The Continuous Time Random Walk and the Finite Difference Method for the Space Time Fractional Diffusion Equations

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Abstract

The space fractional diffusion equations are a linear partial pseudo-differential equation with spatial fractional derivatives in space. This equation arises when the motion of the particle is not Brownian and there are extremely long jumps whose length is distributed according to the Lévy long tail $|x|^{-\alpha}$, $0 < \alpha < 2$. Some physical, biological and chemical models exhibit a power law with a non integer frequency of order $t^{-\beta}$, $0 < \beta < 1$. In this case, one needs to replace the first order time differential operator by the Caputo time fractional operator. In this paper, I am interested in finding the approximation solution of the space time fractional diffusion equations by using the common finite difference rules beside using the Gruenwald-Letnikov difference scheme for the fractional differential operators. The approximation solution is proved to be conditionally stable. Finally, some numerical examples are given based on this method.

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Introduction

In 1827 an English botanist, Robert Brown, noticed that small particles suspended in fluids perform peculiarly erratic movements. This phenomenon, which can also be observed in gases, is referred to as Brownian motion [1]. It was not until 1905 that Albert Einstein first advanced a satisfactory theory. Einstein considered the case of the free particle, that is, a particle in which no forces other than those due to the molecules of the surrounding medium are acting. He was able to show that the probability density $u(x, t)$ must satisfy the partial differential equation

$$\frac{\partial u(x,t)}{\partial t} = a \frac{\partial^2 u(x,t)}{\partial x^2}, \quad (1.1)$$

where $a > 0$ is a certain physical constant. This equation is called the diffusion equation or the free diffusion. The conditions imposed on $u$ are $u(x,t) > 0$, $\int u(x,t)dx = 1$.

The solution $u(x,t)$ of equation (1.1) with the initial condition $u(x,0) = \delta(x-x_0)$ is well known as the corresponding Green function or the fundamental solution. As soon as the theory for the free particle was established, a natural question arose how it should be modified in order to take into account the outside forces $F(x)$, for example, gravity which acts in the direction of the x-axis and forces the particle to go back to the origin. When the external force is proportional to the distance from the origin, it has shown that equation (1.1) should be replaced by

$$\frac{\partial u(x,t)}{\partial t} = a \frac{\partial^2 u(x,t)}{\partial x^2} + (b u(x,t)), a > 0, b > 0, -\infty < x < \infty, t > 0 \quad (1.2)$$

This partial differential equation describes the elastic diffusive motion of a bounded particle (for example, small pendulum) and being a special case of the general (diffusion-convection equation), see [2-4]. equation (1.2) is a special case from Fokker Planck equation which reads...
\[
\frac{\partial u(x,t)}{\partial t} = L_u u(x,t), a > 0, b > 0, -\infty < x < \infty, t > 0. \tag{1.3}
\]

Where
\[
L_u u(x,t) = \frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial F(x) u(x,t)}{\partial x}. \tag{1.4}
\]

It is well known that the Ehrenfest Model is mathematically modelled by the Fokker Planck equation. The Fokker-Planck equation (FPE) is one of the most widely used equations of statistical physics for studying the dynamic behaviour of stochastic differential equations driven by Gaussian noises, see [5-7]. However, it turns out that many other physical phenomena are outside this frame work. Especially solutes that move through fractal media commonly exhibits large deviations from the stochastic processes of Brownian motion and do not require finite velocity. The extension to Lévy stable motion is a straight forward generalization due to the common properties of Lévy stable motion and Brownian motion, but the Lévy flights differ from the regular Brownian motion by the occurrence of extremely long jumps whose length is distributed according to the Lévy long tail \( -1 < \alpha < 2 \). Many physical, biological, medical, and chemical models exhibits a power law with a non integer frequency of order \( \beta \), where \( 0 < \beta < 1 \), for diffusion processes and \( 0 < \beta < 2 \) for wave propagation. Also in a complex inhomogeneous conducting medium experimental evidence shows that the sound waves propagate with power law of non integer order \( 1 < \beta < 2 \).

Such processes have a memory. In this paper, I give a review about the approximate, analytical and the continuous time random walk of the space time fractional diffusion processes under the action of constant and linear forces. Therefore, this paper is written in 6 sections. Section 1 is devoted to the introduction. Section 2 is to the important used notations. In section 3, I study the continuous time random walk of the space fractional diffusion equations. In section 4, the approximate and reversibility of the time fractional Ehrenfest model are discussed. Sections 5 and 6 are devoted to the explicit and implicit approximate solutions of the diffusion equations under the action of a constant force.

**Important notations**

In this research papers, I use the space fractional operator \( \partial^\alpha u(x,t) \)

which is called the Feller space-fractional differentiation operator of order \( \alpha \) where and I adopt the notation introduced by Załadusky, who considered it as a power of the positive definite operator \( \partial^\alpha = \frac{\partial}{\partial v^\alpha} \), see Oldham & Spanier [8], Ross & Miller [9], and recently Gorenflo & Mainardi [10-13]. This form must not be confused with a power of the first order differential operator \( \partial^\alpha \). The Fourier transform of \( \partial^\alpha \) reads

\[
f\{D^\alpha_{\xi}\phi(x) ; k\} = -\left|k\right|^\alpha \phi(k), 0 < \alpha \leq 2, k \in \mathbb{R}, \tag{2.1}\]

While

\[
f\left\{\frac{d^\alpha}{dx^\alpha} \phi(x) ; k\right\} = - (i)^\alpha \phi(k), n = 7, \alpha \in \mathbb{R} \tag{2.2}\]

The operator \( D^\alpha_{0} \) is expressed as the negative inverse of the suitable integral operator (Riesz potential) \( I^\alpha_{0} \) whose symbol is \( \left(k^\alpha\right) \) and can be written as

\[
\frac{d^\alpha}{dx^\alpha} = - I^\alpha_{0}, 0 < \alpha \leq 2, \alpha \neq 1, \tag{2.3}\]

Where \( I^\alpha_{0} \) is the inverse of the symmetric Riesz potential. Fractional integral operators \( I^\alpha_{0} \) is defined as

\[
I^\alpha_{0} \Phi(x) = c(\alpha) I^\alpha_{0} \Phi(x) + c_\alpha I^\alpha_{0} \Phi(x), \alpha \neq 1, \tag{2.4}\]

where

\[
c(-\alpha) = c_\alpha = \frac{1}{2 \cos \frac{\alpha \pi}{2}}. \tag{2.5}\]

Therefore, the symmetric Riesz potential can be written as

\[
I^\alpha_{0} \Phi(x) = \frac{1}{2 \cos \frac{\alpha \pi}{2}} \left( I^\alpha_{0} \Phi(x) + I^\alpha_{0} \Phi(x) \right), 0 < \alpha \leq 2, \alpha \neq 1. \tag{2.6}\]

Where \( I^\alpha_{0} \) denote the Riemann-Liouville fractional integral operators, by some people called Weyl integrals. Because of equation (5.3), the approximation solution of this equation are studied at \( \alpha = 2, 0 < \alpha < 1 < \alpha < 2 \) and \( \alpha = 1 \) separately.

**Grünwald-Letnikov Scheme for all Values of \( \alpha \)**

The approximating of \( I^\alpha_{x} \) in the Grünwald-Letnikov scheme for the different values of \( \alpha \) is listed below. Firstly for \( 0 < \alpha < 1 \)

\[
I^\alpha_{-x} \phi(x) = \frac{1}{\alpha \pi m} \sum_{\mathbb{Z} \neq 0} \left( \frac{\alpha}{x} \right)^{\phi(\alpha, x; m \pi k)}, \tag{2.7}\]

secondly for \( 1 < \alpha < 2 \)

\[
I^\alpha_{-x} \phi(x) = \frac{1}{k \pi} \sum_{\mathbb{Z} \neq 0} \left( \frac{\alpha}{x} \right)^{\phi(\alpha, x; (x-k) \pi k)}. \tag{2.8}\]

Third for \( \alpha = 1 \), One cannot use the Grünwald-Letnikov discretization of \( D^\alpha_{x} \) as \( \alpha = 1 \), because the denominator in equation (5.3). Instead of the Grünwald-Letnikov discretization, I use the discretization used by R. Gorenlo, who replaced the factor \( (\alpha) \) by \( \frac{1}{k \pi} \) for \( k = 0 \) and

\[
\frac{1}{k \pi |k| (|k|+1)} \tag{2.9}\]

**Caputo time-fractional derivative**

The time fractional derivative operator of order \( \alpha \) is defined as

\[
D^\alpha_{x} f(t) = \gamma_{\alpha} \left\{ \int_{0}^{t} f^{(m)} (\tau) K_{\alpha} (\tau) d\tau \right\} \tag{2.9}\]

With

\[
K_{\alpha} (\tau) = \frac{(\tau - \alpha)^{\beta-1}}{\tau^{(m-\alpha)}}, \tag{2.9}\]

being called the memory function, see [14-18]. This kernel enables us to reflect the memory effects of many physical processes. The Laplace transform of it reads

\[
\mathcal{L}\{D^\alpha_{x} f(t) ; s\} = s^\beta f(0)-s^{\beta-1} f(0)-s^{\beta-2} f^{(1)}(0)-...-s^{\beta-n} f^{(n-1)}(0). \tag{2.9}\]
We call them iid. Furthermore the waiting times and the jumps \( X \) and \( W \) are independent of each other. The new position at time \( t \) before moving instantaneously to the next location with jump \( X \) is

\[
T_n = x_n = x_{n+1} + X_n, \quad \text{which equals to}
\]

\[
x_0 = 0, \quad x_n = \sum_{k=1}^{n} T_k, \quad (3.8)
\]

and the particle remains resting at \( x = x_{n+1} \) in the time interval \( t < T_n \). For generating the random variable \( X_n \), i.e. the jump, having the Cauchy or the Gaussian distributions, we use the method of inversion which seems to be simple and most effective. We also use the same method to simulate the random variable \( W \), i.e. the waiting time, having an exponential distribution with mean 1. For simulating the jump \( X \) corresponding stable distribution, \( \alpha \in (0,2) \), we use the method given in the book of Jancik [21], in order to simulate the random variable \( X \) having a symmetric and nonsymmetric \( \alpha - \text{stable} \) distribution. Firstly, for the symmetric \( \alpha - \text{stable} \) random variable \( X \), i.e. \( \beta = 0 \) we follow the steps

a) Generate a random variable \( V \) uniformly distributed on \( \left(-\frac{\pi}{2}, \frac{\pi}{2}\right) \) and an exponential random variable \( W \) with mean 1,

b) Compute

\[
X = \sin(\alpha V) \left( \frac{\cos(V)}{\cos(V')^{\alpha}} \right)^{\frac{\alpha - 1}{\alpha}}, \quad (3.10)
\]

Secondly, for the non-symmetric \( \alpha - \text{stable} \) random variables \( X \) with \( \beta' \in [-1,1] \), one has to follow the following steps

1. Generate a random variable \( V \) uniformly distributed on \( \left(-\frac{\pi}{2}, \frac{\pi}{2}\right) \) and an exponential random variable \( W \) with mean 1,

2. Compute

\[
X = D_{\alpha,\beta'} \sin(\alpha V + V') \left( \frac{\cos(V')^{\beta'}}{\cos(V')^{\beta' \alpha}} \right)^{\frac{\alpha - 1}{\alpha}}, \quad (3.11)
\]

Where

\[
D_{\alpha,\beta'} = \left[ \cos \left( \arctan \left( \beta \tan \left( \frac{\pi \alpha}{2} \right) \right) \right) \right]^{\frac{\alpha - 1}{\alpha}} .
\]

This transformation enables to transfer the solution of the space-fractional diffusion equation to be a solution of the space-fractional Fokker-Planck equation. In [19], I use the Monte Carlo method to simulate the random walk of the discussed model. For this purpose, I generate two random variables \( \{X_n, T_n\} \). First we suppose that a particle starts at the origin \( x_n = 0 \), and waits a period of time \( T_n \), at a particular location \( x_n, T_n \) before moving instantaneously to the next location with jump width \( X_n, V_n \). We call \( T_n \) the waiting times, where \( T_n = t_n - t_{n-1}, t_n > t_{n+1} \). The waiting times \( T_n \) are iid and likewise the jumps \( X_n \) are iid. Furthermore the waiting times and the jumps are independent of each other. The new position at \( t_n = t_{n+1} + t_n \) which is equivalent to

\[
t_0 = 0, t_n = \sum_{k=1}^{n} T_k, \quad (3.8)
\]

\[
X_n = x_n + X_n, \quad \text{which equals to}
\]

\[
x_0 = 0, x_n = \sum_{k=1}^{n} X_n, \quad (3.9)
\]

Figure 1: Cauchy, \( \alpha = 1 \), for DE and FPE.
In the numerical result section, I give some numerical results for the jumps of the diffused particles, see Figures [1-4]. The first column represents the CTRW of the diffusion, DE and the second column represents the CTRW of the diffusion under the action of attractive linear force, FPE.

**Time fractional Ehrenfest model**

The Ehrenfest model, classical case, and the time-fractional Ehrenfest model are considered as stochastic processes and are mathematically modelled by the time-fractional diffusion equation under the action of an attractive linear force, equation (3.4). For more information about the classical Ehrenfest model, see [18]. Equation (3.4) for $\alpha = 2$ has the solution

$$u(\zeta, \tau) = p(\zeta, \tau; \zeta_0, \tau_0) = \frac{1}{\sqrt{2\pi \tau_0 (1 - e^{-2\tau})}} e^{-\left(\frac{\zeta - \zeta_0 e^{-\tau}}{\sqrt{\tau_0 (1 - e^{-2\tau})}}\right)^2}$$

Replace the first order time-derivative by Caputo time-fractional derivative of order $\beta$, where $\beta \in (0,1]$ and replace $(\zeta, \tau)$ by simply $(x,t)$. One gets

$$D_\beta u(x,t) = a \frac{\partial \mu(x,t)}{\partial x} \left( \frac{\partial \mu(x,t)}{\partial x} \right) \frac{\partial u(x,t)}{\partial x}$$

The solution of this equation is getting by using the separation of variables as

$$u(x,t) = \sum_{n=0}^\infty A_n \mathcal{E}_n(x) e^{-x/\lambda},$$

Where $\mathcal{E}_n(x)$ is the Mittag-Leffler function and $D_\beta(x)$ is the Weber function. It is worth to say that in [20], I studied the fundamental solution (Green function) of the space-time fractional Ehrenfest model by replacing $\frac{\partial u(x,t)}{\partial x}$ in equation (4.1) by $D_\beta(x)$. Applying the discretization of the Caputo time fractional operator being given in equation (2.10) besides the common finite difference rule for descretizing $\frac{\partial u(x,t)}{\partial x}$ and

\[
\frac{\partial u(x,t)}{\partial t} = \text{at equation (4.1), then Solving for } y_j^{(\alpha \beta)} \text{, one gets}
\]

\[
y_j^{(\alpha \beta)} = \sum_{k=1}^{R} (-1)^k \binom{\beta}{k} y_j^{(\beta)} + \sum_{k=1}^{R} (-1)^k \binom{\beta}{k} y_j^{(\beta) - k} 
\]

The discrete scheme for the classical case is put in the matrix form

\[
y^{(i+1)} = P^n y^{(i)},
\]

where the matrix \( P = p_{ij} \) is defined as

\[
p_{ij} = \begin{cases} \frac{2\mu}{R} & j \geq i+1, i \geq -R+1, \ldots, R-1 \ \\ \approx (\beta - 2\mu) & j = i, i = -R, \ldots, R \ \\ \mu & j = 1, R+1, \ldots, R-1. \end{cases}
\]

Here \( \sum_{i=-R}^{R} p_{ij} = 1 \) that \( P^n \) means is a stochastic matrix and the classical Ehrenfest forms a Markov chain. While the discrete scheme for the time-fractional Ehrenfest model is put in the matrix form

\[
y^{(i+1)} = Q^n y^{(i)},
\]

where the matrix \( Q = q_{ij} \) is defined as

\[
q_{ij} = \begin{cases} \frac{2\mu}{R} & j \geq i+1, i \geq -R+1, \ldots, R-1 \ \\ \approx (\beta - 2\mu) & j = i, i = -R, \ldots, R \ \\ \mu & j = 1, R+1, \ldots, R-1. \end{cases}
\]

Here \( \sum_{j=-R}^{R} q_{ij} = 1 \) that \( Q^n \) is not a stochastic matrix and therefore its process is not a Markov chain. Both matrices can be written as

\[
P = I + \mu H \quad \text{and} \quad Q = \beta I + \mu H,
\]

where \( H \) is a matrix whose its rows are summed to zero. The elements of the stochastic matrix \( P \) converge to the binomial distribution at \( n \to \infty \) as

\[
\lim_{i=\infty} P^n = (\pi_0, \pi_1, \ldots, \pi_R),
\]

where

\[
\pi_j = 2^{-2j} \binom{2R}{j+R}.
\]

The stationary row of the matrix \( Q \) is getting by using the eigenvector \( y^* \) with eigenvalue zero of the matrix \( H \). Define \( v = cy^* \) to be the stationary solution of the matrix \( Q \), where

\[
\sum_{j=-R}^{R} y_j^* = 1.
\]

Convergence of the Discrete Approximate Solution of both Models

Define, first the vector \( z \) such that

\[
z^{(i)} = \left\{ d(t_0), d(t_1), d(t_2), \ldots \right\},
\]

where

\[
d(t) = \sum_{j=-R}^{R} \left( z_j^{(i)} - \pi_j \right) \delta(t-i).
\]

For the Ehrenfest model, \( d(t) = \delta(t) \).

The space-time fractional diffusion under the action of a constant force

The advection dispersion equations, sfade is mathematically models the particle motion at the earth surface. This equation is obtained from equation (1.3) and equation (1.4) by replacing

\[
\partial_x (x,t) = \text{the time-fractional Ehrenfest is}
\]

\[
\pi_j p_{ik} = \pi_k p_{ij} = \beta_j, j, k \in \mathbb{N}, \quad (4.9)
\]

although the classical is Ehrenfest is Markov and the non classical is Non-Markov.

The space-time fractional diffusion under the action of a constant force

The advection dispersion equations, sfade is mathematically models the particle motion at the earth surface. This equation is obtained from equation (1.3) and equation (1.4) by replacing
Abstract: We study the space-time fractional advection-dispersion equation, which is a generalization of the classical advection-dispersion equation. The fractional derivatives are in the Caputo sense. An explicit finite difference scheme is designed to solve this equation. The Laplace transform is used to simplify the problem and the inverse Laplace transform is then performed to obtain the solution in the original domain. Numerical experiments are carried out to validate the proposed method.

Keywords: Fractional advection-dispersion equation, Explicit finite difference method, Laplace transform.
Where $f_{-O-k}$, $i,j \in [-R,R]$. I have proved in [22] that the discrete schemes of these model converge, in the Fourier-Laplace domain, to the Fourier-Laplace transforms of the corresponding fractional differential equations for all values of $\alpha$ and $\beta$. The bath of the diffused particle $y(n) = y(t_n)$ for different values of the time is simulated at Figures [6-8] and . In Figure [9], I simulated the singular case, i.e. as

**Implicit difference scheme of the space-time fractional advection diffusion equation**

In this section, I study the implicit difference scheme of the advection diffusion equation (5.1), see [23], by using $\theta$—the method which is also known as the weighted method. The idea of the method is to replace $y(n)$ in the right hand side of the solved equation (5.6) by $\left(\theta y(n) + (1-\theta) y(n+1)\right)$.

The implicit method allows to discuss the path of the diffusion in the long run. Therefore, I have numerically compared at this paper the path of the diffusive particles for large values of $t$. The stability analysis of the discrete schemes are discussed and proved for each value of $\alpha$ and $\beta$ according to the Von-Neumann Necessary condition for Stability [24]. I have used here the diffusion and drift constants as variables to adjust the value of $R$ for each values of $\alpha$ and $\beta$. Consequently the value of $\mu$ is also varied. Finally, to simulate the path of the diffused particle for different values of $t, \alpha$ and $\beta$, Figures [10-13].
Figure 11: Implicit time evolution of $y^{(1)}$. 

Figure 12: Implicit time evolution of $y^{(2)}$. 

Figure 13: Implicit time evolution of $y^{(3)}$. 

**Numerical Result**

Figures [1-13].

**References**

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