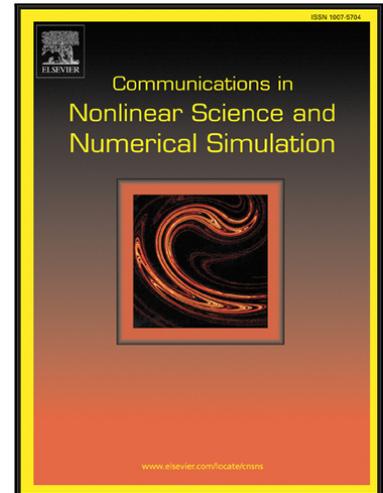


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Highlights

- Model that consists on the time-space fractional Fokker-Planck equation with time dependent coefficients.
- Numerical method for the equation that takes in consideration:
 - (a) Time dependent coefficients;
 - (b) Regularity of the solution.

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Numerical solution of a time-space fractional Fokker Planck equation with variable force field and diffusion

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Abstract

We present a numerical method to solve a time-space fractional Fokker-Planck equation with a space-time dependent force field $F(x, t)$, and diffusion $d(x, t)$. When the problem being modelled includes time dependent coefficients, the time fractional operator, that typically appears on the right hand side of the fractional equation, should not act on those coefficients and consequently the differential equation can not be simplified using the standard technique of transferring the time fractional operator to the left hand side of the equation. We take this into account when deriving the numerical method. Discussions on the unconditional stability and accuracy of the method are presented, including results that show the order of convergence is affected by the regularity of solutions. The numerical experiments confirm that the convergence of the method is second order in time and space for sufficiently regular solutions and they also illustrate how the order of convergence can depend on the regularity of the solutions. In this case, the rate of convergence can be improved by considering a non-uniform mesh.

Keywords: Fokker-Planck equation, time-dependent force field and diffusion, fractional derivatives, finite differences, Fourier analysis.

1. The model

Anomalous diffusion problems under the influence of an external force field $V'(x)$ can be described by the fractional Fokker-Planck equation [17, 18]

$$\frac{\partial u}{\partial t}(x, t) = {}_0D_t^{1-\alpha} \left[d \frac{\partial^2 u}{\partial x^2}(x, t) + \frac{\partial [V'(x)u(x, t)]}{\partial x} \right], \quad (1)$$

where $d > 0$ is the generalized diffusion coefficient and the operator ${}_0D_t^{1-\alpha}$ with $0 < \alpha < 1$ is the fractional Riemann-Liouville derivative defined as

$${}_0D_t^{1-\alpha} u(x, t) = \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t (t-s)^{\alpha-1} u(x, s) ds, \quad (2)$$

where $\Gamma(\cdot)$ is the Gamma function.

These equations describe the evolution in time of the probability density function of a subdiffusive process with sublinear in time mean square displacement. For $\alpha \rightarrow 1$, the standard Fokker-Planck equation is recovered. The fractional operator introduces a convolution integral with a slowly decaying power-law

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kernel, which is typical for memory effects in complex systems. The appearance of the fractional equation corresponds to the trapping events in the underlying motion of the test particle characteristic of subdiffusive dynamics [17]. In the general case of $0 < \alpha < 1$, initial conditions are strongly persistent due to the slow decay of the sticking probability of not moving, that is, one observes characteristic cusps at the location of a sharp initial probability condition, e.g., $f_0(x) = \delta(x - x_0)$ [18].

Equation (1) was first derived in [16] in the framework of continuous-time random walk with heavy-tailed waiting times and since then this equation became the standard physical equation describing subdiffusive dynamics. It can also appear written in a different form [17], such as,

$${}_0D_t^\alpha u(x, t) - \frac{t^{-\alpha}}{\Gamma(1-\alpha)} u(x, 0) = d \frac{\partial^2 u}{\partial x^2}(x, t) + \frac{\partial[V'(x)u(x, t)]}{\partial x}. \quad (3)$$

This equation is obtained by applying the fractional operator ${}_0D_t^{\alpha-1}$ on both sides of (1) and noting that

$${}_0D_t^{\alpha-1} \left(\frac{\partial}{\partial t} u(x, t) \right) = {}_0D_t^\alpha u(x, t) - \frac{t^{-\alpha}}{\Gamma(1-\alpha)} u(x, 0) \quad \text{and} \quad {}_0D_t^{\alpha-1} ({}_0D_t^{1-\alpha} u(x, t)) = u(x, t).$$

Equation (3) can also be written using the Caputo fractional derivative. This derivative is defined as

$${}^C D_t^\alpha u(x, t) := \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u}{\partial t}(x, s) (t-s)^{-\alpha} ds.$$

Since

$${}_0D_t^\alpha [u(x, t) - u(x, 0)] = {}^C D_t^\alpha u(x, t)$$

equation (3) can be written in the simplified form

$${}^C D_t^\alpha u(x, t) = d \frac{\partial^2 u}{\partial x^2}(x, t) + \frac{\partial[V'(x)u(x, t)]}{\partial x}. \quad (4)$$

A considerable number of numerical methods have been developed for this equation with and without force field as can be seen, for instance, in [1, 2, 4, 11, 25].

For the case of a time dependent external force, equation (1) has a slightly different form and it was first derived in [20]. The derivation was based on the generalized master equation with two balance conditions: the probability conservation in a given state and under transition between different states. The main difference from equation (1) lies in the fact that the time fractional operator does not act on the time-dependent force. As a result the force is not modified full-filling the physical requirement that the external time-dependent force cannot be influenced by the environment.

In recent works the time fractional Fokker-Planck equation with space and time dependent force and diffusion has been studied, such as, in [7, 13, 14], where physical and stochastic interpretations have been analyzed. In [7, 24] this type of equation has been discussed using Langevin and continuous-time random walk approaches, which clarified some of the issues addressed in [6] for time dependent coefficients. For a space-time dependent field the equation has the form

$$\frac{\partial u}{\partial t}(x, t) = d \frac{\partial^2}{\partial x^2} ({}_0D_t^{1-\alpha} u(x, t)) - \frac{\partial}{\partial x} (F(x, t) {}_0D_t^{1-\alpha} u(x, t)), \quad 0 < \alpha < 1. \quad (5)$$

A more general equation with space time dependent force and diffusion is given by

$$\frac{\partial u}{\partial t}(x, t) = \frac{\partial^2}{\partial x^2} (d(x, t) {}_0D_t^{1-\alpha} u(x, t)) - \frac{\partial}{\partial x} (F(x, t) {}_0D_t^{1-\alpha} u(x, t)) + g(x, t), \quad (6)$$

where $d(x, t) > 0$ and $g(x, t)$ is a source term. Note that the fractional operator does not act in the time dependent force and diffusion and consequently we can not return to an equation similar to (4).

In this work, we propose a numerical method for an equation that includes a time and space dependent force, but additionally to the time fractional operator it also includes a space fractional operator. Let us

define the left and right Riemann-Liouville fractional derivatives of order $1 < \beta < 2$, $-\infty \leq a < b \leq \infty$, given respectively by

$$\frac{\partial^\beta u}{\partial x^\beta}(x, t) = \frac{1}{\Gamma(2-\beta)} \frac{\partial^2}{\partial x^2} \int_a^x u(\xi, t)(x-\xi)^{1-\beta} d\xi, \quad (1 < \beta < 2) \quad (7)$$

$$\frac{\partial^\beta u}{\partial(-x)^\beta}(x, t) = \frac{(-1)^2}{\Gamma(2-\beta)} \frac{\partial^2}{\partial x^2} \int_x^b u(\xi, t)(\xi-x)^{1-\beta} d\xi, \quad (1 < \beta < 2). \quad (8)$$

The spatial fractional operator is given by

$$\nabla^\beta u = p \frac{\partial^\beta u}{\partial x^\beta} + q \frac{\partial^\beta u}{\partial(-x)^\beta}, \quad p + q = 1, \quad 1 < \beta < 2. \quad (9)$$

The more general equation we study in this work can finally be written as

$$\frac{\partial u}{\partial t}(x, t) = \nabla^\beta (d(x, t)_0 D_t^{1-\alpha} u(x, t)) - \frac{\partial}{\partial x} (F(x, t)_0 D_t^{1-\alpha} u(x, t)) + g(x, t). \quad (10)$$

2. The numerical method

In this section we present the numerical method. We first start by describing the discretisation in time that includes a discretisation of the time fractional operator. Then we discuss the discretization in space, that includes a discretisation of the spatial fractional operator.

2.1. Time discretisation

We denote the integral involved in the definition of the time fractional derivative (2) as

$$\mathcal{I}^\alpha u(x, t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} u(x, s) ds, \quad (11)$$

that is,

$${}_0 D_t^{1-\alpha} u(x, t) = \frac{\partial}{\partial t} \mathcal{I}^\alpha u(x, t).$$

We consider the time discretization $0 = t_0 < t_1 < t_2 < \dots < t_n = T$ and denote $\Delta t_n = t_n - t_{n-1}$ the non-uniform time step. The maximum step is denoted by $\Delta t = \max_n \Delta t_n$.

Integrating equation (10) over $I_n = (t_{n-1}, t_n)$, as done in [12, 26], we obtain

$$\begin{aligned} u(x, t_n) - u(x, t_{n-1}) &= \int_{I_n} \nabla^\beta \left(d(x, t) \frac{\partial}{\partial t} \mathcal{I}^\alpha u(x, t) \right) dt - \int_{I_n} \frac{\partial}{\partial x} \left(F(x, t) \frac{\partial}{\partial t} \mathcal{I}^\alpha u(x, t) \right) dt \\ &\quad + \int_{I_n} g(x, t) dt. \end{aligned} \quad (12)$$

In each interval I_n we approximate the function $d(x, t)$ and $F(x, t)$ by

$$d^{n+1/2}(x) = \frac{d(x, t_n) + d(x, t_{n-1})}{2}, \quad F^{n+1/2}(x) = \frac{F(x, t_n) + F(x, t_{n-1})}{2}.$$

We get

$$\begin{aligned}
u(x, t_n) - u(x, t_{n-1}) &\approx \int_{I_n} \frac{\partial}{\partial t} \nabla^\beta \left(d^{n+1/2}(x) \mathcal{I}^\alpha u(x, t) \right) dt \\
&\quad - \int_{I_n} \frac{\partial}{\partial t} \frac{\partial}{\partial x} \left(F^{n+1/2}(x) \mathcal{I}^\alpha u(x, t) \right) dt + \int_{I_n} g(x, t) dt, \\
&= \nabla^\beta \left(d^{n+1/2}(x) \mathcal{I}^\alpha u(x, t_n) \right) - \nabla^\beta \left(d^{n+1/2}(x) \mathcal{I}^\alpha u(x, t_{n-1}) \right) \\
&\quad - \frac{d}{dx} \left(F^{n+1/2}(x) \mathcal{I}^\alpha u(x, t_n) \right) + \frac{d}{dx} \left(F^{n+1/2}(x) \mathcal{I}^\alpha u(x, t_{n-1}) \right) \\
&\quad + \int_{I_n} g(x, t) dt.
\end{aligned}$$

Regarding time discretisation it remains to discuss how we approximate $\mathcal{I}^\alpha u(x, t_n)$. In what follows, for clarity, we omit the x and denote $\mathcal{I}^\alpha u(t_n) := \mathcal{I}^\alpha u(x, t_n)$. We consider the non-uniform time step $t_n = t_{n-1} + \Delta t_n$, $n > 0$. To compute the integral (11) we can approximate the function u by a linear spline $S^n(\tau)$, that is, a piecewise linear interpolation, whose nodes and knots are chosen at t_k , $k \leq n$, that is, by doing in a non-uniform mesh a similar approach done for uniform meshes in [3, 21, 23]. Therefore, an approximation to (11) becomes

$$I^\alpha u(t_n) = \frac{1}{\Gamma(\alpha)} \int_0^{t_n} S^n(\tau) (t_n - \tau)^{\alpha-1} d\tau, \quad (13)$$

where the spline $S^n(\tau)$ interpolates $\{u(x, t_k), k \leq n\}$ in the interval $[0, t_n]$ and is of the form

$$S^n(\tau) = \sum_{k=0}^n u(x, t_k) s_k(\tau), \quad (14)$$

with $s_k(\tau)$, in each interval $[t_{k-1}, t_{k+1}]$, for $1 \leq k \leq n-1$, given by

$$s_k(\tau) = \begin{cases} \frac{\tau - t_{k-1}}{t_k - t_{k-1}}, & t_{k-1} \leq \tau \leq t_k \\ \frac{t_{k+1} - \tau}{t_{k+1} - t_k}, & t_k \leq \tau \leq t_{k+1} \\ 0 & \text{otherwise.} \end{cases}$$

For $k=0$ in the interval $[0, t_1]$ and for $k=n$ in the interval $[t_{n-1}, t_n]$, $s_k(\tau)$ is of the form respectively

$$s_0(\tau) = \begin{cases} \frac{t_1 - \tau}{t_1 - t_0}, & t_0 \leq \tau \leq t_1 \\ 0 & \text{otherwise,} \end{cases} \quad s_n(\tau) = \begin{cases} \frac{\tau - t_{n-1}}{t_n - t_{n-1}}, & t_{n-1} \leq \tau \leq t_n \\ 0 & \text{otherwise.} \end{cases}$$

Therefore an approximation to \mathcal{I}^α , that we denote by I^α , is given by

$$I^\alpha u(t_n) = \frac{1}{\Gamma(2+\alpha)} \sum_{k=0}^n u(x, t_k) a_{n,k}, \quad n \geq 1, \quad (15)$$

where the $a_{n,k}$ are defined by

$$a_{n,0} = (1+\alpha)(t_n - t_0)^\alpha + \frac{(t_n - t_1)^{1+\alpha} - (t_n - t_0)^{1+\alpha}}{\Delta t_1}, \quad (16)$$

$$a_{n,n} = \Delta t_n^\alpha \quad (17)$$

and for $1 \leq k \leq n-1$, with $n \geq 2$,

$$a_{n,k} = \frac{\Delta t_{k+1}(t_n - t_{k-1})^{1+\alpha} - (\Delta t_k + \Delta t_{k+1})(t_n - t_k)^{1+\alpha} + \Delta t_k(t_n - t_{k+1})^{1+\alpha}}{\Delta t_k \Delta t_{k+1}}. \quad (18)$$

We assume $a_{0,0} = 0$.

Note that for $\alpha = 1$ we get

$$a_{n,0} = \Delta t_1, \quad a_{n,k} = \Delta t_k + \Delta t_{k+1}, \quad a_{n,n} = \Delta t_n$$

and the formula (15) matches the trapezian rule to approximate the integral for $\alpha = 1$, that is given by

$$I^1 u(x, t) = \int_0^t u(x, s) ds.$$

We have so far the approximation

$$\begin{aligned} u(x, t_n) - u(x, t_{n-1}) &\approx \nabla^\beta \left(d^{n+1/2}(x) I^\alpha u(x, t_n) \right) - \nabla^\beta \left(d^{n+1/2}(x) I^\alpha u(x, t_{n-1}) \right) \\ &\quad - \frac{d}{dx} \left(F^{n+1/2}(x) I^\alpha u(x, t_n) \right) + \frac{d}{dx} \left(F^{n+1/2}(x) I^\alpha u(x, t_{n-1}) \right) + \int_{I_n} g(x, t) dt. \end{aligned}$$

We can re-write that as

$$\begin{aligned} u(x, t_n) - u(x, t_{n-1}) &\approx \frac{1}{\Gamma(2+\alpha)} \sum_{k=0}^n a_{n,k} \nabla^\beta \left(d^{n+1/2}(x) u(x, t_k) \right) \\ &\quad - \frac{1}{\Gamma(2+\alpha)} \sum_{k=0}^{n-1} a_{n-1,k} \nabla^\beta \left(d^{n+1/2}(x) u(x, t_k) \right) - \frac{1}{\Gamma(2+\alpha)} \sum_{k=0}^n a_{n,k} \frac{d}{dx} \left(F^{n+1/2}(x) u(x, t_k) \right) \\ &\quad + \frac{1}{\Gamma(2+\alpha)} \sum_{k=0}^{n-1} a_{n-1,k} \frac{d}{dx} \left(F^{n+1/2}(x) u(x, t_k) \right) + \int_{I_n} g(x, t) dt. \end{aligned}$$

When $\alpha = 1$, since $\Gamma(3) = 2$ and

$$\begin{aligned} a_{n,k} - a_{n-1,k} &= 0, & \text{for } k = 0, \dots, n-2 \\ a_{n,n-1} - a_{n-1,n-1} &= \Delta t_n \\ a_{n,n} &= \Delta t_n \end{aligned}$$

the numerical method becomes

$$\begin{aligned} u(x, t_n) - u(x, t_{n-1}) &\approx \frac{1}{2} \left(\Delta t_n \nabla^\beta \left(d^{n+1/2}(x) u(x, t_n) \right) + \Delta t_n \nabla^\beta \left(d^{n+1/2}(x) u(x, t_{n-1}) \right) \right) \\ &\quad - \frac{1}{2} \left(\Delta t_n \frac{d}{dx} \left(F^{n+1/2}(x) u(x, t_n) \right) + \Delta t_n \frac{d}{dx} \left(F^{n+1/2}(x) u(x, t_{n-1}) \right) \right) + \int_{I_n} g(x, t) dt. \end{aligned}$$

This method is similar to a Crank-Nicolson discretisation if we approximate the integral of the source term by

$$\int_{I_n} g(x, t) dt \approx \frac{1}{2} (g(x, t_n) + g(x, t_{n-1})).$$

In the next section we discuss the spatial discretization.

2.2. The spatial discretization

We assume the domain is the real line, and that additionally to the initial condition

$$u(x, 0) = u_0(x), \quad x \in \mathbb{R}$$

we have

$$\lim_{|x| \rightarrow \infty} u(x, t) = 0.$$

We consider a uniform mesh, $x_j, j \in \mathbb{Z}$, where $x_{j+1} = x_j + \Delta x$. We approximate the fractional derivatives by the method discussed in [21, 22] for a uniform mesh. This approximation is obtained by approximating the integral involved in the definition of the fractional derivatives through a linear spline in order to obtain a second order approximation for the fractional operator similarly to what has been described in the previous section in relation to the approximation of the time fractional integral. Additionally, the second order derivative outside the integral is approximated by a central second order approximation.

The approximations for the left and right fractional derivatives, defined in (7) and (8) are in this way given by the formulas

$$\frac{\delta_l^\beta u(x_j, t)}{\Delta x^\beta}, \quad \frac{\delta_r^\beta u(x_j, t)}{\Delta x^\beta}$$

respectively, where the discrete operators are defined by

$$\delta_l^\beta u(x_j, t) = \frac{1}{\Gamma(4-\beta)} \sum_{m=-1}^{\infty} q_m u(x_{j-m}, t), \quad (19)$$

$$\delta_r^\beta u(x_j, t) = \frac{1}{\Gamma(4-\beta)} \sum_{m=-1}^{\infty} q_m u(x_{j+m}, t). \quad (20)$$

The coefficients q_m are defined as

$$q_m = \begin{cases} b_{m-1} - 2b_m + b_{m+1}, & m \geq 1 \\ -2b_0 + b_1, & m = 0 \\ b_0, & m = -1, \end{cases} \quad (21)$$

where

$$b_m = \begin{cases} (m+1)^{3-\beta} - 2m^{3-\beta} + (m-1)^{3-\beta}, & m \geq 1 \\ 1, & m = 0. \end{cases} \quad (22)$$

Hence, we define the discrete operator $\delta^\beta u$, that approximates $\nabla^\beta u$, as

$$\delta^\beta u(x_j, t) = p\delta_l^\beta u(x_j, t) + q\delta_r^\beta u(x_j, t). \quad (23)$$

When $\beta = 2$ this operator is the central second order operator

$$\delta^2 u(x_j, t) = u(x_{j+1}, t) - 2u(x_j, t) + u(x_{j-1}, t).$$

To approximate the first order derivative, included in equation (10), we use the central approximation, that is,

$$\Delta_0 u(x_j, t) = u(x_{j+1}, t) - u(x_{j-1}, t).$$

Let us denote U_j^n the approximation function of $u(x_j, t_n)$. We get the following numerical method

$$\begin{aligned} U_j^n - U_j^{n-1} &= \frac{1}{\Gamma(2+\alpha)\Delta x^\beta} \sum_{k=0}^n a_{n,k} \delta^\beta \left(d_j^{n+1/2} U_j^k \right) \\ &- \frac{1}{\Gamma(2+\alpha)\Delta x^\beta} \sum_{k=0}^{n-1} a_{n-1,k} \delta^\beta \left(d_j^{n+1/2} U_j^k \right) - \frac{1}{\Gamma(2+\alpha)2\Delta x} \sum_{k=0}^n a_{n,k} \Delta_0 \left(F_j^{n+1/2} U_j^k \right) \\ &+ \frac{1}{\Gamma(2+\alpha)2\Delta x} \sum_{k=0}^{n-1} a_{n-1,k} \Delta_0 \left(F_j^{n+1/2} U_j^k \right) + \int_{I_n} g(x_j, t) dt, \end{aligned} \quad (24)$$

where

$$d_j^{n+1/2} := d^{n+1/2}(x_j) \quad F_j^{n+1/2} := F^{n+1/2}(x_j).$$

Or more specifically

$$\begin{aligned} U_j^n - U_j^{n-1} &= \frac{1}{\Gamma(2+\alpha)\Gamma(4-\beta)\Delta x^\beta} \sum_{k=0}^n a_{n,k} \left[p \sum_{m=-1}^{\infty} q_m d_{j-m}^{n+1/2} U_{j-m}^k + q \sum_{m=-1}^{\infty} q_m d_{j+m}^{n+1/2} U_{j+m}^k \right] \\ &\quad - \frac{1}{\Gamma(2+\alpha)\Gamma(4-\beta)\Delta x^\beta} \sum_{k=0}^{n-1} a_{n-1,k} \left[p \sum_{m=-1}^{\infty} q_m d_{j-m}^{n+1/2} U_{j-m}^k + q \sum_{m=-1}^{\infty} q_m d_{j+m}^{n+1/2} U_{j+m}^k \right] \\ &\quad - \frac{1}{\Gamma(2+\alpha)2\Delta x} \sum_{k=0}^n a_{n,k} \left[F_{j+1}^{n+1/2} U_{j+1}^k - F_{j-1}^{n+1/2} U_{j-1}^k \right] \\ &\quad + \frac{1}{\Gamma(2+\alpha)2\Delta x} \sum_{k=0}^{n-1} a_{n-1,k} \left[F_{j+1}^{n+1/2} U_{j+1}^k - F_{j-1}^{n+1/2} U_{j-1}^k \right] + \int_{I_n} g(x_j, t) dt. \end{aligned} \quad (25)$$

This approximation can be also applied to the problem defined in an interval $\Omega = (a, b)$ and where we have $u(x, t) = 0$ for $x \notin \Omega$. In this case we can consider the discretization space as

$$x_j = a + j\Delta x, \quad \Delta x = \frac{b-a}{N}.$$

The infinite sums involved in the numerical method can be written as finite sums and the numerical method becomes

$$\begin{aligned} U_j^n - U_j^{n-1} &= \frac{1}{\Gamma(2+\alpha)\Gamma(4-\beta)\Delta x^\beta} \sum_{k=0}^n a_{n,k} \left[p \sum_{m=-1}^j q_m d_{j-m}^{n+1/2} U_{j-m}^k + q \sum_{m=-1}^{N-j} q_m d_{j+m}^{n+1/2} U_{j+m}^k \right] \\ &\quad - \frac{1}{\Gamma(2+\alpha)\Gamma(4-\beta)\Delta x^\beta} \sum_{k=0}^{n-1} a_{n-1,k} \left[p \sum_{m=-1}^j q_m d_{j-m}^{n+1/2} U_{j-m}^k + q \sum_{m=-1}^{N-j} q_m d_{j+m}^{n+1/2} U_{j+m}^k \right] \\ &\quad - \frac{1}{\Gamma(2+\alpha)2\Delta x} \sum_{k=0}^n a_{n,k} \left[F_{j+1}^{n+1/2} U_{j+1}^k - F_{j-1}^{n+1/2} U_{j-1}^k \right] \\ &\quad + \frac{1}{\Gamma(2+\alpha)2\Delta x} \sum_{k=0}^{n-1} a_{n-1,k} \left[F_{j+1}^{n+1/2} U_{j+1}^k - F_{j-1}^{n+1/2} U_{j-1}^k \right] + \int_{I_n} g(x_j, t) dt. \end{aligned}$$

Additionally, to implement the numerical method, a finite computational domain needs to be considered. The matricial form is given by

$$(\mathbf{I} - a_{1,1}\mathbf{B}^1)\mathbf{U}^1 = (\mathbf{I} + a_{1,0}\mathbf{B}^1)\mathbf{U}^0 + \mathbf{G}^1, \quad (26)$$

$$(\mathbf{I} - a_{n,n}\mathbf{B}^n)\mathbf{U}^n = \mathbf{I}\mathbf{U}^{n-1} + \sum_{k=0}^{n-1} (a_{n,k} - a_{n-1,k})\mathbf{B}^n \mathbf{U}^k + \mathbf{G}^n, \quad n > 1, \quad (27)$$

where \mathbf{U}^0 is the initial vector $\mathbf{U}^0 = [U_1^0, \dots, U_{N-1}^0]^T$, that is, $U_j^0 := u_0(x_j)$; the matrix \mathbf{B}^n , $n \geq 1$ is such that

$$\mathbf{B}^n = \mathbf{B}_1^n + \mathbf{B}_2^n,$$

where $\mathbf{B}_1^n := (B_1^n)_{i,j}$ is the full $(N-1) \times (N-1)$ matrix associated with the fractional diffusion operator, that is,

$$(B_1^n)_{j,j+m} = pq_{-m} d_{j+m}^{n+1/2} / (\Gamma(2+\alpha)\Gamma(4-\beta)\Delta x^\beta), \quad m = -j+1, \dots, -2, \quad (28)$$

$$(B_1^n)_{j,j+m} = (pq_{-m} d_{j+m}^{n+1/2} + qq_m d_{j+m}^{n+1/2}) / (\Gamma(2+\alpha)\Gamma(4-\beta)\Delta x^\beta), \quad m = -1, 0, 1, \quad (29)$$

$$(B_1^n)_{j,j+m} = qq_m d_{j+m}^{n+1/2} / (\Gamma(2+\alpha)\Gamma(4-\beta)\Delta x^\beta), \quad m = 2, \dots, N-j+1. \quad (30)$$

The matrix $\mathbf{B}_2^n := (B_2^n)_{i,j}$ associated with the force field is a tridiagonal $(N-1) \times (N-1)$ matrix given by,

$$(B_2^n)_{j,j+1} = -\frac{F_{j+1}^{n+1/2}}{2\Delta x \Gamma(2+\alpha)}, \quad (B_2^n)_{j,j} = 0, \quad (B_2^n)_{j,j-1} = \frac{F_{j-1}^{n+1/2}}{2\Delta x \Gamma(2+\alpha)}.$$

The vector \mathbf{G}^n contains the values of the integral of the source term in I_n . The integral of the source term is computed using a quadrature rule that can be the trapezium formula or, in the case of a discontinuity at the initial point $t = t_0$, the middle point rule.

The non-locality character of fractional derivatives in time and space leads to a numerical method with increasing storage requirements and computational costs when compared with numerical methods for differential equations with integer order derivatives. The increase of storage requirements is directly related to the time fractional derivative where all the previous time levels need to be considered at each time. Regarding the fractional space derivatives, they lead to dense matrices, although the coefficients of the approximations of the fractional derivatives, which are the entries of those matrices, converges towards zero very quickly for all β . To solve the linear systems (26)–(27) a direct method can be used. For one dimensional problems this numerical approach presents no significant difficulties regarding the computational costs or storage requirements. However, for a higher dimensional setting these aspects will require more attention.

3. Convergence analysis

In this section we discuss properties related to the convergence of the numerical method, namely, consistency of the approximations of the fractional operators and stability properties of the numerical method. We start with consistency and will focus our attention in how the regularity of the solution in relation to time affects the consistency of the time fractional operator.

3.1. Accuracy of the numerical method

The local truncation error for the numerical method (25), for the particular case, $\alpha = 1$ and $\beta = 2$, is known to be second order, that is, $\mathcal{O}(\Delta t^2 + \Delta x^2)$, when the solution is $C^4(\mathbb{R})$ in space and $C^2(0, T)$ in time, that is, $u \in C^{4,2}(\mathbb{R} \times (0, T))$.

For the fractional time integral we have the following result.

Theorem 1. [3] (Order of accuracy of the approximation for the time fractional integral): Let $u \in C^2(0, t_n)$. Then there is a constant C_α that depends only on α such that

$$|\mathcal{I}^\alpha u(t_n) - I^\alpha u(t_n)| \leq C_\alpha \sup_{t \in (0, t_n)} |u''(t)| t_n^\alpha \Delta t^2.$$

The next result concerns the approximation of the spacial left fractional Riemann-Liouville operator.

Theorem 2. [22] (Order of accuracy of the approximation for the left fractional derivative): Let $u \in C^{(4)}(\mathbb{R})$ and such that $u^{(4)}(x) = 0$, for $x \leq a$, being a a real constant. We have that

$$\frac{\partial^\beta u}{\partial x^\beta}(x_j) - \frac{\delta_l^\beta u}{\Delta x^\beta}(x_j) = \epsilon_1(x_j) + \epsilon_2(x_j),$$

where

$$|\epsilon_1(x_j)| \leq C_1 \Delta x^2 \quad |\epsilon_2(x_j)| \leq C_2 \Delta x^2,$$

and C_1 and C_2 are independent of Δx .

A similar result is valid for the right fractional Riemann-Liouville derivative. The previous result can also be proved by assuming that u is a function with sufficiently many continuous derivatives that vanish at infinity in an appropriate manner, see [21].

If the regularity of the function decreases then the order of accuracy diminishes. We will study this aspect, in particular, for the time discretization, similarly to what has been done in [23] for a weakly singular kernel. We have the following result.

Theorem 3. Let $u \in C^1[0, t_n] \cap C^2(0, t_n)$ satisfying $u = O(t^{\alpha+1})$ as $t \rightarrow 0^+$. Then, there is a constant C_α that depends only on α such that

$$|\mathcal{I}^\alpha u(t_n) - I^\alpha u(t_n)| \leq C_\alpha t_n^\alpha \Delta t^{1+\alpha}.$$

Proof: Let $u \in C^2(t_{k-1}, t_k)$. For $\xi \in [t_{k-1}, t_k]$

$$|s_k(\xi) - u(\xi)| \leq \frac{1}{2}|u''(\xi_k)|\Delta t_k^2, \quad t_{k-1} \leq \xi_k \leq t_k.$$

We have

$$\mathcal{I}^\alpha u(t_n) - I^\alpha u(t_n) = \frac{1}{\Gamma(\alpha)} \sum_{k=1}^n \int_{t_{k-1}}^{t_k} (s_k(\tau) - u(\tau))(t_n - \tau)^{\alpha-1} d\tau$$

and

$$|\mathcal{I}^\alpha u(t_n) - I^\alpha u(t_n)| \leq \frac{1}{\Gamma(\alpha)} \sum_{k=1}^n \int_{t_{k-1}}^{t_k} \frac{1}{2}|u''(\xi_k)|\Delta t_k^2 (t_n - \tau)^{\alpha-1} d\tau$$

Therefore, using the mean integral value theorem, for $\eta_k \in (t_{k-1}, t_k)$ and $\Delta t = \max_k \Delta t_k$,

$$\begin{aligned} |\mathcal{I}^\alpha u(t_n) - I^\alpha u(t_n)| &\leq \frac{1}{2\Gamma(\alpha)} \left[\int_{t_0}^{t_1} \Delta t_1^2 O(\Delta t_1^{\alpha-1})(t_n - \tau)^{\alpha-1} d\tau \right. \\ &\quad \left. + \Delta t^2 \sum_{k=2}^n |u''(\eta_k)| \frac{1}{2\Gamma(\alpha)} \int_{t_{k-1}}^{t_k} (t_n - \tau)^{\alpha-1} d\tau \right] \\ &\leq C_\alpha t_n^\alpha \Delta t^{\alpha+1}. \end{aligned}$$

□

Additionally we have the following result, which proof follows the same steps of the previous proof.

Theorem 4. Let $u \in C^0[0, t_n] \cap C^2(0, t_n)$ satisfying $u = O(t^\alpha)$ as $t \rightarrow 0^+$. Then, there is a constant C_α that depends only on α such that

$$|\mathcal{I}^\alpha u(t_n) - I^\alpha u(t_n)| \leq C_\alpha t_n^\alpha \Delta t^\alpha.$$

These results will be confirmed by the numerical experiments in the section titled numerical results.

3.2. Fourier decomposition of the error

For simplicity in this section we assume the source term $g(x, t) = 0$. Our aim is to prove that the numerical method is unconditionally stable for all $0 < \alpha \leq 1$ and $1 < \beta \leq 2$.

When $\alpha = 1$ and $\beta = 2$ we have the following method

$$\begin{aligned} U_j^n - U_j^{n-1} &= \frac{1}{2}\Delta t_n \left(\delta^2(d_j^{n+1/2}U_j^n) + \delta^2(d_j^{n+1/2}U_j^{n-1}) \right) \\ &\quad - \frac{1}{2}\Delta t_n \left(\Delta_0(F_j^{n+1/2}U_j^n) + \Delta_0(F_j^{n+1/2}U_j^{n-1}) \right). \end{aligned}$$

This method is equivalent to a Crank-Nicolson discretization in time and central differences in space for the first and second order derivatives. It is known to be a second order accurate numerical method and unconditionally stable [10].

For the particular case, $\alpha = 1$, $1 < \beta < 2$ and the fractional operator (9) with $p = 1, q = 0$, where the force field $F(x, t) = 0$ and $d(x, t)$ constant, the numerical method is also unconditionally stable, see [22].

In order to derive stability conditions for a more general case we apply the von Neumann analysis or Fourier analysis. Fourier analysis assumes that we have a solution defined in the whole real line. It is also applied to problems defined in finite domains with periodic boundary conditions since the solution is seen as a periodic function in \mathbb{R} .

If u_j^n is the exact solution $u(x_j, t_n)$, let

$$e_j^n = U_j^n - u_j^n \quad (31)$$

be the error at time level n in mesh point j . Considering the numerical method (24) and inserting equation (31) into that equation leads to

$$\begin{aligned} e_j^n - e_j^{n-1} &= \frac{1}{\Gamma(2+\alpha)\Delta x^\beta} \sum_{k=0}^n a_{n,k} \delta^\beta \left(d_j^{n+1/2} e_j^k \right) - \frac{1}{\Gamma(2+\alpha)\Delta x^\beta} \sum_{k=0}^{n-1} a_{n-1,k} \delta^\beta \left(d_j^{n+1/2} e_j^k \right) \\ &\quad - \frac{1}{\Gamma(2+\alpha)2\Delta x} \sum_{k=0}^n a_{n,k} \Delta_0 \left(F_j^{n+1/2} e_j^k \right) + \frac{1}{\Gamma(2+\alpha)2\Delta x} \sum_{k=0}^{n-1} a_{n-1,k} \Delta_0 \left(F_j^{n+1/2} e_j^k \right). \end{aligned} \quad (32)$$

Assuming a uniform mesh in space and time, the force field and the diffusion only dependent on time, we get

$$\begin{aligned} e_j^n - e_j^{n-1} &= \frac{a_{n,n} d^{n+1/2}}{\Gamma(2+\alpha)\Delta x^\beta} \delta^\beta e_j^n + \frac{d^{n+1/2}}{\Gamma(2+\alpha)\Delta x^\beta} \sum_{k=0}^{n-1} (a_{n,k} - a_{n-1,k}) \delta^\beta e_j^k \\ &\quad - \frac{a_{n,n} F^{n+1/2}}{\Gamma(2+\alpha)2\Delta x} \Delta_0 e_j^n - \frac{F^{n+1/2}}{\Gamma(2+\alpha)2\Delta x} \sum_{k=0}^{n-1} (a_{n,k} - a_{n-1,k}) \Delta_0 e_j^k. \end{aligned}$$

We can re-write this method as

$$\begin{aligned} e_j^n &- \frac{a_{n,n} d^{n+1/2}}{\Gamma(2+\alpha)\Delta x^\beta} \delta^\beta e_j^n + \frac{a_{n,n} F^{n+1/2}}{\Gamma(2+\alpha)2\Delta x} \Delta_0 e_j^n \\ &= e_j^{n-1} + \frac{d^{n+1/2}}{\Gamma(2+\alpha)\Delta x^\beta} \sum_{k=0}^{n-1} c_{n,k} \delta^\beta e_j^k - \frac{F^{n+1/2}}{\Gamma(2+\alpha)2\Delta x} \sum_{k=0}^{n-1} c_{n,k} \Delta_0 e_j^k, \end{aligned}$$

with $c_{n,k} = a_{n,k} - a_{n-1,k}$. We have

$$\begin{aligned} c_{n,k} &= \Delta t^\alpha [(n-k+1)^{1+\alpha} - 3(n-k)^{1+\alpha} + 3(n-k-1)^{1+\alpha} - (n-k-2)^{1+\alpha}], \\ &\quad 1 \leq k \leq n-2, \\ c_{n,n-1} &= a_{n,n-1} - a_{n-1,n-1} \\ &= \Delta t^\alpha (2^{1+\alpha} - 3), \\ c_{n,0} &= a_{n,0} - a_{n-1,0} \\ &= \Delta t^\alpha [(1+\alpha)(n^\alpha - (n-1)^\alpha) - n^{1+\alpha} + 2(n-1)^{1+\alpha} - (n-2)^{1+\alpha}], \quad n \geq 2. \end{aligned}$$

We can simplify the notation of the constants $c_{n,k}$ by writing

$$\begin{aligned} e_j^n &- \frac{\Delta t^\alpha d^{n+1/2}}{\Gamma(2+\alpha)\Delta x^\beta} \delta^\beta e_j^n + \frac{\Delta t^\alpha F^{n+1/2}}{\Gamma(2+\alpha)2\Delta x} \Delta_0 e_j^n \\ &= e_j^{n-1} + \frac{d^{n+1/2} \Delta t^\alpha}{\Gamma(2+\alpha)\Delta x^\beta} \sum_{l=1}^n c_l \delta^\beta e_j^{n-l} - \frac{F^{n+1/2} \Delta t^\alpha}{\Gamma(2+\alpha)2\Delta x} \sum_{l=1}^n c_l \Delta_0 e_j^{n-l}, \end{aligned} \quad (33)$$

where, for $n \geq 2$,

$$\begin{aligned} c_1 &= 2^{1+\alpha} - 3, \\ c_l &= (l+1)^{1+\alpha} - 3l^{1+\alpha} + 3(l-1)^{1+\alpha} - (l-2)^{1+\alpha}, \quad l = 2, \dots, n-1, \\ c_n &= (1+\alpha)(n^\alpha - (n-1)^\alpha) - n^{1+\alpha} + 2(n-1)^{1+\alpha} - (n-2)^{1+\alpha}. \end{aligned} \quad (34)$$

Remarks: For the case $k = 0$ and $n = 1$, the sum of the constants c_l in (33) is equal to a $s^* = a_{n,k} - a_{n-1,k} = a_{1,0} - a_{0,0} = \Delta t^\alpha [(1 + \alpha)n^\alpha - n^{1+\alpha}] = \alpha$. Note also that as we change n , the c_l 's need to be redefined according to (34).

The von Neumann analysis assumes that any finite mesh function, such as, the error e_j^n will be decomposed into a Fourier series as

$$e_j^n = \sum_p \kappa_p^n e^{ij\xi_p \Delta x},$$

where κ_p^n is the amplitude of the p -th harmonic and the product $\xi_p \Delta x$ is often called the phase angle $\phi = \xi_p \Delta x$.

Considering a single mode $\kappa^n e^{ij\phi}$, its time evolution is determined by the same numerical scheme as the error e_j^n . The stability conditions will be satisfied if the amplitude of any error harmonic κ^n does not grow in time [5, 8], that is, if the ratio

$$G(\phi) = |\kappa^{n+1}/\kappa^n| \leq 1, \quad \text{for all } \phi.$$

If $|G(\phi)| > 1$ for some ϕ , then the solution grows to infinity and the mode is unstable. An arbitrary mode can be singled out and stability requires that no harmonic should be allowed to increase in time without bound. Hence inserting a representation of a single mode $\kappa^n e^{ij\phi}$ into a numerical scheme we obtain stability conditions. By substituting e_j^n by $\kappa^n e^{ij\phi}$ we get

$$\begin{aligned} & \kappa^n e^{ij\phi} - \kappa^n \frac{\Delta t^\alpha d^{n+1/2}}{\Gamma(2+\alpha)\Delta x^\beta} \delta^\beta e^{ij\phi} + \kappa^n \frac{\Delta t^\alpha F^{n+1/2}}{\Gamma(2+\alpha)2\Delta x} \Delta_0 e^{ij\phi} \\ = & \kappa^{n-1} e^{ij\phi} + \frac{d^{n+1/2}\Delta t^\alpha}{\Gamma(2+\alpha)\Delta x^\beta} \sum_{l=1}^n c_l \kappa^{n-l} \delta^\beta e^{ij\phi} - \frac{F^{n+1/2}\Delta t^\alpha}{\Gamma(2+\alpha)2\Delta x} \sum_{l=1}^n c_l \kappa^{n-l} \Delta_0 e^{ij\phi}. \end{aligned} \quad (35)$$

Let

$$\nu^\alpha = F^{n+1/2} \frac{\Delta t^\alpha}{\Delta x} \quad \mu_\beta^\alpha = d^{n+1/2} \frac{\Delta t^\alpha}{\Delta x^\beta}.$$

Dividing (35) by κ^{n-1} we get

$$\begin{aligned} & \frac{\kappa^n}{\kappa^{n-1}} \left(e^{ij\phi} - \frac{\mu_\beta^\alpha}{\Gamma(2+\alpha)} \delta^\beta e^{ij\phi} + \frac{\nu^\alpha}{2\Gamma(2+\alpha)} \Delta_0 e^{ij\phi} \right) \\ = & e^{ij\phi} + \frac{\mu_\beta^\alpha}{\Gamma(2+\alpha)} \sum_{l=1}^n c_l \frac{\kappa^{n-l}}{\kappa^{n-1}} \delta^\beta e^{ij\phi} - \frac{\nu^\alpha}{\Gamma(2+\alpha)2} \sum_{l=1}^n c_l \frac{\kappa^{n-l}}{\kappa^{n-1}} \Delta_0 e^{ij\phi}. \end{aligned} \quad (36)$$

We have

$$\begin{aligned} \delta^\beta e^{ij\phi} &= p\delta_l^\beta e^{ij\phi} + q\delta_r^\beta e^{ij\phi} \\ &= p \frac{1}{\Gamma(4-\beta)} \sum_{m=-1}^{\infty} q_m e^{ij\phi} (e^{-im\phi}) + q \frac{1}{\Gamma(4-\beta)} \sum_{m=-1}^{\infty} q_m e^{ij\phi} (e^{im\phi}) \\ &= \frac{e^{ij\phi}}{\Gamma(4-\beta)} \left((p+q) \sum_{m=-1}^{\infty} q_m \cos(m\phi) + (q-p)i \sum_{m=-1}^{\infty} q_m \sin(m\phi) \right) \end{aligned} \quad (37)$$

and

$$\Delta_0 e^{ij\phi} = e^{ij\phi} (e^{i\phi} - e^{-i\phi}) = e^{ij\phi} 2i \sin(\phi). \quad (38)$$

Therefore from (36), (37) and (38) we get

$$\begin{aligned}
& \frac{\kappa^n}{\kappa^{n-1}} \left(1 - \frac{\mu_\beta^\alpha}{\Gamma(2+\alpha)\Gamma(4-\beta)} \left((p+q) \sum_{m=-1}^{\infty} q_m \cos(m\phi) + (q-p)i \sum_{m=-1}^{\infty} q_m \sin(m\phi) \right) \right. \\
& \quad \left. + \frac{\nu^\alpha}{2\Gamma(2+\alpha)} 2i \sin(\phi) \right) \\
= & 1 + \frac{\mu_\beta^\alpha}{\Gamma(2+\alpha)\Gamma(4-\beta)} \sum_{l=1}^n c_l \frac{\kappa^{n-l}}{\kappa^{n-1}} \left((p+q) \sum_{m=-1}^{\infty} q_m \cos(m\phi) + (q-p)i \sum_{m=-1}^{\infty} q_m \sin(m\phi) \right) \\
& - \frac{\nu^\alpha}{\Gamma(2+\alpha)2} \sum_{l=1}^n c_l \frac{\kappa^{n-l}}{\kappa^{n-1}} 2i \sin(\phi). \tag{39}
\end{aligned}$$

Let

$$\begin{aligned}
A = & \frac{\mu_\beta^\alpha}{\Gamma(2+\alpha)\Gamma(4-\beta)} \left((p+q) \sum_{m=-1}^{\infty} q_m \cos(m\phi) + (q-p)i \sum_{m=-1}^{\infty} q_m \sin(m\phi) \right) \\
& - \frac{\nu^\alpha}{\Gamma(2+\alpha)} i \sin(\phi). \tag{40}
\end{aligned}$$

We can write (39) in the simplified form

$$\frac{\kappa^n}{\kappa^{n-1}} (1 - A) = 1 + A \sum_{l=1}^n c_l \frac{\kappa^{n-l}}{\kappa^{n-1}}. \tag{41}$$

In what follows we present theoretical results for some particular cases.

Theorem 5. For $\alpha = 1$ and $1 < \beta < 2$, the method (24) is von Neumann unconditionally stable.

Proof: For $\alpha = 1$, from equation (39) and for $\kappa^n = G\kappa^{n-1}$ we get

$$\begin{aligned}
G & \left(1 - \frac{\mu_\beta^\alpha}{\Gamma(2+\alpha)\Gamma(4-\beta)} \left((p+q) \sum_{m=-1}^{\infty} q_m \cos(m\phi) + (q-p)i \sum_{m=-1}^{\infty} q_m \sin(m\phi) \right) \right. \\
& \quad \left. + \frac{\nu^\alpha}{\Gamma(2+\alpha)} i \sin(\phi) \right) \\
= & 1 + \frac{\mu_\beta^\alpha}{\Gamma(2+\alpha)\Gamma(4-\beta)} \left((p+q) \sum_{m=-1}^{\infty} q_m \cos(m\phi) + (q-p)i \sum_{m=-1}^{\infty} q_m \sin(m\phi) \right) \\
& - \frac{\nu^\alpha}{\Gamma(2+\alpha)} i \sin(\phi) \tag{42}
\end{aligned}$$

Therefore, we have

$$G = \frac{1+A}{1-A},$$

where A is defined by (40). If the real part of A is negative then $|G| \leq 1$ for all ϕ , since $|1+A| \leq |1-A|$. The real part of A is negative since we have [22],

$$\sum_{m=-1}^{\infty} q_m \cos(m\phi) \leq 0$$

and therefore the method is unconditionally stable. \square

Lemma 6. The coefficients c_l defined in (34) satisfy:

$$-1 < c_1 < 1, \quad |c_{l+1}| < |c_l| \text{ and } -1 < c_l < 0, \quad l \geq 2 \quad (43)$$

$$c_1 + \sum_{l=2}^{n-1} c_l + c_n = -1 + (1 + \alpha)(n^\alpha - (n-1)^\alpha) \quad (44)$$

$$-1 \leq \sum_{l=1}^n c_l \leq 1 \text{ and } \lim_{n \rightarrow \infty} \sum_{l=1}^n c_l = -1 \quad (45)$$

Proof: The second inequality of (43) can be proved by developing into a series the fractional power terms that appear in the constants c_l and the other two inequalities are straightforward.

The equality (44) comes immediately after noting that

$$\sum_{l=2}^{n-1} c_l = 2 - 2^{1+\alpha} + (n-2)^{1+\alpha} - 2(n-1)^{1+\alpha} + n^\alpha.$$

Lastly, equality (45) follows from (43), (44) and the fact that

$$\lim_{n \rightarrow \infty} (n^\alpha - (n-1)^\alpha) = 0.$$

□

Theorem 7. For $0 < \alpha < \alpha^*$, where $\alpha^* = \log(3)/\log(2) - 1 \approx 0.585$ and $1 < \beta < 2$, the method (24) is von Neumann unconditionally stable for the case of a free force, that is, $F(x, t) = 0$ and for a symmetric fractional operator (9), that is, when $p = q$.

Proof: By assuming that $\kappa^n = G\kappa^{n-1}$, for all n , [8, 25], from (39) we get a closed form for the amplification factor $G(\phi)$. We have $\kappa^n = G\kappa^{n-1}$ and $\kappa^{n-l} = G^{-l+1}\kappa^{n-1}$. Therefore

$$\begin{aligned} & G \left(1 - \frac{\mu_\beta^\alpha}{\Gamma(2+\alpha)\Gamma(4-\beta)} \left((p+q) \sum_{m=-1}^{\infty} q_m \cos(m\phi) + (q-p)i \sum_{m=-1}^{\infty} q_m \sin(m\phi) \right) \right. \\ & \left. + \frac{\nu^\alpha}{\Gamma(2+\alpha)} i \sin(\phi) \right) \\ = & 1 + \frac{\mu_\beta^\alpha}{\Gamma(2+\alpha)\Gamma(4-\beta)} \sum_{l=1}^n c_l G^{-l+1} \left((p+q) \sum_{m=-1}^{\infty} q_m \cos(m\phi) + (q-p)i \sum_{m=-1}^{\infty} q_m \sin(m\phi) \right) \\ & - \frac{\nu^\alpha}{\Gamma(2+\alpha)} \sum_{l=1}^n c_l G^{-l+1} i \sin(\phi). \end{aligned} \quad (46)$$

From equation (46) and for A defined by (40) we have

$$G(1-A) = 1 + A \sum_{l=1}^n c_l G^{-l+1}, \quad (47)$$

where the constants c_l are defined by (34). If for all ϕ the parameter G that satisfies this equation is less than one, then the method is unconditionally stable.

If we multiply by G^{n-1} equation (47), we get

$$G^n(1-A) = G^{n-1} + A \sum_{l=1}^n c_l G^{n-l}, \quad (48)$$

that is,

$$G^n - \frac{1 + Ac_1}{1 - A} G^{n-1} - \frac{A}{1 - A} (c_2 G^{n-2} + \dots + c_{n-2} G^2 + c_{n-1} G + c_n) = 0. \quad (49)$$

The roots G^* of the polynomial (49) verify [15]

$$|G^*| \leq \max \left\{ 1, \left| \frac{1 + Ac_1}{1 - A} \right| + \left| \frac{A}{1 - A} \right| \sum_{l=2}^n |c_l| \right\}.$$

For the case under discussion, that is, $\nu^\alpha = 0$ (free force case) and $p = q$ (symmetric spatial fractional operator) there is no imaginary part in A defined by (40). Additionally, if $c_1 = 2^{1+\alpha} - 3 \leq 0$ we have $1 + c_1 A \geq 0$, because $A \leq 0$. We have $c_l \leq 0$ for all $l \geq 2$, see Lemma 6, and therefore

$$\left| \frac{1 + Ac_1}{1 - A} \right| + \left| \frac{A}{1 - A} \right| \sum_{l=2}^n |c_l| = \frac{1 + Ac_1}{1 - A} + \frac{A}{1 - A} \sum_{l=2}^n c_l = \frac{1}{1 - A} + \frac{A}{1 - A} \sum_{l=1}^n c_l.$$

Since $A \leq 0$ and $\sum_{l=1}^n c_l$ is less than one in absolute value, then $1 + A \sum_{l=1}^n c_l \leq 1 - A$. Therefore $|G^*| \leq 1$. \square

In [9] stability results, in the L_∞ norm, are proved under similar restrictions for α , for a simpler case with $\beta = 2$ and non-dependent time coefficients.

Now we turn to the general case $0 < \alpha < 1$ and $1 < \beta < 2$. To analyse if the numerical method is von Neumann stable, we need to check if the roots of the polynomial

$$G^n - \frac{1 + Ac_1}{1 - A} G^{n-1} - \frac{A}{1 - A} (c_2 G^{n-2} + \dots + c_{n-2} G^2 + c_{n-1} G + c_n) = 0 \quad (50)$$

are in modulus less than one. The roots of this polynomial are the same as the eigenvalues of the companion matrix [15],

$$C_G = \begin{bmatrix} \frac{1 + Ac_1}{1 - A} & \frac{Ac_2}{1 - A} & \dots & \frac{Ac_{n-1}}{1 - A} & \frac{Ac_n}{1 - A} \\ 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \end{bmatrix}.$$

Therefore, if the eigenvalues of the matrix C_G are all less or equal to one, for $0 < \alpha < 1$ and $1 < \beta < 2$, the method (24) is unconditionally stable. The companion matrix C_G depends on $p, q, \alpha, \beta, \nu^\alpha, \mu_\beta^\alpha, \phi$ and we have checked computationally that the eigenvalues of C_G are less than one for a big set of values, indicating the method is unconditionally stable for $0 < \alpha \leq 1$ and $1 < \beta \leq 2$. This is also confirmed by the numerical tests in the next section. We illustrate in Figures 1(a) and 1(b) the eigenvalues of the matrix C_G for fixed values of $\mu_\beta^\alpha, \nu^\alpha, \alpha, \beta$ and a fixed ϕ . Note that the value $\phi = \pi$ corresponds to the highest frequency resolvable in the mesh and that ν^α is similar to the Courant number. In Figures 1(a) and 1(b) we have considered $n = 20$ and $n = 200$ respectively. If, for instance, we consider $n = 500$ we obtain a similar figure to 1(b), with a more dense black region, since the number of eigenvalues increases.

4. Numerical results

We consider the one-dimensional fractional Fokker-Planck equation,

$$u_t(x, t) - \nabla^\beta (d(x, t) {}_0D_t^{1-\alpha} u(x, t)) + (F(x, t) {}_0D_t^{1-\alpha} u(x, t))_x = g(x, t), \quad x \in \Omega \times (0, T],$$

for $0 < \alpha \leq 1$ and $1 < \beta \leq 2$.

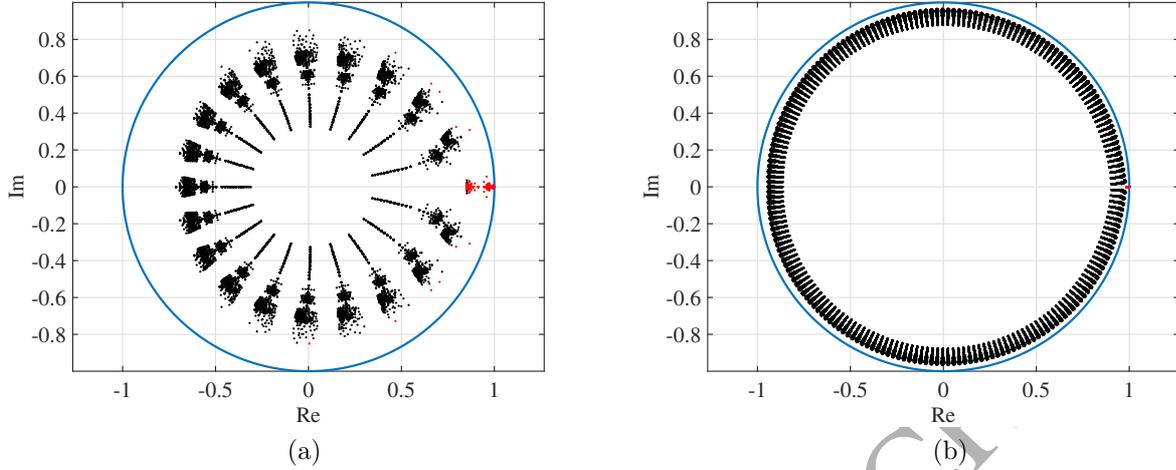


Figure 1: Eigenvalues for the companion matrix C_G for $p = 0.2$ ($q = 1 - p$) and a range of values for $\alpha, \beta, \nu^\alpha, \mu_\beta^\alpha, \phi$, namely, $\alpha = 0.1, 0.5, 0.9$, $\beta = 1.1, 1.5, 1.9$, $\nu^\alpha = -2, -1, -0.25, 0.25, 1, 2$, $\mu_\beta^\alpha = 0.25, 0.5, 1, 2$, $\phi = -\pi, -\pi/2, \pi/2, \pi$. The red dots denote the maximum value for each fixed value of $\alpha, \beta, \nu^\alpha, \mu_\beta^\alpha, \phi$. The blue circle is the unitary circle. (a) $n = 20$; (b) $n = 200$.

For the numerical simulations we assume $\Omega = (a, b)$ and a uniform mesh in space, that is, $x_j = a + j\Delta x$, for $j = 0, \dots, N$, with $x_N = b$. In time, we consider the case of a uniform mesh, and also an example with a non-uniform mesh. For the non-uniform case we have $t_n = t_{n-1} + \Delta t_n$, for $n = 0, \dots, M$, with $t_M = T$ and in the cases of a uniform mesh we denote the time step by Δt . The error is defined by,

$$\text{error} = \max_{n=1, \dots, M} \left(\Delta x \sum_{j=1}^{N-1} (U_j^n - u(x_j, t_n))^2 \right)^{1/2},$$

where U_j^n is the numerical approximation of the exact solution $u(x_j, t_n)$.

Problem 1. In this first example we have a diffusion parameter that depends on x and a force that depends on x and t . We assume $\Omega = (0, 2)$, $T = 1$, $d(x, t) = x$, $F(x, t) = x + \sin(t)$, and the source term $g(x, t)$ and initial solution $u_0(x)$ are defined, such that, the exact solution of this problem is given by

$$u(x, t) = t^{2+\alpha} x^4 (2 - x)^4.$$

The problem can be interpreted as defined in the real line with

$$u(x, t) = 0 \quad x \notin \Omega.$$

In this case, the regularity of the solution is in space $C^3(\mathbb{R})$ and in time is $C^2([0, T])$, that is, $C^{3,2}(\mathbb{R} \times [0, T])$. It is shown that the order of convergence of the numerical method is second order accurate in space and time in Table 1 and Table 2 respectively. We also observe in Table 2 that the time steps we have considered are significantly larger when compared with the space step and this is in agreement with the discussion in Section 3 about the unconditional stability of the numerical method. This can also be verified in the next example.

Problem 2. We assume $\beta = 2$ and therefore we do not have a non-local operator in space, only in time. We consider $\Omega = (0, 1)$, $T = 1$, $d(x, t) = \frac{\Gamma(3+\alpha)}{2}$, $F(x, t) = x + \sin(t)$, and define the source term $g(x, t)$ and the initial condition $u_0(x)$, such that, the exact solution is given by

$$u(x, t) = t^{\alpha+2} e^x.$$

	β	$\Delta x = 2/40$	$\Delta x = 2/80$	Rate
$\alpha = 0.2$	1.2	2.5514e-03	6.3422e-04	2.0082
	1.4	2.3981e-03	5.9864e-04	2.0021
	1.6	2.3289e-03	5.8877e-04	1.9838
	1.8	2.1534e-03	5.5150e-04	1.9652
	2.0	1.5200e-03	3.7890e-04	2.0041
$\alpha = 0.4$	1.2	2.4934e-03	6.1983e-04	2.0082
	1.4	2.3241e-03	5.8009e-04	2.0024
	1.6	2.2499e-03	5.6870e-04	1.9841
	1.8	2.0868e-03	5.3435e-04	1.9654
	2.0	1.4869e-03	3.7061e-04	2.0043
$\alpha = 0.6$	1.2	2.4316e-03	6.0450e-04	2.0081
	1.4	2.2426e-03	5.5975e-04	2.0023
	1.6	2.1632e-03	5.4681e-04	1.9841
	1.8	2.0129e-03	5.1552e-04	1.9651
	2.0	1.4474e-03	3.6075e-04	2.0044
$\alpha = 0.8$	1.2	2.3612e-03	5.8708e-04	2.0079
	1.4	2.1462e-03	5.3580e-04	2.0020
	1.6	2.0626e-03	5.2155e-04	1.9836
	1.8	1.9276e-03	4.9395e-04	1.9644
	2.0	1.3992e-03	3.4874e-04	2.0043
$\alpha = 1.0$	1.2	2.2723e-03	5.6519e-04	2.0074
	1.4	2.0240e-03	5.0555e-04	2.0013
	1.6	1.9413e-03	4.9119e-04	1.9826
	1.8	1.8264e-03	4.6846e-04	1.9630
	2.0	1.3397e-03	3.3396e-04	2.0042

Table 1: Results concerning Problem 1. Convergence rate in space for different values of α and β with $\Delta t = 1/800$. The solution is regular enough in space and therefore we get second order convergence.

In Table 3 and Table 4 we observe second order convergence in space and time respectively. The regularity of the solutions is $C^{\infty,2}([0, 1] \times [0, T])$.

Problem 3. In this example we consider a problem with a solution with lower regularity than the previous problem. We assume, $\Omega = (0, 2)$, $T = 1$, $d(x, t) = \frac{\Gamma(5-\beta)}{2}$, $F(x, t) = x + \sin(t)$, and define $g(x, t)$ and $u_0(x)$, such that, the exact solution is given by

$$u(x, t) = t^{1+\alpha} 4x^2(2-x)^2.$$

We have a fractional operator also in space and the problem can be interpreted as defined in the real line with

$$u(x, t) = 0 \quad x \notin \Omega.$$

In this case the regularity of the solution in time is $C^1([0, T])$. We observe, in Table 5, that the convergence is approximately of order $\Delta t^{\alpha+1}$. This is in agreement with the discussion in Section 3.1 and in particular with Theorem 3.

Problem 4. In this example we further reduce the regularity of the solution in time and we assume $\beta = 2$. This example is also included in [12]. We consider $\Omega = (0, \pi)$, $T = 1$, $d(x, t) = 1$, $F(x, t) = x + \sin(t)$,

	β	$\Delta t = 1/10$	$\Delta t = 1/20$	Rate
$\alpha = 0.2$	1.2	2.1073e-03	5.2759e-04	1.9979
	1.4	1.9439e-03	4.8647e-04	1.9985
	1.6	1.7778e-03	4.4470e-04	1.9991
	1.8	1.6523e-03	4.1333e-04	1.9991
	2.0	1.5187e-03	3.8038e-04	1.9974
$\alpha = 0.4$	1.2	2.1073e-03	5.2759e-04	1.9979
	1.4	1.9439e-03	4.8647e-04	1.9985
	1.6	1.7778e-03	4.4470e-04	1.9991
	1.8	1.6523e-03	4.1333e-04	1.9991
	2.0	1.5187e-03	3.8038e-04	1.9974
$\alpha = 0.6$	1.2	2.0842e-03	5.1786e-04	2.0089
	1.4	1.9798e-03	4.9151e-04	2.0101
	1.6	1.8761e-03	4.6536e-04	2.0113
	1.8	1.8082e-03	4.4850e-04	2.0114
	2.0	1.7278e-03	4.2896e-04	2.0100
$\alpha = 0.8$	1.2	2.1725e-03	5.4257e-04	2.0015
	1.4	2.0760e-03	5.1799e-04	2.0028
	1.6	1.9838e-03	4.9440e-04	2.0045
	1.8	1.9284e-03	4.8030e-04	2.0054
	2.0	1.8694e-03	4.6585e-04	2.0046
$\alpha = 1.0$	1.2	2.3783e-03	5.9608e-04	1.9963
	1.4	2.2814e-03	5.7129e-04	1.9977
	1.6	2.1895e-03	5.4760e-04	1.9994
	1.8	2.1348e-03	5.3343e-04	2.0007
	2.0	2.0936e-03	5.2321e-04	2.0005

Table 2: Results concerning Problem 1. Convergence rate in time for different values of α and β with $\Delta x = 2/800$. The solution is regular enough in time and therefore we get second order convergence.

α	$\Delta x = 1/10$	$\Delta x = 1/20$	Rate
0.2	6.5175e-04	1.6259e-04	2.0031
0.4	5.2336e-04	1.3062e-04	2.0025
0.6	4.0707e-04	1.0163e-04	2.0019
0.8	3.0495e-04	7.6154e-05	2.0016
1.0	2.1766e-04	5.4362e-05	2.0014

Table 3: Results concerning Problem 2. Convergence rate in space for different values of α and $\beta = 2$ with $\Delta t = 1/800$. The solution is regular enough in space and therefore we get second order convergence.

and define $g(x, t)$ and $u_0(x)$, such that, the exact solution of this problem is given by

$$u(x, t) = \left(1 + \frac{t^\alpha}{\Gamma(1 + \alpha)}\right) \sin(x).$$

In this example, we also include the results we obtain when a nonuniform mesh in time is considered, that is, we assume $t_n = (n/M)^\gamma T$, where $\gamma \geq 1$. Note that for $\gamma = 1$ we obtain a uniform mesh.

For this solution we see that $u_t = \mathcal{O}(t^{\alpha-1})$ as $t \rightarrow 0$ and therefore it presents a singularity behavior. The regularity of the solution is $C^{\infty,0}([0, \pi] \times [0, T])$. For a uniform mesh the order of convergence in time is

α	$\Delta t = 1/10$	$\Delta t = 1/20$	Rate
0.2	6.5734e-04	1.6444e-04	1.9991
0.4	6.1647e-04	1.5346e-04	2.0061
0.6	5.5681e-04	1.3844e-04	2.0079
0.8	5.0006e-04	1.2430e-04	2.0083
1.0	4.5011e-04	1.1194e-04	2.0076

Table 4: Results concerning Problem 2. Convergence rate in time for different values of α and $\beta = 2$ with $\Delta x = 1/200$. The solution is regular enough in time and therefore we get second order convergence.

	β	$\Delta t = 1/10$	$\Delta t = 1/20$	Rate
$\alpha = 0.2$	1.2	7.9734e-02	3.5276e-02	1.1765
	1.4	7.8981e-02	3.4822e-02	1.1815
	1.6	7.8515e-02	3.4563e-02	1.1837
	1.8	7.8275e-02	3.4431e-02	1.1848
	2.0	7.8223e-02	3.4397e-02	1.1853
$\alpha = 0.4$	1.2	3.5666e-02	1.4085e-02	1.3404
	1.4	3.4561e-02	1.3641e-02	1.3411
	1.6	3.3930e-02	1.3390e-02	1.3414
	1.8	3.3608e-02	1.3261e-02	1.3417
	2.0	3.3522e-02	1.3225e-02	1.3419
$\alpha = 0.6$	1.2	1.5247e-02	5.3238e-03	1.5180
	1.4	1.4558e-02	5.1283e-03	1.5052
	1.6	1.4161e-02	5.0139e-03	1.4979
	1.8	1.3955e-02	4.9541e-03	1.4941
	2.0	1.3896e-02	4.9371e-03	1.4929
$\alpha = 0.8$	1.2	5.0490e-03	1.5836e-03	1.6728
	1.4	4.8284e-03	1.4829e-03	1.7031
	1.6	4.6975e-03	1.4564e-03	1.6895
	1.8	4.6283e-03	1.4423e-03	1.6821
	2.0	4.6077e-03	1.4385e-03	1.6795
$\alpha = 1.0$	1.2	3.7635e-03	9.4709e-04	1.9905
	1.4	2.7431e-03	6.9172e-04	1.9876
	1.6	2.1755e-03	5.5022e-04	1.9833
	1.8	1.8495e-03	4.6987e-04	1.9768
	2.0	1.6716e-03	4.2669e-04	1.9700

Table 5: Results concerning Problem 3. Convergence rate in time for different values of α and β with $\Delta x = 2/800$. The solution is not regular enough in time and therefore we get approximately $1 + \alpha$ order of convergence. This is in agreement with Theorem 3.

approximately $O(\Delta t^\alpha)$. This is according to the analysis done in Section 3.1 and in particular with Theorem 4. A non-uniform mesh improves the order of convergence as expected. In Table 6 and 7 we compare the performance of a non-uniform mesh versus a uniform mesh. In Table 8 we consider a very small time step to see that the method is second order convergent in space.

Problem 5. In order to observe the dynamical behavior of the fractional Fokker-Planck equation with a time dependent force, we consider equation (10) without the source term, for $p = q$, and with the initial

M	$\alpha = 0.25$	Rate	$\alpha = 0.50$	Rate	$\alpha = 0.75$	Rate
80	5.2235e-01	-	1.1051e-01	-	1.5103e-02	-
160	4.6086e-01	0.18071	8.2666e-02	0.41888	9.3432e-03	0.69288
320	4.0466e-01	0.18761	6.1090e-02	0.43634	5.7081e-03	0.71089
640	3.5374e-01	0.19404	4.4725e-02	0.44985	3.4851e-03	0.71184

Table 6: Results concerning Problem 4. Convergence rate in time for different values of α and $\beta = 2$ with $\Delta x = \pi/5120$ and $\gamma = 1$. Uniform time step. The solution is not regular enough in time. We have approximately α order convergence. This is in agreement with Theorem 4.

M	$\gamma = 1.0$	Rate	$\gamma = \alpha^{-1} = 1.6$	Rate	$\gamma = 2.0$	Rate
80	4.4207e-02	-	1.0396e-02	-	4.4297e-03	-
160	3.0110e-02	0.55402	5.4931e-03	0.92039	1.9917e-03	1.1532
320	2.0242e-02	0.57294	2.8629e-03	0.94015	8.8090e-04	1.1769
640	1.3478e-02	0.58671	1.4778e-03	0.95404	3.8482e-04	1.1948

Table 7: Results concerning Problem 4. Convergence rate in time for $\alpha = 0.625$ and $\beta = 2$ with $\Delta x = \pi/5120$. Non-uniform mesh. The convergent rate improves with a non-uniform time step.

Δx	$\alpha = 0.25$	Rate	$\alpha = 0.50$	Rate	$\alpha = 0.75$	Rate
$\pi/4$	3.5158e-01	-	3.6313e-01	-	3.6018e-01	-
$\pi/8$	8.1629e-02	2.1067	8.5220e-02	2.0912	8.5007e-02	2.0831
$\pi/16$	1.9009e-02	2.1024	2.0671e-02	2.0436	2.0875e-02	2.0258
$\pi/32$	4.5141e-03	2.0741	4.8261e-03	2.0987	5.1233e-03	2.0266

Table 8: Results concerning Problem 4. Convergence rate in space for different values of α and $\beta = 2$ with $M = 1000$ and $\gamma = \alpha^{-1}$. Non-uniform time space.

condition

$$u(x, 0) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right).$$

We assume $\sigma = 0.1$ and $x_0 = 2$.

We start to show, in Figure 2, the dynamics of the Fokker-Planck equation (10) without a force field, that is, for $F(x, t) = 0$ with $d(x, t) = 1$, to visualize the effect of the diffusion. In this case, the solution along time is still symmetric in shape, in relation to $x = 2$, as the initial solution. If we consider a force field different from zero, the solution is greatly influenced by the presence of the force field, as we can see in Figures 3 and 4.

In Figure 3, we show how the solution evolves in time for a force field, periodic in time, $F(x, t) = x + \sin(t)$, and $d(x, t) = 1$. From left to right we can observe the effect of changing α for a fixed β . From top to bottom the effect of changing β for a fixed α .

In Figure 4, the force is of the form $F(x, t) = -2x + 3x^2/(1 + e^{-t})$, related to the commonly named metastable potential [19]. Similarly to the previous figure, from left to right we can observe the effect of changing α for a fixed β and from top to bottom the effect of changing β for a fixed α .

5. Final Remarks

A numerical method is presented for a Fokker-Planck equation with a force field and diffusion depending on space and time. For the general case, $0 < \alpha < 1$ and $1 < \beta < 2$, the stability is discussed through the computation of the eigenvalues of a companion matrix showing the method is unconditionally stable. The numerical method is second order convergent in space and time for sufficiently regular solutions. We present numerical tests that show the rate of convergence is affected when less regular solutions are considered as discussed theoretically in Section 3. In this case, we can improve the rate of convergence by considering a

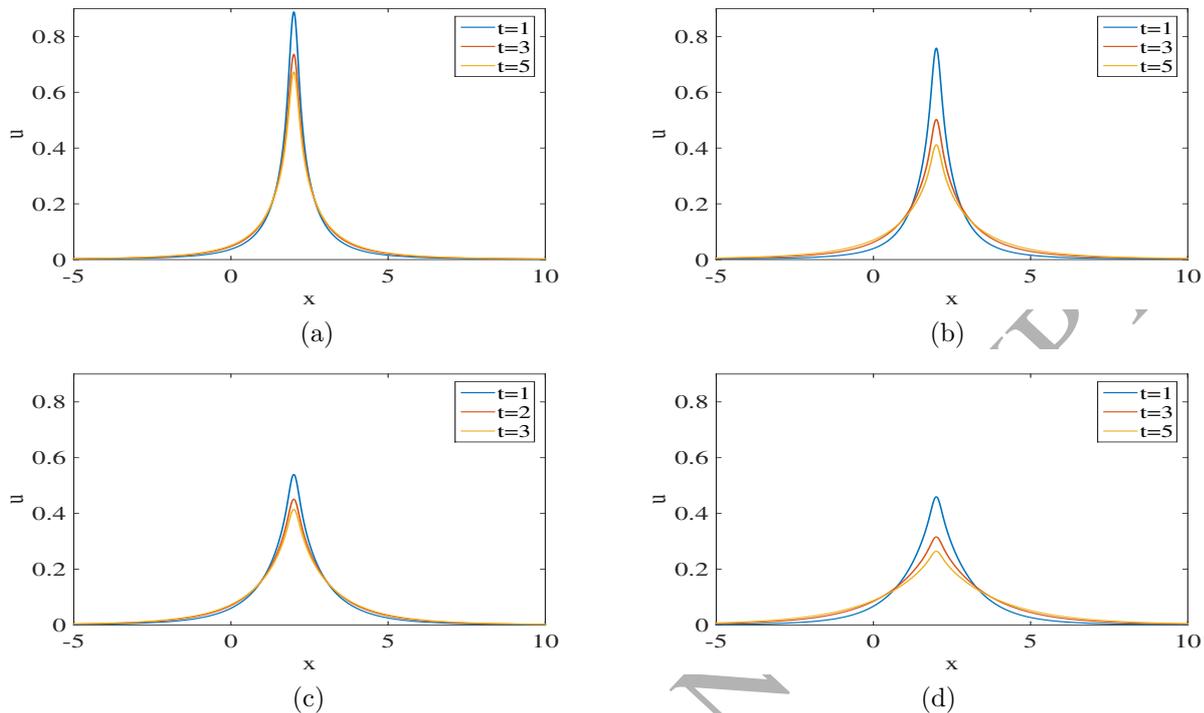


Figure 2: Time evolution of $u(x, t)$ for $F(x, t) = 0$ with $d(x, t) = 1$: (a) $\alpha = 0.3$, $\beta = 1.3$; (b) $\alpha = 0.6$, $\beta = 1.3$; (c) $\alpha = 0.3$, $\beta = 1.6$, (d) $\alpha = 0.6$, $\beta = 1.6$.

non-uniform mesh. In the end, in order to reveal the dynamics of the equation, we display the time evolution of the solution $u(x, t)$, for different time dependent force fields.

The numerical method presented here can be generalized for the velocity fractional Klein-Kramers equation, defined in the position-velocity space, that is, $x-v$ space, where a fractional operator is considered in the open space v and in the x space different type of boundary conditions can be studied. However, the theoretical analysis presents additional difficulties that will require a separated study.

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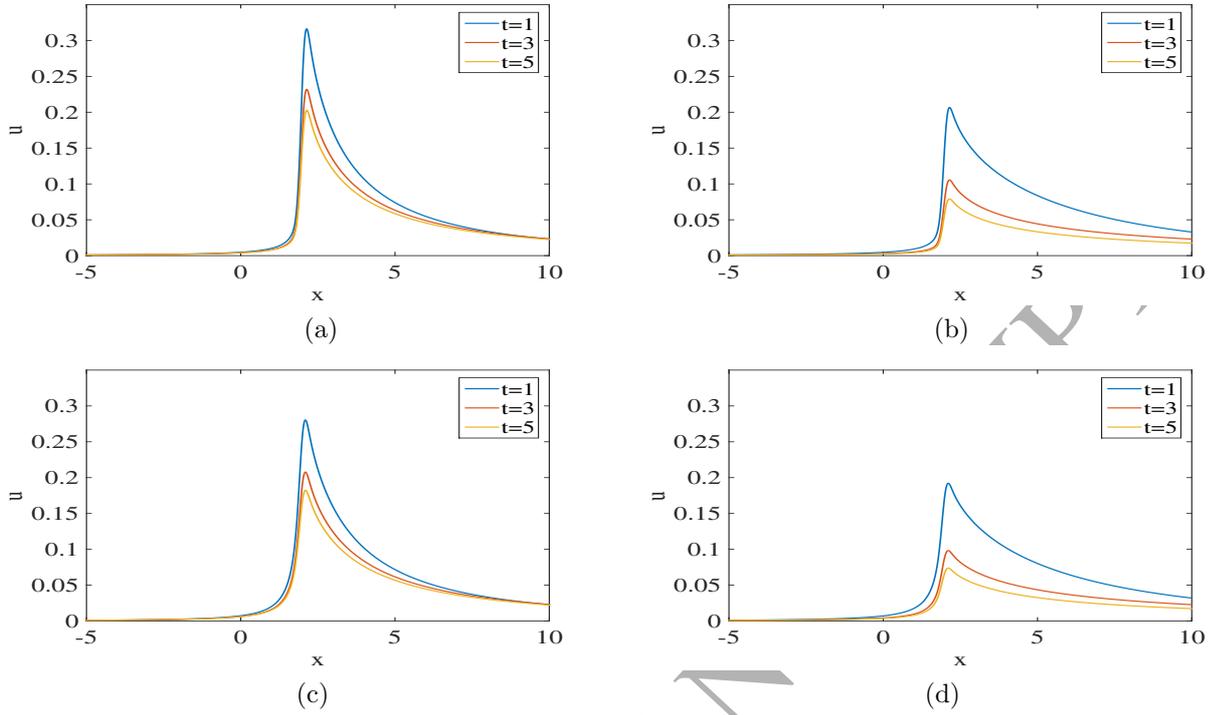


Figure 3: Time evolution of $u(x,t)$ for $F(x,t) = x + \sin(t)$ with $d(x,t) = 1$: (a) $\alpha = 0.3, \beta = 1.3$; (b) $\alpha = 0.6, \beta = 1.3$; (c) $\alpha = 0.3, \beta = 1.6$, (d) $\alpha = 0.6, \beta = 1.6$.

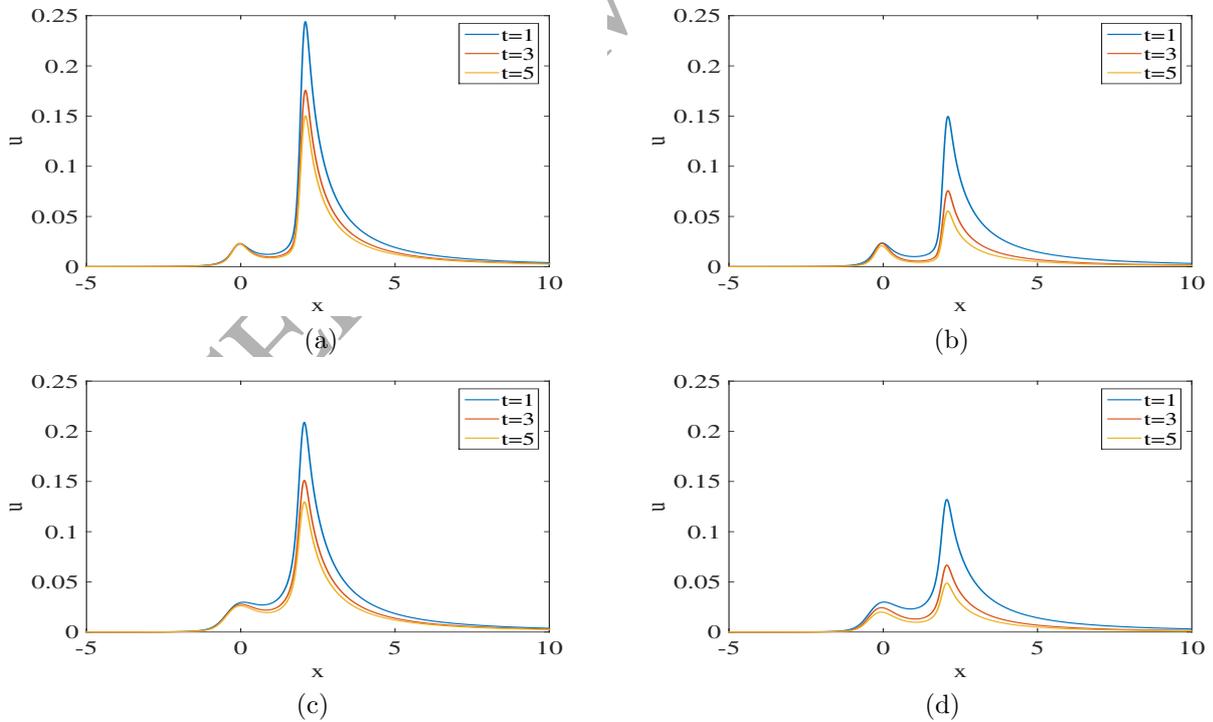


Figure 4: Time evolution of $u(x,t)$ for $F(x,t) = -2x + 3x^2/(1 + e^{-t})$ with $d(x,t) = 1$: (a) $\alpha = 0.3, \beta = 1.3$; (b) $\alpha = 0.6, \beta = 1.3$; (c) $\alpha = 0.3, \beta = 1.6$, (d) $\alpha = 0.6, \beta = 1.6$.

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