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Lattice Monte Carlo simulation of Galilei variant anomalous diffusion

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ABSTRACT

The observation of an increasing number of anomalous diffusion phenomena motivates the study to reveal the actual reason for such stochastic processes. When it is difficult to get analytical solutions or necessary to track the trajectory of particles, lattice Monte Carlo (LMC) simulation has been shown to be particularly useful. To develop such an LMC simulation algorithm for the Galilei variant anomalous diffusion, we derive explicit solutions for the conditional and unconditional first passage time (FPT) distributions with double absorbing barriers. According to the theory of random walks on lattices and the FPT distributions, we propose an LMC simulation algorithm and prove that such LMC simulation can reproduce both the mean and the mean square displacement exactly in the long-time limit. However, the error introduced in the second moment of the displacement diverges according to a power law as the simulation time progresses. We give an explicit criterion for choosing a small enough lattice step to limit the error within the specified tolerance. We further validate the LMC simulation algorithm and confirm the theoretical error analysis through numerical simulations. The numerical results agree with our theoretical predictions very well.

1. Introduction

Diffusion is one of the most important phenomena encountered in numerous physical, chemical and biological systems [1]. However, the picture that has emerged over the last few decades clearly reveals that an increasing number of natural phenomena do not fit into the relatively simple description of normal diffusion [2]. Anomalous diffusion turns out to be quite ubiquitous which is characterized by a non-linear behavior for the mean square displacement (MSD) as a function of time [3].

The actual reason or the very nature of anomalous diffusion may vary significantly and there are several approaches that can be used to describe anomalous diffusion. For example, fractional diffusion equations (FDEs) and continuous time random walk (CTRW) models are frequently used for a wide range of applications [4,5]. When it is difficult to get analytical solutions or necessary to track the trajectory of particles, lattice Monte Carlo (LMC) simulation is particularly useful as one of the most effective microscopic stochastic methods [6,7].

For normal diffusion, such LMC simulation is already developed [8] and the accuracy of the simulation is extensively studied [9]. Anomalous diffusion has been studied, for example using Monte Carlo approach on lattices with fixed obstacles

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[10–13] or hybrid approaches combining reaction–diffusion simulation with potentially interacting individual particles blocking one or several lattice sites [14,15]. However, more sophisticated LMC simulation algorithms are still needed because anomalous diffusion processes described by different models or schemes may exhibit obviously different characteristic behaviors.

For the purpose of this paper, we only consider the anomalous diffusion described by the Galilei variant fractional diffusion–advection equation (FDAE). This model can be used to describe anomalous diffusion processes in porous media or physical systems where trapping occurs, i.e. particles get repeatedly immobilized before getting dragged along the drift again [5]. In particular, we are interested in its application in cell biology and other biological systems [16–20]. For one example, subballistic superdiffusive behavior of the MSD in time was observed in experiments on wild-type and mutated epithelial cells [21] and cancer cells [22]. Such superdiffusive behavior of cell transport has been previously explained by the Galilei variant FDAE [5] or the two-state model with anomalous switching between migrating and proliferating phenotypes of cancer cells [23]. As another example, the Galilei variant FDAE has been used to investigate the intracellular fluid flow in rapidly moving cells with combined diffusion and drift intermittent with brief sticking to or trapping within the actin network [24].

The Galilei variant FDAE with constant diffusivity D_α and drift v_α is given by

$$\frac{\partial}{\partial t}P(x,t) = {}_0\partial_t^{1-\alpha}\left(D_\alpha\frac{\partial^2}{\partial x^2}P(x,t) - v_\alpha\frac{\partial}{\partial x}P(x,t)\right), 0<\alpha<1, \tag{1}$$

with the natural boundary and initial conditions

$$P(-\infty,t)=0,\ P(+\infty,t)=0,\ P(x,0)=\delta(x), \tag{2}$$

where δ is the Dirac delta function and the Riemann–Liouville operator is defined as

$${}_0\partial_t^{1-\alpha}P(x,t) = \frac{\partial}{\partial t}{}_0\partial_t^{-\alpha}P(x,t) = \frac{1}{\Gamma(\alpha)}\frac{\partial}{\partial t}\int_0^t (t-\tau)^{\alpha-1}P(x,\tau)d\tau. \tag{3}$$

Note that $P(x,t)$ is the time dependent concentration and for simplicity we only consider the 1D case. It is known that this FDAE gives the following moments

$$<x> = {}_0\partial_t^{-\alpha}\left(v_\alpha\int_{-\infty}^{+\infty}P(x,t)dx - D_\alpha\int_{-\infty}^{+\infty}\left(\frac{\partial}{\partial x}P(x,t)\right)dx\right) = v_\alpha\,{}_0\partial_t^{-\alpha}(1) = \frac{v_\alpha t^\alpha}{\Gamma(1+\alpha)}, \tag{4}$$

$$\begin{aligned}<x^2> &= 2\,{}_0\partial_t^{-\alpha}\left(v_\alpha\int_{-\infty}^{+\infty}xP(x,t)dx - D_\alpha\int_{-\infty}^{+\infty}\left(x\frac{\partial}{\partial x}P(x,t)\right)dx\right) = 2\,{}_0\partial_t^{-\alpha}\left(\frac{v_\alpha^2 t^\alpha}{\Gamma(1+\alpha)} + D_\alpha\right)\\ &= \frac{2D_\alpha t^\alpha}{\Gamma(1+\alpha)} + \frac{2v_\alpha^2 t^{2\alpha}}{\Gamma(1+2\alpha)},\end{aligned} \tag{5}$$

$$<\Delta x^2> = <(x-<x>)^2> = \frac{2D_\alpha t^\alpha}{\Gamma(1+\alpha)} + \left(\frac{2}{\Gamma(1+2\alpha)} - \frac{1}{\Gamma^2(1+\alpha)}\right)v_\alpha^2 t^{2\alpha}, \tag{6}$$

where we have performed integration by parts and assumed that $x^n P(x,t)=0, x^n(\partial P(x,t)/\partial x)=0, x=\pm\infty, n=1,2$.

Our objective is to derive a valid LMC simulation algorithm that can reproduce the macroscopic dynamical properties of anomalous diffusion characterized by Eqs. (4), (5) and (6) as accurately as possible. It is clear that the process described by Eq. (1) is Gaussian when $\alpha=1$. Strictly speaking, it is not sufficient to describe the same stochastic process if we only reproduce the moments of the particle distribution. However, it is a little difficult to get an analytic solution to Eq. (1). In this case, LMC simulation can be designed and used to reproduce the moments of the particle distribution and the accuracy of LMC simulation is mainly determined by the approximation algorithm.

Such LMC simulation can be derived according to the theory of CTRW and the first passage time (FPT) problem [25–28]. It can be shown that, depending on the specific form of the waiting time distribution and the jump step distribution, the CTRW can produce both subdiffusive and superdiffusive processes as well as normal diffusion [29,30]. Therefore, the key to designing LMC simulation is to calculate the FPT probability distributions and the jump probabilities exactly for random walkers on discrete lattices [31–34]. In principle, LMC simulation will approach the solution of continuous systems arbitrarily close if the algorithm is correctly designed and the lattice step is small enough [9].

At this point we note that one can in fact develop different simulation algorithms according to the balance between accuracy and efficiency once we get the FPT distribution. For example, one can design an asynchronous event-driven First-Passage Kinetic Monte Carlo (FPKMC) algorithm as described in Refs. [7,32,33] if it is required that the individual particles should be modeled with positions in continuous space. FPKMC is an exact algorithm (within numerical precision) because of the sampling from exact analytical solutions for diffusion Green's function (propagators). It is important to keep in mind that particle and pair protections as well as computational techniques such as finding an optimal space partitioning and