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Numerical algorithm for the time fractional Fokker–Planck equation ☆

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Abstract

Anomalous diffusion is one of the most ubiquitous phenomena in nature, and it is present in a wide variety of physical situations, for instance, transport of fluid in porous media, diffusion of plasma, diffusion at liquid surfaces, etc. The fractional approach proved to be highly effective in a rich variety of scenarios such as continuous time random walk models, generalized Langevin equations, or the generalized master equation. To investigate the subdiffusion of anomalous diffusion, it would be useful to study a time fractional Fokker–Planck equation. In this paper, firstly the time fractional, the sense of Riemann–Liouville derivative, Fokker–Planck equation is transformed into a time fractional ordinary differential equation (FODE) in the sense of Caputo derivative by discretizing the spatial derivatives and using the properties of Riemann–Liouville derivative and Caputo derivative. Then combining the predictor–corrector approach with the method of lines, the algorithm is designed for numerically solving FODE with the numerical error $O(k^{\min\{1+2\alpha,2\}}) + O(h^2)$, and the corresponding stability condition is got. The effectiveness of this numerical algorithm is evaluated by comparing its numerical results for $\alpha = 1.0$ with the ones of directly discretizing classical Fokker–Planck equation, some numerical results for time fractional Fokker–Planck equation with several different fractional orders are demonstrated and compared with each other, moreover for $\alpha = 0.8$ the convergent order in space is confirmed and the numerical results with different time step sizes are shown.

Keywords: Riemann–Liouville derivative; Caputo derivative; Fokker–Planck equation; Subdiffusion; Predictor–corrector approach; Method of lines; Convergent order; Numerical stability

1. Introduction

Fractional calculus [5,18,21,24,33,34], a three hundred years old mathematical topic, did not attract enough attention till recent decades. Nowadays the fractional approach has been employed in more and more fields, encompassing materials and mechanical, signal processing and systems identification, control and robotics,

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etc. [1]. Moreover, the rich fractional dynamical appearances are disclosed, for instance, viscoelasticity [22], colored noise [29], boundary layer effects in ducts [37], electromagnetic waves [16], fractional kinetics [23,38], electrode-electrolyte polarization [19], synchronization of chaos [9,10], and multi-directional multi-scroll attractors [7,8]. In particular, the fractional approach also proved to be highly effective in continuous time random walk models, generalized Langevin equations, or the generalized master equation [32]. The advantage of the fractional model basically lies in the straightforward way of including external force terms and of calculating boundary value problems [25].

Anomalous diffusion is one of the most ubiquitous phenomena in nature, and it is present in a wide variety of physical situations, for instance, transport of fluid in porous media, surface growth, diffusion of plasma, diffusion at liquid surfaces, two-dimensional rotating flow [4,15,25,36]. Mathematically, the variance of diffusion behave as $\langle x^2(t)\rangle - \langle x(t)\rangle^2 \sim t^{\gamma}$. The exponent γ is equal to one for the normal diffusion case, for Lévy flights, γ is larger than one (but typically smaller than two), which is called superdiffusion, $\gamma = 2$ corresponds to "allistic" motion, for example the particles of a bomb which is exploding, and it is called subdiffusion if γ is less than one which corresponds to the divergence of microscopic time scales in random walk schemes [4,25,32,36,38]. Fractional derivatives play a key role in characterizing anomalous diffusion, including space fractional Fokker–Planck (advection-dispersion) equation, time fractional Fokker–Planck equation, and space and time fractional Fokker–Planck equation [2,3,15,17,20,23,25,26,30,32,36,38].

The Fokker–Planck equation (named after Adriaan Fokker and Max Planck) describes the time evolution of the probability density function of position and velocity of a particle, which is one of the classical, widely used equations of statistical physics. This paper mainly focuses on the numerical algorithm of time fractional Fokker–Planck equation [2,3,17,31], being used to characterize subdiffusion,

$$\frac{\partial}{\partial t}P(x,t) = {}_0D_t^{1-\alpha}\left[\frac{\partial}{\partial x}\frac{U'(x)}{\eta_\alpha} + \kappa_\alpha\frac{\partial^2}{\partial x^2}\right]P(x,t), \tag{1}$$

where $P(x,t)$ is the probability density, $U(x)$ indicates the potential of overdamped Brownian motion, a prime stands for the derivative w.r.t. the space coordinate, κ_α denotes the anomalous diffusion coefficient with physical dimension $[\mathrm{m}^2\,\mathrm{s}^{-\alpha}]$, η_α represents the generalized friction coefficient possessing the dimension $[\mathrm{kg}\,\mathrm{s}^{\alpha-2}]$, $\alpha \in (0,1)$ throughout the paper except in the Appendix A where $\alpha > 0$, and ${}_0D_t^{1-\alpha}$ stands for the Riemann–Liouville derivative of order $1-\alpha$, which is defined as follows

$${}_0D_t^{1-\alpha}P(x,t) = \frac{1}{\Gamma(\alpha)}\frac{\partial}{\partial t}\int_0^t (t-\tau)^{\alpha-1}P(x,\tau)\,\mathrm{d}\tau.$$

There are already some efforts for the analytical/numerical solution of (1). Using the technique of Laplace transform, the analytical solution of (1) with force free, $U'(x) \equiv 0$, is given in terms of a Fox function in [35], and a simple transformation that maps the solution of the usual Fokker–Planck equation to the FFPE is presented in [3]. Since the time fractional Fokker–Planck equation represents the continuous limit of a continuous-time random walk (CTRW) with the Mittag–Leffler residence time density [15], for arbitrary force field the numerical solution of (1) was given in [17] based on the numerical simulation of CTRW. So far, it seems that no published research takes account of the numerical scheme and detailed numerical error analysis of time fractional Fokker–Planck equation. In the real world, parameters, for example the potential $U(x)$, are usually spatially and/or temporally variable and so the Laplace transform cannot work well. In order to more accurately predict the subdiffusion, a proper numerical model is required. This paper firstly transforms the time fractional, the sense of Riemann–Liouville derivative, Fokker–Planck equation into a fractional ordinary differential equation (FODE) in the sense of Caputo derivative by discretizing the spatial derivatives and using the properties of Riemann–Liouville derivative and Caputo derivative. Then combining the predictor–corrector approach [12,13] with the method of lines [26], the algorithm is designed for numerically solving FODE, and the numerical error is $\mathrm{O}(k^{\min\{1+2\alpha,2\}}) + \mathrm{O}(h^2)$. The stability condition of this algorithm is strictly obtained. The effectiveness of this numerical algorithm is evaluated by comparing its numerical results for $\alpha = 1.0$ with the ones of directly discretizing classical Fokker–Planck equation, some numerical results for time fractional Fokker–Planck equation with several different fractional orders are demonstrated and compared with each other. Moreover, for $\alpha = 0.8$ the convergent order in space is confirmed and the numerical results with different time step sizes are illustrated.

2. Preliminaries

There are three kinds of widely used fractional derivatives, namely the Grünwald–Letnikov derivative, Riemann–Liouville derivative, and the Caputo derivative. The first two fractional derivatives are equivalent if the functions they perform are sufficiently smooth. The Riemann–Liouville integral, the Riemann–Liouville derivative, and the Caputo derivative are defined as follows: the Riemann–Liouville integral

$$ {}_0D_t^{-\beta}x(t) = \frac{1}{\Gamma(\beta)}\int_0^t (t-\tau)^{\beta-1}x(\tau)\,\mathrm{d}\tau, \quad \beta > 0, $$

the Riemann–Liouville derivative

$$ {}_0D_t^{\beta}x(t) = \frac{1}{\Gamma(m-\beta)}\frac{\mathrm{d}^m}{\mathrm{d}t^m}\int_0^t (t-\tau)^{m-\beta-1}x(\tau)\,\mathrm{d}\tau, \quad \beta \in [m-1, m), $$

and the Caputo derivative

$$ D_*^{\beta}x(t) = \frac{1}{\Gamma(m-\beta)}\int_0^t (t-\tau)^{m-\beta-1}\frac{\mathrm{d}^m x(\tau)}{\mathrm{d}\tau^m}\,\mathrm{d}\tau, \quad \beta \in (m-1, m), $$

where $m \in \mathbb{Z}^+$. And they have the following properties, where the limit is in the sense of pointwise and $x(t)$ satisfies the requirements that the corresponding fractional/classical differentiation/integration performed on $x(t)$ are meaningful and t is strictly positive, letting ${}_0D_t^{-n}x(t)$ represent n degree integral in the interval $[0, t]$,

$$ \lim_{\beta\to n} {}_0D_t^{-\beta}x(t) = {}_0D_t^{-n}x(t), \quad \text{where } n \text{ is any natural number;} \quad \lim_{\beta\to(m-1)^+} {}_0D_t^{\beta}x(t) = \frac{\mathrm{d}^{m-1}x(t)}{\mathrm{d}t^{m-1}}; $$

$$ \lim_{\beta\to m^-} {}_0D_t^{\beta}x(t) = \frac{\mathrm{d}^m x(t)}{\mathrm{d}t^m}; \quad \lim_{\beta\to 0} {}_0D_t^{-\beta}x(t) = \lim_{\beta\to 0} {}_0D_t^{\beta}x(t) = x(t), \beta > 0; $$

$$ \lim_{\beta\to(m-1)^+} D_*^{\beta}x(t) = \frac{\mathrm{d}^{m-1}x(t)}{\mathrm{d}t^{m-1}} - \left.\frac{\mathrm{d}^{m-1}x(t)}{\mathrm{d}t^{m-1}}\right|_{t=0} \neq \frac{\mathrm{d}^{m-1}x(t)}{\mathrm{d}t^{m-1}}; \quad \lim_{\beta\to m^-} D_*^{\beta}x(t) = \frac{\mathrm{d}^m x(t)}{\mathrm{d}t^m}, $$

that is classical integrals and derivatives can be continuously "connected" by the Riemann–Liouville integral and derivative $({}_0D_t^{-\beta}, \beta \in \mathbb{R})$ but Caputo derivative can not do this.

Since $P(x,t)$ in (1) is at least a continuous function w.r.t. t, then

$$ {}_0D_t^{\alpha-1}\,{}_0D_t^{1-\alpha}P(x,t) = P(x,t) - \left[{}_0D_t^{\alpha-1}P(x,t)\right]_{t=0}\frac{t^{\alpha-1}}{\Gamma(\alpha)} = P(x,t), $$

this is because

$$ \lim_{t\to 0}\left|{}_0D_t^{\alpha-1}P(x,t)\right| = \lim_{t\to 0}\left|\frac{1}{\Gamma(1-\alpha)}\int_0^t (t-\tau)^{-\alpha}P(x,\tau)\,\mathrm{d}\tau\right| \leqslant \lim_{t\to 0} M\cdot\frac{t^{1-\alpha}}{\Gamma(2-\alpha)} = 0, $$

where $M = \max_{t\in[0,T]}P(x,t)$ for fixed x, and T is any small fixed positive number.

So letting ${}_0D_t^{\alpha-1}$ act on both sides of (1), we find

$$ {}_0D_t^{\alpha-1}\frac{\partial P(x,t)}{\partial t} = \left[\frac{\partial}{\partial x}\frac{U'(x)}{\eta_\alpha} + \kappa_\alpha\frac{\partial^2}{\partial x^2}\right]P(x,t), $$

namely,

$$ D_*^{\alpha}P(x,t) = \left[\frac{\partial}{\partial x}\frac{U'(x)}{\eta_\alpha} + \kappa_\alpha\frac{\partial^2}{\partial x^2}\right]P(x,t). \tag{2} $$

Now recall and slightly improve the predictor–corrector approach for the following fractional ordinary differential equation [12,13,27,28],

$$ D_*^{\alpha}y(t) = f(y(t),t), \quad y(0) = y_0, \tag{3} $$

which is equivalent to the Volterra integral equation [11],

$$y(t) = y_0 + \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} f(y(\tau),\tau)\,\mathrm{d}\tau \tag{4}$$

in the sense that a continuous function is a solution of the initial value problem (3) if and only if it is a solution of (4).

For the numerical computation of (4), use the product trapezoidal quadrature formula to replace the integral, where nodes t_j $(j = 0, 1, 2, \ldots, n+1)$ are taken w.r.t. the weight function $(t_{n+1} - \cdot)^{\alpha-1}$, i.e., apply the approximation

$$\int_0^{t_{n+1}} (t_{n+1}-\tau)^{\alpha-1} g(\tau)\,\mathrm{d}\tau \approx \int_0^{t_{n+1}} (t_{n+1}-\tau)^{\alpha-1} \tilde{g}_{n+1}(\tau)\,\mathrm{d}\tau, \tag{5}$$

where $\tilde{g}_{n+1}$ is the piecewise linear interpolation for g with nodes and knots chosen at t_j, $j = 0, 1, 2, \ldots, n+1$. Using the standard techniques from quadrature theory, the integral on the right hand of (5) can be written as

$$\int_0^{t_{n+1}} (t_{n+1}-\tau)^{\alpha-1} \tilde{g}_{n+1}(\tau)\,\mathrm{d}\tau = \frac{k^\alpha}{\alpha(\alpha+1)} \sum_{j=0}^{n+1} a_{j,n+1} g(t_j), \tag{6}$$

where

$$a_{j,n+1} = \begin{cases} n^{\alpha+1} - (n-\alpha)(n+1)^\alpha, & \text{if } j = 0, \\ (n-j+2)^{\alpha+1} + (n-j)^{\alpha+1} - 2(n-j+1)^{\alpha+1}, & \text{if } 1 \leqslant j \leqslant n, \\ 1, & \text{if } j = n+1 \end{cases} \tag{7}$$

and k is the step length, i.e., $k = t_{j+1} - t_j$. That is to numerically approximate (4) by using the corrector formula

$$y_k(t_{n+1}) = \begin{cases} y_0 + \frac{k^\alpha}{\Gamma(\alpha+2)} \left(f(y_k^{Pr}(t_1), t_1) + \alpha \cdot f(y_k(t_0), t_0) \right), & \text{if } n = 0, \\ y_0 + \frac{k^\alpha}{\Gamma(\alpha+2)} \left(f(y_k^{Pr}(t_{n+1}), t_{n+1}) + (2^{\alpha+1} - 2) \cdot f(y_k(t_n), t_n) \right) & \\ \quad + \frac{k^\alpha}{\Gamma(\alpha+2)} \sum_{j=0}^{n-1} a_{j,n+1} f(y_k(t_j), t_j), & \text{if } n \geqslant 1. \end{cases} \tag{8}$$

The remaining problem is the determination of the predictor formula used to calculate the values $x_k^{Pr}(t_1)$ and $x_k^{Pr}(t_{n+1})$. This needs to apply the numerical approximation, being different from [12,13],

$$\int_0^{t_{n+1}} (t_{n+1}-\tau)^{\alpha-1} g(\tau)\,\mathrm{d}\tau \approx \int_0^{t_n} (t_{n+1}-\tau)^{\alpha-1} \tilde{g}_n(\tau)\,\mathrm{d}\tau + \int_{t_n}^{t_{n+1}} (t_{n+1}-\tau)^{\alpha-1} g(t_n)\,\mathrm{d}\tau, \tag{9}$$

where $\tilde{g}_n$ is the piecewise linear interpolation for g with nodes and knots chosen at t_j, $j = 0, 1, 2, \ldots, n$. Similarly using the standard quadrature technique, the right hand side of (9) can be recast as

$$\int_0^{t_n} (t_{n+1}-\tau)^{\alpha-1} \tilde{g}_n(\tau)\,\mathrm{d}\tau + \int_{t_n}^{t_{n+1}} (t_{n+1}-\tau)^{\alpha-1} g(t_n)\,\mathrm{d}\tau = \frac{k^\alpha}{\alpha(\alpha+1)} \sum_{j=0}^{n} b_{j,n+1} g(t_j), \tag{10}$$

where

$$b_{j,n+1} = \begin{cases} \begin{cases} a_{j,n+1}, & \text{if } 0 \leqslant j \leqslant n-1, \\ 2^{\alpha+1} - 1, & \text{if } j = n, \end{cases} & \text{if } n > 0, \\ b_{0,1} = \alpha + 1, & \text{if } n = 0. \end{cases} \tag{11}$$

So the predictor formula for the numerical approximation of (4) is

$$y_k^{Pr}(t_{n+1}) = \begin{cases} y_0 + \frac{k^\alpha}{\Gamma(\alpha+1)} f(y_k(t_0), t_0), & \text{if } n = 0, \\ y_0 + \frac{k^\alpha}{\Gamma(\alpha+2)} \cdot (2^{\alpha+1} - 1) \cdot f(y_k(t_n), t_n) & \\ \quad + \frac{k^\alpha}{\Gamma(\alpha+2)} \sum_{j=0}^{n-1} a_{j,n+1} f(y_k(t_j), t_j), & \text{if } n \geqslant 1. \end{cases} \tag{12}$$

Combining (8) and (12), the new version predictor–corrector approach for solving (3) is got, which has numerical accuracy $O(k^{\min\{1+2\alpha,2\}})$, for details, see the Appendix A. Comparing with the original version, the present predictor–corrector approach has two benefits: 1. for the predictor formula, the numerical approximation is more accurate since the product trapezoidal quadrature rule is used instead of the product rectangle one for the integral in the interval $[0,t_n]$, and finally the numerical accuracy is improved from $O(k^{\min\{1+\alpha,2\}})$ to $O(k^{\min\{1+2\alpha,2\}})$, 2. almost half of the computational cost is reduced because the most expensive computation $\sum_{j=0}^{n-1} a_{j,n+1} f(y_k(t_j),t_j)$ just need to be computed one times rather than two times. Since fractional derivatives are non-local operators, the computational cost for (3) becomes $O(n^2)$ where n is the number of points used to compute. But based on the short memory principle of fractional derivatives, it is possible to reduce the computational cost to $O(n\log n)$ [6,14].

3. Numerical algorithm for the time fractional Fokker–Planck equation

Combining the predictor–corrector approach with the idea of method of lines, the numerical scheme for (2) is devised and evaluated in this section. First rewrite (2) and present the initial and boundary conditions to (2) as follows:

$$D_*^\alpha P(x,t) = \frac{U''(x)}{\eta_\alpha} P(x,t) + \frac{U'(x)}{\eta_\alpha}\frac{\partial}{\partial x} P(x,t) + \kappa_\alpha \frac{\partial^2}{\partial x^2} P(x,t), \quad x \in (c,d),\ t \in \mathbb{R}^+, \tag{13}$$

$$P(x,0) = \psi(x), \quad x \in [c,d], \tag{14}$$

$$P(c,t) = \varphi_1(t), \quad P(d,t) = \varphi_2(t),\ t \geqslant 0, \tag{15}$$

where $\varphi_1(t), \varphi_2(t),$ and $\psi(x)$ are given functions.

Using the second-order accuracy finite difference scheme to discretize the spatial derivatives $\frac{\partial}{\partial x}$ and $\frac{\partial^2}{\partial x^2}$, and taking the space step length h, (13) can be cast into the following fractional ordinary differential equation

$$\begin{aligned} D_*^\alpha P(x,t) &= \frac{U''(x)}{\eta_\alpha} P(x,t) + \frac{1}{2h}\frac{U'(x)}{\eta_\alpha}\cdot(P(x+h,t) - P(x-h,t)) + \frac{\kappa_\alpha}{h^2}\cdot(P(x+h,t) - 2P(x,t) + P(x-h,t)) \\ &= \left(\frac{\kappa_\alpha}{h^2} - \frac{1}{2h}\frac{U'(x)}{\eta_\alpha}\right)\cdot P(x-h,t) + \left(\frac{U''(x)}{\eta_\alpha} - \frac{2\kappa_\alpha}{h^2}\right)\cdot P(x,t) + \left(\frac{1}{2h}\frac{U'(x)}{\eta_\alpha} + \frac{\kappa_\alpha}{h^2}\right)\cdot P(x+h,t). \end{aligned} \tag{16}$$

Hereafter, denote $x_i = c + ih$, $x_0 = c$, and $x_{L=\frac{(d-c)}{h}} = d$. Based on the predictor–corrector approach for numerical solving fractional ordinary differential equation in the last section and the idea of method of lines, the computational scheme for (16) with initial and boundary conditions (14) and (15) is devised as follow.

The starting (first) predictor step is

$$\begin{cases} P_{h,k}^{Pr}(x_i,t_1) = \psi(x_i) + \frac{k^\alpha}{\Gamma(\alpha+1)}\cdot\left(\left(\frac{\kappa_\alpha}{h^2} - \frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}\right)\cdot\psi(x_{i-1})\left(\frac{U''(x_i)}{\eta_\alpha} - \frac{2\kappa_\alpha}{h^2}\right)\cdot\psi(x_i)\right. \\ \qquad\qquad \left. + \left(\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha} + \frac{\kappa_\alpha}{h^2}\right)\cdot\psi(x_{i+1})\right); \end{cases} \tag{17}$$

where $i = 1,2,\ldots,L-1$.

The starting (first) corrector step has

$$\begin{cases} P_{h,k}(x_i,t_1) = \psi(x_i) + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{\kappa_\alpha}{h^2} - \frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}\right)\cdot\left(P_{h,k}^{Pr}(x_{i-1},t_1) + \alpha\cdot\psi(x_{i-1})\right) \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{U''(x_i)}{\eta_\alpha} - \frac{2\kappa_\alpha}{h^2}\right)\cdot(P_{h,k}^{Pr}(x_i,t_1) + \alpha\cdot\psi(x_i)) \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha} + \frac{\kappa_\alpha}{h^2}\right)\cdot(P_{h,k}^{Pr}(x_{i+1},t_1) + \alpha\cdot\psi(x_{i+1})); \end{cases} \tag{18}$$

where $i = 1,2,\ldots,L-1$, $P_{h,k}^{Pr}(x_0,t_1) = \varphi_1(t_1)$, and $P_{h,k}^{Pr}(x_L,t_1) = \varphi_2(t_1)$.

The remaining predictor and corrector steps are given as follows. First, some temporary variables that need to be computed are: $\text{temp}_0 = \sum_{j=0}^{n-1} a_{j,n+1}\varphi_1(t_j)$; $\text{temp}_i = \sum_{j=0}^{n-1} a_{j,n+1}P_{h,k}(x_i,t_j)$, $i = 1,2,\ldots,L-1$; $\text{temp}_L = \sum_{j=0}^{n-1} a_{j,n+1}\varphi_2(t_j)$.

The remaining predictor steps have

$$\begin{cases} P^{Pr}_{h,k}(x_i,t_{n+1}) = \psi(x_i) + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot(2^{\alpha+1}-1)\cdot\left(\frac{\kappa_\alpha}{h^2}-\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}\right)\cdot P_{h,k}(x_{i-1},t_n) \\ \qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot(2^{\alpha+1}-1)\cdot\left(\frac{U''(x_i)}{\eta_\alpha}-\frac{2\kappa_\alpha}{h^2}\right)\cdot P_{h,k}(x_i,t_n) \\ \qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot(2^{\alpha+1}-1)\cdot\left(\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}+\frac{\kappa_\alpha}{h^2}\right)\cdot P_{h,k}(x_{i+1},t_n) \\ \qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{\kappa_\alpha}{h^2}-\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}\right)\cdot\text{temp}_{i-1}\,\frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{U''(x_i)}{\eta_\alpha}-\frac{2\kappa_\alpha}{h^2}\right)\cdot\text{temp}_i \\ \qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}+\frac{\kappa_\alpha}{h^2}\right)\cdot\text{temp}_{i+1}; \end{cases} \tag{19}$$

where $i = 1,2,\ldots,L-1$, $P_{h,k}(x_0,t_n) = \varphi_1(t_n)$, and $P_{h,k}(x_L,t_n) = \varphi_2(t_n)$.

The remaining corrector steps are

$$\begin{cases} P_{h,k}(x_i,t_{n+1}) = \psi(x_i) + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{\kappa_\alpha}{h^2}-\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}\right)\cdot(P^{Pr}_{h,k}(x_{i-1},t_{n+1})+(2^{\alpha+1}-2)\cdot P_{h,k}(x_{i-1},t_n)) \\ \qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{U''(x_i)}{\eta_\alpha}-\frac{2\kappa_\alpha}{h^2}\right)\cdot(P^{Pr}_{h,k}(x_i,t_{n+1})+(2^{\alpha+1}-2)\cdot P_{h,k}(x_i,t_n)) \\ \qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}+\frac{\kappa_\alpha}{h^2}\right)\cdot\left(P^{Pr}_{h,k}(x_{i+1},t_{n+1})+(2^{\alpha+1}-2)\cdot P_{h,k}(x_{i+1},t_n)\right) \\ \qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\left(\frac{\kappa_\alpha}{h^2}-\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}\right)\cdot\text{temp}_{i-1}+\left(\frac{U''(x_i)}{\eta_\alpha}-\frac{2\kappa_\alpha}{h^2}\right)\cdot\text{temp}_i\right) \\ \qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}+\frac{\kappa_\alpha}{h^2}\right)\cdot\text{temp}_{i+1}; \end{cases} \tag{20}$$

where $i = 1,2,\ldots,L-1$, $P_{h,k}(x_0,t_n) = \varphi_1(t_n)$, $P^{Pr}_{h,k}(x_0,t_{n+1}) = \varphi_1(t_{n+1})$, $P_{h,k}(x_L,t_n) = \varphi_2(t_n)$, and $P^{Pr}_{h,k}(x_L,t_{n+1}) = \varphi_2(t_{n+1})$.

Thus the description of the numerical algorithm for (13) with initial and boundary conditions (14) and (15) has been completed. In the following, we analyze the numerical stability and convergent order of the algorithm. To express (19) and (20) by matrix form, denote

$$d_{l_i} = \frac{\kappa_\alpha}{h^2}-\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha},\quad d_{c_i} = \frac{U''(x_i)}{\eta_\alpha}-\frac{2\kappa_\alpha}{h^2},\quad d_{r_i} = \frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}+\frac{\kappa_\alpha}{h^2},\quad i = 1,2,\ldots,L-1,$$

$$\mathbb{C} = \begin{pmatrix} d_{c_1} & d_{r_1} & 0 & \cdots & 0 & 0 \\ d_{l_2} & d_{c_2} & d_{r_2} & \cdots & 0 & 0 \\ & \ddots & & \ddots & \ddots & \\ 0 & 0 & \cdots & d_{l_{L-2}} & d_{c_{L-2}} & d_{r_{L-2}} \\ 0 & 0 & \cdots & 0 & d_{l_{L-1}} & d_{c_{L-1}} \end{pmatrix},\quad \mathbb{P}_{h,k}(t_n) = \begin{pmatrix} P_{h,k}(x_1,t_n) \\ P_{h,k}(x_2,t_n) \\ \vdots \\ P_{h,k}(x_{L-2},t_n) \\ P_{h,k}(x_{L-1},t_n) \end{pmatrix},$$

$$\mathbb{P}^{Pr}_{h,k}(t_n) = \begin{pmatrix} P^{Pr}_{h,k}(x_1,t_n) \\ P^{Pr}_{h,k}(x_2,t_n) \\ \vdots \\ P^{Pr}_{h,k}(x_{L-2},t_n) \\ P^{Pr}_{h,k}(x_{L-1},t_n) \end{pmatrix},\quad \Phi = \begin{pmatrix} \varphi(x_1) \\ \varphi(x_2) \\ \vdots \\ \varphi(x_{L-2}) \\ \varphi(x_{L-1}) \end{pmatrix},\quad \mathbb{F}(t_n) = \begin{pmatrix} d_{l_1}\varphi_1(t_n) \\ 0 \\ \vdots \\ 0 \\ d_{r_{L-1}}\varphi_2(t_n)) \end{pmatrix},$$

$$\mathbb{P}(t_n) = \begin{pmatrix} P(x_1,t_n) \\ P(x_2,t_n) \\ \vdots \\ P(x_{L-2},t_n) \\ P(x_{L-1},t_n) \end{pmatrix}, \quad \text{and it can be noted that } \mathbb{P}(t_0) = \mathbb{P}_{h,k}(t_0) = \Phi.$$

Now the matrix forms of (19), (20), and their integration are as follows:

$$\mathbb{P}^{Pr}_{h,k}(t_{n+1}) = \Phi + \frac{(2^{\alpha+1}-1)k^\alpha}{\Gamma(\alpha+2)}(\mathbb{C}\mathbb{P}_{h,k}(t_n) + \mathbb{F}(t_n)) + \frac{k^\alpha}{\Gamma(\alpha+2)} um_{j=0}^{n-1} a_{j,n+1}(\mathbb{C}\mathbb{P}_{h,k}(t_j) + \mathbb{F}(t_j)), \tag{19'}$$

$$\mathbb{P}_{h,k}(t_{n+1}) = \Phi + \frac{k^\alpha}{\Gamma(\alpha+2)}(\mathbb{C}\mathbb{P}^{Pr}_{h,k}(t_{n+1}) + \mathbb{F}(t_{n+1})) + \frac{k^\alpha}{\Gamma(\alpha+2)} \sum_{j=0}^{n} a_{j,n+1}(\mathbb{C}\mathbb{P}_{h,k}(t_j) + \mathbb{F}(t_j)). \tag{20'}$$

Substituting (19′) into (20′), we get

$$\begin{aligned} \mathbb{P}_{h,k}(t_{n+1}) = {} & \left(1 + \frac{k^\alpha}{\Gamma(\alpha+2)}\mathbb{C}\right)\Phi + \left(\frac{(2^{\alpha+1}-1)k^{2\alpha}}{\Gamma^2(\alpha+2)}\mathbb{C} + \frac{(2^{\alpha+1}-2)k^\alpha}{\Gamma(\alpha+2)}\right)(\mathbb{C}\mathbb{P}_{h,k}(t_n) + \mathbb{F}(t_n)) \\ & + \left(\frac{k^{2\alpha}\mathbb{C}}{\Gamma^2(\alpha+2)} + \frac{k^\alpha}{\Gamma(\alpha+2)}\right)\sum_{j=0}^{n-1} a_{j,n+1}(\mathbb{C}\mathbb{P}_{h,k}(t_j) + \mathbb{F}(t_j)) + \frac{k^\alpha \mathbb{F}(t_{n+1})}{\Gamma(\alpha+2)}. \end{aligned} \tag{21}$$

Assume matrix $\mathbb{C}$ can be diagonalized, then the necessary and sufficient condition for the stability of computational scheme (21) is:

$$\left|\frac{(2^{\alpha+1}-1)k^{2\alpha}}{\Gamma^2(\alpha+2)}\lambda_i^2 + \frac{(2^{\alpha+1}-2)k^\alpha}{\Gamma(\alpha+2)}\lambda_i\right| \leqslant 1, \tag{22}$$

where $\lambda_i,\ i = 1,2,\ldots,L-1$ are the eigenvalues of $\mathbb{C}$.

In view of Gerschgorin Circle Theorem, $|\lambda_i| \leqslant |d_{l_i}| + |d_{c_i}| + |d_{r_i}|$. So we have the following theorem.

Theorem 3.1. *Assume matrix $\mathbb{C}$ can be diagonalized, the numerical algorithm (17)–(20) (or (21)) for (13) is stable if*

$$\left(\frac{(2^{\alpha+1}-1)k^{2\alpha}}{\Gamma^2(\alpha+2)\tilde{h}^4} + \frac{(2^{\alpha+1}-2)k^\alpha}{\Gamma(\alpha+2)\tilde{h}^2}\right) \leqslant 1,$$

where $1/\tilde{h}^2 = \max_{i=1,2,\ldots,L-1}\{|d_{l_i}| + |d_{c_i}| + |d_{r_i}|\}$.

Remark 3.1. Assume $U''(x)/\eta_\alpha (x \in [c,d])$ is bounded, then the numerical algorithm (17)–(20) is stable if

$$\frac{k^\alpha}{h^2} < C,$$

where C is a suitable constant.

Theorem 3.2. *Let the computational scheme satisfy (22) and assume $D^\alpha_* P(\cdot,t) \in C^2[0,T]$ for some suitable T, then*

$$\max_{i=0,1,\ldots,L;n=0,1,\ldots,N} |P(x_i,t_n) - P_{h,k}(x_i,t_n)| = \mathrm{O}(k^{\min\{1+2\alpha,2\}}) + \mathrm{O}(h^2),$$

where N is the number of steps which are computed in the time direction.

Proof. We will prove that for sufficiently small k and h,

$$\|\mathbb{P}(t_j) - \mathbb{P}_{h,k}(t_j)\| < C_1 k^{\min\{1+2\alpha,2\}} + C_2 h^2 \tag{23}$$

for all $j \in \{0, 1, \cdots, N\}$, where $\|\mathbb{P}(t_j) - \mathbb{P}_{h,k}(t_j)\| = \max_{i=0,1,\ldots,L}|P(x_i, t_j) - P_{h,k}(x_i, t_j)|$, C_1 and C_2 are suitable constants. Assume that (23) holds for $j = 0, 1, \ldots, n$, $n \leqslant N-1$, we prove the inequality is true for $j = n+1$, some of the following estimations are similar to the estimations in Appendix A, so the details are omitted. The error of predictor $\mathbb{P}^{Pr}_{h,k}(t_{n+1})$ can be found that

$$
\begin{aligned}
&\|\mathbb{P}(t_{n+1}) - \mathbb{P}^{Pr}_{h,k}(t_{n+1})\| \\
&\quad = \frac{1}{\Gamma(\alpha)}\left\| \int_0^{t_{n+1}} (t_{n+1}-\tau)^{\alpha-1}(\mathbb{C}\mathbb{P}(\tau) + \mathbb{F}(\tau) + \mathrm{O}(h^2))\,\mathrm{d}\tau - \frac{k^\alpha}{\alpha(\alpha+1)}\sum_{j=0}^{n} b_{j,n+1}(\mathbb{C}\mathbb{P}_{h,k}(t_j) + \mathbb{F}(t_j))\right\| \\
&\quad \leqslant \frac{1}{\Gamma(\alpha)}\left\| \int_0^{t_{n+1}} (t_{n+1}-\tau)^{\alpha-1}(\mathbb{C}\mathbb{P}(\tau) + \mathbb{F}(\tau) + \mathrm{O}(h^2))\,\mathrm{d}\tau - \frac{k^\alpha}{\alpha(\alpha+1)}\sum_{j=0}^{n} b_{j,n+1}(\mathbb{C}\mathbb{P}(t_j) + \mathbb{F}(t_j))\right\| \\
&\qquad + \frac{1}{\Gamma(\alpha)}\left\| \frac{k^\alpha}{\alpha(\alpha+1)}\sum_{j=0}^{n} b_{j,n+1}(\mathbb{C}\mathbb{P}(t_j) + \mathbb{F}(t_j)) - \frac{k^\alpha}{\alpha(\alpha+1)}\sum_{j=0}^{n} b_{j,n+1}(\mathbb{C}\mathbb{P}_{h,k}(t_j) + \mathbb{F}(t_j))\right\| \\
&\quad \leqslant (\widetilde{C}_1 k^{1+\alpha} + \mathrm{O}(h^2)) + (\widetilde{C}_2 k^{1+2\alpha} + \widetilde{C}_3 h^2) \leqslant \widetilde{C}_3 k^{1+\alpha} + \widetilde{C}_4 h^2. \qquad (24)
\end{aligned}
$$

On the basis of the error bound (24) for the predictor, the corrector error is argued as

$$
\begin{aligned}
&\|\mathbb{P}(t_{n+1}) - \mathbb{P}_{h,k}(t_{n+1})\| \\
&\quad = \frac{1}{\Gamma(\alpha)}\left\| \int_0^{t_{n+1}} (t_{n+1}-\tau)^{\alpha-1}(\mathbb{C}\mathbb{P}(\tau) + \mathbb{F}(\tau) + \mathrm{O}(h^2))\,\mathrm{d}\tau - \frac{k^\alpha}{\alpha(\alpha+1)}\sum_{j=0}^{n} a_{j,n+1}(\mathbb{C}\mathbb{P}_{h,k}(t_j) + \mathbb{F}(t_j))\right. \\
&\qquad \left. - \frac{k^\alpha}{\alpha(\alpha+1)}\left(\mathbb{C}\mathbb{P}^{Pr}_{h,k}(t_{n+1}) + \mathbb{F}(t_n)\right)\right\| \\
&\quad \leqslant \frac{1}{\Gamma(\alpha)}\left\| \int_0^{t_{n+1}} (t_{n+1}-\tau)^{\alpha-1}(\mathbb{C}\mathbb{P}(\tau) + \mathbb{F}(\tau) + \mathrm{O}(h^2))\,\mathrm{d}\tau - \frac{k^\alpha}{\alpha(\alpha+1)}\sum_{j=0}^{n+1} a_{j,n+1}(\mathbb{C}\mathbb{P}(t_j) + \mathbb{F}(t_j))\right\| \\
&\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\sum_{j=0}^{n} a_{j,n+1}\left\|\mathbb{C}\mathbb{P}(t_j) - \mathbb{C}\mathbb{P}_{h,k}(t_j)\right\| + \frac{k^\alpha}{\Gamma(\alpha+2)}\left\|\mathbb{C}\mathbb{P}(t_{n+1}) - \mathbb{C}\mathbb{P}^{Pr}_{h,k}(t_{n+1})\right\| \\
&\quad \leqslant (\widetilde{C}_5 k^2 + \mathrm{O}(h^2)) + (\widetilde{C}_6 k^{1+2\alpha} + \widetilde{C}_7 h^2) + (\widetilde{C}_8 k^{1+2\alpha} + \widetilde{C}_9 k^\alpha h^2) \leqslant C_1 k^{\min\{1+2\alpha,2\}} + C_2 h^2.
\end{aligned}
$$

The proof is complete. □

Remark 3.2. The computational scheme (17)–(20) can be changed to the version presented in Appendix B.

Remark 3.3. Our algorithm has an $\mathrm{O}(LN^2)$ arithmetic complexity because of the non-local property of fractional derivatives. As being pointed out in the preliminary section, based on the short memory principle of fractional derivatives it is possible to reduce the computation cost to $\mathrm{O}(LN\log N)$, for more details, the reader can refer to [6,14].

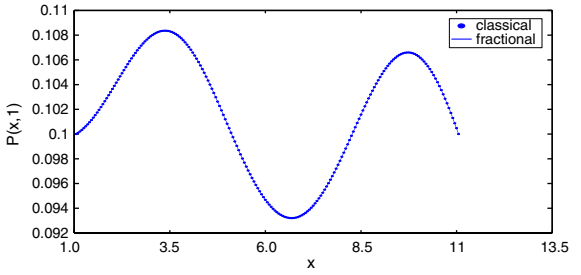


Fig. 1. The comparison of numerical solutions of our algorithm with the ones of directly discretizing the corresponding classical Fokker–Planck equation, where '·' stands for the solution of directly discretizing the classical equation and '—' stands for the solution of this paper's algorithm with $\alpha = 1.0$. The parameter values $h = 0.05$, $k = 0.0001$, and $N = 10000$ are taken in these two algorithms.

4. Effectiveness of numerical algorithm

We first take smooth initial and boundary conditions to verify our theoretical analysis, then simulate the real physical cases with initial δ distribution.

The numerical solutions of Eq. (13) with initial and boundary conditions (14) and (15) are considered with

$$U(x) = \cos x - Fx, \quad F = 6, \quad \eta_\alpha = 6, \quad \kappa_\alpha = 2, \quad c = 1, \quad d = 11, \quad \psi(x) \equiv 0.10, \quad \varphi_1(t) \equiv 0.10, \quad \varphi_2(t) \equiv 0.10.$$

Using above parameter values, Fig. 1 shows the comparison of the numerical results for our algorithm, choosing $\alpha = 1.0$, with the counterpart of directly discretizing the corresponding classical Fokker–Planck equation. Here we suppose the numerical solution with $k = 0.000015$ and $h = 0.03125$ is exactly equals to the analytical solution $P(x_i, t_n)$. Table 4.1 includes numerical calculations for $\alpha = 0.8,\ k = 0.000015,$ and $T = 0.3$ with different space step sizes which support the predicted order of convergence in space, and in Table 4.2 we take $\alpha = 0.8,\ h = 0.0625,\ T = 0.3$, and use different time step sizes, the numerical results show the error induced in the time discretization is immerged by the error aroused in the space discretization for ensuring the stability of the numerical scheme.

To simulate the real physical systems with absorbing boundary conditions, we take the values of parameters as (the initial condition is δ distribution)

$$U(x) = \cos x - Fx,\ F = 6,\ \eta_\alpha = 6,\ \kappa_\alpha = 2,\ c = -2.8,\ d = 3.2,\ \psi(x) = \delta(x - 0.2),\ \varphi_1(t) = \varphi_2(t) \equiv 0.$$

Fig. 2 displays the results with fractional order $\alpha = 0.4,\ 0.5,\ 0.6,\ 0.7,\ 0.8,\ 0.9,\ 1.0$, respectively, as it can be seen that the cusps are appeared for the non-classical cases: $\alpha \neq 1.0$, and when α becomes smaller the decay grows slower.

5. Conclusions

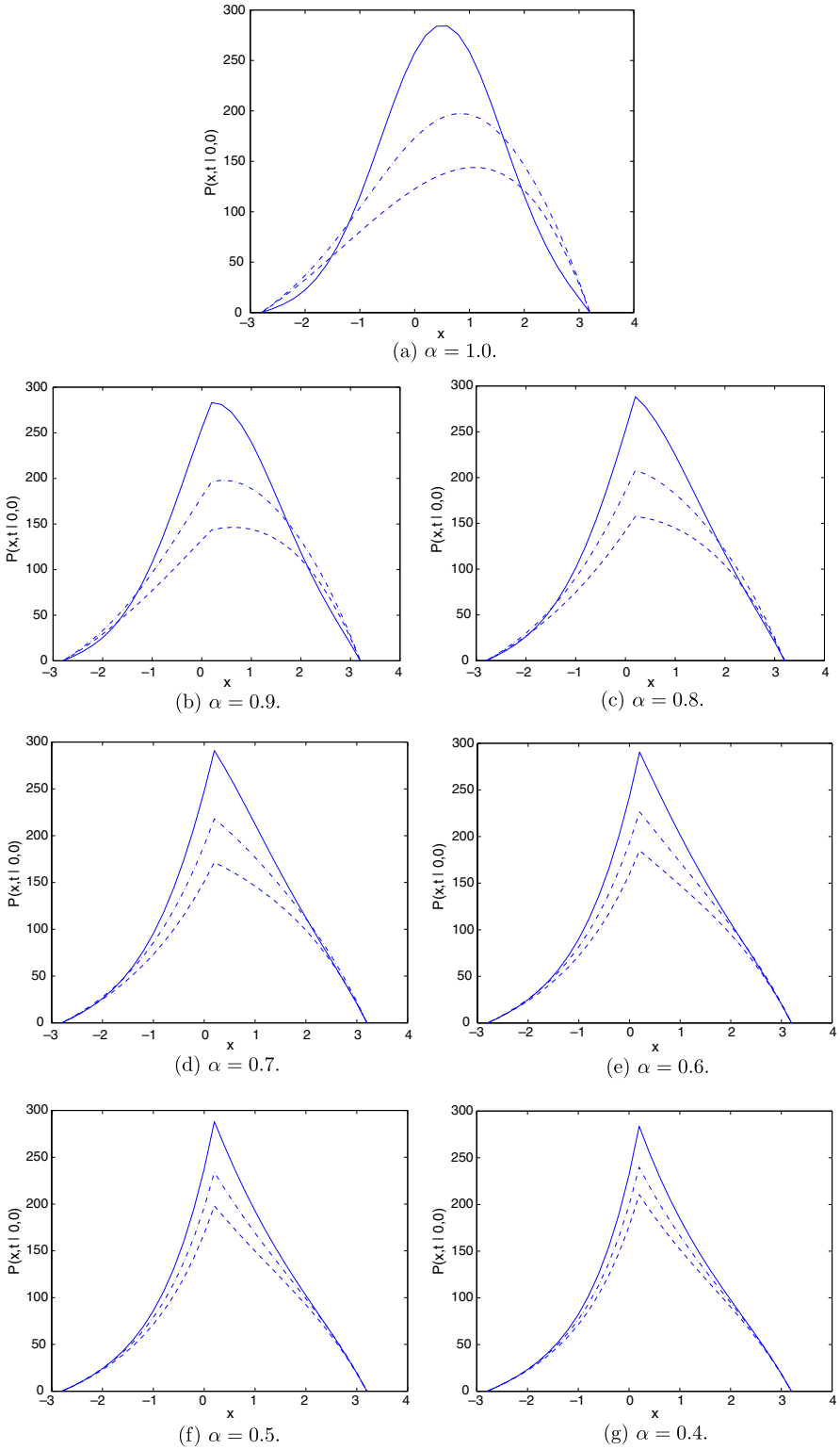
In this paper, a numerical algorithm for solving time fractional Fokker–Planck equation has been described and demonstrated. First based on the properties of Riemann–Liouville derivative and Caputo derivative, the original time fraction Fokker–Planck equation with Riemann–Liouville derivative is transformed into a FODE with time Caputo derivative, then combining the fractional predictor–corrector approach with the idea of method of lines, the numerical scheme is designed and its numerical stability condition and convergent rate are rigorously proved. This algorithm has been tested against the time fractional Fokker–Planck equation with $\alpha = 1.0$. Good agreement between the numerical solutions of this algorithm and the ones of directly discretizing the classical Fokker–Planck equation has been noted. Some numerical results for several different fractional

Table 4.1
Experimental results for $\alpha = 0.8$, $k = 0.000015$, and $T = 0.3$

h	$\max_{i=0,1,\ldots,L}\lvert P(x_i, 0.3) - P_{h,k}(x_i, 0.3)\rvert$	Convergent rate
1.0000	0.0352	
0.5000	0.0088	2.0000
0.2500	0.0022	2.0000
0.1250	5.1969×10^{-4}	2.0818
0.0625	1.0394×10^{-4}	2.3219

Table 4.2
Experimental results for $\alpha = 0.8$, $h = 0.0625$, and $T = 0.3$

k	$\max_{i=0,1,\ldots,L}\lvert P(x_i, 0.3) - P_{h,k}(x_i, 0.3)\rvert$
0.00012	2.0425×10^{-4}
0.00006	1.4622×10^{-4}
0.00003	1.1795×10^{-4}
0.000015	1.0394×10^{-4}



(a) $\alpha = 1.0$.

(b) $\alpha = 0.9$.

(c) $\alpha = 0.8$.

(d) $\alpha = 0.7$.

(e) $\alpha = 0.6$.

(f) $\alpha = 0.5$.

(g) $\alpha = 0.4$.

Fig. 2. The evolution of $P(x, t|0.2, 0)$ with absorbing boundary conditions, where the solid line '—' stands for the solution when $t = 0.3$, the dashdot line '–·–' stands for the solution when $t = 0.6$, and the dashed line '– –' stands for the solution when $t = 1.0$.

orders have also been displayed and compared with each other. Moreover, the convergent rate in the space direction is confirmed by the numerical calculations and it should especially be noted that for ensuring the numerical scheme's stability the error aroused in time discretization is immerged by the error in the space discretization. At last but not the least, the algorithm of this paper can be easily extended to the general time fractional partial differential equation that can be converted into a system of FODE with time Caputo derivatives.

Acknowledgments

The author wishes to express his sincere thanks for Professor P. Degond and the reviewers' constructive suggestions.

Appendix A

First, we prove the approximation accuracy of (9). Using the Mean Value Theorem of differential calculus, we have the quadrature error of the second term of the right hand side of (9),

$$\left|\int_{t_n}^{t_{n+1}}(t_{n+1}-\tau)^{\alpha-1}(g(\tau)-g(t_n))\,\mathrm{d}\tau\right| \leqslant \|g'\|_\infty \int_{t_n}^{t_{n+1}}(t_{n+1}-\tau)^{\alpha-1}(\tau-t_n)\,\mathrm{d}\tau = \frac{\|g'\|_\infty}{\alpha(\alpha+1)}k^{\alpha+1} \tag{25}$$

and for the quadrature error of the first term, we derive

$$\begin{aligned}
&\left|\int_0^{t_n}(t_{n+1}-\tau)^{\alpha-1}(g(\tau)-\tilde{g}_n(\tau))\,\mathrm{d}\tau\right| \leqslant \frac{\|g''\|}{2}\sum_{j=1}^{n}\int_{t_{j-1}}^{t_j}(t_{n+1}-\tau)^{\alpha-1}(t_j-\tau)(\tau-t_{j-1})\,\mathrm{d}\tau.\\
&= \frac{\|g''\|k^{\alpha+2}}{2\alpha(\alpha+1)}\sum_{j=1}^{n}\left((n-j+2)^{\alpha+1}+(n-j+1)^{\alpha+1}+\frac{2}{\alpha+2}\left((n-j+1)^{\alpha+2}-(n-j+2)^{\alpha+2}\right)\right)\\
&= \frac{\|g''\|k^{\alpha+2}}{2\alpha(\alpha+1)}\left(\sum_{j=1}^{n}((j+1)^{\alpha+1}+j^{\alpha+1})+\frac{2}{\alpha+2}(1-(n+1)^{\alpha+2})\right)\\
&= \frac{\|g''\|k^{\alpha+2}}{2\alpha(\alpha+1)}\left(2\int_1^{n+1}\tau^{\alpha+1}\,\mathrm{d}\tau-\sum_{j=1}^{n}\left((j+1)^{\alpha+1}+j^{\alpha+1}\right)\right) \leqslant \begin{cases}\frac{\|g''\|k^{\alpha+2}}{24}\sum_{j=1}^{n}j^{\alpha-1}, & \text{if } \alpha<1,\\ \frac{\|g''\|k^{\alpha+2}}{24}\sum_{j=1}^{n}(j+1)^{\alpha-1}, & \text{if } \alpha\geqslant 1\end{cases}\\
&\leqslant \begin{cases}\frac{\|g''\|k^{\alpha+2}}{24}\int_0^n\tau^{\alpha-1}\,\mathrm{d}\tau, & \text{if } \alpha<1,\\ \frac{\|g''\|k^{\alpha+2}}{24}\int_2^{n+2}\tau^{\alpha-1}\,\mathrm{d}\tau, & \text{if } \alpha\geqslant 1\end{cases} \leqslant Ck^2,
\end{aligned} \tag{26}$$

where C is a constant.

So, the approximation accuracy of (9) is $\mathrm{O}(k^{\min\{1+\alpha,2\}})$. Now in view of Theorem 2.5 and Lemma 3.1 of [13], we get the following theorem.

Theorem A. *For the fractional initial value problem*

$$D_*^\alpha y(t) = f(t,y(t)), \quad y^{(i)}(0)=y_0^{(i)}, \quad i=0,1,\ldots,\lceil\alpha\rceil-1,$$

assume $D_*^\alpha y \in C^2[0,T]$ *for some suitable* T, *then*

$$\max_{0\leqslant j\leqslant N}|y(t_j)-y_j| = \begin{cases}\mathrm{O}(k^2), & \text{if } \alpha\geqslant 0.5,\\ \mathrm{O}(k^{1+2\alpha}), & \text{if } 0<\alpha<0.5.\end{cases}$$

Appendix B

The computational scheme (17)–(20) is changed, maybe improved, under the guidelines: the product trapezoidal formula is used rather than the product rectangle formula, and the updating value obtained from corrector formula is applied in place of the value computed from predictor formula. It appears below.

The starting (first) predictor step is

$$\begin{cases} P^{Pr}_{h,k}(x_i,t_1) = \psi(x_i) + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{\kappa_\alpha}{h^2} - \frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}\right)\cdot\left(P^{Pr}_{h,k}(x_{i-1},t_1) + \alpha\cdot\psi(x_{i-1})\right) \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+1)}\cdot\left(\left(\frac{U''(x_i)}{\eta_\alpha} - \frac{2\kappa_\alpha}{h^2}\right)\cdot\psi(x_i) + \left(\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha} + \frac{\kappa_\alpha}{h^2}\right)\cdot\psi(x_{i+1})\right); \\ P^{Pr}_{h,k}(x_{L-1},t_1) = \psi(x_{L-1}) + \frac{k^\alpha}{\Gamma(\alpha+1)}\cdot\left(\frac{U''(x_{L-1})}{\eta_\alpha} - \frac{2\kappa_\alpha}{h^2}\right)\cdot\psi(x_{L-1}) \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{\kappa_\alpha}{h^2} - \frac{1}{2h}\frac{U'(x_{L-1})}{\eta_\alpha}\right)\cdot\left(P^{Pr}_{h,k}(x_{L-2},t_1) + \alpha\cdot\psi(x_{L-2})\right) \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{1}{2h}\frac{U'(x_{L-1})}{\eta_\alpha} + \frac{\kappa_\alpha}{h^2}\right)\cdot(\varphi_2(t_1) + \alpha\cdot\varphi_2(0)); \end{cases}$$

where $i = 1,2,\ldots,L-2$, and $P^{Pr}_{h,k}(x_0,t_1) = \varphi_1(t_1)$.

The starting (first) corrector step has

$$\begin{cases} P_{h,k}(x_i,t_1) = \psi(x_i) + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{\kappa_\alpha}{h^2} - \frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}\right)\cdot\left(P_{h,k}(x_{i-1},t_1) + \alpha\cdot\psi(x_{i-1})\right) \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{U''(x_i)}{\eta_\alpha} - \frac{2\kappa_\alpha}{h^2}\right)\cdot\left(P^{Pr}_{h,k}(x_i,t_1) + \alpha\cdot\psi(x_i)\right) \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha} + \frac{\kappa_\alpha}{h^2}\right)\cdot\left(P^{Pr}_{h,k}(x_{i+1},t_1) + \alpha\cdot\psi(x_{i+1})\right); \end{cases}$$

where $i = 1,2,\ldots,L-1$, $P_{h,k}(x_0,t_1) = \varphi_1(t_1)$, and $P^{Pr}_{h,k}(x_L,t_1) = \varphi_2(t_1)$.

The remaining predictor and corrector steps are given as follows. The remaining corrector steps are

$$\begin{cases} P_{h,k}(x_i,t_{n+1}) = \psi(x_i) + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{\kappa_\alpha}{h^2} - \frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}\right) \\ \qquad\qquad \cdot\left(P_{h,k}(x_{i-1},t_{n+1}) + (2^{\alpha+1}-2)\cdot P_{h,k}(x_{i-1},t_n)\right) \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{U''(x_i)}{\eta_\alpha} - \frac{2\kappa_\alpha}{h^2}\right)\cdot\left(P^{Pr}_{h,k}(x_i,t_{n+1}) + (2^{\alpha+1}-2)\cdot P_{h,k}(x_i,t_n)\right) \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha} + \frac{\kappa_\alpha}{h^2}\right)\cdot\left(P^{Pr}_{h,k}(x_{i+1},t_{n+1}) + (2^{\alpha+1}-2)\cdot P_{h,k}(x_{i+1},t_n)\right) \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\left(\frac{\kappa_\alpha}{h^2} - \frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}\right)\cdot\mathrm{temp}_{i-1} + \left(\frac{U''(x_i)}{\eta_\alpha} - \frac{2\kappa_\alpha}{h^2}\right)\cdot\mathrm{temp}_i\right) \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha} + \frac{\kappa_\alpha}{h^2}\right)\cdot\mathrm{temp}_{i+1}; \end{cases}$$

where $i = 1,2,\ldots,L-1$, $P_{h,k}(x_0,t_n) = \varphi_1(t_n)$, $P_{h,k}(x_0,t_{n+1}) = \varphi_1(t_{n+1})$, $P_{h,k}(x_L,t_n) = \varphi_2(t_n)$, and $P^{Pr}_{h,k}(x_L,t_{n+1}) = \varphi_2(t_{n+1})$.

The remaining predictor steps have

$$\begin{cases} P^{Pr}_{h,k}(x_i,t_{n+1}) = \psi(x_i) + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{\kappa_\alpha}{h^2} - \frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}\right)\cdot\left(P^{Pr}_{h,k}(x_{i-1},t_{n+1}) + (2^{\alpha+1}-2)\cdot P_{h,k}(x_{i-1},t_n)\right) \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot(2^{\alpha+1}-1)\cdot\left(\frac{U''(x_i)}{\eta_\alpha} - \frac{2\kappa_\alpha}{h^2}\right)\cdot P_{h,k}(x_i,t_n) + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot(2^{\alpha+1}-1)\cdot\left(\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha} + \frac{\kappa_\alpha}{h^2}\right) \\ \qquad\qquad \cdot P_{h,k}(x_{i+1},t_n) + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\left(\frac{\kappa_\alpha}{h^2} - \frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha}\right)\cdot\mathrm{temp}_{i-1} + \left(\frac{U''(x_i)}{\eta_\alpha} - \frac{2\kappa_\alpha}{h^2}\right)\cdot\mathrm{temp}_i\right) \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{1}{2h}\frac{U'(x_i)}{\eta_\alpha} + \frac{\kappa_\alpha}{h^2}\right)\cdot\mathrm{temp}_{i+1}; \\ P^{Pr}_{h,k}(x_{L-1},t_{n+1}) = \psi(x_{L-1}) + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{\kappa_\alpha}{h^2} - \frac{1}{2h}\frac{U'(x_{L-1})}{\eta_\alpha}\right)\cdot\left(P^{Pr}_{h,k}(x_{L-2},t_{n+1}) + (2^{\alpha+1}-2)\cdot P_{h,k}(x_{L-2},t_n)\right) \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot(2^{\alpha+1}-1)\cdot\left(\frac{U''(x_{L-1})}{\eta_\alpha} - \frac{2\kappa_\alpha}{h^2}\right)\cdot P(x_{L-1},t_n) + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{1}{2h}\frac{U'(x_{L-1})}{\eta_\alpha} + \frac{\kappa_\alpha}{h^2}\right) \\ \qquad\qquad \cdot(\varphi_2(t_{n+1}) + (2^{\alpha+1}-2)\cdot\varphi_2(t_n)) + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{\kappa_\alpha}{h^2} - \frac{1}{2h}\frac{U'(x_{L-1})}{\eta_\alpha}\right)\cdot\mathrm{temp}_{L-2} \\ \qquad\qquad + \frac{k^\alpha}{\Gamma(\alpha+2)}\left(\frac{U''(x_{L-1})}{\eta_\alpha} - \frac{2\kappa_\alpha}{h^2}\right)\cdot\mathrm{temp}_{L-1} + \frac{k^\alpha}{\Gamma(\alpha+2)}\cdot\left(\frac{1}{2h}\frac{U'(x_{L-1})}{\eta_\alpha} + \frac{\kappa_\alpha}{h^2}\right)\cdot\mathrm{temp}_L; \end{cases}$$

where $i = 1,2,\ldots,L-2, P^{Pr}_{h,k}(x_0,t_{n+1}) = \varphi_1(t_{n+1})$, and $P_{h,k}(x_0,t_n) = \varphi_1(t_n)$.

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