3.114e-3	2.83	3.232e-3	2.70	3.320e-3	2.59
16×16	8.531e-4	1.86	6.917e-4	2.17	7.112e-4	2.18	8.142e-4	2.03

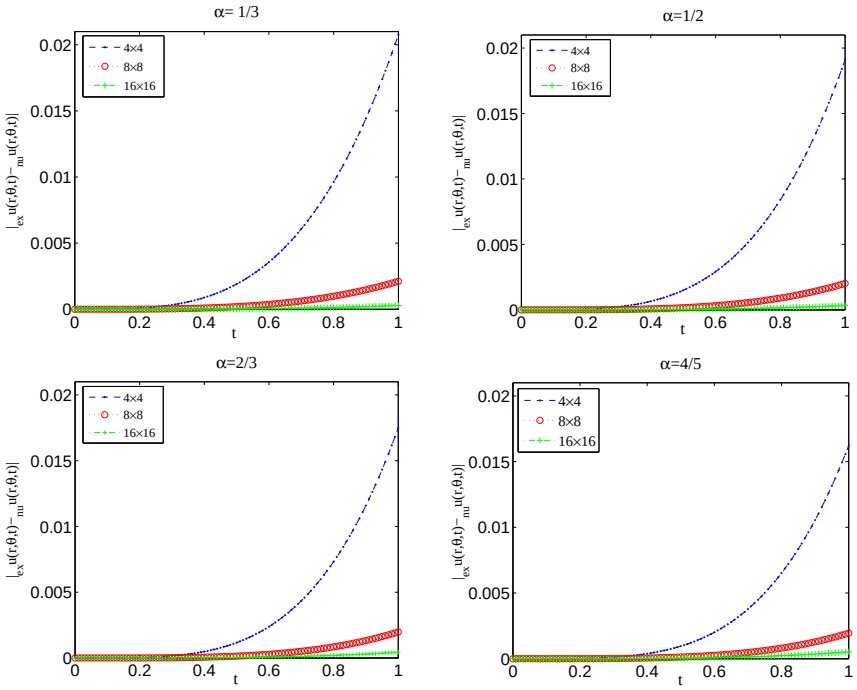


Figure 5: The L_∞-error with several spatial mesh sizes for several α and fixed $\theta = \frac{\pi}{3}$ in Example 4.2.

5. Conclusion

The high-order LABCs on the introduced circular artificial boundary were designed for the time-fractional sub-diffusion equation on two-dimensional unbounded domains by invoking the Laplace transform and a Fourier series expansion. In order to avoid the high-order derivatives in the ABCs, auxiliary variables were introduced. The original problem defined on unbounded domain was reduced to an IBV problem on a bounded computational domain. The finite difference method was then constructed to solve the reduced problem. Numerical results for two examples illustrate the effectiveness and accuracy of the proposed LABCs.

In future, fast evaluation of the Caputo fractional derivative will be considered to reduce the computation cost. The smoothness of the convolution kernel away from the origin

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admits an efficient sum-of-exponentials approximation. At each time step, the convolution with the exponential kernel can be evaluated via an O(1) recurrence relation, implying that the convolution of the Caputo fractional derivative needs $O(N_T \log^2 N_T)$ time and only $O(\log^2 N_T)$ history modes [39–44]. There are also some important theoretical issues to explore — including a rigorous stability analysis of the reduced problem with LABCs, and the design of LABCs for nonlinear time-fractional diffusion equation on unbounded domains.

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