

Fractional Fokker-Planck dynamics: Stochastic representation and computer simulation

Marcin Magdziarz* and Aleksander Weron

*Hugo Steinhaus Center, Institute of Mathematics and Computer Science, Wrocław University of Technology,
Wyb. Wyspińskiego 27, 50-370 Wrocław, Poland*

Karina Weron

Institute of Physics, Wrocław University of Technology, Wyb. Wyspińskiego 27, 50-370 Wrocław, Poland

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A computer algorithm for the visualization of sample paths of anomalous diffusion processes is developed. It is based on the stochastic representation of the fractional Fokker-Planck equation describing anomalous diffusion in a nonconstant potential. Monte Carlo methods employing the introduced algorithm will surely provide tools for studying many relevant statistical characteristics of the fractional Fokker-Planck dynamics.

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I. INTRODUCTION

Many physical transport problems take place under the influence of an external field. A framework for the treatment of anomalous diffusion problems under the influence of an external force field is developed in terms of the fractional Fokker-Planck equation (FFPE). It provides a useful approach for the description of transport dynamics in complex systems which are governed by anomalous diffusion [1] and nonexponential relaxation patterns [2]. The FFPE can be rigorously derived from the generalized master equation or the continuous-time random walk (CTRW) models as shown in [3,4]. The numerical simulation of the anomalous transport in a tilted periodic potential within the framework of the FFPE through the underlying CTRW was presented recently in [5].

Several methods of solution of the FFPE in terms of the probability density function are described in [1]. However, the limitation of such an approach is that it does not allow one to construct and analyze sample paths of the underlying stochastic process. Here, we introduce a simple and efficient method for computer simulation of sample paths of the anomalous diffusion process described by the FFPE. This lets us numerically investigate statistical properties of the physical system under consideration, such as quantile lines and the time evolution of the corresponding probability density function (PDF). The proposed simulation method is a consequence of a stochastic representation of the anomalous diffusion process $Y(t)$ described by the FFPE in terms of the PDF function $w(x, t)$: namely, $Y(t) = X(S_t)$, where $X(\tau)$ is the solution of a certain Itô stochastic differential equation and S_t is the inverse-time α -stable subordinator. A basic feature arising in this context is the random change of time of the system. It reflects the fact that the distribution of waiting times between successive jumps of a particle in the underlying CTRW scenario is heavy tailed. Moreover, the process $X(\tau)$ described by Langevin-type dynamics with standard Brownian motion $B(\tau)$ sheds some light on the fractional dynamics. Summing up, the stochastic representation of the

anomalous diffusion process described by the FFPE gives another link to the foundation of microscopic dynamics within the Langevin picture. A related problem for the fractional Fokker-Planck dynamics for Lévy flights via the corresponding Langevin equation in the context of resonant activation was numerically studied in [6]; see also [7].

The article is structured as follows. In Sec. II we show that a stochastic process, whose PDF obeys the dynamics of the fractional Fokker-Planck equation, can be identified as the subordination of two fundamental processes: the solution of a certain Itô stochastic differential equation and the inverse-time α -stable subordinator. Taking advantage of the obtained representation, in Sec. III we find an efficient method of simulating sample paths of the anomalous diffusion process. We show that the introduced algorithm and Monte Carlo methods allow us to detect and examine many relevant statistical properties of the fractional Fokker-Planck dynamics, such as quantile lines, evolution in time of the PDF's, asymptotic stationarity, self-similarity, etc.

II. STOCHASTIC REPRESENTATION OF THE FFPE

The celebrated FFPE, describing anomalous diffusion in the presence of an external potential $V(x)$, is given by the following formula:

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

It was derived explicitly in [1], where methods of its solution were introduced and for some special cases exact solutions were calculated. Here, the operator ${}_0D_t^{1-\alpha}$, $\alpha \in (0, 1)$, is the fractional derivative of the Riemann-Liouville type [8]. It is known that ${}_0D_t^{1-\alpha}$ introduces a convolution integral with a slowly decaying power-law kernel, which is typical for memory effects in complex systems [9]. In Eq. (1), $w(x, t)$ denotes the PDF and the prime stands for the derivative with respect to the space coordinates relating the force $F(x)$ and the potential through $F(x) = -V'(x)$. The constant K denotes the anomalous diffusion coefficient, whereas η is the generalized friction constant. For $\alpha \rightarrow 1$, Eq. (1) becomes the ordinary Fokker-Planck equation. The FFPE describes subdif-

*Electronic address: marcin.magdziarz@pwr.wroc.pl

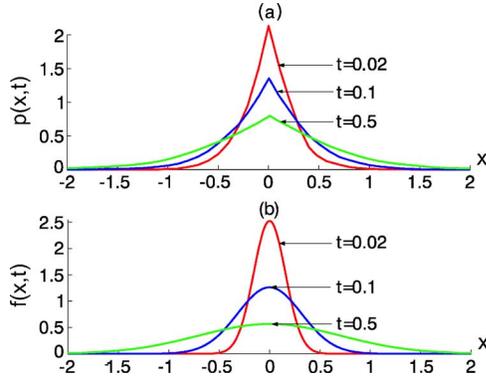


FIG. 1. (Color online) Evolution in time of the PDF of (a) the anomalous diffusion $X(S_t)$ with parameters $V(x)=\text{const}$, $\alpha=0.6$, $K=1/2$, and $\eta=1$ and (b) the standard diffusion (Brownian motion). The cusp shape of the PDF in the anomalous diffusion case confirms the correctness of the simulation algorithm (cf. [1]). The results in (a) were obtained by Monte Carlo methods using the introduced algorithm.

fusion in accordance with the mean-squared displacement in the force-free limit, and it obeys some generalized fluctuation-dissipation theorem. Moreover, a generalization of the Einstein-Stokes-Smoluchowski relation $K=k_B T/\eta$ connects the generalized friction and diffusion coefficients [1].

The main aim of this section is to show that the solution $w(x,t)$ of the FFPE (1) is equal to the PDF $p(x,t)$ (see Fig. 1) of the subordinated process $Y(t)$ obtained by a random change of time,

$$Y(t) = X(S_t), \quad (2)$$

where the process $X(\tau)$ is the solution of the Itô stochastic differential equation

$$dX(\tau) = -V'(X(\tau))\eta^{-1}d\tau + (2K)^{1/2}dB(\tau) \quad (3)$$

driven by standard Brownian motion $B(\tau)$. The subordinator S_t , called the *inverse-time α -stable subordinator*, $\alpha \in (0, 1)$, is defined [10,11] as

$$S_t = \inf\{\tau: U(\tau) > t\}, \quad (4)$$

where $U(\tau)$ denotes a strictly increasing α -stable Lévy motion [14]—i.e., an α -stable process with Laplace transform

$$\langle e^{-kU(\tau)} \rangle = e^{-\tau k^\alpha}. \quad (5)$$

Moreover, the processes $X(\tau)$ and S_t are assumed to be independent. Observe that both processes $U(\tau)$ and $X(\tau)$ are indexed by the internal time τ . The time is not real, physical time. In order to find a position of a particle at the observable time t , we have to introduce the inverse-time α -stable subordinator S_t relating the internal time τ and the observable time t .

The physical properties of the subordinator S_t have been discussed in detail in recent papers [10,11]. It is worth mentioning that S_t appears in a natural way and can be explicitly

TABLE I. Key processes and the corresponding notation.

| Process | Description | Density |
|---------------|--|--------------|
| $X(\tau)$ | standard diffusion | $f(x, \tau)$ |
| S_t | inverse-time α -stable subordinator | $g(\tau, t)$ |
| $Y(t)=X(S_t)$ | anomalous diffusion | $p(x, t)$ |
| $U(\tau)$ | α -stable Lévy motion | $u(t, \tau)$ |

derived when considering the CTRW scenario with heavy-tailed waiting-time distributions between successive jumps of the particle.

The advantage of the stochastic representation (2) relative to other popular subordination methodologies, expressed in the language of PDF's through an integral transform [12,13], follows from the possibility of a straightforward computer simulation [14] of sample paths of the anomalous diffusion process $X(S_t)$.

Now, let us pass on to the main problem of the section. Let the potential $V(x)$ be an arbitrary nonconstant function. First, we establish the relationship between the PDF $g(\tau, t)$ of S_t and the PDF $u(t, \tau)$ of $U(\tau)$ (see Table I for the notation used). Since $U(\tau)$ is the strictly increasing α -stable Lévy motion, it is $\frac{1}{\alpha}$ self-similar [15]; i.e., its PDF fulfills the scaling relation

$$u(t, \tau) = \frac{1}{\tau^{1/\alpha}} u\left(\frac{t}{\tau^{1/\alpha}}, \tau\right),$$

where $u(t) = u(t, 1)$. From Eq. (4) we get that $\Pr(S_t < \tau) = \Pr(U(\tau) \geq t)$, and therefore

$$\begin{aligned} g(\tau, t) &= -\frac{\partial}{\partial \tau} \int_0^t u(y, \tau) dy \\ &= -\frac{\partial}{\partial \tau} \int_0^t \frac{1}{\tau^{1/\alpha}} u\left(\frac{y}{\tau^{1/\alpha}}, \tau\right) dy \\ &= -\frac{\partial}{\partial \tau} \int_0^{t\tau^{1/\alpha}} u(y) dy \\ &= \frac{t}{\alpha \tau^{1+1/\alpha}} u\left(\frac{t}{\tau^{1/\alpha}}, \tau\right) \\ &= \frac{t}{\alpha \tau} u(t, \tau). \end{aligned} \quad (6)$$

Now, using the fact that $\langle e^{-kU(\tau)} \rangle = \hat{u}(k, \tau) = \int_0^\infty e^{-kt} u(t, \tau) dt = e^{-\tau k^\alpha}$, we calculate the Laplace transform

$$\begin{aligned} \hat{g}(\tau, k) &= \int_0^\infty e^{-kt} g(\tau, t) dt \\ &= \int_0^\infty e^{-kt} \frac{t}{\alpha \tau} u(t, \tau) dt \\ &= -\frac{1}{\alpha \tau} \frac{\partial}{\partial k} \int_0^\infty e^{-kt} u(t, \tau) dt \end{aligned}$$

$$\begin{aligned}
 &= -\frac{1}{\alpha\tau} \frac{\partial}{\partial k} e^{-\tau k^\alpha} \\
 &= k^{\alpha-1} e^{-\tau k^\alpha}.
 \end{aligned} \tag{7}$$

Using the total probability formula and the independence of $X(\tau)$ and S_t , we get that the PDF $p(x, t)$ of $X(S_t)$ is given by

$$p(x, t) = \int_0^\infty f(x, \tau) g(\tau, t) d\tau,$$

where $f(x, \tau)$ and $g(\tau, t)$ are the PDF's of $X(\tau)$ and S_t , respectively. Consequently, in the Laplace space, the above formula and Eq. (7) yield

$$\begin{aligned}
 \hat{p}(x, k) &= \int_0^\infty e^{-kt} p(x, t) dt \\
 &= \int_0^\infty f(x, \tau) \hat{g}(\tau, k) d\tau \\
 &= \int_0^\infty f(x, \tau) k^{\alpha-1} e^{-\tau k^\alpha} d\tau.
 \end{aligned} \tag{8}$$

Since the process $X(\tau)$ is given by the Itô stochastic differential equation (3), its PDF $f(x, \tau)$ obeys the ordinary Fokker-Planck equation [1]

$$\frac{\partial f(x, \tau)}{\partial \tau} = \left[\frac{\partial}{\partial x} \frac{V'(x)}{\eta} + K \frac{\partial^2}{\partial x^2} \right] f(x, \tau);$$

thus, in the Laplace space the following scaling relationship between $f(x, \tau)$ and the solution $w(x, t)$ of Eq. (1) holds [12,16]:

$$\hat{w}(x, k) = k^{\alpha-1} \hat{f}(x, k^\alpha).$$

Now, using Eq. (8) we finally obtain

$$\hat{w}(x, k) = k^{\alpha-1} \hat{f}(x, k^\alpha) = \int_0^\infty f(x, \tau) k^{\alpha-1} e^{-\tau k^\alpha} d\tau = \hat{p}(x, k). \tag{9}$$

The last formula gives us the desired relation

$$w(x, t) = p(x, t). \tag{10}$$

Thus, we have shown that the solution $w(x, t)$ of the FFPE (1) describes the dynamics of the PDF of the subordinated process $X(S_t)$ defined in Eq. (2). This result provides a physical interpretation of the anomalous diffusion phenomenon as the process obtained by replacing the operational time τ [12], in the standard diffusion $X(\tau)$, by the inverse-time α -stable subordinator S_t . This change of the operational time of the system is related to the fact that the distribution of the waiting times between successive jumps of the particle in the underlying CTRW scenario is heavy tailed.

In the special case of a constant potential $V(x) = \text{const}$, the Fourier transform of $w(x, t)$ is, in terms of the Mittag-Leffler function $E_\alpha(\cdot)$ [8], given by

$$\tilde{w}(k, t) = \int_{-\infty}^{\infty} e^{ikx} w(x, t) dx = E_\alpha(-Kk^2 t^\alpha).$$

As shown in [10,11], the same formula applies to the PDF $p(x, t)$ of $X(S_t)$, which confirms that the general result (10) is physically correct. A closed-form solution of the FFPE can be found in terms of the H-Fox functions [1]. Unfortunately, these functions can be numerically evaluated only in a few special cases.

In the next section we use the stochastic representation (2) of the FFPE to construct a method of simulating sample paths of the underlying anomalous diffusion process.

III. NUMERICAL APPROXIMATION OF SAMPLE PATHS

Below, we show how to numerically approximate sample paths of the anomalous diffusion $X(S_t)$. In a recent paper [5], the authors present a method of simulating sample paths of the anomalous diffusion via the underlying CTRW. In their approach, it is necessary to generate successive residence times of the particle, which are Mittag-Leffler distributed. Since computer generation of Mittag-Leffler-distributed random variables is troublesome, the authors suggest that one can replace the Mittag-Leffler distribution by the Pareto one. However, these two distributions, in spite of their obvious similarities (i.e., asymptotic behavior), have some distinct differences, especially when the parameter α is close to 1.

Our method originates from a different concept; it explicitly uses representation (2). It does not require generating Mittag-Leffler-distributed random variables. In our algorithm every trajectory is obtained as a subordination of two trajectories of the processes $X(\tau)$ and S_t — i.e., the solution of the stochastic differential equation (3) and the subordinator defined as $S_t = \inf\{\tau: U(\tau) > t\}$, where $U(\tau)$ is a strictly increasing α -stable Lévy motion.

The proposed algorithm of approximation of the process $X(S_t)$ on the lattice $\{t_i = i\Delta t: i=0, 1, \dots, N\}$, where $\Delta t = \frac{T}{N}$ and T is the time horizon, consists of two steps.

(I) Our first goal is to approximate the values $S_{t_0}, S_{t_1}, \dots, S_{t_N}$ of the subordinator S_t . Therefore, we begin with approximating a realization of the strictly increasing α -stable Lévy motion $U(\tau)$ on the mesh $\tau_j = j\Delta\tau$, $j=0, 1, \dots, M$ (it is recommended to choose $\Delta\tau < \Delta t$). Using the standard method of summing increments of the process $U(\tau)$ we get

$$U(\tau_0) = 0,$$

$$U(\tau_j) = U(\tau_{j-1}) + \Delta\tau^{1/\alpha} \xi_j, \tag{11}$$

where ξ_j are the i.i.d. totally skewed positive α -stable random variables. The procedure of generating realizations of ξ_j is the following [17–19]:

$$\xi_j = c_1 \frac{\sin[\alpha(V + c_2)]}{[\cos(V)]^{1/\alpha}} \times \left(\frac{\cos[V - \alpha(V + c_2)]}{W} \right)^{(1-\alpha)/\alpha},$$

where $c_1 = [\cos(\pi\alpha/2)]^{-1/\alpha}$, $c_2 = \pi/2$, the random variable V is uniformly distributed on $(-\pi/2, \pi/2)$, and W has expo-

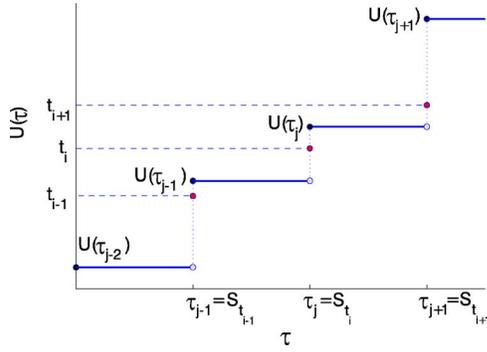


FIG. 2. (Color online) Visualization of the method of finding the values S_i used in the first step of the algorithm. If $U(\tau_{j-1}) < t_i \leq U(\tau_j)$, then $S_i = \tau_j$ (see text for details).

nential distribution with mean 1. The iteration (11) ends when $U(\tau)$ crosses the level T — i.e., when for some $j_0 =: M$ we get $U(\tau_{M-1}) \leq T < U(\tau_M)$. Since $U(\tau)$ is strictly increasing, such M always exists.

Now, for every element t_i of the lattice $\{t_i = i\Delta t : i = 0, 1, \dots, N\}$, we find the element τ_j such that $U(\tau_{j-1}) < t_i \leq U(\tau_j)$, and finally, from definition (4), we get that in such a case (see Fig. 2)

$$S_{t_i} = \tau_j.$$

It is worth emphasizing that, since $U(\tau)$ is a strictly increasing function, the above procedure of finding the values S_{t_i} , $i = 0, 1, \dots, N$, can be implemented efficiently.

(II) In the second step, our aim is to find the approximated values $X(S_{t_0}), X(S_{t_1}), \dots, X(S_{t_N})$ of the subordinated process $X(S_t)$. From the first step of the algorithm already we have at our disposal the approximations $S_{t_0}, S_{t_1}, \dots, S_{t_N}$. We start with employing the classical Euler scheme to approximate the solution $X(\tau)$ of the stochastic differential equation (3) on the lattice $\{\bar{\tau}_k = k\Delta\bar{\tau} : k = 0, 1, \dots, L\}$ (it is also recommended to choose $\Delta\bar{\tau} < \Delta t$). Here L is equal to the first integer that

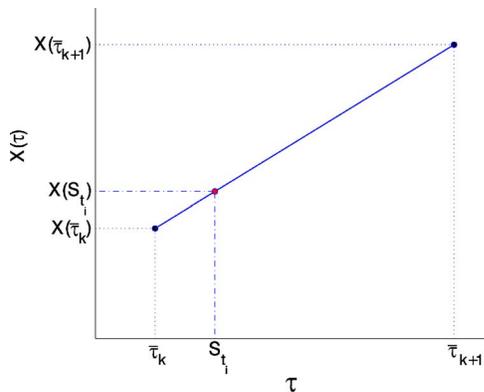


FIG. 3. (Color online) Visualization of the linear interpolation method used to find the values $X(S_i)$ in the second step of the algorithm. In this case, $X(S_{t_i}) = \frac{X(\bar{\tau}_{k+1}) - X(\bar{\tau}_k)}{\bar{\tau}_{k+1} - \bar{\tau}_k} (S_{t_i} - \bar{\tau}_k) + X(\bar{\tau}_k)$ (see text for details).

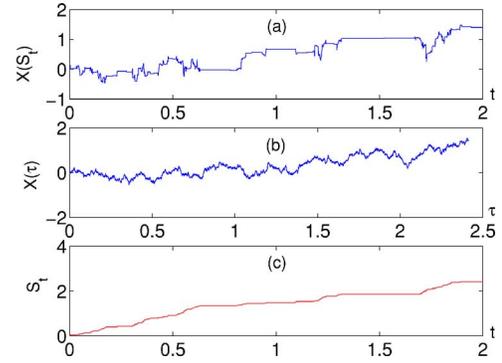


FIG. 4. (Color online) Sample realizations of (a) the anomalous diffusion $X(S_t)$, (b) the normal diffusion $X(\tau)$, and (c) the inverse-time α -stable subordinator S_t , in the presence of a constant potential. The parameters are $\alpha = 0.6$, $K = 1/2$, and $\eta = 1$. The intervals with $X(S_t)$ being constant indicate the heavy-tailed residence times of the underlying CTRW. The similarities between the constant intervals of $X(S_t)$ and S_t and the similarities between $X(S_t)$ and $X(\tau)$ in the remaining domain are distinct.

exceeds the value $S_{t_N} / \Delta\bar{\tau}$. From the Euler scheme [14] we get

$$X(\bar{\tau}_0) = 0,$$

$$X(\bar{\tau}_k) = X(\bar{\tau}_{k-1}) + \frac{V'(X(\bar{\tau}_{k-1}))}{\eta} \Delta\bar{\tau} + (2K)^{1/2} \Delta\bar{\tau}^{1/2} \bar{\xi}_k, \quad (12)$$

for $k = 1, 2, \dots, L$. Here $\bar{\xi}_k$ are i.i.d. random variables with standard normal distribution, $\bar{\xi}_k \sim N(0, 1)$. Now, since the realizations of $X(\tau)$ are continuous functions and since from the iteration scheme (12) we have at our disposal the values $X(\bar{\tau}_0), X(\bar{\tau}_1), \dots, X(\bar{\tau}_L)$, we use the standard linear interpolation in order to obtain the approximate values $X(S_{t_0}), X(S_{t_1}), \dots, X(S_{t_N})$. Thus, for every t_i from the lattice

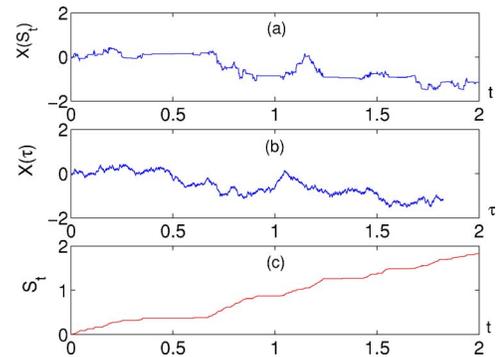


FIG. 5. (Color online) Sample realizations of (a) the anomalous diffusion $X(S_t)$, (b) the normal diffusion $X(\tau)$, and (c) the inverse-time α -stable subordinator S_t , in the presence of the external potential $V(x) = x^2/2$ (Ornstein-Uhlenbeck process). The parameters are $\alpha = 0.7$, $K = 1/2$, and $\eta = 1$. The intervals with $X(S_t)$ being constant indicate the heavy-tailed residence times of the underlying CTRW. Note the similarities between the constant intervals of $X(S_t)$ and S_t and the similarities between $X(S_t)$ and $X(\tau)$ in the remaining domain.

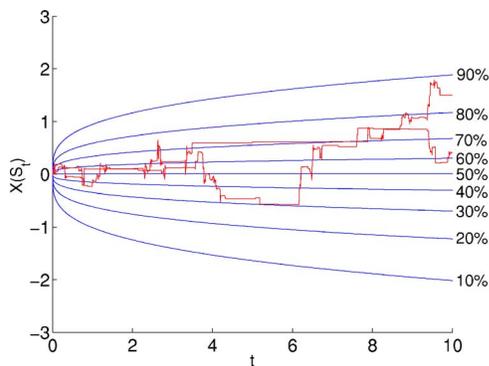


FIG. 6. (Color online) Estimated quantile lines and two sample trajectories of the anomalous diffusion $X(S_t)$ in the constant potential with parameters $\alpha=0.6$, $K=1/2$, and $\eta=1$. Since in this case the process is $\alpha/2$ self-similar, every quantile line is of the form $c_i t^{\alpha/2}$, where c_i are the appropriate constants. Clearly, the model is not asymptotically stationary (compare with Fig. 7).

$\{t_i = i\Delta t : i=0, 1, \dots, N\}$, we find such an index k that the condition $\bar{\tau}_k \leq S_{t_i} \leq \bar{\tau}_{k+1}$ holds true, and finally, through the linear interpolation (see Fig. 3), we get that

$$X(S_{t_i}) = \frac{X(\bar{\tau}_{k+1}) - X(\bar{\tau}_k)}{\bar{\tau}_{k+1} - \bar{\tau}_k} (S_{t_i} - \bar{\tau}_k) + X(\bar{\tau}_k).$$

The above algorithm allows us to simulate sample paths of the process $X(S_t)$ (see Figs. 4 and 5), for the whole range of the parameter $\alpha \in (0, 1)$ and for an arbitrary potential $V(x)$. Let us note that the realizations obtained of the anomalous diffusion process displayed in the top panels of both figures do not allow for distinguishing the type of underlying stochastic process. In order to see the essential differences we need to perform a statistical analysis of the realizations. Monte Carlo methods using the algorithm enable us to find many relevant statistical characteristics of the model. It works in the following way. For a time evolution of the PDF $p(x, t)$ (see Fig. 1), we simulate 10^4 realizations and construct a kernel density estimator using the Rozenblatt-Parzen method [14]. The cusp shape of the pdf estimator confirms the correctness of our algorithm by comparison with the exact result for $\alpha=1/2$ obtained in [1].

A very useful tool for investigation of sample path dynamics was introduced in [14,18]. A p -quantile line, $p \in (0, 1)$, for a stochastic process $Y(t)$ is a function $q_p(t)$ given by the relationship $\Pr(Y(t) \leq q_p(t)) = p$. In Fig. 6 nine quantile lines (10%, 20%, ..., 90%) are constructed from 10^4 realizations of the anomalous diffusion process $Y(t) = X(S_t)$ with a constant potential $V(x) = \text{const}$. In Fig. 7 results for the external potential $V(x) = x^2/2$ are displayed. Different shape of the quantile lines indicates $\alpha/2$ self-similarity (lines of the

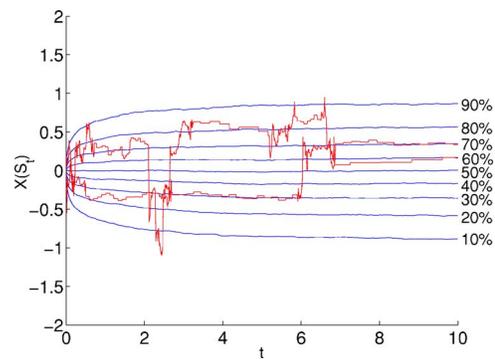


FIG. 7. (Color online) Estimated quantile lines and two sample trajectories of the anomalous diffusion $X(S_t)$ with parameters $\alpha=0.7$, $K=1/2$, and $\eta=1$. In this case the external potential $V(x) = x^2/2$ is used. The shape of the quantile lines (asymptotically parallel lines) indicates the asymptotic stationarity of the model, which confirms the correctness of the algorithm used. The stationary PDF is given by the Gibbs-Boltzmann distribution $p(x) = c_1 \exp[-c_2 V(x)]$, where $c_1 > 0$ and $c_2 > 0$ are appropriate normalizing constants.

form $c_i t^{\alpha/2}$) in Fig. 6 and asymptotic stationarity (asymptotically parallel lines) in Fig. 7.

IV. CONCLUSIONS

We have introduced an efficient method for computer simulation of sample paths of the subdiffusive process described by the FFPE. This permits investigations of the fractional Fokker-Planck dynamics of complex systems by Monte Carlo methods.

We have shown that the solution $w(x, t)$ of the FFPE (1) is equal to the PDF $p(x, t)$ of the subordinated process $X(S_t)$, where $X(\tau)$ is the standard diffusion described by Eq. (3) and S_t is the so-called inverse-time α -stable subordinator (4). The process S_t is a new operational time of the system and originates from the heavy-tailed residence times of the underlying CTRW. The obtained stochastic representation is crucial in constructing an algorithm of simulating sample paths of the anomalous diffusion $X(S_t)$, which, in turn, allows us to detect and examine many relevant properties of the system under consideration. The algorithm can be applied for an arbitrary potential $V(x)$ and for any value of the parameter $\alpha \in (0, 1)$. This is a great advantage of the proposed method, since the exact solution of the FFPE is known only in terms of the H-Fox functions [1], and this function can be numerically evaluated only in a few special cases. Additionally, since the algorithm uses stochastic representation (2), we avoid all the difficulties related to the simulation of the Mittag-Leffler distribution, which appeared in the method presented in [5].

We expect that statistical tools proposed here will contribute to a better understanding of subdiffusion transport and its dynamical foundation.

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