Journal of Computational Physics 293 (2015) 53–69

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A discrete time random walk model for anomalous diffusion

C.N. Angstmann, I.C. Donnelly, B.I. Henry *, J.A. Nichols

School of Mathematics and Statistics, UNSW Australia, 2052, Australia

ARTICLE INFO

Article history:
Received 8 May 2014
Received in revised form 10 July 2014
Accepted 3 August 2014
Available online 7 August 2014

Keywords:
Fractional diffusion
Fractional Fokker–Planck equation
Continuous time random walk
Finite difference method
Anomalous diffusion

ABSTRACT

The continuous time random walk, introduced in the physics literature by Montroll and Weiss, has been widely used to model anomalous diffusion in external force fields. One of the features of this model is that the governing equations for the evolution of the probability density function, in the diffusion limit, can generally be simplified using fractional calculus. This has in turn led to intensive research efforts over the past decade to develop robust numerical methods for the governing equations, represented as fractional partial differential equations.

Here we introduce a discrete time random walk that can also be used to model anomalous diffusion in an external force field. The governing evolution equations for the probability density function share the continuous time random walk diffusion limit. Thus the discrete time random walk provides a novel numerical method for solving anomalous diffusion equations in the diffusion limit, including the fractional Fokker–Planck equation. This method has the clear advantage that the discretisation of the diffusion limit equation, which is necessary for numerical analysis, is itself a well defined physical process. Some examples using the discrete time random walk to provide numerical solutions of the probability density function for anomalous subdiffusion, including forcing, are provided.

1. Introduction

Following the seminal *Physics Reports* article by Metzler and Klafter in 2000 [1] there has been an explosion of literature on using the physically motivated continuous time random walk (CTRW) model of Montroll and Weiss [2] together with the mathematics of fractional calculus [3] to provide mathematical models of anomalous diffusion [4–12]. Further interest has been stimulated by large numbers of papers reporting findings of anomalous diffusion in experimental systems [1,13–18] and large numbers of papers seeking to provide numerical solutions of the models [19–29]; ultimately to compare with experimental observations.

Anomalous diffusion, in this research field, has been taken to be stochastic particle motion where the variance, in the position of the particle, scales other than linearly with time. In the following we focus on so-called subdiffusion in which the variance scales as a sublinear power law in time, i.e.,

$$\langle x(t)^2\rangle - \langle x(t)\rangle^2 \sim t^\alpha \tag{1}$$

where $0 < \alpha < 1$.

In the CTRW model, particles wait for a time t, selected from a waiting time probability density $\psi(t)$, before jumping through a distance x, selected from a jump probability density $\lambda(x)$. Here it is assumed that the waiting time density and the jump density are decoupled. The evolution of the probability density function describing the position of the random

* Corresponding author.
E-mail address: b.henry@unsw.edu.au (B.I. Henry).

http://dx.doi.org/10.1016/j.jcp.2014.08.003
0021-9991/

walk on a lattice at subsequent times is given by a generalised master equation [30]

$$\frac{du(x,t)}{dt} = \sum_{x'} \int_0^t K\left(x-x', t-t'\right) u\left(x', t'\right) dt' \tag{2}$$

where the kernel is related to the waiting time density and the jump density in Laplace space by

$$\hat{K}\left(x-x', s\right) = s\hat{\psi}(s) \frac{\lambda(x-x') - \delta_{x,0}}{1-\hat{\psi}(s)}. \tag{3}$$

The hat denotes a Laplace transform with respect to time. In the case of nearest neighbour jumps on a lattice of spacing Δx, the jump density

$$\lambda\left(x-x'\right) = \frac{1}{2}(\delta_{x-x',\Delta x} + \delta_{x-x',-\Delta x}) \tag{4}$$

has a finite variance. The generalised master equation for CTRWs with nearest neighbour jumps provides a model for standard diffusion if the waiting time density is exponential,

$$\psi(t) = \frac{1}{\tau} \exp\left(-\frac{t}{\tau}\right), \tag{5}$$

and it provides a model for subdiffusion if the waiting time density is Mittag–Leffler,

$$\psi(t) = \frac{t^{\alpha-1}}{\tau^\alpha} E_{\alpha,\alpha}\left[-\left(\frac{t}{\tau}\right)^\alpha\right] \quad \text{for } 0 < \alpha < 1. \tag{6}$$

The essential difference is that the exponential waiting time density is Markovian and the Mittag–Leffler density is non-Markovian with an infinite first moment [1].

The diffusion limit of the generalised master equation is found by taking the time and space scales of the random walk, characterised by τ and Δx respectively, to zero in a way that preserves the scaling relation $\Delta x^2 \sim \tau^\alpha$, where $\alpha = 1$ for standard diffusion. With the exponential waiting time density the diffusion limit of the generalised master equation results in the standard diffusion equation

$$\frac{\partial u(x,t)}{\partial t} = D \frac{\partial^2 u(x,t)}{\partial x^2} \tag{7}$$

with

$$D = \lim_{\Delta x \to 0, \tau \to 0} \frac{\Delta x^2}{2\tau}. \tag{8}$$

With the Mittag–Leffler waiting time density, the diffusion limit of the generalised master equation results in the fractional diffusion equation

$$\frac{\partial u(x,t)}{\partial t} = D_\alpha {}_0D_t^{1-\alpha} \frac{\partial^2 u(x,t)}{\partial x^2}, \tag{9}$$

with [5]

$$D = \lim_{\Delta x \to 0, \tau \to 0} \frac{\Delta x^2}{2\tau^\alpha}, \tag{10}$$

and the operator ${}_0D_t^{1-\alpha}$ is the Riemann–Liouville fractional derivative defined by [3]

$${}_0D_t^{1-\alpha} y(x,t) = \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t \frac{y(x,t')}{(t-t')^{1-\alpha}} dt'. \tag{11}$$

In the limit $\alpha \to 1^-$, Eq. (11) recovers the standard diffusion equation.

The CTRW model has been extended to model anomalous diffusion in an external force field by introducing a bias probability for the direction of each step [5]. The bias probability is determined by evaluating the external force field at the instant of jumping. In the case where the force field, $F(x,t)$, varies in both space and time, in the diffusion limit, the evolution of the probability density function is given by the fractional Fokker–Planck equation [10],

$$\frac{\partial u(x,t)}{\partial t} = D_\alpha {}_0D_t^{1-\alpha}\left(\frac{\partial^2 u(x,t)}{\partial x^2}\right) - \frac{1}{\eta_\alpha} \frac{\partial}{\partial x}\left(F(x,t) {}_0D_t^{1-\alpha}\left(u(x,t)\right)\right). \tag{12}$$

Here $\eta_\alpha = (2\beta D_\alpha)^{-1}$ is a fractional friction coefficient and β is a parameter quantifying the strength of the effect of the force. If $\beta = 0$, Eq. (12) simplifies to Eq. (9). The CTRW formalism has also been extended to model subdiffusion in an external force field with reactions [12].