Finite difference method for time-fractional Klein-Gordon equation on an unbounded domain using artificial boundary conditions

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Peng Ding · Yubin Yan · Zongqi Liang · Yuyuan Yan

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Abstract A finite difference method for time-fractional Klein-Gordon equation with the fractional order $\alpha \in (1, 2]$ on an unbounded domain is studied. The artificial boundary conditions involving the generalized Caputo derivative are derived using the Laplace transform technique. Stability and error estimates of the proposed finite difference scheme are proved in detail by using the discrete energy method. Numerical examples show that the artificial boundary method is a robust and efficient method for solving the time-fractional Klein-Gordon equation on an unbounded domain.

Keywords Time-fractional Klein-Gordon equation · artificial boundary conditions · the generalized Caputo derivative · stability · convergence.

Mathematics Subject Classification (2000) 65M15 · 65M60 · 65M12 · 45K05

Peng Ding
School of Sciences, Jimei University, Xiamen 361021, China
E-mail: 3065757659@qq.com

Yubin Yan
Department of Mathematical and Physical Sciences, University of Chester, CH1 4BJ
E-mail: y.yan@chester.ac.uk

Zongqi Liang
School of Sciences, Jimei University, Xiamen 361021, China
E-mail: zqliang@jmu.edu.cn

Yuyuan Yan
School of Sciences, Jimei University, Xiamen 361021, China
E-mail: 624557441@qq.com
Zongqi Liang is the corresponding author.

1 Introduction

The aim of this paper is to derive the artificial boundary conditions and study a robust and efficient finite difference scheme for approximating the following time-fractional Klein-Gordon equation

$$ {}_0^C D_t^\alpha u(x,t) - p^2 \frac{\partial^2 u(x,t)}{\partial x^2} + q^2 u(x,t) = f(x,t), \quad x \in \mathbb{R}, 0 \le t \le T, \tag{1} $$

$$ u(x,0) = \varphi(x), \quad u_t(x,0) = \psi(x), \quad x \in \mathbb{R}, \tag{2} $$

$$ u(x,t) \to 0, \quad |x| \to \infty, \quad 0 \le t \le T, \tag{3} $$

where supp $\{\psi, \varphi\} \subseteq [x_l, x_r]$, supp$\{f\} \subseteq [x_l, x_r] \times [0,T]$, $1 < \alpha \le 2$ and p, q are positive constants. The Caputo derivative is defined by [35], with $\alpha \in (1,2]$,

$$ {}_0^C D_t^\alpha u(t) = \frac{1}{\Gamma(2-\alpha)} \int_0^t \frac{1}{(t-\tau)^{\alpha-1}} \frac{d^2 u(\tau)}{d\tau^2} d\tau. $$

Many problems in physical and engineering sciences can be described by Klein-Gordon equations. The applications of Klein-Gordon equations in propagation of fluxion between superconductors, motion of pendule, and dislocations in crystal can be found in [1], [2], [3]. There is a trend of modeling problems by fractional differential equations instead of the classical integer order differential equations. Some problems are described more accurately using fractional derivatives.

The analytical solutions of fractional differential equations mostly contain the special functions such as Mittag-Leffler function, H-function, hypergeometric function, Wright function, etc. which makes the analytical solutions of fractional differential equations are difficult to find explicitly. Many efficient numerical methods for approximating the fractional partial differential equation on the bounded domains are presented, for example, finite difference methods [4], [8], [9], [10], [13], [20], [21], [22], [25], finite element methods [26], [27], [28], [29],[30] and spectral methods [11], [12], [23], [24]. However, it is challenging to numerically solve and analyze time-fractional partial differential equations on the unbounded domains due to the non-locality of time-fractional derivative and the unboundedness of spatial domain.

The unbounded domain brings the essential difficulties to the numerical solutions of the fractional partial differential equations. Neither the finite difference method nor the finite element method can be directly applied to solve such problems. One of the methods for solving such problem is to apply the artificial boundary method, which divides the unbounded physical domain into a bounded computational domain and the remaining unbounded domain. By deriving the exact or approximate boundary conditions, the original problems on spatial unbounded domains can be reduced to the initial-boundary value problems on spatial bounded computational domains. For the artificial boundary methods for integer order partial differential equations, we refer to [34].

Let us first review some numerical methods for approximating the time fractional partial differential equations on the unbounded domains. Gao and

Sun [14],[15] studied the artificial boundary conditions of time-fractional subdiffusion equation on the unbounded domain and presented a finite difference scheme based on the L1 approximation for time-fractional derivatives and compact difference scheme for spatial derivatives and proved that the convergence order of the proposed scheme is $O(\Delta t^{2-\alpha} + h^4)(0 < \alpha \leq 1)$. Using the order reduction method, Zhang [16] studied the artificial boundary conditions of the time-fractional linear KdV equation on the unbounded domains and constructed the finite difference scheme and analyzed its stability and convergence. The artificial boundary conditions of the time-fractional Schrödinger equation on the unbounded domains for the potential function $V_c = 0$ was studied by Li and Zhang [17]. Sun and Zhang [18] further improved the proof of convergence and gave the optimal convergence order when $V_c = 0$. In [19], the artificial boundary conditions of the time-fractional nonlinear Schrödinger equation on the unbounded domain was obtained by the operator splitting method and Padé approximation. The value of α in the artificial boundary conditions mentioned above for the time-fractional partial differential equation on the unbounded domains are all less than or equal to 1. In this paper, we will derive the artificial boundary condition for the time-fractional Klein-Gordon equation with $1 < \alpha \leq 2$.

To obtain the artificial boundary conditions for (1)-(3), we perform the Laplace transform on (1) to get an ordinary differential equation. The artificial boundary conditions can be derived by solving this ordinary differential equation. We then introduce a finite difference scheme for approximating the time-fractional Klein-Gordon equation on the bounded domain with the proposed artificial boundary conditions. The stability and convergence of the scheme are proved using the discrete energy method.

The main contributions of this paper are as follows.

1. The artificial boundary condition for time-fractional Klein-Gordon equation on the unbounded domain is derived, which transformed the original problem on the unbounded domain into the initial boundary value problem on the bounded domain.
2. The L1 scheme of the generalized Caputo derivative is constructed and the truncation error is studied in detail.
3. A finite difference method of time-fractional Klein-Gordon equation with exact artificial boundary conditions is established and the convergence and stability of the proposed method are proved by the discrete energy method.

The paper is organized as follows. In Section 2, the exact artificial boundary conditions of time-fractional Klein-Gordon equation on the unbounded domains are derived by using the Laplace transform method. In Section 3, the difference scheme for approximating the time-fractional Klein-Gordon equation on the bounded domain is constructed. In Section 4, the lower bound of the approximation to the generalized Caputo derivative is given and the convergence and stability of the finite difference scheme for approximating the time-fractional Klein-Gordon equation on the bounded domain are analyzed.

In section 5, several numerical examples are given to show that the numerical results are consistent with the theoretical findings.

2 The artificial boundary condition for (1)-(3)

In this section, we shall introduce the artificial boundary conditions for (1)-(3). Denote

$$\Sigma_r = \{(x,t)|x = x_r, 0 \le t \le T\}, \qquad \Sigma_l = \{(x,t)|x = x_l, 0 \le t \le T\},$$

which divides the unbounded domain into three parts

$$\Omega_{in} = (x_l, x_r) \times [0,T], \qquad \Omega_r = [x_r, +\infty) \times [0,T], \qquad \Omega_l = (-\infty, x_l] \times [0,T].$$

We further denote $\Omega_{out} = (-\infty, x_l] \cup [x_r, +\infty) \times [0,T]$.

Since $\text{supp}\{\psi, \varphi\} \subseteq [x_l, x_r]$, $\text{supp}\{f\} \subseteq [x_l, x_r] \times [0,T]$, the constraint of the problem (1)-(3) on the domain Ω_{out} takes the form of

$$ {}_0^C D_t^\alpha u(x,t) - p^2 \frac{\partial^2 u(x,t)}{\partial x^2} + q^2 u(x,t) = 0, \quad (x,t) \in \Omega_{out}, \tag{4}$$

$$u(x,0) = 0, \quad u_t(x,0) = 0, \quad x \in (-\infty, x_l] \cup [x_r, +\infty), \tag{5}$$

$$u(x,t) \to 0, \quad \big|x\big| \to \infty, \quad t \in [0,T]. \tag{6}$$

Let $\widehat{u}(x,s)$ be the Laplace transform of $u(x,t)$, i.e.

$$\widehat{u}(x,s) = \int_0^{+\infty} e^{-st} u(x,t) dt, \quad \Re(s) > 0.$$

Recalling the result of Laplace transform for the Caputo derivatives in the form of

$$\widehat{{}_0^C D_t^\alpha v}(s) = s^\alpha \widehat{v}(s) - s^{\alpha-1} v(0) - s^{\alpha-2} v_t(0).$$

From (4)-(6) , we have

$$\begin{cases} s^\alpha \widehat{u}(x,s) - p^2 \dfrac{\partial^2 \widehat{u}(x,s)}{\partial x^2} + q^2 \widehat{u}(x,s) = 0, \quad x \in (-\infty, x_l] \cup [x_r, +\infty), \\ \widehat{u}(x,s) \to 0, \quad |x| \to \infty. \end{cases}$$

Solving the above ordinary differential equation, one gets

$$\widehat{u}(x,s) = \begin{cases} c_1(s) e^{-\frac{\sqrt{s^\alpha + q^2}}{p} x}, \quad x \in [x_r, +\infty), \\ c_2(s) e^{\frac{\sqrt{s^\alpha + q^2}}{p} x}, \quad x \in (-\infty, x_l], \end{cases} \tag{7}$$

where $c_1(s)$ and $c_2(s)$ are undetermined functions.

Formula (7) is equivalent to

$$\frac{\partial \widehat{u}(x,s)}{\partial x} = \begin{cases} -\dfrac{1}{p}\dfrac{s^\alpha+q^2}{\sqrt{s^\alpha+q^2}}\widehat{u}(x,s), & x\in[x_r,+\infty), \\ \dfrac{1}{p}\dfrac{s^\alpha+q^2}{\sqrt{s^\alpha+q^2}}\widehat{u}(x,s), & x\in(-\infty,x_l]. \end{cases} \tag{8}$$

When $x \in [x_r, +\infty)$, from (8), we get

$$\begin{aligned}\frac{\partial \widehat{u}(x_r,s)}{\partial x} &= -\frac{1}{p}\frac{s^\alpha+q^2}{\sqrt{s^\alpha+q^2}}\widehat{u}(x_r,s) \\ &= -\frac{1}{p}\{\frac{s^{\frac{\alpha}{2}-(1-\frac{\alpha}{2})}}{\sqrt{s^\alpha+q^2}}s\widehat{u}(x_r,s)+q^2\frac{s^{\frac{\alpha}{2}-(1+\frac{\alpha}{2})}}{\sqrt{s^\alpha+q^2}}s\widehat{u}(x_r,s)\}.\end{aligned} \tag{9}$$

Taking the inverse Laplace transform of the problem (9), we get

$$\begin{aligned}\frac{\partial u(x_r,t)}{\partial x} &= -\frac{1}{p}t^{-\frac{\alpha}{2}}\Big[E^{\frac{1}{2}}_{\alpha,1-\frac{\alpha}{2}}(-q^2t^\alpha)*\frac{\partial u(x_r,t)}{\partial t}+q^2t^\alpha E^{\frac{1}{2}}_{\alpha,1+\frac{\alpha}{2}}(-q^2t^\alpha)*\frac{\partial u(x_r,t)}{\partial t}\Big] \\ &= -\frac{1}{p}\Big\{t^{-\frac{\alpha}{2}}\Big[E^{\frac{1}{2}}_{\alpha,1-\frac{\alpha}{2}}(-q^2t^\alpha)+q^2t^\alpha E^{\frac{1}{2}}_{\alpha,1+\frac{\alpha}{2}}(-q^2t^\alpha)\Big]\Big\}*\frac{\partial u(x_r,t)}{\partial t} \\ &= -\frac{1}{p}\int_0^t \frac{G_{\alpha,q}(t-\tau)}{(t-\tau)^{\frac{\alpha}{2}}}\frac{\partial u(x_r,\tau)}{\partial \tau}d\tau \\ &= -\frac{1}{p}\Gamma(1-\frac{\alpha}{2}){}_0^GD_t^{\frac{\alpha}{2}}u(x_r,t),\end{aligned} \tag{10}$$

where

$${}_0^GD_t^{\frac{\alpha}{2}}u(x_r,t) = \frac{1}{\Gamma(1-\frac{\alpha}{2})}\int_0^t \frac{G_{\alpha,q}(t-\tau)}{(t-\tau)^{\frac{\alpha}{2}}}\frac{\partial u(x_r,\tau)}{\partial \tau}d\tau, \tag{11}$$

$$G_{\alpha,q}(t) = E^{\frac{1}{2}}_{\alpha,1-\frac{\alpha}{2}}(-q^2t^\alpha)+q^2t^\alpha E^{\frac{1}{2}}_{\alpha,1+\frac{\alpha}{2}}(-q^2t^\alpha). \tag{12}$$

Here the generalized Mittag-Leffler function $E^{\gamma}_{\alpha,\beta}(z)$ is defined by, with $\alpha,\beta\in\mathbb{C}$ and $\Re(\alpha)>0,\Re(\beta)>0,\gamma>0$, [35],

$$E^{\gamma}_{\alpha,\beta}(z) = \sum_{k=0}^{\infty}\frac{(\gamma)_k}{\Gamma(k+1)\Gamma(k\alpha+\beta)}z^k, \quad z\in\mathbb{C},$$

where $(\gamma)_k = \Gamma(\gamma+k)/\Gamma(\gamma)$. Further we have

$$\mathcal{L}^{-1}\left[\frac{s^{\alpha\gamma-\beta}}{(\lambda+s^\alpha)^\gamma}\right] = t^{\beta-1}E^{\gamma}_{\alpha,\beta}(-\lambda t^\alpha),$$

where $\mathcal{L}^{-1}$ denotes the inverse Laplace transform.

Similarly to the derivation of (10), one may obtain

$$\frac{\partial u(x_l,t)}{\partial x} = \frac{1}{p}\Gamma(1-\frac{\alpha}{2}){}_0^G D_t^{\frac{\alpha}{2}} u(x_l,t).$$

Thus the problem (1)-(3) is equivalent to the following time-fractional Klein-Gordon equation with the exact artificial boundary conditions

$${}_0^C D_t^{\alpha} u(x,t) - p^2 \frac{\partial^2 u(x,t)}{\partial x^2} + q^2 u(x,t) = f(x,t), \quad (x,t) \in (x_l,x_r)\times[0,T], \tag{13}$$

$$u(x,0) = \varphi(x), \quad u_t(x,0) = \psi(x), \quad x \in [x_l,x_r], \tag{14}$$

$$\frac{\partial u(x_r,t)}{\partial x} = -\frac{1}{p}\Gamma(1-\frac{\alpha}{2}){}_0^G D_t^{\frac{\alpha}{2}} u(x_r,t), \quad t\in[0,T], \tag{15}$$

$$\frac{\partial u(x_l,t)}{\partial x} = \frac{1}{p}\Gamma(1-\frac{\alpha}{2}){}_0^G D_t^{\frac{\alpha}{2}} u(x_l,t), \quad t\in[0,T]. \tag{16}$$

Remark 1 The equations (15), (16) contain the generalized Caputo fractional derivative ${}_0^G D_t^{\frac{\alpha}{2}} u(x,t)$ defined by, with $n-1<\alpha\le n$, $n\in\mathbb{Z}^+$, [31] [35],

$${}_0^G D_t^{\alpha} f(t) := \frac{1}{\Gamma(n-\alpha)}\int_0^t \frac{G_{\alpha,q}(t-\tau) f^{(n)}(\tau)}{(t-\tau)^{\alpha-n+1}} d\tau.$$

Obviously, ${}_0^G D_t^{\frac{\alpha}{2}} u(x,t) = {}_0^C D_t^{\frac{\alpha}{2}} u(x,t)$ when $G_{\alpha,q}(t)=1$.

Remark 2 In general, the solution of (13)-(16) has the weak singularity near the initial time. In this work, we will mainly focus on the formulation of the artificial boundary conditions of (13)-(16) under the assumptions that the solutions are sufficiently smooth. In literature, there are lots of works to consider the numerical methods for time fractional partial differential equations by using the graded meshes which can recover the optimal convergence orders of the proposed numerical methods. One may also use the graded meshes to solve (13)-(16) numerically.

Remark 3 In (13), the equation involves the Caputo fractional derivative which makes the solution have the singularity near the initial time. In the artificial boundary conditions (14)-(15), the generalize Caputo fractional derivatives are also involved which also contains the initial singularity.

3 The finite difference scheme of (13)-(16)

In this section, we shall construct the finite difference scheme for approximating (13)-(16). To do this, we first need to study the approximation scheme of the generalized Caputo derivative in (15), (16).

Let M and N be two positive integers. We introduce a mesh $\Omega_h \times \Omega_{\Delta t}$ defined by

$$\Omega_h = \{x_i | x_i = x_0 + ih, x_0 = x_l, x_M = x_r, 0 \le i \le M\},$$
$$\Omega_{\Delta t} = \{t_n | t_n = t_0 + n\Delta t, t_0 = 0, t_N = T, 0 \le n \le N\}.$$

The domain Ω_{in} is then covered by $\Omega_h \times \Omega_{\Delta t}$. For any mesh function $u = \{u_i^n | 0 \le i \le M, 0 \le n \le N\}$ defined on $\Omega_h \times \Omega_{\Delta t}$, we introduce the following notations:

$$u_i^{n-\frac{1}{2}} = \frac{u_i^n + u_i^{n-1}}{2}, \quad \delta_t u_i^{n-\frac{1}{2}} = \frac{u_i^n - u_i^{n-1}}{\Delta t}, \quad 0 \le i \le M, 1 \le n \le N,$$
$$\delta_x u_{i+\frac{1}{2}}^n = \frac{u_{i+1}^n - u_i^n}{h}, \quad \delta_x^2 u_i^n = \frac{\delta_x u_{i+\frac{1}{2}}^n - \delta_x u_{i-\frac{1}{2}}^n}{h}, \quad 1 \le i \le M-1, 0 \le n \le N.$$

Let

$$S_M = \big\{u | u = (u_0, u_1, ..., u_M)\big\}.$$

For any $u, v \in S_M$, the inner product and norm are defined by

$$(u,v) = h(\frac{1}{2}u_0 v_0 + \sum_{i=1}^{M-1} u_i v_i + \frac{1}{2}u_M v_M), \quad \|u\| = \sqrt{(u,u)},$$
$$\|\delta_x u\| = \sqrt{h\sum_{i=1}^{M}(\delta_x u_{i-\frac{1}{2}})^2}, \quad \|u\|_\infty = \max_{0\le i\le M} |u_i|.$$

Lemma 1 *[33] Suppose $y(x) \in C^3[x_l, x_r]$, where $x_l = x_0, x_r = x_M$, then*

$$y''(x_0) - \frac{2}{h}\left[\frac{y(x_1) - y(x_0)}{h} - y'(x_0)\right] = -\frac{h}{3}y'''(x_0 + \theta_1 h), \quad \theta_1 \in (0,1),$$
$$y''(x_M) - \frac{2}{h}\left[y'(x_M) - \frac{y(x_M) - y(x_{M-1})}{h}\right] = -\frac{h}{3}y'''(x_M - \theta_1 h), \quad \theta_1 \in (0,1).$$

Lemma 2 *[32] Suppose $1 < \alpha \le 2$, $u(t) \in C^3[t_0, t_n]$, with $n = 1, 2, \cdots, N$,*

$$\bar{R}^{n-\frac{1}{2}} = {}_0^C D_t^\alpha u(t)|_{t=t_{n-\frac{1}{2}}} - \mathbb{D}_t^\alpha u^{n-\frac{1}{2}},$$

then

$$\left|\bar{R}^{n-\frac{1}{2}}\right| \le \left\{\frac{1}{6\Gamma(3-\alpha)} + \frac{1}{2\Gamma(2-\alpha)}\left[\frac{1}{4} + \frac{\alpha-1}{(2-\alpha)(3-\alpha)}\right]\right\} \max_{t_0\le t\le t_n}\left|u'''(t)\right|\Delta t^{3-\alpha},$$

where

$$\mathbb{D}_t^\alpha u^{n-\frac{1}{2}} = \frac{\Delta t^{1-\alpha}}{\Gamma(3-\alpha)}\left[b_0^{(\alpha)}\delta_t u^{n-\frac{1}{2}} - \sum_{j=1}^{n-1}(b_{n-j-1}^{(\alpha)} - b_{n-j}^{(\alpha)})\delta_t u^{j-\frac{1}{2}} - b_{n-1}^{(\alpha)}u'(t_0)\right],$$

$$b_l^{(\alpha)} = (l+1)^{2-\alpha} - l^{2-\alpha}, \quad l = 0, 1, 2, \cdots, n-1.$$

Below we shall approximate the generalized Caputo derivatives ${}_0^G D_t^{\frac{\alpha}{2}} u(t)$ in (15), (16) by using the L1 scheme. Note that, at $t = t_{n-\frac{1}{2}}$,

$$
{}_0^G D_t^{\frac{\alpha}{2}} u(t)|_{t=t_{n-\frac{1}{2}}} = \frac{1}{\Gamma(1-\frac{\alpha}{2})} \int_0^{t_{n-\frac{1}{2}}} \frac{G_{\alpha,q}(t_{n-\frac{1}{2}}-\tau)u'(\tau)}{(t_{n-\frac{1}{2}}-\tau)^{\frac{\alpha}{2}}} d\tau
$$

$$
= \frac{1}{\Gamma(1-\frac{\alpha}{2})} \Big[\sum_{j=1}^{n-1} \int_{t_{j-1}}^{t_j} \frac{G_{\alpha,q}(t_{n-\frac{1}{2}}-\tau)u'(\tau)}{(t_{n-\frac{1}{2}}-\tau)^{\frac{\alpha}{2}}} d\tau + \int_{t_{n-1}}^{t_{n-\frac{1}{2}}} \frac{G_{\alpha,q}(t_{n-\frac{1}{2}}-\tau)u'(\tau)}{(t_{n-\frac{1}{2}}-\tau)^{\frac{\alpha}{2}}} d\tau \Big].
$$

Performing the linear interpolation of $u(t)$ in the interval $[t_{j-1}, t_j] (1 \le j \le n-1)$ on the nodes t_{j-1} and t_j $(1 \le j \le n-1)$ and the linear interpolation of $u(t)$ in the interval $[t_{n-1}, t_{n-\frac{1}{2}}]$ on the nodes t_{n-1} and t_n, respectively, we obtain the approximation scheme $\mathbb{D}_t^{G,\frac{\alpha}{2}} u^{n-\frac{1}{2}}$ defined by (17) of ${}_0^G D_t^{\frac{\alpha}{2}} u(t)|_{t=t_{n-\frac{1}{2}}}$. We have the following lemma for the truncation error of the approximation $\mathbb{D}_t^{G,\frac{\alpha}{2}} u^{n-\frac{1}{2}}$.

Lemma 3 *Let $1 < \alpha \le 2$ and $u(t) \in C^3[0,T]$. There exist positive constants $M_i(T,\alpha) (i = 1, 2, \cdots, 5)$ which only depend on T and α, such that*

$$
\begin{aligned}
\left|\tilde{R}^{n-\frac{1}{2}}\right| &= \left| {}_0^G D_t^{\frac{\alpha}{2}} u(t)|_{t=t_{n-\frac{1}{2}}} - \mathbb{D}_t^{G,\frac{\alpha}{2}} u^{n-\frac{1}{2}} \right| \\
&\le \frac{\Delta t^{2-\frac{\alpha}{2}}}{8\Gamma(1-\frac{\alpha}{2})} \max_{t_0 \le t \le t_{n-1}} |u''(t)| \sum_{i=1}^{2} M_i(T,\alpha) \\
&\quad + \frac{2\Delta t^{2-\frac{\alpha}{2}}}{\Gamma(1-\frac{\alpha}{2})} \max_{t_{n-1} \le t \le t_n} \left|u'''(t)\right| \sum_{i=3}^{5} M_i(T,\alpha).
\end{aligned}
$$

Here

$$
\mathbb{D}_t^{G,\frac{\alpha}{2}} u^{n-\frac{1}{2}} = \frac{1}{\Gamma(1-\frac{\alpha}{2})} \sum_{j=1}^{n} a_{n-j}^{(\alpha)} \delta_t u^{j-\frac{1}{2}}, \quad n \ge 1, \tag{17}
$$

where

$$
a_j^{(\alpha)} = \begin{cases} \sum_{k=0}^{+\infty} \Big[\tilde{A}_k^{(\alpha)} (\frac{\Delta t}{2})^{k\alpha - \frac{\alpha}{2}+1} - \tilde{B}_k^{(\alpha)} (\frac{\Delta t}{2})^{k\alpha+\frac{\alpha}{2}+1} \Big], \quad j = 0, \\ \sum_{k=0}^{+\infty} \tilde{A}_k^{(\alpha)} \Delta t^{k\alpha-\frac{\alpha}{2}+1} \Big[(j+\frac{1}{2})^{k\alpha-\frac{\alpha}{2}+1} - (j-\frac{1}{2})^{k\alpha-\frac{\alpha}{2}+1} \Big] \\ \quad - \sum_{k=0}^{+\infty} \tilde{B}_k^{(\alpha)} \Delta t^{k\alpha+\frac{\alpha}{2}+1} \Big[(j+\frac{1}{2})^{k\alpha+\frac{\alpha}{2}+1} - (j-\frac{1}{2})^{k\alpha+\frac{\alpha}{2}+1} \Big], \\ \qquad\qquad 1 \le j \le n-1, \end{cases}
$$

and

$$
\tilde{A}_k^{(\alpha)} = \frac{\Gamma(k+\frac{1}{2})(-q^2)^k}{\Gamma(k\alpha+2-\frac{\alpha}{2})\Gamma(k+1)\Gamma(\frac{1}{2})}, \quad \tilde{B}_k^{(\alpha)} = \frac{\Gamma(k+\frac{1}{2})(-q^2)^{k+1}}{\Gamma(k\alpha+2+\frac{\alpha}{2})\Gamma(k+1)\Gamma(\frac{1}{2})}. \tag{18}
$$

Proof See Appendix.

The coefficients $\{a_j^{(\alpha)}\}(j=0,1,\cdots,n-1)$ defined in (17) satisfy the following Lemma.

Lemma 4 *Let $1<\alpha<2$, $\{a_j^{(\alpha)}\}(0\le j\le n-1, n\ge 1)$ be defined in (17). Then there exists a positive $T>0$ such that, with $t_j=j\Delta t\le T$,*

$$a_j^{(\alpha)}\ge 0,\quad 0\le j\le n-1.$$

Proof For $j=0$, we have

$$a_0^{(\alpha)}=\frac{1}{\Gamma(2-\frac{\alpha}{2})}(\frac{\Delta t}{2})^{1-\frac{\alpha}{2}}+\sum_{k=1}^{+\infty}(-1)^{k+1}\frac{q^{2k}\Gamma(k-\frac{1}{2})}{2\sqrt{\pi}\Gamma(k\alpha-\frac{\alpha}{2}+2)\Gamma(k+1)}(\frac{\Delta t}{2})^{k\alpha-\frac{\alpha}{2}+1}. \tag{19}$$

It is easy to show the first term in the right side of (19) is positive. Now we consider the second term in the right side of (19). Let

$$g_k=\frac{q^{2k}\Gamma(k-\frac{1}{2})}{2\sqrt{\pi}\Gamma(k\alpha-\frac{\alpha}{2}+2)\Gamma(k+1)}(\frac{\Delta t}{2})^{k\alpha-\frac{\alpha}{2}+1}.$$

When Δt is small enough, we have

$$\begin{aligned}\frac{g_{k+1}}{g_k}&=\frac{q^{2k+2}\Gamma(k+\frac{1}{2})(\frac{\Delta t}{2})^{k\alpha+\frac{\alpha}{2}+1}}{2\sqrt{\pi}\Gamma(k\alpha+\frac{\alpha}{2}+2)\Gamma(k+2)}\Bigg/\frac{q^{2k}\Gamma(k-\frac{1}{2})(\frac{\Delta t}{2})^{k\alpha-\frac{\alpha}{2}+1}}{2\sqrt{\pi}\Gamma(k\alpha-\frac{\alpha}{2}+2)\Gamma(k+1)}\\&=q^2(\frac{\Delta t}{2})^{\alpha}\left(\frac{k-\frac{1}{2}}{k+1}\right)\frac{\Gamma(k\alpha-\frac{\alpha}{2}+2)}{\Gamma(k\alpha+\frac{\alpha}{2}+2)}\le q^2(\frac{\Delta t}{2})^{\alpha}\le 1,\quad k=1,2,\cdots.\end{aligned}$$

That is, $\{g_k\}$ is a descending sequence. Consequently, $g_1-g_2+g_3-g_4+\cdots\ge 0$. Reorganizing (19), we have

$$a_0^{(\alpha)}=\frac{1}{\Gamma(2-\frac{\alpha}{2})}(\frac{\Delta t}{2})^{1-\frac{\alpha}{2}}+\sum_{k=1}^{+\infty}(-1)^{k+1}g_k\ge 0.$$

For $1\le j\le n-1$, one obtains

$$\begin{aligned}a_j^{(\alpha)}&=\frac{1}{\Gamma(2-\frac{\alpha}{2})}(t_{j+\frac{1}{2}}^{1-\frac{\alpha}{2}}-t_{j-\frac{1}{2}}^{1-\frac{\alpha}{2}})\\&+\sum_{k=1}^{+\infty}(-1)^{k+1}\frac{q^{2k}\Gamma(k-\frac{1}{2})}{2\sqrt{\pi}\Gamma(k\alpha-\frac{\alpha}{2}+2)\Gamma(k+1)}(t_{j+\frac{1}{2}}^{k\alpha-\frac{\alpha}{2}+1}-t_{j-\frac{1}{2}}^{k\alpha-\frac{\alpha}{2}+1}).\end{aligned} \tag{20}$$

Obviously, the first term in the right side of (20) is positive. For the second term on the right side of (20), let

$$z_k=\frac{q^{2k}\Gamma(k-\frac{1}{2})}{2\sqrt{\pi}\Gamma(k\alpha-\frac{\alpha}{2}+2)\Gamma(k+1)}(t_{j+\frac{1}{2}}^{k\alpha-\frac{\alpha}{2}+1}-t_{j-\frac{1}{2}}^{k\alpha-\frac{\alpha}{2}+1}),$$

we get

$$\frac{z_{k+1}}{z_k} = \frac{q^{2k+2}\Gamma(k+\frac{1}{2})}{2\sqrt{\pi}\Gamma(k\alpha+\frac{\alpha}{2}+2)\Gamma(k+2)} \Big/ \frac{q^{2k}\Gamma(k-\frac{1}{2})}{2\sqrt{\pi}\Gamma(k\alpha-\frac{\alpha}{2}+2)\Gamma(k+1)} \times \frac{(t_{j+\frac{1}{2}}^{k\alpha+\frac{\alpha}{2}+1} - t_{j-\frac{1}{2}}^{k\alpha+\frac{\alpha}{2}+1})}{(t_{j+\frac{1}{2}}^{k\alpha-\frac{\alpha}{2}+1} - t_{j-\frac{1}{2}}^{k\alpha-\frac{\alpha}{2}+1})}$$

$$= q^2 \frac{k-\frac{1}{2}}{k+1} \frac{\Gamma(k\alpha-\frac{\alpha}{2}+1)}{\Gamma(k\alpha+\frac{\alpha}{2}+1)} \frac{\int_{t_{j-\frac{1}{2}}}^{t_{j+\frac{1}{2}}} t^{k\alpha+\frac{\alpha}{2}}\,dt}{\int_{t_{j-\frac{1}{2}}}^{t_{j+\frac{1}{2}}} t^{k\alpha-\frac{\alpha}{2}}\,dt}.$$

Note that

$$\frac{\int_{t_{j-\frac{1}{2}}}^{t_{j+\frac{1}{2}}} t^{k\alpha+\frac{\alpha}{2}}\,dt}{\int_{t_{j-\frac{1}{2}}}^{t_{j+\frac{1}{2}}} t^{k\alpha-\frac{\alpha}{2}}\,dt} = \frac{\int_{t_{j-\frac{1}{2}}}^{t_{j+\frac{1}{2}}} t^{\alpha}\cdot t^{k\alpha-\frac{\alpha}{2}}\,dt}{\int_{t_{j-\frac{1}{2}}}^{t_{j+\frac{1}{2}}} t^{k\alpha-\frac{\alpha}{2}}\,dt} \le T^{\alpha} \frac{\int_{t_{j-\frac{1}{2}}}^{t_{j+\frac{1}{2}}} t^{k\alpha-\frac{\alpha}{2}}\,dt}{\int_{t_{j-\frac{1}{2}}}^{t_{j+\frac{1}{2}}} t^{k\alpha-\frac{\alpha}{2}}\,dt} = T^{\alpha},$$

there exists a suitable $T > 0$, such that

$$\frac{z_{k+1}}{z_k} = q^2 \frac{k-\frac{1}{2}}{k+1} \frac{\Gamma(k\alpha-\frac{\alpha}{2}+1)}{\Gamma(k\alpha+\frac{\alpha}{2}+1)} \frac{\int_{t_{j-\frac{1}{2}}}^{t_{j+\frac{1}{2}}} t^{k\alpha+\frac{\alpha}{2}}\,dt}{\int_{t_{j-\frac{1}{2}}}^{t_{j+\frac{1}{2}}} t^{k\alpha-\frac{\alpha}{2}}\,dt} \le \frac{q^2 T^{\alpha}}{k\alpha-\frac{\alpha}{2}+1} \le 1, \quad k \ge 1.$$

Hence $\{z_k\}$ is a descending sequence and we show that $a_j^{(\alpha)} \ge 0$.

Remark 4 To show $a_j^{(\alpha)} \ge 0$, we need to assume that $j\Delta t \le T$ for a suitable T. This restriction comes from the argument of the proof. Our numerical simulation show that $a_j^{(\alpha)} \ge 0$ for a sufficiently large $T > 0$.

Applying the L1 schemes to approximate the Caputo fractional derivative and the generalized Caputo fractional derivative and applying the central difference scheme to approximate the spatial derivative, we obtain the following finite difference method for (13)-(16), with $U_i^n = u(x_i, t_n)$, $f_i^n = f(x_i, t_n)$,

$$\mathbb{D}_t^{\alpha} U_i^{n-\frac{1}{2}} - p^2 \delta_x^2 U_i^{n-\frac{1}{2}} + q^2 U_i^{n-\frac{1}{2}} = f_i^{n-\frac{1}{2}} + R_i^{n-\frac{1}{2}}, \quad 1 \le i \le M-1, 1 \le n \le N, \tag{21}$$

$$\mathbb{D}_t^{\alpha} U_M^{n-\frac{1}{2}} + \frac{2p^2}{h}\left[\frac{1}{p}\Gamma(1-\frac{\alpha}{2})\mathbb{D}_t^{G,\frac{\alpha}{2}} U_M^{n-\frac{1}{2}} + \delta_x U_{M-\frac{1}{2}}^{n-\frac{1}{2}}\right] + q^2 U_M^{n-\frac{1}{2}} = f_M^{n-\frac{1}{2}} + R_M^{n-\frac{1}{2}}, 1 \le n \le N, \tag{22}$$

$$\mathbb{D}_t^{\alpha} U_0^{n-\frac{1}{2}} - \frac{2p^2}{h}\left[\delta_x U_{\frac{1}{2}}^{n-\frac{1}{2}} - \frac{1}{p}\Gamma(1-\frac{\alpha}{2})\mathbb{D}_t^{G,\frac{\alpha}{2}} U_0^{n-\frac{1}{2}}\right] + q^2 U_0^{n-\frac{1}{2}} = f_0^{n-\frac{1}{2}} + R_0^{n-\frac{1}{2}}, 1 \le n \le N, \tag{23}$$

$$U_i^0 = \varphi(x_i), \quad 0 \le i \le M. \tag{24}$$

By Taylor theorem, there exists a positive constant C such that

$$\left|R_i^{n-\frac{1}{2}}\right| \leq C(\Delta t^{3-\alpha} + h^2), \quad 1 \leq i \leq M-1, 1 \leq n \leq N, \tag{25}$$

$$\left|R_M^{n-\frac{1}{2}}\right| \leq C(\Delta t^{3-\alpha} + h + \frac{\Delta t^{2-\frac{\alpha}{2}}}{h}), \quad 1 \leq n \leq N, \tag{26}$$

$$\left|R_0^{n-\frac{1}{2}}\right| \leq C(\Delta t^{3-\alpha} + h + \frac{\Delta t^{2-\frac{\alpha}{2}}}{h}), \quad 1 \leq n \leq N. \tag{27}$$

Omitting the small term $R_i^{n-\frac{1}{2}}(0 \leq i \leq M, 1 \leq n \leq N)$, we obtain the following finite difference scheme for (13)-(16),

$$\mathbb{D}_t^{\alpha} u_i^{n-\frac{1}{2}} - p^2 \delta_x^2 u_i^{n-\frac{1}{2}} + q^2 u_i^{n-\frac{1}{2}} = f_i^{n-\frac{1}{2}}, \quad 1 \leq i \leq M-1, 1 \leq n \leq N, \tag{28}$$

$$\mathbb{D}_t^{\alpha} u_M^{n-\frac{1}{2}} + \frac{2p^2}{h}\left[\frac{1}{p}\Gamma(1-\frac{\alpha}{2})\mathbb{D}_t^{G,\frac{\alpha}{2}} u_M^{n-\frac{1}{2}} + \delta_x u_{M-\frac{1}{2}}^{n-\frac{1}{2}}\right] + q^2 u_M^{n-\frac{1}{2}} = f_M^{n-\frac{1}{2}}, \tag{29}$$

$$1 \leq n \leq N,$$

$$\mathbb{D}_t^{\alpha} u_0^{n-\frac{1}{2}} - \frac{2p^2}{h}\left[\delta_x u_{\frac{1}{2}}^{n-\frac{1}{2}} - \frac{1}{p}\Gamma(1-\frac{\alpha}{2})\mathbb{D}_t^{G,\frac{\alpha}{2}} u_0^{n-\frac{1}{2}}\right] + q^2 u_0^{n-\frac{1}{2}} = f_0^{n-\frac{1}{2}}, \tag{30}$$

$$1 \leq n \leq N,$$

$$u_i^0 = \varphi(x_i), \quad 0 \leq i \leq M. \tag{31}$$

For each temporal level $t = t_{n-\frac{1}{2}}$, the difference scheme (28)-(31) is a tridiagonal system of linear algebraic equations with respect to the unknowns $\{u_i^n | 0 \leq i \leq M, 1 \leq n \leq N\}$, and the coefficient matrix is strictly diagonally dominant. Thus the solution of (28)-(31) is unique and Thomas algorithm [36] can be used for computing of (28)-(31) .

Remark 5 Compared with the direct discretizations of the boundary conditions (15)-(16), we found that the discretizations (29)-(30) have some advantages which make the discretizaed matrix to be tridiagonal and also make the space convergence order to be higher.

4 Stability and convergence of (28)-(31)

In this section, the stability and convergence of the finite difference scheme (28)-(31) is analyzed using the discrete energy method. Before presenting the theoretical analysis, we introduce some important Lemmas.

Lemma 5 *[4] Let $b_l^{(\alpha)}$, $l = 0, 1, \ldots, n-1$ be defined in Lemma 3 with $1 < \alpha \leq 2$. For any grid function $u = \{u^k | 0 \leq k \leq n\}$ defined on $\Omega_{\Delta t}$, it holds*

$$\Delta t \sum_{n=1}^{N} \frac{\Delta t^{1-\alpha}}{\Gamma(3-\alpha)}\left[b_0^{(\alpha)} u^n - \sum_{j=1}^{n-1}(b_{n-j-1}^{(\alpha)} - b_{n-j}^{(\alpha)})u^j - b_{n-1}^{(\alpha)} u^0\right] u^n$$

$$\geq \frac{t_N^{1-\alpha}}{2\Gamma(2-\alpha)} \Delta t \sum_{n=1}^{N} (u^n)^2 - \frac{t_N^{2-\alpha}}{2\Gamma(3-\alpha)} (u^0)^2, \quad 1 \leq n \leq N.$$

Lemma 6 *Let $1<\alpha\le 2$. For any grid function $u=\{u^k|0\le k\le n\}$ defined on $\Omega_{\Delta t}$, it holds, with some positive constants $M_6(T,\alpha), M_7(T,\alpha)$ which only depend on T and α,*

$$\Delta t\sum_{n=1}^{N}\left(\mathbb{D}_t^{G,\frac{\alpha}{2}}u^{n-\frac{1}{2}}\right)(\delta_t u^{n-\frac{1}{2}})\ge -\frac{\Delta t}{2\Gamma(1-\frac{\alpha}{2})}\left[M_6(T,\alpha)+M_7(T,\alpha)\right]\sum_{n=1}^{N}(\delta_t u^{n-\frac{1}{2}})^2.$$

Proof Using the inequality $ab\ge -\frac{1}{2}(a^2+b^2)$, we get, noting $a_j^{(\alpha)}\ge 0$ by Lemma 4,

$$\begin{aligned}\Delta t\sum_{n=1}^{N}\left(\mathbb{D}_t^{G,\frac{\alpha}{2}}u^{n-\frac{1}{2}}\right)(\delta_t u^{n-\frac{1}{2}}) &= \frac{\Delta t}{\Gamma(1-\frac{\alpha}{2})}\sum_{n=1}^{N}\left[\sum_{j=1}^{n}a_{n-j}^{(\alpha)}\left(\delta_t u^{j-\frac{1}{2}}\right)\right]\delta_t u^{n-\frac{1}{2}}\\ &\ge -\frac{\Delta t}{2\Gamma(1-\frac{\alpha}{2})}\sum_{n=1}^{N}\sum_{j=1}^{n}a_{n-j}^{(\alpha)}\left[(\delta_t u^{j-\frac{1}{2}})^2+(\delta_t u^{n-\frac{1}{2}})^2\right]\\ &= -\frac{\Delta t}{2\Gamma(1-\frac{\alpha}{2})}\sum_{n=1}^{N}\left[\sum_{j=1}^{n}a_{n-j}^{(\alpha)}\right](\delta_t u^{j-\frac{1}{2}})^2-\frac{\Delta t}{2\Gamma(1-\frac{\alpha}{2})}\sum_{n=1}^{N}\left[\sum_{j=1}^{n}a_{n-j}^{(\alpha)}\right](\delta_t u^{n-\frac{1}{2}})^2.\end{aligned} \tag{32}$$

Exchanging the summation order of the first term in the right hand of (32), we obtain

$$\begin{aligned}\Delta t\sum_{n=1}^{N}\mathbb{D}_t^{G,\frac{\alpha}{2}}u^{n-\frac{1}{2}}(\delta_t u^{n-\frac{1}{2}})\ge &-\frac{\Delta t}{2\Gamma(1-\frac{\alpha}{2})}\sum_{j=1}^{N}\left[\sum_{n=j}^{N}a_{n-j}^{(\alpha)}\right](\delta_t u^{j-\frac{1}{2}})^2\\ &-\frac{\Delta t}{2\Gamma(1-\frac{\alpha}{2})}\sum_{n=1}^{N}\left[\sum_{j=1}^{n}a_{n-j}^{(\alpha)}\right](\delta_t u^{n-\frac{1}{2}})^2.\end{aligned} \tag{33}$$

Using (17), we have

$$\begin{aligned}&\sum_{j=1}^{n}a_{n-j}^{(\alpha)}=a_0^{(\alpha)}+a_1^{(\alpha)}+\cdots+a_{n-1}^{(\alpha)}\\ &=\sum_{k=0}^{+\infty}\Bigg\{\left[\tilde{A}_k^{(\alpha)}(\frac{\Delta t}{2})^{k\alpha-\frac{\alpha}{2}+1}-\tilde{B}_k^{(\alpha)}(\frac{\Delta t}{2})^{k\alpha+\frac{\alpha}{2}+1}\right]\\ &\quad+\tilde{A}_k^{(\alpha)}\left[(\frac{3\Delta t}{2})^{k\alpha-\frac{\alpha}{2}+1}-(\frac{\Delta t}{2})^{k\alpha-\frac{\alpha}{2}+1}\right]-\tilde{B}_k^{(\alpha)}\left[(\frac{3\Delta t}{2})^{k\alpha+\frac{\alpha}{2}+1}-(\frac{\Delta t}{2})^{k\alpha+\frac{\alpha}{2}+1}\right]\\ &\quad+\cdots+\tilde{A}_k^{(\alpha)}\left[\left((n-\frac{1}{2})\Delta t\right)^{k\alpha-\frac{\alpha}{2}+1}-\left((n-\frac{3}{2})\Delta t\right)^{k\alpha-\frac{\alpha}{2}+1}\right]\\ &\quad-\tilde{B}_k^{(\alpha)}\left[\left((n-\frac{1}{2})\Delta t\right)^{k\alpha+\frac{\alpha}{2}+1}-\left((n-\frac{3}{2})\Delta t\right)^{k\alpha+\frac{\alpha}{2}+1}\right]\Bigg\}.\end{aligned} \tag{34}$$

Reorganizing (34), we obtain

$$\sum_{j=1}^{n} a_{n-j}^{(\alpha)} = \sum_{k=0}^{+\infty} \tilde{A}_k^{(\alpha)} t_{n-\frac{1}{2}}^{k\alpha-\frac{\alpha}{2}+1} - \sum_{k=0}^{+\infty} \tilde{B}_k^{(\alpha)} t_{n-\frac{1}{2}}^{k\alpha+\frac{\alpha}{2}+1}.$$

Hence

$$\sum_{j=1}^{n} a_{n-j}^{(\alpha)} \leq \Big|\sum_{j=1}^{n} a_{n-j}^{(\alpha)}\Big| \leq \sum_{k=0}^{+\infty} |\tilde{A}_k^{(\alpha)}| T^{k\alpha-\frac{\alpha}{2}+1} + \sum_{k=0}^{+\infty} |\tilde{B}_k^{(\alpha)}| T^{k\alpha+\frac{\alpha}{2}+1}.$$

Noting that

$$\lim_{k\to\infty} \frac{|\tilde{A}_{k+1}^{(\alpha)}| T^{k\alpha+\frac{\alpha}{2}+1}}{|\tilde{A}_k^{(\alpha)}| T^{k\alpha-\frac{\alpha}{2}+1}} = \lim_{k\to\infty} q^2 T^{\alpha} \frac{\Gamma(k\alpha-\frac{\alpha}{2}+2)(k+\frac{1}{2})}{\Gamma(k\alpha+\frac{\alpha}{2}+2)(k+1)} = 0,$$

and

$$\lim_{k\to\infty} \frac{|\tilde{B}_{k+1}^{(\alpha)}| T^{k\alpha+\frac{\alpha}{2}+1}}{|\tilde{B}_k^{(\alpha)}| T^{k\alpha-\frac{\alpha}{2}+1}} = \lim_{k\to\infty} q^2 T^{\alpha} \frac{\Gamma(k\alpha+\frac{\alpha}{2}+2)(k+\frac{1}{2})}{\Gamma(k\alpha+\frac{3\alpha}{2}+2)(k+1)} = 0,$$

we see that $\sum\limits_{k=0}^{+\infty} |\tilde{A}_k^{(\alpha)}| T^{k\alpha-\frac{\alpha}{2}+1}$, $\sum\limits_{k=0}^{+\infty} |\tilde{B}_k^{(\alpha)}| T^{k\alpha+\frac{\alpha}{2}+1}$ are convergent which implies that $\Big|\sum\limits_{j=1}^{n} a_{n-j}^{(\alpha)}\Big|$ is convergent. Hence there exists a positive constant $M_6(T,\alpha)$, which only depend on T, α, such that

$$\sum_{j=1}^{n} a_{n-j}^{(\alpha)} \leq M_6(T,\alpha), \quad n \geq 1. \tag{35}$$

Similarly, $\sum\limits_{n=j}^{N} a_{n-j}^{(\alpha)}$ is convergent, and there exists a positive constant $M_7(T,\alpha)$, which only depend on T, α, such that

$$\sum_{n=j}^{N} a_{n-j}^{(\alpha)} \leq M_7(T,\alpha), \quad n \geq j. \tag{36}$$

Combining (33) with (35), (36), we get

$$\Delta t \sum_{n=1}^{N} \mathbb{D}_t^{G,\frac{\alpha}{2}} u^{n-\frac{1}{2}} (\delta_t u^{n-\frac{1}{2}}) \geq -\frac{\Delta t}{2\Gamma(1-\frac{\alpha}{2})} \big[M_6(T,\alpha) + M_7(T,\alpha)\big] \sum_{n=1}^{N} (\delta_t u^{n-\frac{1}{2}})^2.$$

Remark 6 By the series comparison rule, we see that $\sum\limits_{k=0}^{+\infty} |\tilde{A}_k^{(\alpha)}| T^{k\alpha-\frac{\alpha}{2}+1}$ and $\sum\limits_{k=0}^{+\infty} |\tilde{B}_k^{(\alpha)}| T^{k\alpha+\frac{\alpha}{2}+1}$ are convergent. Hence there exists a positive constant $M_6(T,\alpha)$ which only depends on T and α such that

$$\sum_{k=0}^{+\infty} |\tilde{A}_k^{(\alpha)}| T^{k\alpha-\frac{\alpha}{2}+1} + \sum_{k=0}^{+\infty} |\tilde{B}_k^{(\alpha)}| T^{k\alpha+\frac{\alpha}{2}+1} \leq M_6(T,\alpha).$$

Lemma 7 *[33] For any function u defined on S_M, it holds*

$$\|u\|_\infty^2 \le \varepsilon\|\delta_x u\|^2 + (\frac{1}{\varepsilon} + \frac{1}{L})\|u\|^2, \quad \varepsilon > 0,$$

where $L = x_r - x_l$.

Theorem 1 *Assume $\{u_i^m, 0 \le i \le M, 1 \le m \le N\}$ satisfy the difference scheme* (28)-(31)*, when Δt satisfy $\frac{\Delta t^\alpha}{h} \le \frac{1}{4p\Gamma(2-\alpha)\left[M_6(T,\alpha)+M_7(T,\alpha)\right]}$, then*

$$\|u^m\|_\infty^2 \le \frac{p^2\Big(1+\sqrt{1+\frac{4L^2q^2}{p^2}}\Big)}{2Lq^2}\Big[\|\delta_x u^0\|^2 + \frac{q^2}{p^2}\|\varphi\|^2 + \frac{T^{2-\alpha}}{2p^2\Gamma(3-\alpha)}\|\psi\|^2 + \frac{2}{p^2}T^{\alpha-1}\Gamma(2-\alpha)\Delta t\sum_{n=1}^{m}\|f^{n-\frac{1}{2}}\|^2\Big], \quad 1 \le m \le N.$$

Proof Multiplying $h\delta_t u_i^{n-\frac{1}{2}}$ on both sides of (28) and summing up for i from 1 to $M-1$, multiplying $\frac{h}{2}\delta_t u_M^{n-\frac{1}{2}}$, $\frac{h}{2}\delta_t u_0^{n-\frac{1}{2}}$ on both sides of (29) and (30) respectively, one obtains

$$\begin{aligned}
&\big(\mathbb{D}_t^\alpha u^{n-\frac{1}{2}}, \delta_t u^{n-\frac{1}{2}}\big) + p\Gamma(1-\frac{\alpha}{2})\Big[(\mathbb{D}_t^{G,\frac{\alpha}{2}}u_0^{n-\frac{1}{2}})\delta_t u_0^{n-\frac{1}{2}} + (\mathbb{D}_t^{G,\frac{\alpha}{2}}u_M^{n-\frac{1}{2}})\delta_t u_M^{n-\frac{1}{2}}\Big] \\
&- p^2\Big[(\delta_x u_{\frac{1}{2}}^{n-\frac{1}{2}})\delta_t u_0^{n-\frac{1}{2}} + h\sum_{i=1}^{M-1}(\delta_x^2 u_i^{n-\frac{1}{2}})\delta_t u_i^{n-\frac{1}{2}} - (\delta_x u_{M-\frac{1}{2}}^{n-\frac{1}{2}})\delta_t u_M^{n-\frac{1}{2}}\Big] \\
&+ q^2 h\Big[\frac{1}{2}(u_0^{n-\frac{1}{2}})\delta_t u_0^{n-\frac{1}{2}} + \sum_{i=1}^{M-1}(u_i^{n-\frac{1}{2}})\delta_t u_i^{n-\frac{1}{2}} + \frac{1}{2}(u_M^{n-\frac{1}{2}})\delta_t u_M^{n-\frac{1}{2}}\Big] \\
&= (f^{n-\frac{1}{2}}, \delta_t u^{n-\frac{1}{2}}).
\end{aligned} \tag{37}$$

Using the summation formula by parts, we have

$$\begin{aligned}
&q^2 h\Big[\frac{1}{2}(u_0^{n-\frac{1}{2}})\delta_t u_0^{n-\frac{1}{2}} + \sum_{i=1}^{M-1}(u_i^{n-\frac{1}{2}})\delta_t u_i^{n-\frac{1}{2}} + \frac{1}{2}(u_M^{n-\frac{1}{2}})\delta_t u_M^{n-\frac{1}{2}}\Big] \\
&= \frac{hq^2}{2\Delta t}\Big[\frac{1}{2}(u_0^n + u_0^{n-1})(u_0^n - u_0^{n-1}) + \sum_{i=1}^{M-1}(u_i^n + u_i^{n-1})(u_i^n - u_i^{n-1}) \\
&\quad + \frac{1}{2}(u_M^n + u_M^{n-1})(u_M^n - u_M^{n-1})\Big] \\
&= \frac{q^2}{2\Delta t}\Big[\frac{h}{2}(u_0^n)^2 + h\sum_{i=1}^{M-1}(u_i^n)^2 + \frac{h}{2}(u_M^n)^2\Big] \\
&\quad - \frac{q^2}{2\Delta t}\Big[\frac{h}{2}(u_0^{n-1})^2 + h\sum_{i=1}^{M-1}(u_i^{n-1})^2 + \frac{h}{2}(u_M^{n-1})^2\Big] \\
&= \frac{q^2}{2\Delta t}(\|u^n\|^2 - \|u^{n-1}\|^2),
\end{aligned} \tag{38}$$

and

$$
\begin{aligned}
&-p^2\Big[(\delta_x u_{\frac{1}{2}}^{n-\frac{1}{2}})\delta_t u_0^{n-\frac{1}{2}} + h\sum_{i=1}^{M-1}(\delta_x^2 u_i^{n-\frac{1}{2}})\delta_t u_i^{n-\frac{1}{2}} - (\delta_x u_{M-\frac{1}{2}}^{n-\frac{1}{2}})\delta_t u_M^{n-\frac{1}{2}}\Big]\\
&= p^2\sum_{i=1}^{M}(\delta_x u_{i-\frac{1}{2}}^{n-\frac{1}{2}})\big(\delta_t u_i^{n-\frac{1}{2}} - \delta_t u_{i-1}^{n-\frac{1}{2}}\big)\\
&= \frac{p^2 h}{2\Delta t}\sum_{i=1}^{M}\big(\delta_x u_{i-\frac{1}{2}}^{n} + \delta_x u_{i-\frac{1}{2}}^{n-1}\big)\big(\delta_x u_{i-\frac{1}{2}}^{n} - \delta_x u_{i-\frac{1}{2}}^{n-1}\big)\\
&= \frac{p^2}{2\Delta t}\Big[h\sum_{i=1}^{M}(\delta_x u_{i-\frac{1}{2}}^{n})^2 - h\sum_{i=1}^{M}(\delta_x u_{i-\frac{1}{2}}^{n-1})^2\Big] = \frac{p^2}{2\Delta t}(\|\delta_x u^n\|^2 - \|\delta_x u^{n-1}\|^2).
\end{aligned} \tag{39}
$$

Substituting (38), (39) into (37), we get

$$
\begin{aligned}
&\big(\mathbb{D}_t^{\alpha} u^{n-\frac{1}{2}}, \delta_t u^{n-\frac{1}{2}}\big) + p\Gamma(1-\frac{\alpha}{2})\Big[\,(\mathbb{D}_t^{G,\frac{\alpha}{2}} u_0^{n-\frac{1}{2}})\delta_t u_0^{n-\frac{1}{2}} + (\mathbb{D}_t^{G,\frac{\alpha}{2}} u_M^{n-\frac{1}{2}})\delta_t u_M^{n-\frac{1}{2}}\Big]\\
&+\frac{p^2}{2\Delta t}(\|\delta_x u^n\|^2 - \|\delta_x u^{n-1}\|^2) + \frac{q^2}{2\Delta t}(\|u^n\|^2 - \|u^{n-1}\|^2) = (f^{n-\frac{1}{2}}, \delta_t u^{n-\frac{1}{2}}).
\end{aligned} \tag{40}
$$

Multiplying Δt on both sides of (40), summing up for n from 1 to m, it follows

$$
\begin{aligned}
&\Delta t\sum_{n=1}^{m}(\mathbb{D}_t^{\alpha} u^{n-\frac{1}{2}}, \delta_t u^{n-\frac{1}{2}}) + \frac{p^2}{2}(\|\delta_x u^m\|^2 - \|\delta_x u^0\|^2) + \frac{q^2}{2}(\|u^m\|^2 - \|u^0\|^2)\\
&+\Delta t\sum_{n=1}^{m} p\Gamma(1-\frac{\alpha}{2})\Big[\,(\mathbb{D}_t^{G,\frac{\alpha}{2}} u_0^{n-\frac{1}{2}})\delta_t u_0^{n-\frac{1}{2}} + (\mathbb{D}_t^{G,\frac{\alpha}{2}} u_M^{n-\frac{1}{2}})\delta_t u_M^{n-\frac{1}{2}}\Big]\\
&= \Delta t\sum_{n=1}^{m}(f^{n-\frac{1}{2}}, \delta_t u^{n-\frac{1}{2}}).
\end{aligned} \tag{41}
$$

By Lemmas 5 and 6, one obtains

$$
\Delta t\sum_{n=1}^{m}\big(\mathbb{D}_t^{\alpha} u^{n-\frac{1}{2}}, \delta_t u^{n-\frac{1}{2}}\big) \ge \frac{t_m^{1-\alpha}}{2\Gamma(2-\alpha)}\Delta t\sum_{n=1}^{m}\|\delta_t u^{n-\frac{1}{2}}\|^2 - \frac{t_m^{2-\alpha}}{2\Gamma(3-\alpha)}\|\psi\|^2, \tag{42}
$$

and

$$
\begin{aligned}
&\Delta t\sum_{n=1}^{m} p\Gamma(1-\frac{\alpha}{2})\Big[\,(\mathbb{D}_t^{G,\frac{\alpha}{2}} u_0^{n-\frac{1}{2}})\delta_t u_0^{n-\frac{1}{2}} + (\mathbb{D}_t^{G,\frac{\alpha}{2}} u_M^{n-\frac{1}{2}})\delta_t u_M^{n-\frac{1}{2}}\Big]\\
&\ge -\frac{p}{2}\Delta t\big[M_6(T,\alpha) + M_7(T,\alpha)\big]\sum_{n=1}^{m}\Big((\delta_t u_0^{n-\frac{1}{2}})^2 + (\delta_t u_M^{n-\frac{1}{2}})^2\Big).
\end{aligned} \tag{43}
$$

Substituting (42), (43) into (41), we get

$$\frac{t_m^{1-\alpha}\Delta t}{2\Gamma(2-\alpha)}\sum_{n=1}^{m}\|\delta_t u^{n-\frac{1}{2}}\|^2-\frac{t_m^{2-\alpha}}{2\Gamma(3-\alpha)}\|\psi\|^2+\frac{p^2}{2}(\|\delta_x u^m\|^2-\|\delta_x u^0\|^2)$$
$$+\frac{q^2}{2}(\|u^m\|^2-\|u^0\|^2)-\frac{p}{2}\Delta t\big[M_6(T,\alpha)+M_{7,\alpha}(T)\big]\sum_{n=1}^{m}\Big((\delta_t u_0^{n-\frac{1}{2}})^2$$
$$+(\delta_t u_M^{n-\frac{1}{2}})^2\Big)\le\Delta t\sum_{n=1}^{m}(f^{n-\frac{1}{2}},\delta_t u^{n-\frac{1}{2}}),$$

or

$$\Delta t\sum_{n=1}^{m}\left[\frac{t_m^{1-\alpha}}{4\Gamma(2-\alpha)}\|\delta_t u^{n-\frac{1}{2}}\|^2-\frac{p}{2}\Delta t(M_6(T,\alpha)+M_7(T,\alpha))\Big((\delta_t u_0^{n-\frac{1}{2}})^2\right.$$
$$\left.+(\delta_t u_M^{n-\frac{1}{2}})^2\Big)\right]+\frac{t_m^{1-\alpha}\Delta t}{4\Gamma(2-\alpha)}\sum_{n=1}^{m}\|\delta_t u^{n-\frac{1}{2}}\|^2+\frac{p^2}{2}\|\delta_x u^m\|^2+\frac{q^2}{2}\|u^m\|^2$$
$$\le\frac{t_m^{2-\alpha}}{2\Gamma(3-\alpha)}\|\psi\|^2+\frac{p^2}{2}\|\delta_x u^0\|^2+\frac{q^2}{2}\|u^0\|^2+\Delta t\sum_{n=1}^{m}(f^{n-\frac{1}{2}},\delta_t u^{n-\frac{1}{2}}).\quad(44)$$

When Δt satisfy $\frac{\Delta t^\alpha}{h}\le\frac{1}{4p\Gamma(2-\alpha)\big[M_6(T,\alpha)+M_7(T,\alpha)\big]}$, the first term for the left side of (44) satisfies

$$\Delta t\sum_{n=1}^{m}\left[\frac{t_m^{1-\alpha}}{4\Gamma(2-\alpha)}\|\delta_t u^{n-\frac{1}{2}}\|^2-\frac{p}{2}\Delta t\big[M_6(T.\alpha)+M_7(T,\alpha)\big]\Big((\delta_t u_0^{n-\frac{1}{2}})^2+(\delta_t u_M^{n-\frac{1}{2}})^2\Big)\right]$$
$$=\Delta t\sum_{n=1}^{m}\left[\frac{ht_m^{1-\alpha}}{8\Gamma(2-\alpha)}-\frac{p}{2}\Delta t\big[M_6(T,\alpha)+M_7(T,\alpha)\big]\right]\left[(\delta_t u_0^{n-\frac{1}{2}})^2+(\delta_t u_M^{n-\frac{1}{2}})^2\right]$$
$$+\frac{t_m^{1-\alpha}\Delta t}{4\Gamma(2-\alpha)}\sum_{n=1}^{m}h\sum_{i=1}^{M-1}(\delta_t u_i^{n-\frac{1}{2}})^2\ge 0,\quad 1\le m\le N.$$

Thus (44) can be rewritten as

$$\frac{t_m^{1-\alpha}\Delta t}{4\Gamma(2-\alpha)}\sum_{n=1}^{m}\|\delta_t u^{n-\frac{1}{2}}\|^2+\frac{p^2}{2}\|\delta_x u^m\|^2+\frac{q^2}{2}\|u^m\|^2$$
$$\le\frac{t_m^{2-\alpha}}{2\Gamma(3-\alpha)}\|\psi\|^2+\frac{p^2}{2}\|\delta_x u^0\|^2+\frac{q^2}{2}\|u^0\|^2+\Delta t\sum_{n=1}^{m}(f^{n-\frac{1}{2}},\delta_t u^{n-\frac{1}{2}}).\quad(45)$$

By Cauchy-Schwarz inequality, it yields

$$\Delta t\sum_{n=1}^{m}(f^{n-\frac{1}{2}},\delta_t u^{n-\frac{1}{2}})$$
$$\le\frac{t_m^{1-\alpha}\Delta t}{4\Gamma(2-\alpha)}\sum_{n=1}^{m}\|\delta_t u^{n-\frac{1}{2}}\|^2+t_m^{\alpha-1}\Gamma(2-\alpha)\Delta t\sum_{n=1}^{m}\|f^{n-\frac{1}{2}}\|^2.\quad(46)$$

The substitution of (46) into (45) produces that

$$\begin{aligned}&\left\|\delta_x u^m\right\|^2+\frac{q^2}{p^2}\left\|u^m\right\|^2\\ \le\ &\frac{t_m^{2-\alpha}}{\Gamma(3-\alpha)p^2}\left\|\psi\right\|^2+\left\|\delta_x u^0\right\|^2+\frac{q^2}{p^2}\left\|u^0\right\|^2+\frac{2}{p^2}t_m^{\alpha-1}\Gamma(2-\alpha)\Delta t\sum_{n=1}^{m}\left\|f^{n-\frac{1}{2}}\right\|^2.\end{aligned} \tag{47}$$

Taking $\varepsilon>0$ such that $\frac{\frac{1}{\varepsilon}+\frac{1}{L}}{\varepsilon}=\frac{q^2}{p^2}$, that is, $\varepsilon=\frac{p^2\left(1+\sqrt{1+\frac{4L^2q^2}{p^2}}\right)}{2Lq^2}$, it follows from Lemma 7 that

$$\begin{aligned}\left\|u^m\right\|_\infty^2\le\ &\frac{p^2\left(1+\sqrt{1+\frac{4L^2q^2}{p^2}}\right)}{2Lq^2}\Big[\left\|\delta_x u^0\right\|^2+\frac{q^2}{p^2}\left\|\varphi\right\|^2\\ &+\frac{T^{2-\alpha}}{2p^2\Gamma(3-\alpha)}\left\|\psi\right\|^2+\frac{2}{p^2}T^{\alpha-1}\Gamma(2-\alpha)\Delta t\sum_{n=1}^{m}\left\|f^{n-\frac{1}{2}}\right\|^2\Big],\quad 1\le m\le N.\end{aligned}$$

This completes the proof.

From Theorem 1, the convergence analysis of the difference equation (28)-(31) can be obtained.

Theorem 2 *Let* $u(x,t)\in C_{x,t}^{4,3}([x_l,x_r]\times[0,T])$ *be the solution of the problem* (21)-(24) *and* $\{u_i^m,0\le i\le M,1\le m\le N\}$ *the solutions of the difference scheme* (28)-(31), *respectively. Assume that*

$$e_i^m=u(x_i,t_m)-u_i^m,\quad 0\le i\le M,1\le m\le N.$$

When Δt *satisfies* $\frac{\Delta t^\alpha}{h}\le\frac{1}{4p\Gamma(2-\alpha)\left[M_6(T,\alpha)+M_7(T,\alpha)\right]}$, *we have*

$$\left\|e^m\right\|_\infty\le c_2\left[(h^{3/2}+\frac{\Delta t^{2-\frac{\alpha}{2}}}{h^{1/2}})+\sqrt{L}(\Delta t^{3-\alpha}+h^2)\right],\quad 1\le m\le N.$$

Proof Subtracting (21)-(24) from (28)-(31), we get the following error equation,

$$\mathbb{D}_t^\alpha e_i^{n-\frac{1}{2}}-p^2\delta_x^2 e_i^{n-\frac{1}{2}}+q^2 e_i^{n-\frac{1}{2}}=R_i^{n-\frac{1}{2}},\quad 1\le i\le M-1,1\le n\le N, \tag{48}$$

$$\mathbb{D}_t^\alpha e_M^{n-\frac{1}{2}}+\frac{2p^2}{h}\left[\frac{1}{p}\Gamma(1-\frac{\alpha}{2})\mathbb{D}_t^{G,\frac{\alpha}{2}}e_M^{n-\frac{1}{2}}+\delta_x e_{M-\frac{1}{2}}^{n-\frac{1}{2}}\right]+q^2 e_M^{n-\frac{1}{2}}=R_M^{n-\frac{1}{2}},\quad 1\le n\le N, \tag{49}$$

$$\mathbb{D}_t^\alpha e_0^{n-\frac{1}{2}}-\frac{2p^2}{h}\left[\delta_x e_{\frac{1}{2}}^{n-\frac{1}{2}}-\frac{1}{p}\Gamma(1-\frac{\alpha}{2})\mathbb{D}_t^{G,\frac{\alpha}{2}}e_0^{n-\frac{1}{2}}\right]+q^2 e_0^{n-\frac{1}{2}}=R_0^{n-\frac{1}{2}},\quad 1\le n\le N, \tag{50}$$

$$e_i^0=0,\quad 0\le i\le M. \tag{51}$$

Applying Theorem 1, it yields that

$$\begin{aligned}\left\|e^m\right\|_\infty^2 &\le \frac{\left(1+\sqrt{1+\frac{4L^2q^2}{p^2}}\right)}{Lq^2}T^{\alpha-1}\Gamma(2-\alpha)\Delta t\sum_{n=1}^{m}\left\|R^{n-\frac{1}{2}}\right\|^2\\
&= \frac{\left(1+\sqrt{1+\frac{4L^2q^2}{p^2}}\right)}{Lq^2}T^{\alpha-1}\Gamma(2-\alpha)\Delta t\sum_{n=1}^{m}\left[\frac{h}{2}(R_0^{n-\frac{1}{2}})^2\right.\\
&\quad\left.+h\sum_{i=1}^{M-1}(R_i^{n-\frac{1}{2}})^2+\frac{h}{2}(R_M^{n-\frac{1}{2}})^2\right]. \qquad (52)\end{aligned}$$

From (25)-(27), we have

$$\begin{aligned}&\frac{h}{2}(R_0^{n-\frac{1}{2}})^2+h\sum_{i=1}^{M-1}(R_i^{n-\frac{1}{2}})^2+\frac{h}{2}(R_M^{n-\frac{1}{2}})^2\\
&\le c_1^2\left[h(\Delta t^{2-\frac{\alpha}{2}}+h+\frac{\Delta t^{2-\frac{\alpha}{2}}}{h})^2+L\left(\Delta t^{3-\alpha}+h^2\right)^2\right]\\
&\le c_1^2\left[(h^{3/2}+\frac{\Delta t^{2-\frac{\alpha}{2}}}{h^{1/2}})^2+L(\Delta t^{3-\alpha}+h^2)^2\right]. \qquad (53)\end{aligned}$$

The substitution of (53) into (52) produces that

$$\begin{aligned}\left\|e^m\right\|_\infty^2 &\le \frac{\left(1+\sqrt{1+\frac{4L^2q^2}{p^2}}\right)}{Lq^2}T^{\alpha-1}\Gamma(2-\alpha)\Delta t\sum_{n=1}^{m}c_1^2\left[(h^{3/2}+\frac{\Delta t^{2-\frac{\alpha}{2}}}{h^{1/2}})^2\right.\\
&\quad\left.+L(\Delta t^{3-\alpha}+h^2)^2\right]\\
&= \frac{\left(1+\sqrt{1+\frac{4L^2q^2}{p^2}}\right)}{Lq^2}c_1^2T^{\alpha}\Gamma(2-\alpha)\left[(h^{3/2}+\frac{\Delta t^{2-\frac{\alpha}{2}}}{h^{1/2}})^2\right.\\
&\quad\left.+L(\Delta t^{3-\alpha}+h^2)^2\right]. \qquad (54)\end{aligned}$$

Hence, the inequality (54) can be rewritten as $\left\|e^m\right\|_\infty \le c_2\left[(h^{3/2}+\frac{\Delta t^{2-\frac{\alpha}{2}}}{h^{1/2}})+\sqrt{L}(\Delta t^{3-\alpha}+h^2)\right]$, where $c_2 = \sqrt{\frac{\left(1+\sqrt{1+\frac{4L^2q^2}{p^2}}\right)}{Lq^2}c_1^2T^{\alpha}\Gamma(2-\alpha)}$, which completes the proof.

Remark 7 In the error estimates in Theorem 2, there exists a term $\frac{\Delta t^{2-\frac{\alpha}{2}}}{h^{1/2}}$ which is due to the approximation of the temporal convolution arising in the exact artificial boundary conditions. We can not improve this convergence order in theoretical analysis. When $\alpha = 2$, this order is meaningless when $\frac{\Delta t^{\alpha}}{h} \le C$. However the numerical simulation shows that the convergence order is almost $3-\alpha$ when $\alpha \to 2$, see Table 1.

5 Numerical simulations

In this section, to verify the validity of the numerical scheme and theoretical analysis of the finite difference scheme for time-fractional Klein-Gordon equation with exact artificial boundary conditions, we shall illustrate several experiments to show the error and the numerical accuracy for the difference scheme (28)-(31).

Denote

$$E_2(h,\Delta t)=\sqrt{h\sum_{i=0}^{M}\big(u(x_i,t_N)-u_i^N)^2},\quad E_\infty(h,\Delta t)=\max_{0\le i\le M}\big|u(x_i,t_N)-u_i^N\big|.$$

The temporal convergence order can be calculated by $\mathrm{Order}_\infty=log_2\left(\frac{E_\infty(h,\Delta t)}{E_\infty(h,\frac{\Delta t}{2})}\right)$,, $\mathrm{Order}_2=log_2\left(\frac{E_2(h,\Delta t)}{E_2(h,\frac{\Delta t}{2})}\right)$, and the spatial convergence order can be calculated by $\mathrm{Order}_1=log_2\left(\frac{E_\infty(h,\Delta t)}{E_\infty(\frac{h}{2},\Delta t)}\right)$.

Example 1 For $\alpha\in(1,2]$, we consider the time fractional Klein-Gordon equation (13)-(16). Taking $T=1,\ x_l=-\pi,x_r=\pi,\ p=q=1$, K is the cutoff number of the generalized Mittag-Leffler function, i. e. $\sum_{k=0}^{K}\frac{(\gamma)_k}{\Gamma(k+1)\Gamma(k\alpha+\beta)}z^k\approx\sum_{k=0}^{\infty}\frac{(\gamma)_k}{\Gamma(k+1)\Gamma(k\alpha+\beta)}z^k$. The exact solution is $u(x,t)=e^{-x^2}t^3$ with $\varphi(x)=\psi(x)=0$, $f(x,t)=\frac{6e^{-x^2}}{\Gamma(4-\alpha)}t^{3-\alpha}-e^{-x^2}(4x^2-2)t^3+e^{-x^2}t^3$.

Firstly, we compute the numerical accuracy for temporal direction. Fixing the spatial stepsize h sufficiently small($M=1000$), and the temporal step size is reduced to $\frac{1}{2}$ times. Table 1 presents the computational error and covergence order with different temporal stepsizes($\Delta t=\frac{1}{10},\ \frac{1}{20},\ \frac{1}{40},\ \frac{1}{80},\ \frac{1}{160}$) when $K=10$, $\alpha=1.3,\ 1.5,\ 1.8,1.9,1.99$. From the table, we can see that numerical accuracy in temporal is $O(\Delta t^{3-\alpha})$ for the difference scheme (28)-(31). In addition, we see that the numerical scheme has the optimal convergence order ($O(\Delta t^{3-\alpha})$) when α approaches 2.

Secondly, the numerical accuracy in spatial direction is verified in Table 2 when $N=1000$, $K=10$, $\alpha=1.2,1.4,1.6,1.8$. It shows that the spatial accuracy of the difference scheme (28)-(31) has the second order convergence.

We now illustrate that a suitable T does not affect the numerical solution of difference scheme (28)-(31). Tables 3 and 4 show the numerical accuracies in temporal direction when T takes the different values.

From (11)-(12), we see that the artificial boundary condition of time-fractional Klein-Gordon equation contains an infinite series. A graph of the numerical solution of the finite difference scheme (28)-(31) is presented when the series is truncated to K terms. Figures 1-4 show the exact solution for $K=50$ and the numerical solutions for $K=10,\ 15,\ 20,\ 25,\ 30$ with different

α	Δt	$E_2(h,\Delta t)$	$Order_2$	$E_\infty(h,\Delta t)$	$Order_\infty$
1.3	1/10	1.11e-02	-	8.38e-03	-
	1/20	3.44e-03	1.69	2.59e-03	1.69
	1/40	1.06e-03	1.69	8.03e-04	1.69
	1/80	3.29e-04	1.69	2.49e-04	1.68
	1/160	1.04e-04	1.65	7.87e-05	1.66
1.5	1/10	2.51e-02	-	1.93e-02	-
	1/20	8.99e-03	1.48	6.92e-03	1.48
	1/40	3.19e-03	1.49	2.46e-03	1.49
	1/80	1.13e-03	1.49	8.74e-04	1.49
	1/160	4.02e-04	1.49	3.11e-04	1.49
1.8	1/10	7.43e-02	-	5.95e-02	-
	1/20	3.28e-02	1.18	2.63e-02	1.17
	1/40	1.43e-02	1.18	1.15e-02	1.18
	1/80	6.28e-03	1.19	5.04e-03	1.19
	1/160	2.74e-03	1.19	2.20e-03	1.19
1.9	1/10	3.46e-01	-	2.21e-01	-
	1/20	1.73e-01	1.07	1.07e-01	1.06
	1/40	8.64e-02	1.08	5.05e-02	1.08
	1/80	4.29e-02	1.09	2.38e-02	1.09
	1/160	2.13e-02	1.10	1.11e-02	1.09
1.99	1/10	3.46e-01	-	2.78e-01	-
	1/20	1.73e-01	0.994	1.41e-01	0.980
	1/40	8.64e-02	1.005	7.09e-02	0.960
	1/80	4.29e-02	1.008	3.53e-02	1.007
	1/160	2.13e-02	1.009	1.76e-02	1.008

Table 1 Time convergence orders in Example 1 at $T = 1$

α	h	$E_\infty(h,\Delta t)$	$Order_1$
1.2	$2\pi/10$	3.14e-02	-
	$2\pi/20$	7.54e-03	2.06
	$2\pi/40$	1.86e-03	2.02
	$2\pi/80$	4.66e-04	2.00
1.4	$2\pi/10$	2.75e-02	-
	$2\pi/20$	6.70e-03	2.04
	$2\pi/40$	1.67e-03	2.01
	$2\pi/80$	4.23e-04	2.00
1.6	$2\pi/10$	2.33e-02	-
	$2\pi/20$	5.82e-03	2.00
	$2\pi/40$	1.46e-03	2.00
	$2\pi/80$	3.66e-04	1.99
1.8	$2\pi/10$	1.91e-02	-
	$2\pi/20$	4.78e-03	2.00
	$2\pi/40$	1.46e-03	2.00
	$2\pi/80$	3.06e-04	1.97

Table 2 Spatial convergence orders in Example 1 at $T = 1$

T	Δt	$E_2(h, \Delta t)$	$Order_2$	$E_\infty(h, \Delta t)$	$Order_\infty$
1	1/10	7.09e-02	-	5.42e-02	-
	1/20	2.40e-02	1.56	1.83e-02	1.57
	1/40	8.02e-03	1.58	6.10e-03	1.58
	1/80	2.66e-03	1.59	2.03e-03	1.59
	1/160	8.81e-04	1.59	6.71e-04	1.59
2	1/10	1.13e-01	-	7.85e-02	-
	1/20	3.77e-02	1.58	2.60e-02	1.59
	1/40	1.25e-02	1.59	8.63e-03	1.59
	1/80	4.18e-03	1.58	2.87e-03	1.59
	1/160	1.46e-03	1.52	9.67e-04	1.57
3	1/10	1.20e-01	-	8.03e-02	-
	1/20	3.98e-02	1.59	2.65e-02	1.60
	1/40	1.35e-02	1.56	8.83e-03	1.59
	1/80	4.60e-03	1.54	2.98e-03	1.56
	1/160	1.63e-03	1.52	1.03e-03	1.53
4	1/10	1.14e-01	-	7.62e-02	-
	1/20	3.88e-02	1.56	2.53e-02	1.59
	1/40	1.33e-02	1.55	1.15e-02	1.56
	1/80	4.67e-03	1.53	4.00e-03	1.54
	1/160	1.62e-03	1.51	1.42e-03	1.51

Table 3 Time convergence orders in Example 1 at $\alpha = 1.4$

T	Δt	$E_2(h, \Delta t)$	$Order_2$	$E_\infty(h, \Delta t)$	$Order_\infty$
1	1/10	2.15e-01	-	1.71e-01	-
	1/20	9.66e-02	1.16	7.72e-02	1.15
	1/40	4.27e-02	1.18	3.43e-02	1.17
	1/80	1.88e-02	1.18	1.51e-02	1.19
	1/160	8.20e-03	1.19	6.59e-03	1.19
2	1/10	4.65e-01	-	3.23e-01	-
	1/20	2.09e-01	1.15	1.44e-01	1.16
	1/40	9.24e-02	1.18	6.37e-02	1.18
	1/80	4.05e-02	1.19	2.79e-02	1.19
	1/160	1.77e-02	1.19	1.22e-02	1.19
3	1/10	5.21e-01	-	3.31e-01	-
	1/20	2.31e-01	1.17	1.45e-01	1.19
	1/40	1.02e-01	1.19	6.34e-02	1.19
	1/80	4.46e-02	1.19	2.77e-02	1.20
	1/160	1.98e-02	1.18	1.21e-02	1.19
4	1/10	4.2e-01	-	2.66e-01	-
	1/20	1.81e-01	1.21	1.14e-01	1.22
	1/40	7.94e-02	1.19	4.94e-02	1.21
	1/80	3.59e-02	1.15	2.16e-02	1.19
	1/160	1.62e-02	1.15	9.58e-03	1.17

Table 4 Time convergence orders in Example 1 at $\alpha = 1.8$

α. We observe that the value of K does not affect the numerical solutions of (28)-(31).

Example 2 In this example, we choose $T = 1,\ \ x_l = -\pi, x_r = \pi,\ p = q = 1.$ Taking $\varphi(x) = \sin[2\pi(x-\pi)(x+\pi)],\ \psi(x) = \sin[\frac{\pi}{2}(x-\pi)(x+\pi)]$ and

$$f(x,t) = \begin{cases} 1, & x \in [-\pi, \pi], \\ 0, & \text{otherwise.} \end{cases}$$

Figures 5-8 show the numerical solutions for $N = 10,\ 20,\ 40,\ 80,\ 160$ where the exact solution is calculated with $N = 640$ for the different α. One may see the approximations for the different N.

6 Conclusion

In this paper, we introduce a new finite difference scheme for solving the time-fractional Klein-Gordon equation using artificial boundary conditions. The stability and the error estimates are proved by using the discrete energy method. Numerical examples are given to show that the numerical results are consistent with the theoretical findings. In our future work, we shall use the artificial boundary conditions to consider the numerical method for approximating the nonlinear Klein-Gordon equation on an unbounded domain.

7 Declarations

Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

References

1. A. Wazwaz, *The tanh method: exact solutions of the sine-Gordon and the sinh-Gordon equations*, Appl Math Comput, 167(2005), pp. 1196-1210.
2. E. Yusufoğlu, *The variational iteration method for studying the Klein-Gordon equationt*, Appl Math Lett, 21 (2008), pp. 669-674.
3. A.Golmankhaneh, A.Golmankhaneh and D. Baleanu, *On nonlinear fractional Klein-Gordon equation*, Signal Process, 91(2011), pp. 446-451.
4. Z. Sun and X. Wu, *A fully discrete scheme for a diffusion wave system*, Appl. Numer. Math., 56(2011), pp. 193-209.
5. H. Liao, D. Li and J. Zhang,*Sharp error estimate of the nonuniform L1 formula for linear reaction subdiffusion equations*, SIAM J. Numer. Anal., 56(2018), pp. 1112-1133.
6. B. Jin, R. Lazarov and Z. Zhou, *An analysis of the L1 scheme for the subdiffusion equation with nonsmooth data* ,IMA J. Numer. Anal., 36(2016), pp. 197-221.
7. P. Lyu, S. Vong, *A high-order method with a temporal nonuniform mesh for a time-fractional Benjamin Bona-Mahony equation.* J. Sci. Comput., 80(2019), PP.1607-1628.
8. A. Alikhanov, *A new difference scheme for the time fractional diffusion equation*, Journal of Computational Physics, 280(2015), pp. 424-438.
9. H. Sun, Z. Sun and G. Gao, *Some temporal second order difference schemes for fractional wave equations*, Numer Methods Partial Differential Equations, 32 (2016), pp. 870-1001.

10. R. Du, Y. Yan and Z. Liang, *A high-order scheme to approximate the Caputo fractional derivative and its application to solve the fractional diffusion wave equation*, J. Comput. Phys., 376(2019), pp. 1312-1330.
11. Y. Lin and C. Xu, *Finite difference/spectral approximations for the time-fractional diffusion equation*, J. Comput. Phys., 225(2007), pp. 1533-1552.
12. X. Li and C. Xu, *A space-time spectral method for the time fractional diffusion equation*, SIAM Journal Numerical Analysis, 47 (2009), pp. 2108-2131.
13. G. Gao, Z. Sun and H. Zhang, *A new fractional numerical differentiation formula to approximate the Caputo fractional derivative and its applications*, Journal of Computational Physics, 259(2014), pp. 33-50.
14. G. Gao and Z. Sun, *The finite difference approximation for a class of fractional sub-diffusion equations on a space unbounded domain*, Journal of Computa tional Physics, 236(2013), pp. 443-460.
15. G. Gao, Z. Sun and Y. Zhang, *A finite difference scheme for fractional sub-diffusion equations on an unbounded domain using artificial boundary conditions*, Journal of Computational Physics, 231(2012), pp. 2865-2879.
16. Q. Zhang, J.Zhang, S. Jiang and Z. Zhang, *Numerical solution to a linearized time fractional KdV equation on unbounded domains*, Mathematics of Computation, 87(2017), pp. 693-719.
17. D. Li, J. Zhang and Z. Zhang, *The numerical computation of the time fractional Schrodinger equation on an unbounded domain*, Computational Methods in Applied Mathematics, 18(2018), pp. 77-94.
18. Z. Sun, J. Zhang and Z. Zhang, *Optimal error estimates in numerical solution of time fractional Schrodinger equations on unbounded domains*, East Asian Journal on Applied Mathematics, 8(2018), pp. 634-655.
19. J. Zhang, D. Li and X. Antoine, *Efficient numerical computation of time-fractional nonlinear Schrodinger equations in unbounded domain*, Communications in Computational Physics, 25(2019). pp. 218-243.
20. S. Vong and Z. Wang, *A compact difference scheme for a two dimensional fractional Klein-Gordon equation with Neumann boundary conditions*, Journal of Computational Physics, 274(2014), pp. 268-282.
21. S. Vong and Z. Wang, *A high-order compact scheme for the nonlinear fractional Klein-Gordon equation*, Numerical Methods for Partial Differential Equations, 38(2014), pp. 706-722.
22. P. Lyu and S. Vong, *A linearized second-order scheme for nonlinear time fractional Klein-Gordon type equations*, Numerical Algorithms, 78(2018), pp. 485-511.
23. H. Chen, S. Lu and W. Chen, *A fully discrete spectral method for the nonlinear time fractional Klein-Gordon equation*, Taiwanese Journal Of Mathematics, 21(2017), pp.231-251.
24. Y. Yang, X. Yang, J. Wang and J. Liu, *The numerical solution of the time-fractional non-linear Klein-Gordon equation via spectral collocation method*, Thermal Science, 23(2019), pp. 1529-1537.
25. Z. Sun, C. Ji and R. Du, *A new analytical technique of the L-type difference schemes for time fractional mixed sub-diffusion and diffusion-wave equations*, Applied Mathematics Letters, 102(2020), pp. 106-115.
26. Y. Yan, B. Egwu, Z. Liang and Y. Yan, *Error estimates of a continuous Galerkin time stepping method for subdiffusion problem*, J Scientific Computing, 68 (2021), pp. 1-30.
27. W. Kang, B. Egwu, Y. Yan and A. K. Pani, *Galerkin finite element approximation of a stochastic semilinear fractional subdiffusion with fractionally integrated additive noise*, IMA Journal of Numerical Analysis, 6 (2021), pp. 1-35.
28. Y. Wang, Y. Yan, Y. Yan, and A. K. Pani, *Higher order time stepping methods for subdiffusion problems based on weighted and shifted Grünwald-Letnikov formulae with nonsmooth data*, J. Sci. Comput., (2020), 83:40.
29. Y. Wang, Y. Yan and Y. Yang, *Two high-order time discretization schemes for subdiffusion problems with nonsmooth data*, Fract. Calc. Appl. Anal., 23(2020), 1349-1380.
30. Y. Xing and Y. Yan, *A higher order numerical method for time fractional partial differential equations with nonsmooth data*, J. Comput. Phys., 357(2018), pp. 305-323.
31. K. Oldham and J. Spanier, *The Fractional Calculus*, Academic Press, New York, 1974.

32. Z. Sun and G. Gao, *Fractional Differential Equations. Finite Difference Methods*, Science Press, Beijing. 2020.

33. Z. Sun, *Numerical Methods Of Partial Differential Equations (in Chinese, 2nd version)*, Science Press, Beijing, 2012.

34. H. Han and X. Wu, *Artificial Boundary Method-Numerical Solution Of Partial Differential Equations On Unbounded Domains*, Tsinghua University Pres, Beijing, 2009.

35. A. Kilbas, H. Srivastava and J. Trujillo, *Theory And Applications Of Fractional Differential Equations*, Elsevier Science, Amsterdam, 2006.

36. A. Neumaier, *Introduction To Numerical Analysis*, Cambridge University Press, 2001.

8 Appendix

In this Appendix, we shall prove Lemma 3.

Proof (Proof of Lemma 3) It is easy to show the conclusion is true for $n = 1$. We now consider the case with $n \geq 2$. Note that, by (18),

$$
\begin{aligned}
&{}_0^G D_t^{\frac{\alpha}{2}} u(t)|_{t=t_{n-\frac{1}{2}}} \\
&= \frac{1}{\Gamma(1-\frac{\alpha}{2})} \int_0^{t_{n-\frac{1}{2}}} \frac{G_{\alpha,q}(t_{n-\frac{1}{2}} - \tau) u'(\tau)}{(t_{n-\frac{1}{2}} - \tau)^{\frac{\alpha}{2}}} d\tau \\
&= \frac{1}{\Gamma(1-\frac{\alpha}{2})} \sum_{j=1}^{n-1} \sum_{k=0}^{+\infty} \Bigg[(k\alpha - \frac{\alpha}{2} + 1) \tilde{A}_k^{(\alpha)} \int_{t_{j-1}}^{t_j} (t_{n-\frac{1}{2}} - \tau)^{k\alpha - \frac{\alpha}{2}} u'(\tau) d\tau \\
&\quad - (k\alpha + \frac{\alpha}{2} + 1) \tilde{B}_k^{(\alpha)} \int_{t_{j-1}}^{t_j} (t_{n-\frac{1}{2}} - \tau)^{k\alpha + \frac{\alpha}{2}} u'(\tau) d\tau \Bigg] \\
&\quad + \frac{1}{\Gamma(1-\frac{\alpha}{2})} \sum_{k=0}^{+\infty} \Bigg[(k\alpha - \frac{\alpha}{2} + 1) \tilde{A}_k^{(\alpha)} \int_{t_{n-1}}^{t_{n-\frac{1}{2}}} (t_{n-\frac{1}{2}} - \tau)^{k\alpha - \frac{\alpha}{2}} u'(\tau) d\tau \\
&\quad - (k\alpha + \frac{\alpha}{2} + 1) \tilde{B}_k^{(\alpha)} \int_{t_{n-1}}^{t_{n-\frac{1}{2}}} (t_{n-\frac{1}{2}} - \tau)^{k\alpha + \frac{\alpha}{2}} u'(\tau) d\tau \Bigg]. \qquad (55)
\end{aligned}
$$

We now consider the L1 approximation of the generalized Caputo derivative ${}_0^G D_t^{\frac{\alpha}{2}} u(t)$ on the grid point $\{t_{j-1}, t_j\}(1 \leq j \leq n)$. With $\delta_t u^{j-\frac{1}{2}} = \frac{u^j - u^{j-1}}{\Delta t}$, one gets

$$
\begin{aligned}
&{}_0^G D_t^{\frac{\alpha}{2}} u(t)|_{t=t_{n-\frac{1}{2}}} \\
&= \frac{1}{\Gamma(1-\frac{\alpha}{2})} \sum_{j=1}^{n-1} \sum_{k=0}^{+\infty} \Big[(k\alpha - \frac{\alpha}{2} + 1) \tilde{A}_k^{(\alpha)} \int_{t_{j-1}}^{t_j} (t_{n-\frac{1}{2}} - \tau)^{k\alpha - \frac{\alpha}{2}} d\tau \\
&\quad - (k\alpha + \frac{\alpha}{2} + 1) \tilde{B}_k^{(\alpha)} \int_{t_{j-1}}^{t_j} (t_{n-\frac{1}{2}} - \tau)^{k\alpha + \frac{\alpha}{2}} d\tau \Big] \delta_t u^{j-\frac{1}{2}} \\
&\quad + \frac{1}{\Gamma(1-\frac{\alpha}{2})} \sum_{k=0}^{+\infty} \Big[(k\alpha - \frac{\alpha}{2} + 1) \tilde{A}_k^{(\alpha)} \int_{t_{n-1}}^{t_{n-\frac{1}{2}}} (t_{n-\frac{1}{2}} - \tau)^{k\alpha - \frac{\alpha}{2}} d\tau \\
&\quad - (k\alpha + \frac{\alpha}{2} + 1) \tilde{B}_k^{(\alpha)} \int_{t_{n-1}}^{t_{n-\frac{1}{2}}} (t_{n-\frac{1}{2}} - \tau)^{k\alpha + \frac{\alpha}{2}} d\tau \Big] \delta_t u^{n-\frac{1}{2}} + \tilde{R}^{n-\frac{1}{2}} \\
&= \frac{1}{\Gamma(1-\frac{\alpha}{2})} \sum_{j=1}^{n-1} \sum_{k=0}^{+\infty} \Big\{ \tilde{A}_k^{(\alpha)} \Delta t^{k\alpha - \frac{\alpha}{2} + 1} \Big[(n-j+\frac{1}{2})^{k\alpha - \frac{\alpha}{2} + 1} - (n-j-\frac{1}{2})^{k\alpha - \frac{\alpha}{2} + 1} \Big] \\
&\quad - \tilde{B}_k^{(\alpha)} \Delta t^{k\alpha + \frac{\alpha}{2} + 1} \Big[(n-j+\frac{1}{2})^{k\alpha + \frac{\alpha}{2} + 1} - (n-j-\frac{1}{2})^{k\alpha + \frac{\alpha}{2} + 1} \Big] \Big\} \delta_t u^{j-\frac{1}{2}} \\
&\quad + \frac{1}{\Gamma(1-\frac{\alpha}{2})} \sum_{k=0}^{+\infty} \Big[\tilde{A}_k^{(\alpha)} (\frac{\Delta t}{2})^{k\alpha - \frac{\alpha}{2} + 1} - \tilde{B}_k^{(\alpha)} (\frac{\Delta t}{2})^{k\alpha + \frac{\alpha}{2} + 1} \Big] \delta_t u^{n-\frac{1}{2}} + \tilde{R}^{n-\frac{1}{2}} \\
&=: \mathbb{D}_t^{G,\frac{\alpha}{2}} u(t)|_{t=t_{n-\frac{1}{2}}} + \tilde{R}^{n-\frac{1}{2}}. \qquad (56)
\end{aligned}
$$

Here

$$
\mathbb{D}_t^{G,\frac{\alpha}{2}} u(t)|_{t=t_{n-\frac{1}{2}}} = \frac{1}{\Gamma(1-\frac{\alpha}{2})} \sum_{j=1}^{n} a_{n-j}^{(\alpha)} \delta_t u^{j-\frac{1}{2}},
$$

where

$$
a_j^{(\alpha)} = \left\{ \begin{aligned}
&\sum_{k=0}^{+\infty} \Big[\tilde{A}_k^{(\alpha)} (\frac{\Delta t}{2})^{k\alpha - \frac{\alpha}{2} + 1} - \tilde{B}_k^{(\alpha)} (\frac{\Delta t}{2})^{k\alpha + \frac{\alpha}{2} + 1} \Big], \quad j = 0, \\
&\sum_{k=0}^{+\infty} \tilde{A}_k^{(\alpha)} \Delta t^{k\alpha - \frac{\alpha}{2} + 1} \Big[(j+\frac{1}{2})^{k\alpha - \frac{\alpha}{2} + 1} - (j-\frac{1}{2})^{k\alpha - \frac{\alpha}{2} + 1} \Big] \\
&\quad - \sum_{k=0}^{+\infty} \tilde{B}_k^{(\alpha)} \Delta t^{k\alpha + \frac{\alpha}{2} + 1} \Big[(j+\frac{1}{2})^{k\alpha + \frac{\alpha}{2} + 1} - (j-\frac{1}{2})^{k\alpha + \frac{\alpha}{2} + 1} \Big], \\
&\qquad\qquad\qquad\qquad\qquad\qquad 1 \le j \le n-1.
\end{aligned} \right\}
$$

Using integration by parts, it yields that, with $L_{1,j}u$ denoting the linear interpolation function of u at t_{j-1} and t_j, $j = 1, 2, \dots, n$,

$$
\begin{aligned}
\tilde{R}^{n-\frac{1}{2}} &= {}_0^G D_t^{\frac{\alpha}{2}} u(t)|_{t=t_{n-\frac{1}{2}}} - \mathbb{D}_t^{G,\frac{\alpha}{2}} u(t)|_{t=t_{n-\frac{1}{2}}} \\
&= \frac{1}{\Gamma(1-\frac{\alpha}{2})} \sum_{j=1}^{n-1} \sum_{k=0}^{+\infty} \Big[(k\alpha + 1 - \frac{\alpha}{2}) \tilde{A}_k^{(\alpha)} \int_{t_{j-1}}^{t_j} (t_{n-\frac{1}{2}} - \tau)^{k\alpha - \frac{\alpha}{2}} \big[u(\tau) - L_{1,j}u(\tau)\big]' d\tau \\
&\quad - (k\alpha + 1 + \frac{\alpha}{2}) \tilde{B}_k^{(\alpha)} \int_{t_{j-1}}^{t_j} (t_{n-\frac{1}{2}} - \tau)^{k\alpha + \frac{\alpha}{2}} \big[u(\tau) - L_{1,j}u(\tau)\big]' d\tau \Big] \\
&\quad + \frac{1}{\Gamma(1-\frac{\alpha}{2})} \sum_{k=0}^{+\infty} \Big[(k\alpha + 1 - \frac{\alpha}{2}) \tilde{A}_k^{(\alpha)} \int_{t_{n-1}}^{t_{n-\frac{1}{2}}} (t_{n-\frac{1}{2}} - \tau)^{k\alpha - \frac{\alpha}{2}} \big[u(\tau) - L_{1,n}u(\tau)\big]' d\tau \\
&\quad - (k\alpha + 1 + \frac{\alpha}{2}) \tilde{B}_k^{(\alpha)} \int_{t_{n-1}}^{t_{n-\frac{1}{2}}} (t_{n-\frac{1}{2}} - \tau)^{k\alpha + \frac{\alpha}{2}} \big[u(\tau) - L_{1,n}u(\tau)\big]' d\tau \Big] \\
&= \frac{1}{\Gamma(1-\frac{\alpha}{2})} \sum_{j=1}^{n-1} \sum_{k=0}^{+\infty} \Big[(k\alpha + 1 - \frac{\alpha}{2})(k\alpha - \frac{\alpha}{2}) \tilde{A}_k^{(\alpha)} \int_{t_{j-1}}^{t_j} (t_{n-\frac{1}{2}} - \tau)^{k\alpha - \frac{\alpha}{2} - 1} \big[u(\tau) - L_{1,j}u(\tau)\big] d\tau \\
&\quad - (k\alpha + 1 + \frac{\alpha}{2})(k\alpha + \frac{\alpha}{2}) \tilde{B}_k^{(\alpha)} \int_{t_{j-1}}^{t_j} (t_{n-\frac{1}{2}} - \tau)^{k\alpha + \frac{\alpha}{2} - 1} \big[u(\tau) - L_{1,j}u(\tau)\big] d\tau \Big] \\
&\quad + \frac{1}{\Gamma(1-\frac{\alpha}{2})} \sum_{k=0}^{+\infty} \Big[(k\alpha + 1 - \frac{\alpha}{2}) \tilde{A}_k^{(\alpha)} \int_{t_{n-1}}^{t_{n-\frac{1}{2}}} (t_{n-\frac{1}{2}} - \tau)^{k\alpha - \frac{\alpha}{2}} \big[u'(\tau) - (L_{1,n}u(\tau))'\big] d\tau \\
&\quad - (k\alpha + 1 + \frac{\alpha}{2}) \tilde{B}_k^{(\alpha)} \int_{t_{n-1}}^{t_{n-\frac{1}{2}}} (t_{n-\frac{1}{2}} - \tau)^{k\alpha + \frac{\alpha}{2}} \big[u'(\tau) - (L_{1,n}u(\tau))'\big] d\tau \Big] \\
&\equiv \tilde{R}_1^{n-\frac{1}{2}} + \tilde{R}_2^{n-\frac{1}{2}},
\end{aligned} \tag{57}
$$

For $\tilde{R}_1^{n-\frac{1}{2}}$, we have, with $r(\tau)$ denoting the interpolation error,

$$
\begin{aligned}
\big|\tilde{R}_1^{n-\frac{1}{2}}\big| &= \frac{1}{\Gamma(1-\frac{\alpha}{2})} \Bigg| \sum_{j=1}^{n-1} \sum_{k=0}^{+\infty} \Big[(k\alpha + 1 - \frac{\alpha}{2})(k\alpha - \frac{\alpha}{2}) \tilde{A}_k^{(\alpha)} \int_{t_{j-1}}^{t_j} (t_{n-\frac{1}{2}} - \tau)^{k\alpha - \frac{\alpha}{2} - 1} r(\tau) d\tau \\
&\quad - (k\alpha + 1 + \frac{\alpha}{2})(k\alpha + \frac{\alpha}{2}) \tilde{B}_k^{(\alpha)} \int_{t_{j-1}}^{t_j} (t_{n-\frac{1}{2}} - \tau)^{k\alpha + \frac{\alpha}{2} - 1} r(\tau) d\tau \Big] \Bigg| \\
&= \frac{u''(t_\xi)}{2\Gamma(1-\frac{\alpha}{2})} \Bigg| \sum_{j=1}^{n-1} \sum_{k=0}^{+\infty} \Big[(k\alpha + 1 - \frac{\alpha}{2})(k\alpha - \frac{\alpha}{2}) \tilde{A}_k^{(\alpha)} \int_{t_{j-1}}^{t_j} (t_{n-\frac{1}{2}} - \tau)^{k\alpha - \frac{\alpha}{2} - 1} (\tau - t_{j-1})(t_j - \tau) d\tau \\
&\quad - (k\alpha + 1 + \frac{\alpha}{2})(k\alpha + \frac{\alpha}{2}) \tilde{B}_k^{(\alpha)} \int_{t_{j-1}}^{t_j} (t_{n-\frac{1}{2}} - \tau)^{k\alpha + \frac{\alpha}{2} - 1} \frac{u''(t_\xi)}{2} (\tau - t_{j-1})(t_j - \tau) d\tau \Bigg|.
\end{aligned}
$$

Hence we obtain

$$\big|\tilde{R}_1^{n-\frac{1}{2}}\big| \le \frac{\Delta t^{2-\frac{\alpha}{2}}}{8\Gamma(1-\frac{\alpha}{2})}\max_{t_0\le t\le t_{n-1}}|u''(t)|\Big[(1-\frac{\alpha}{2})|\tilde{A}_0^{(\alpha)}|+\sum_{k=1}^{+\infty}(k\alpha+1-\frac{\alpha}{2})|\tilde{A}_k^{(\alpha)}|T^{k\alpha-\frac{\alpha}{2}}\Big]$$
$$+\frac{\Delta t^2}{8\Gamma(1-\frac{\alpha}{2})}\max_{t_0\le t\le t_{n-1}}|u''(t)|\sum_{k=0}^{+\infty}(k\alpha+1+\frac{\alpha}{2})|\tilde{B}_k^{(\alpha)}|T^{k\alpha+\frac{\alpha}{2}},\quad (58)$$

where

$$\sum_{k=1}^{+\infty}(k\alpha+1-\frac{\alpha}{2})\Big|\tilde{A}_k^{(\alpha)}\Big|T^{k\alpha-\frac{\alpha}{2}}=\sum_{k=1}^{+\infty}\frac{\Gamma(k+\frac{1}{2})q^{2k}}{\Gamma(\frac{1}{2})\Gamma(k\alpha-\frac{\alpha}{2}+1)\Gamma(k+1)}T^{k\alpha-\frac{\alpha}{2}},$$

which is convergent since

$$\lim_{k\to\infty}\frac{\Gamma(k+\frac{3}{2})q^{2k+2}T^{k\alpha+\frac{\alpha}{2}}}{\Gamma(\frac{1}{2})\Gamma(k\alpha+\frac{\alpha}{2}+1)\Gamma(k+2)}\cdot\frac{\Gamma(\frac{1}{2})\Gamma(k\alpha-\frac{\alpha}{2}+1)\Gamma(k+1)}{\Gamma(k+\frac{1}{2})q^{2k}T^{k\alpha-\frac{\alpha}{2}}}$$
$$=\lim_{k\to\infty}q^2T^\alpha\frac{\Gamma(k\alpha-\frac{\alpha}{2}+1)(k+\frac{1}{2})}{\Gamma(k\alpha+\frac{\alpha}{2}+1)(k+1)}=0<1.\quad (59)$$

Further note that $(1-\frac{\alpha}{2})\Big|\tilde{A}_0^{(\alpha)}\Big|=\frac{1}{\Gamma(1-\frac{\alpha}{2})}$ is bounded. Hence there exists a positive constant $M_1(T,\alpha)$ which only depends on T,α such that

$$(1-\frac{\alpha}{2})\Big|\tilde{A}_0^{(\alpha)}\Big|+\sum_{k=1}^{+\infty}(k\alpha+1-\frac{\alpha}{2})\Big|\tilde{A}_k^{(\alpha)}\Big|T^{k\alpha-\frac{\alpha}{2}}\le M_1(T,\alpha).\quad (60)$$

Similarly there exists a positive constant $M_2(T,\alpha)$ such that $\sum\limits_{k=0}^{+\infty}(k\alpha+1+\frac{\alpha}{2})|\tilde{B}_k^{(\alpha)}|T^{k\alpha+\frac{\alpha}{2}}\le M_2(T,\alpha)$. Hence one gets

$$\big|\tilde{R}_1^{n-\frac{1}{2}}\big|\le\frac{\Delta t^{2-\frac{\alpha}{2}}}{8\Gamma(1-\frac{\alpha}{2})}\max_{t_0\le t\le t_{n-1}}|u''(t)|\big[M_1(T,\alpha)+M_2(T,\alpha)\big].\quad (61)$$

For $\tilde{R}_2^{n-\frac{1}{2}}$, we have

$$\big|\tilde{R}_2^{n-\frac{1}{2}}\big|$$
$$=\frac{1}{\Gamma(1-\frac{\alpha}{2})}\Bigg|\sum_{k=0}^{+\infty}\Big\{(k\alpha+1-\frac{\alpha}{2})\tilde{A}_k^{(\alpha)}\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(t_{n-\frac{1}{2}}-\tau)^{k\alpha-\frac{\alpha}{2}}\big[u'(\tau)-(L_{1,n}u(\tau))'\big]d\tau$$
$$-(k\alpha+1+\frac{\alpha}{2})\tilde{B}_k^{(\alpha)}\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(t_{n-\frac{1}{2}}-\tau)^{k\alpha+\frac{\alpha}{2}}\big[u'(\tau)-(L_{1,n}u(\tau))'\big]d\tau\Big\}\Bigg|$$
$$\le\frac{1}{\Gamma(1-\frac{\alpha}{2})}\sum_{k=0}^{+\infty}\Big|(k\alpha+1-\frac{\alpha}{2})\tilde{A}_k^{(\alpha)}\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(t_{n-\frac{1}{2}}-\tau)^{k\alpha-\frac{\alpha}{2}}\big[u'(\tau)-(L_{1,n}u(\tau))'\big]d\tau\Big|$$
$$+\frac{1}{\Gamma(1-\frac{\alpha}{2})}\sum_{k=0}^{+\infty}\Big|(k\alpha+1+\frac{\alpha}{2})\tilde{B}_k^{(\alpha)}\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(t_{n-\frac{1}{2}}-\tau)^{k\alpha+\frac{\alpha}{2}}\big[u'(\tau)-(L_{1,n}u(\tau))'\big]d\tau\Big|$$
$$=I_1+I_2.\quad (62)$$

Using Taylor's expansion,

$$u'(t) = u'(t_{n-\frac{1}{2}}) + (t - t_{n-\frac{1}{2}})u''(t_{n-\frac{1}{2}}) + \frac{1}{2}(t - t_{n-\frac{1}{2}})^2 u'''(\eta_n), \quad \eta_n \in (t_{n-1}, t_{n-\frac{1}{2}}),$$

one gets

$$\begin{aligned}
I_1 &= \frac{1}{\Gamma(1-\frac{\alpha}{2})}\sum_{k=0}^{+\infty}\left|(k\alpha+1-\frac{\alpha}{2})\tilde{A}_k^{(\alpha)}\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(t_{n-\frac{1}{2}}-\tau)^{k\alpha-\frac{\alpha}{2}}\left[u'(\tau)-(L_{1,n}u(\tau))'\right]d\tau\right| \\
&= \frac{1}{\Gamma(1-\frac{\alpha}{2})}\sum_{k=0}^{+\infty}\left|(k\alpha+1-\frac{\alpha}{2})\tilde{A}_k^{(\alpha)}\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(t_{n-\frac{1}{2}}-\tau)^{k\alpha-\frac{\alpha}{2}}\left[u'(t_{n-\frac{1}{2}})-\delta_t u^{n-\frac{1}{2}}\right]d\tau\right| \\
&\quad + \frac{1}{\Gamma(1-\frac{\alpha}{2})}\sum_{k=0}^{+\infty}\left|(k\alpha+1-\frac{\alpha}{2})\tilde{A}_k^{(\alpha)}\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(t_{n-\frac{1}{2}}-\tau)^{k\alpha-\frac{\alpha}{2}}(\tau-t_{n-\frac{1}{2}})u''(t_{n-\frac{1}{2}})d\tau\right| \\
&\quad + \frac{1}{\Gamma(1-\frac{\alpha}{2})}\sum_{k=0}^{+\infty}\left|(k\alpha+1-\frac{\alpha}{2})\tilde{A}_k^{(\alpha)}\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(t_{n-\frac{1}{2}}-\tau)^{k\alpha-\frac{\alpha}{2}}\frac{1}{2}(\tau-t_{n-\frac{1}{2}})^2u'''(\eta_n)d\tau\right|.
\end{aligned} \tag{63}$$

Calculating the three integrals in the above formula (63), we get

$$\begin{aligned}
&\frac{1}{\Gamma(1-\frac{\alpha}{2})}\sum_{k=0}^{+\infty}\left|(k\alpha+1-\frac{\alpha}{2})\tilde{A}_k^{(\alpha)}\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(t_{n-\frac{1}{2}}-\tau)^{k\alpha-\frac{\alpha}{2}}\left[u'(t_{n-\frac{1}{2}})-\delta_t u^{n-\frac{1}{2}}\right]d\tau\right| \\
&\le \frac{1}{\Gamma(1-\frac{\alpha}{2})}\left|u'(t_{n-\frac{1}{2}})-\delta_t u^{n-\frac{1}{2}}\right|\left|\sum_{k=0}^{+\infty}\right|(k\alpha+1-\frac{\alpha}{2})\tilde{A}_k^{(\alpha)}\left|\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(t_{n-\frac{1}{2}}-\tau)^{k\alpha-\frac{\alpha}{2}}d\tau\right. \\
&\le \frac{\Delta t^{3-\frac{\alpha}{2}}}{24\Gamma(1-\frac{\alpha}{2})}\max_{t_{n-1}\le t\le t_n}\left|u'''(t)\right|\sum_{k=0}^{+\infty}\left|\tilde{A}_k^{(\alpha)}\right|(\frac{1}{2})^{k\alpha-\frac{\alpha}{2}+1}T^{k\alpha},
\end{aligned} \tag{64}$$

and

$$\begin{aligned}
&\frac{1}{\Gamma(1-\frac{\alpha}{2})}\sum_{k=0}^{+\infty}\left|(k\alpha+1-\frac{\alpha}{2})\tilde{A}_k^{(\alpha)}\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(t_{n-\frac{1}{2}}-\tau)^{k\alpha-\frac{\alpha}{2}}(\tau-t_{n-\frac{1}{2}})u''(t_{n-\frac{1}{2}})d\tau\right| \\
&\le \frac{1}{\Gamma(1-\frac{\alpha}{2})}\max_{t_{n-1}\le t\le t_n}\left|u''(t)\right|\sum_{k=0}^{+\infty}(k\alpha+1-\frac{\alpha}{2})\left|\tilde{A}_k^{(\alpha)}\right|\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(t_{n-\frac{1}{2}}-\tau)^{k\alpha-\frac{\alpha}{2}+1}d\tau \\
&\le \frac{\Delta t^{2-\frac{\alpha}{2}}}{\Gamma(1-\frac{\alpha}{2})}\max_{t_{n-1}\le t\le t_n}\left|u''(t)\right|\sum_{k=0}^{+\infty}\frac{k\alpha-\frac{\alpha}{2}+1}{k\alpha-\frac{\alpha}{2}+2}\left|\tilde{A}_k^{(\alpha)}\right|(\frac{1}{2})^{k\alpha-\frac{\alpha}{2}+2}T^{k\alpha},
\end{aligned} \tag{65}$$

and

$$\frac{1}{\Gamma(1-\frac{\alpha}{2})}\sum_{k=0}^{+\infty}\left|(k\alpha+1-\frac{\alpha}{2})\tilde{A}_k^{(\alpha)}\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(t_{n-\frac{1}{2}}-\tau)^{k\alpha-\frac{\alpha}{2}}\frac{1}{2}(\tau-t_{n-\frac{1}{2}})^2u'''(\eta_n)d\tau\right|$$
$$\leq\frac{\Delta t^2}{8\Gamma(1-\frac{\alpha}{2})}\max_{t_{n-1}\leq t\leq t_n}\left|u'''(t)\right|\sum_{k=0}^{+\infty}(k\alpha+1-\frac{\alpha}{2})\left|\tilde{A}_k^{(\alpha)}\right|\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(t_{n-\frac{1}{2}}-\tau)^{k\alpha-\frac{\alpha}{2}}d\tau$$
$$\leq\frac{\Delta t^{3-\frac{\alpha}{2}}}{8\Gamma(1-\frac{\alpha}{2})}\max_{t_{n-1}\leq t\leq t_n}\left|u'''(t)\right|\sum_{k=0}^{+\infty}\left|\tilde{A}_k^{(\alpha)}\right|(\frac{1}{2})^{k\alpha-\frac{\alpha}{2}+1}T^{k\alpha}. \quad (66)$$

Similarly we may show that there exist positive constant $M_3(T,\alpha)$, $M_4(T,\alpha)$ and $M_5(T,\alpha)$ such that

$$\sum_{k=0}^{+\infty}\left|\tilde{A}_k^{(\alpha)}\right|(\frac{1}{2})^{k\alpha-\frac{\alpha}{2}+1}T^{k\alpha}\leq M_3(T,\alpha), \quad (67)$$
$$\sum_{k=0}^{+\infty}\frac{k\alpha-\frac{\alpha}{2}+1}{k\alpha-\frac{\alpha}{2}+2}\left|\tilde{A}_k^{(\alpha)}\right|(\frac{1}{2})^{k\alpha-\frac{\alpha}{2}+2}T^{k\alpha}\leq M_4(T,\alpha), \quad (68)$$
$$\sum_{k=0}^{+\infty}\left|\tilde{A}_k^{(\alpha)}\right|(\frac{1}{2})^{k\alpha-\frac{\alpha}{2}+1}T^{k\alpha}\leq M_5(T,\alpha). \quad (69)$$

Hence we obtain, combining (63) with (64)-(69),

$$I_1\leq\frac{\Delta t^{2-\frac{\alpha}{2}}}{\Gamma(1-\frac{\alpha}{2})}\max_{t_{n-1}\leq t\leq t_n}\left|u'''(t)\right|\big[M_3(T,\alpha)+M_4(T,\alpha)+M_5(T,\alpha)\big]. \quad (70)$$

Further we may show, following the same approach as for the estimate of I_1 above,

$$I_2\leq\frac{\Delta t^{2+\frac{\alpha}{2}}}{\Gamma(1-\frac{\alpha}{2})}\max_{t_{n-1}\leq t\leq t_n}\left|u'''(t)\right|\big[M_3(T,\alpha)+M_4(T,\alpha)+M_5(T,\alpha)\big]. \quad (71)$$

Substitute (70)-(71) into (62), we obtain

$$\left|\tilde{R}_2^{n-\frac{1}{2}}\right|\leq\frac{2\Delta t^{2-\frac{\alpha}{2}}}{\Gamma(1-\frac{\alpha}{2})}\max_{t_{n-1}\leq t\leq t_n}\left|u'''(t)\right|\big[M_3(T,\alpha)+M_4(T,\alpha)+M_5(T,\alpha)\big]. \quad (72)$$

Hence, combining (61) and (72),

$$\left|\tilde{R}^{n-\frac{1}{2}}\right|\leq\frac{\Delta t^{2-\frac{\alpha}{2}}}{8\Gamma(1-\frac{\alpha}{2})}\max_{t_0\leq t\leq t_{n-1}}|u''(t)|\sum_{i=1}^{2}M_i(T,\alpha)$$
$$+\frac{2\Delta t^{2-\frac{\alpha}{2}}}{\Gamma(1-\frac{\alpha}{2})}\max_{t_{n-1}\leq t\leq t_n}\left|u'''(t)\right|\sum_{i=3}^{5}M_i(T,\alpha).$$

Together these estimates complete the proof of Lemma 3.

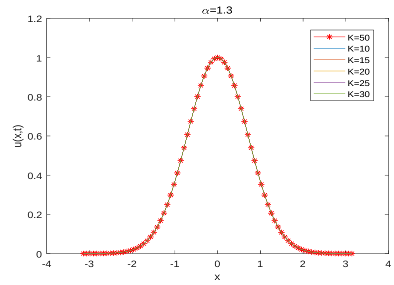

Fig. 1 Exact solution and numerical solution for $\alpha = 1.3$

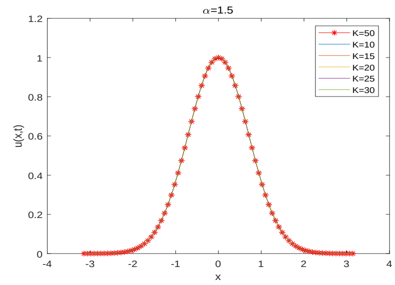

Fig. 2 Exact solution and numerical solution for $\alpha = 1.5$

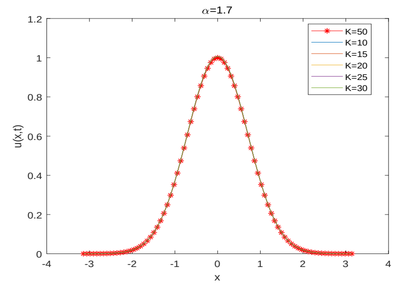

Fig. 3 Exact solution and numerical solution for $\alpha = 1.7$

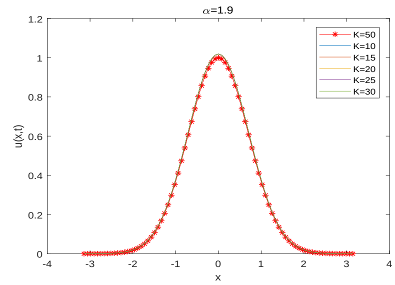

Fig. 4 Exact solution and numerical solution for $\alpha = 1.9$

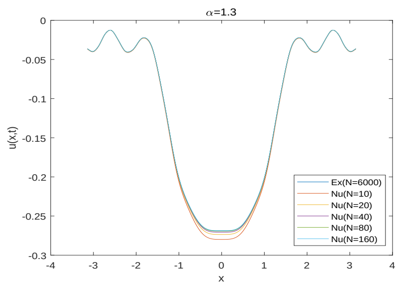

Fig. 5 Exact solution and numerical solution for $\alpha = 1.3$

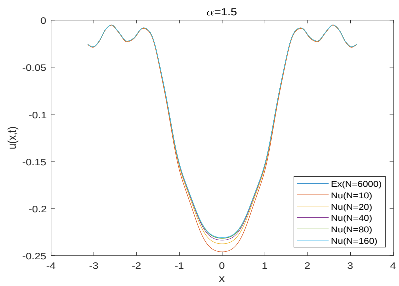

Fig. 6 Exact solution and numerical solution for $\alpha = 1.5$

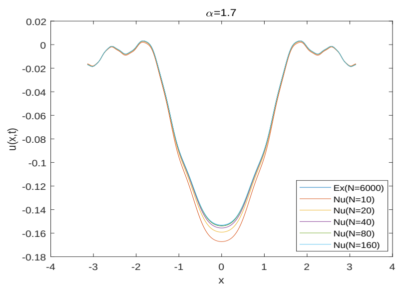

Fig. 7 Exact solution and numerical solution for $\alpha = 1.7$

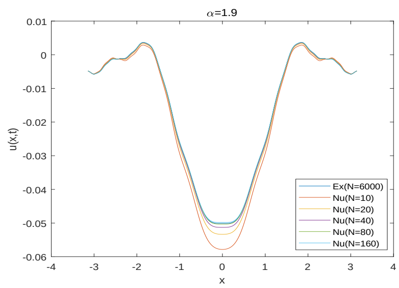

Fig. 8 Exact solution and numerical solution for $\alpha = 1.9$