Continuous Time Random Walks: Simulation of continuous trajectories

D. Kleinhans and R. Friedrich
Westfälische Wilhelms-Universität Münster, Institut für Theoretische Physik, D-48149 Münster, Germany
(Dated: February 1, 2008)

Continuous time random walks have been developed as a straightforward generalisation of classical random walk processes. Some 10 years ago, Fogedby introduced a continuous representation of these processes by means of a set of Langevin equations [H. C. Fogedby, Phys. Rev. E 50 (1994)]. The present work is devoted to a detailed discussion of Fogedby’s model and presents its application for the robust numerical generation of sample paths of continuous time random walk processes.

PACS numbers: 05.40.Fb, 45.10.Hj, 02.60.Cb

I. INTRODUCTION

The analysis of stochastic processes by Bachelier, Einstein and Langevin extensively has inspired scientist in the last century. First, Fokker-Planck equations describing the time evolution of probability density functions (pdfs) emerged. In addition, mathematical methods for proper interpretation of the associated Langevin equations have been developed, that allow access to the trajectories of individual particles. An intrinsic feature of these processes is, that they obey Markov properties. Therefore, two point statistics are sufficient for a complete description of these processes.

In recent years, processes exhibiting anomalous diffusion, \( \langle x^2(t) \rangle \sim t^\xi \) with \( \xi \neq 1 \), increasingly have attracted attention. Such processes typically are realised in complex environments such as porous and disordered media, see e.g. \cite{6} and references therein. In contrast to ordinary diffusion, Markov properties do not hold for these processes. Therefore, multipoint joint statistics have to be considered for proper description of the dynamics. On the other hand, these processes can be described by means of fractional Fokker-Planck equations, that contain fractional derivatives with non-local character. On the other hand, Continuous Time Random Walk (CTRW) processes have been proposed for the analysis of the microscopic properties of anomalous diffusion processes \cite{8}. In general, they are specified by the iterative discrete equations \cite{2}.

\[
\begin{align*}
  x_{i+1} &= x_i + \eta_i \\
  t_{i+1} &= t_i + \tau_i
\end{align*}
\]

where \( (\eta_i, \tau_i) \) is a set of random numbers drawn from the pdf \( \Psi(\eta, \tau) \), that vanishes for negative values of \( \tau \) for reasons of causality. Frequently, equations (1) are used to model time-continuous processes with the additional assignment \cite{2}.

\[
x(t) = x_i \quad \text{with} \quad t_i \leq t < t_{i+1}
\]

With the aid of CTRWs, limiting behaviour and ensemble statistics of anomalous diffusion processes become accessible through Monte-Carlo simulations. For details, the reader is referred to recent works by Dentz et al. \cite{9}, Heinsalu et al. \cite{10} and Gorenflo et al. \cite{11}.

Recently, Fogedby formulated a continuous description of CTRWs, that is based on a set of stochastic differential equations \cite{12}.

\[
\begin{align*}
  \frac{dx}{ds} &= F(x) + \eta(s) \\
  \frac{dt}{ds} &= \tau(s)
\end{align*}
\]

Here, the discrete variable \( i \) of equations (1) is generalised to the continuous variable \( s \), that can be associated with an intrinsic time of the CTRW. A number of publications addressed statistical properties of trajectories of this approach \cite{13, 14, 15}. It is the aim of the present work, to present a robust algorithm for the generation of continuous sample paths from Fogedby’s equations. By this means trajectories can be obtained, that properly exhibit the anomalous dynamics of CTRWs on any time scale.

This work is structured as follows. In the next section, some general remarks are made on the definition of continuous CTRWs, equations (3). Section IV is dedicated to the properties of the process \( t(s) \), equation (3b), that typically is driven by Levy noise. The numerical simulation of continuous CTRW processes is presented in section V and exemplified by means of some results in section VI. We conclude with section VII that summarizes our results and suggests future applications.

II. CTRWS IN THE SPIRIT OF FOGEDBY: SOME REMARKS

First of all, the character of the distributions of the random variables \( \eta \) for the jump length and \( \tau \) for the waiting time has to be addressed. In case of the discrete definition, equations (1), a broad class of distributions is feasible for this purpose. The continuous Langevin formulation of Fogedby, equations (3), however, requires the associated distributions to be stable in order to be properly defined. For a short introduction into the concept of stable distributions we refer to \cite{5}. In the long time limit, however, both approaches are equivalent.

In 1994, Fogedby introduced the stochastic differential equations (3) for CTRWs as the continuum limit of the
path parameter or arc length $s$ along the trajectory $[12]$. He considered independent random variables $\eta(s)$ and $\tau(s)$ with power law behaviour, that is

$$\Psi(\eta, \tau) \sim \eta^{-1-\xi}, \tau^{-1-\xi}, \text{ for } \eta, \tau \gg 1.$$  

(4a)

For reasons of normability, Fogedby used cutoffs at low values of $|\eta|$ and $\tau$, respectively. He mainly was interested in the properties of the process $x(t)$, that can be obtained from equations (3) by inversion of the latter process. By means of his modified power-law distributions, the long-time behaviour of processes with power law waiting jump length and waiting time distributions could be derived. In this context, first properties of the inverse process $s(t)$ of equation (3b) have been addressed.

Baule et al. investigated the properties of the inverse process $s(t)$ in greater detail [13]. In particular, multiple joint probabilities could be calculated. The waiting times $\tau$ were considered to obey one-sided Levy distributions with tail parameter $\alpha$, that are discussed in greater detail in the following section. In absence of external force terms ($F = 0$ in equation (3a)) analytical expressions for correlations functions could be derived by application of the inverse Fourier- and Laplace-transforms. Recently, these results could be extended to Ornstein-Uhlenbeck like processes with a linear repelling term, thus $F(x) = -\gamma x$ [15].

Both works, however, focus on the ensemble statistics, whereas the Langevin approach of Fogedby, that is interesting itself, has not attracted much attention yet.

III. PROPERTIES OF $t(s)$ AND ITS INVERSE PROCESS $s(t)$

In this section, we concentrate on the process $t(s)$. Due to causality, this process has to be strictly monotonically increasing. The increments $dt(s) = t(s + ds) - t(s)$, therefore, have to obey fully skewed stable distributions.

Generally, stable distribution are assigned to the $\alpha$-stable probability distribution functions (pdfs). $\alpha$-stable Levy distributions typically are not available in a closed form but are only accessible by means of their Fourier transform. We especially consider the distribution

$$L_\alpha(x) = \frac{1}{\pi} Re \left\{ \int_0^\infty dz \exp \left( -i k x - z^\alpha \exp \left[ -\frac{\alpha \pi}{2} \right] \right) \right\}.$$  

(5)

Here, $i$ is the imaginary unit and $0 < \alpha \leq 1$ the stability index, that specifies the asymptotic behaviour $L_\alpha(x) \sim x^{-(1+\alpha)}$ at $x \gg 1$. This pdf complies with a common parametrization of $\alpha$-stable pdfs $[5, 14, 17],$

$$L_{\alpha, c}^\beta(x) = \frac{1}{2\pi} \int_{-\infty}^\infty dz \exp \left( -i k x - cz^\alpha \left( 1 - i \beta \frac{z}{|z|} \tan \frac{\alpha \pi}{2} \right) \right),$$  

(6)

for the parameters $\beta = 1$ and $c = \left( 1 + \tan^2 \frac{\alpha \pi}{2} \right)^{-1/2}$. Some examples for this distribution are depicted in figure 1. An important feature of this representation is, that it according to equation (5) is defined even for $\alpha = 1$ by means of $L_{1,1}(x) = \delta(x-1)$. From the theory of stable processes it follows, that the increment $dt$ has to obey the distribution $ds^{-\alpha} L_{\alpha}(dt/ds)$ [10]. The case $\alpha = 1$ with $dt = ds$ complies with a stochastic processes, that solely can be described by equation (3a) with $s = t$.

An intrinsic feature of Levy processes is, that trajectories contain finite jumps in terms of discontinuities with a probability greater than zero. They are continuous only from the right [18], that is

$$\lim_{\Delta s \rightarrow 0} t(s + \Delta s) = t(s).$$  

(7)

A sample of a fully skewed Levy process with characteristic exponent $\alpha = 0.9$ is depicted in the upper panel of figure 2. Due to these jumps, the range of values $t(s)$ does not cover the full interval $[0, \infty)$. Rather, the range can be specified by means of a set of intervals. Due to the monotonic increase of the process $t(s)$ a inverse process $s(t)$ exists. This process has been applied for construction of the process $x(t) = x(s(t))$ in the past. It, however, a priori is not properly defined for $t \in [0, \infty]$, due to the jump characteristic of the Levy process. A sample of the inverse process is depicted in the lower panel of figure 2.

In general, the meaning of the inverse function has to be specified in order to be properly defined on $t \in [0, \infty]$. Appropriate definitions for the inverse function e.g. are

$$s(t) := \inf \{ s : t(s) \geq t \} \quad \text{or} \quad (8a)$$  

$$s(t) := \sup \{ s : t(s) \leq t \} \quad . (8b)$$

If the process $x(s)$, is steady, these definitions are equivalent in the limit $\Delta s \rightarrow 0$ for at $t \in [0, \infty[$: Since
FIG. 2: Trajectories of the process $t(s)$ (upper panel) and the associated inverse process $s(t)$ (lower panel) simulated for $\alpha = 0.9$. The finite jumps of the process $t(s)$, that are characteristic for Levy processes, are evident. Due to these jumps the inverse process $s(t)$, however, a priori is not defined on $[0, \infty]$.

$x(s)$ is steady,

$$\lim_{\Delta s \to 0} x(s - \Delta s) = \lim_{\Delta s \to 0} x(s + \Delta s) = x(s)$$

(9)
is valid by definition. Due to the monotonic character of the process $t(s)$, $t(s) \leq t(s + \Delta s)$ for $\Delta s \geq 0$. Consequently, $s \leq s(t') \leq s + \Delta s$ if $t(s) \leq t' \leq t(s + \Delta s)$. Then,

$$\lim_{\Delta s \to 0} x(s) = x(s(t')) = x(s + \Delta s)$$

(10)
is valid for $t(s) \leq t' \leq t(s + \Delta s)$. Here, for the process $t(s)$ only the continuity from the rights has been used. For steady processes $x(s)$ in the limit of infinitesimal $\Delta s$, thus, no additional definition for proper interpretation of the inverse function is required.

If unsteady jumps of $x(s)$ coincide with those of $t(s)$, the latter argumentation is not feasible. We, however, restrict to stochastic processes $x(s)$ with Gaussian noise, that are steady with probability 1 for $s \in [0, \infty]$.

IV. NUMERICAL SIMULATION OF SAMPLE PATHS

An equivalent formulation of equations (9) is given by the integral equations

$$x(s) = x(0) + \int_0^s ds' F(x(s')) + \int_0^s dW(s')$$

(11a)

$$t(s) = t(0) + \int_0^s dL_\alpha(s')$$

(11b)

where $dW$ and $dL_\alpha$ are the infinitesimal increments of Wiener and $\alpha$-stable Levy processes, respectively. For numerical integration these equations have to be discretized with an adequate discrete increment $\Delta s$. Application of the Euler scheme for numerical evaluation of equations (11) then yields

$$x(s + \Delta s) = x(s) + \Delta s F(x(s)) + \eta(s, \Delta s)$$

(12a)

$$t(s + \Delta s) = t(s) + \tau_\alpha(s, \Delta s)$$

(12b)

Here, the random variables $\eta(s, \Delta s)$ independently have to be drawn from a Gaussian pdf with variance $\sigma^2 = \Delta s$.

The variables $\tau_\alpha(s_i, \Delta s)$ have to comply with the distribution $1/(\Delta s) L_\alpha(\Delta L_\alpha/\Delta s)$. The efficient numerical generation of these random numbers is addressed in appendix A. Due to the absence of forcing and the purely additive character of the noise, the integration of $t(s)$ by means of the Euler scheme is exact. For numerical integration of the process $x(s)$ with Gaussian noise, alternatively advanced discretization schemes can be applied [1].

For numerical simulation of trajectories $x(t)$ at discrete times $t_j := j \Delta t, j = 0, \ldots, N$, the inverse $s(t)$ does not have to be calculated explicitly. Instead, the following algorithm can be applied, that incorporates definition (5a) for the inverse process:

- Initialisation of $x_s(0)$ and $t_s(0)$, set $s = 0$
- for every $j = 0$ to $N$:
  1. while $(t_s(s) < t_j)$:
     - (a) calculate $x_s(s + \Delta s)$ and $t_s(s + \Delta s)$ from eqns. (12)
     - (b) increase $s$ by $\Delta s$
  2. set $x(t_j) := x_s(s)$

The discretization of $t$, $\Delta t$, is given by the desired sampling rate of the simulated process. The optimal value for the discretization of the intrinsic variable $s$, $\Delta s$, depends on characteristic length scales of the process $x(s)$ and the desired accuracy of the resulting process $x(t)$. Typically, $\Delta s$ has to be adjusted, such that the right hand side term of the discrete equation, $\Delta s F(x(s_i)) + \eta(s_i, \Delta s)$, with a sufficient probability is less than the desired accuracy of the simulation. This argument is illustrated within the scope of the following section. Too small values for $\Delta s$, in
FIG. 3: Determination of the intrinsic increment Δs. From the transition pdf of Ornstein-Uhlenbeck processes, that is available in a closed form, the square root of the means square deviation of the increment Δx as function of the increment Δs can be derived. From inspection of this graph, Δs = 0.0001 seems to be sufficient for the current purpose.

10000 data points with time increment Δt = 0.001 have been generated for several values of α. The trajectories of the respective processes are exhibited in figure 4. From the sample paths, the influence of the subordinating process t(s) on the dynamics becomes evident. For α = 1 an Ornstein-Uhlenbeck process is recovered. With decreasing α waiting events start to dominate the process. This also can be seen from the evolution of the increment pdfs, that is depicted in figure 5.

Recently, the fractional extension of Ornstein-Uhlenbeck processes has been investigated by Baule et al. 15, starting from the fractional Fokker-Planck equation for the time evolution of ensembles of particles. For the Ornstein-Uhlenbeck process x(s) with initial value x(0) = 1, that has been considered in this section, for t_2 > t_1 eventually an analytical expression for the correlation function could be derived,

$$\langle x(t_2)x(t_1) \rangle = \frac{t_1^\alpha}{\Gamma(\alpha + 1)} \sum_{n=0}^{\infty} \frac{(-t_2^\alpha)^n}{\Gamma(\alpha n + 1)}$$

$$\times \text{hypergeom}_2(\alpha, -\alpha n, \alpha + 1; \frac{t_1}{t_2}; E_\alpha(-t_2^\alpha))$$

Here, Γ denotes the Gamma function, E_α the one-parameter Mittag-Leffler function and \text{hypergeom}_2(a, b, c; z) the Gaussian hypergeometric function. For details see the references provided by Baule et al. 15.

On the other hand, the correlations can be estimated from ensemble averages of simulated trajectories x(t). A comparison of the analytical result by Baule et al. with the correlations estimated from our simulated trajectories is exhibited in figure 6. Perfect coincidence of these two approaches is observed, that never could be compared before.

VI. SUMMARY AND CONCLUSIONS

A method for the accurate and efficient simulation of continuous trajectories of Continuous Time Random Walk (CTRW) processes has been proposed, that relies on the representation through Langevin equations proposed by Fogedby. It is based on the simultaneous simulation of two stochastic processes, one of which is driven by Levy noise.

Within the scope of section 111 the construction of the process x(t) = x(s(t)) with the aid of the inverse s(t) of the Levy process t(s) has been discussed in great detail. The unique existence of the inverse of t(s) for any t typically has been assumed in the past 13. However, the meaning of the inverse process in fact has to be specified in detail at discontinuities of t(s) in order to guarantee for unique existence, see e.g. equations 8. We would like to emphasize, that these additional specifications influence neither the trajectories x(t) nor the ensemble statistics, if the trajectories x(s) are continuous with probability 1. In the subsequent sections, we mainly focused on this specific case.
Comparison with recent analytical results by Baule et al. [15] has been used for validation of the simulation procedure and showed compliance of the results. Due to the non-Markovian character of fractional processes, higher order joint statistics are of great interest [20]. We propose the use of probabilistic methods for numerical calculation of these functions.

**Acknowledgements**

The authors kindly acknowledge intensive discussions with Adrian Baule, Stephan Eule, Michael Wilczek and Eli Barkai. Adrian Baule provided the numerical evaluation of equation (15), that has been used in figure 6 for comparison with our numerical results. Financial support was granted by the Bundesministerium für Bildung, Forschung und Wissenschaft (BMBF) within the project Windturbulenzen und deren Bedeutung für die Windenergie.
FIG. 5: Increments distributions for $\Delta x := x(t + \tau) - x(t)$ with $\tau = 0.001$ for some processes depicted in figure 4. For reasons of clearness the individual pdfs are shifted in vertical direction by a constant factor. It is evident, that with decreasing stability index $\alpha$ a central peaks evolves, that corresponds to persistent regions due to waiting events. On the other hand, the distributions broaden indicating a higher probability of the occurrence of extreme increments.

FIG. 6: Correlation function of the process depicted in figure 4 for $\alpha = 0.8$. The solid line marks the analytical solution (15) derived by Baule et al. [15]. The circles indicate the correlation obtained from the analysis of an ensemble of 500000 trajectories. Since a perfect coincidence is observed, this evaluation is proposed as a benchmark for accuracy of the numerical implementation.

APPENDIX A: GENERATION OF RANDOM VARIABLES WITH SKEWED $\alpha$-STABLE PDF ACCORDING TO EQUATION (5)

Skewed Levy-stable random numbers efficiently can be generated by means of the algorithm proposed in [16,17]. We adapted this algorithm to our definition of the skewed Levy distributions, (5).

The random numbers $\tau_\alpha(s_i, \Delta s)$, that are required for numerical integration of the process $t(s)$, then for $0 < \alpha \leq 1$ efficiently can be generated by means of this algorithm:

- Generate a random variable $V_i$ uniformly distributed on $]-\pi/2, \pi/2[$ and an independent exponential random variable $W_i$ with mean 1. Several optimized random number generators are available for this purpose. In case of doubt, $V$ and $W$ can be obtained from two independent variables $u_1$ and $u_2$, that are uniformly distributed on $]0, 1[$, by means of

  $$ V_i = \pi \left( u_1 - \frac{1}{2} \right) \quad \text{(A1)} $$

  $$ W_i = -\log(u_2) \quad . \text{(A2)} $$

- Set

  $$ \tau_\alpha(s_i, \Delta s) = (\Delta s)^\frac{\alpha}{\pi} \sin \left[ \frac{\alpha(V_i + \frac{\pi}{2})}{\cos(V_i)^{(1/\alpha)}} \right] \quad (A3) $$

  \times \left\{ \cos \left[ V_i - \alpha(V_i + \frac{\pi}{2}) \right] \right\}^{-\frac{1-\alpha}{\alpha}} \frac{W_i}{W_i} .$$

In case of $\alpha = 1$, $\tau_1(s_i, \Delta s) = \Delta s$ is recovered. If adequate random number generators are applied for generation of the variables $V_i$ and $W_i$, the resulting random numbers $\tau_\alpha$ are uncorrelated. From figure 7 it becomes evident, that the desired skewed $\alpha$-stable Levy pdf (5) is matched. This algorithm therefore can be applied for efficient numerical simulation of the process $t(s)$ according to equation (12b).
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