ARTICLE IN PRESS
YJCPH:5413

Journal of Computational Physics ••• (••••) •••–•••

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 xxxx

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/

Please cite this article in press as: C.N. Angstmann et al., A discrete time random walk model for anomalous diffusion, J. Comput. Phys. (2014), http://dx.doi.org/10.1016/j.jcp.2014.08.003

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

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

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].

Please cite this article in press as: C.N. Angstmann et al., A discrete time random walk model for anomalous diffusion, J. Comput. Phys. (2014), http://dx.doi.org/10.1016/j.jcp.2014.08.003

In general, it is not possible to obtain explicit algebraic solutions for the fractional Fokker–Planck equation, Eq. (12), and related fractional partial differential equations, except in special cases. This has stimulated enormous interest in the development of numerical methods of approximation, including explicit finite difference methods [19], implicit finite difference methods [20], spectral methods [26], and Galerkin methods [27].

In this paper, we introduce a discrete time random walk (DTRW) model for anomalous diffusion in an external space- and time-dependent force field. In an earlier series of papers, Gorenflo, Mainardi and co-workers [31,32] introduced a discrete time random walk for anomalous diffusion by using the backward Grünwald–Letnikov summation to replace the time fractional Caputo derivative in the time fractional diffusion equation. Our DTRW model for subdiffusion starts with the physical description of a random walk on a lattice with the steps of the walk selected from a jump probability distribution with a finite variance, and with waiting times, between steps, selected from a discrete time power law waiting time probability distribution with an infinite first moment. The forcing is again realised through bias probabilities in the step directions. We have derived the generalised master equations for the probability distribution of the DTRW and we show that the diffusion limit is equivalent to the diffusion limit of the corresponding CTRW model.

The DTRW, which is itself a well defined physical process, provides a novel explicit numerical scheme for solving the fractional Fokker–Planck equation. In Section 2 we derive the generalised master equations for DTRWs. We find the diffusion limit for these equations and show that they limit to the diffusion limit equations for CTRWs. In Section 3 we describe our numerical scheme for solving fractional Fokker–Planck equations, based on the DTRW model. Some illustrative examples are provided in Section 4. We conclude with a summary in Section 5.

2. The master equation for discrete time random walks

In this section we derive the master equation for the stochastic motion of a particle traversing a lattice $\{x_{-L}, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_L\}$ in discrete time $n \in \mathbb{N}$. At each discrete time the particle either remains at the current site or transitions to a new site. If a particle arrives at a site x_i at time m then the transition to another site x_j at time n is governed by a transition probability distribution function $\Psi(x_j, n|x_i, m)$. In the following we assume that

$$\Psi(x_j, n|x_i, m) = \lambda(x_j, n|x_i)\psi(n-m) \tag{13}$$

where $\psi(n-m)$ is the probability distribution function for waiting a time $(n-m)$ before jumping and $\lambda(x_j, n|x_i)$ is the probability distribution function for jumping from x_i to x_j at time n. The probability distributions are normalised as follows:

$$\sum_{n=0}^{\infty} \psi(n) = 1 \tag{14}$$

and

$$\sum_{j=-L}^{L} \lambda(x_j, n|x_i) = 1. \tag{15}$$

The effect of a space- and time-dependent force can be included in the probability distribution for jumping by biasing the jump probabilities in proportion to the external force. It is also possible to include spatial heterogeneity by having ψ vary as a function of the lattice site, but, in order to simplify the presentation, we have not included this generalisation in the following.

The probability of a particle arriving at a site x_i after n time steps is recursively defined by

$$Q(x_i, n) = \sum_{j=-L}^{L} \sum_{m=0}^{n-1} \Psi(x_i, n|x_j, m) Q(x_j, m) \tag{16}$$

where $Q(x_i, 0) = \delta_{x_i, x^*}$ and x^* is the lattice site the random walker started from at time $n = 0$. The probability of a particle remaining at x_i at time n given the particle arrived at the earlier time m is given by the survival probability

$$\Phi(n-m) = 1 - \sum_{k=0}^{n-m} \psi(k). \tag{17}$$

The probability of a particle being at site x_i after the nth time step is given by

$$X(x_i, n) = \sum_{m=0}^{n} \Phi(n-m) Q(x_i, m), \tag{18}$$

which expresses the probability that the particle arrived at x_i at some earlier time m, and has not yet jumped away.

Conservation of probability leads to the condition that the difference in probability on a site after one time step is just the probability of a particle arriving, minus the probability of a particle leaving,

Please cite this article in press as: C.N. Angstmann et al., A discrete time random walk model for anomalous diffusion, J. Comput. Phys. (2014), http://dx.doi.org/10.1016/j.jcp.2014.08.003

$$X(x_i,n) - X(x_i,n-1) = Q(x_i,n) - \sum_{j=-L}^{L}\sum_{m=0}^{n-1}\Psi(x_j,n|x_i,m)Q(x_i,m). \tag{19}$$

Substituting Eq. (16) into Eq. (19) gives

$$X(x_i,n) - X(x_i,n-1) = \sum_{j=-L}^{L}\sum_{m=0}^{n-1}\Psi(x_i,n|x_j,m)Q(x_j,m) - \sum_{j=-L}^{L}\sum_{m=0}^{n-1}\Psi(x_j,n|x_i,m)Q(x_i,m). \tag{20}$$

Restricting further analysis to biased nearest neighbour steps we have

$$\lambda(x_i,n|x_j) = p_r(x_i,n|x_j)\delta_{x_j,x_{i-1}} + p_\ell(x_i,n|x_j)\delta_{x_j,x_{i+1}}, \tag{21}$$

$$\lambda(x_j,n|x_i) = p_r(x_j,n|x_i)\delta_{x_j,x_{i+1}} + p_\ell(x_j,n|x_i)\delta_{x_j,x_{i-1}}, \tag{22}$$

where $p_r(x_i,n|x_{i-1})$ is the bias probability of jumping to the right and $p_\ell(x_i,n|x_{i+1})$ is the bias probability of jumping to the left. Substituting Eq. (13) with the above jump probabilities into Eq. (20), and using the normalisation

$$p_r(x_{i+1},n|x_i) + p_\ell(x_{i-1},n|x_i) = 1, \tag{23}$$

we arrive at

$$X(x_i,n) - X(x_i,n-1) = p_r(x_i,n|x_{i-1})\sum_{m=0}^{n-1}\psi(n-m)Q(x_{i-1},m) + p_\ell(x_i,n|x_{i+1})\sum_{m=0}^{n-1}\psi(n-m)Q(x_{i+1},m)$$
$$- \sum_{m=0}^{n-1}\psi(n-m)Q(x_i,m). \tag{24}$$

To obtain the generalised master equation (GME) from the flux balance we make use of the single-sided Z transform [33] defined by

$$\hat{Y}(z) = Z\{Y(n)\} = \sum_{n=0}^{\infty}Y(n)z^{-n}. \tag{25}$$

The Z transform of Eq. (18) gives

$$\hat{X}(x_i,z) = \hat{\Phi}(z)\hat{Q}(x_i,z). \tag{26}$$

Similarly to the analysis of CTRWs in [34], it is convenient to define a discrete memory kernel $K(n)$ by the Z transform relation

$$\hat{K}(z) = \frac{\hat{\psi}(z)}{\hat{\Phi}(z)}. \tag{27}$$

Note that $K(0) = 0$. This enables us to replace the convolutions involving ψ and Q, with convolutions involving K and X. Explicitly we have

$$\sum_{m=0}^{n-1}\psi(n-m)Q(x,m) = \sum_{m=0}^{n-1}K(n-m)X(x,m), \tag{28}$$

which can readily be verified by taking the Z transform of each side of the equation and using Eqs. (26) and (27). Replacing the $\psi \star Q$ convolutions with $K \star X$ convolutions in Eq. (24) we arrive at the GME for DTRWs with biased step directions

$$X(x_i,n) - X(x_i,n-1) = p_r(x_i,n|x_{i-1})\sum_{m=0}^{n-1}K(n-m)X(x_{i-1},m) + p_\ell(x_i,n|x_{i+1})\sum_{m=0}^{n-1}K(n-m)X(x_{i+1},m)$$
$$- \sum_{m=0}^{n-1}K(n-m)X(x_i,m). \tag{29}$$

The sum of the bias probabilities at a lattice site is normalised

$$p_r(x_{i+1},n|x_i) + p_\ell(x_{i-1},n|x_i) = 1, \tag{30}$$

and the difference in bias probabilities at a lattice site can be represented as a bias force function

$$f(x_i,n) = p_r(x_{i+1},n|x_i) - p_\ell(x_{i-1},n|x_i). \tag{31}$$

Please cite this article in press as: C.N. Angstmann et al., A discrete time random walk model for anomalous diffusion, J. Comput. Phys. (2014), http://dx.doi.org/10.1016/j.jcp.2014.08.003

Using these results in Eq. (29) we can obtain the Generalised Master Equation (GME) for DTRWs with space- and time-dependent forcing

$$\begin{aligned} X(x_i,n)-X(x_i,n-1) = {} & \sum_{m=0}^{n-1}\frac{K(n-m)}{2}\big(X(x_{i-1},m)+X(x_{i+1},m)-2X(x_i,m)\big) \\ & -\sum_{m=0}^{n-1}\frac{K(n-m)}{2}\big(f(x_{i+1},n)X(x_{i+1},m)-f(x_{i-1},n)X(x_{i-1},m)\big). \end{aligned} \tag{32}$$

2.1. Diffusion limit of the GMEs for DTRWs

The diffusion limit is found by taking the time and space scales of the random walk to zero, effectively having an infinite number of size zero jumps in every instant in time.

We can introduce the time scale limit by transforming the Z transform variable via

$$z^{-1}=e^{-s\Delta t}. \tag{33}$$

The Z transform is then a so called star transform

$$\hat{Y}^{\star}(s|\Delta t)=\sum_{n=0}^{\infty}Y(n)e^{-sn\Delta t} \tag{34}$$

which can be considered as a discrete time sampled Laplace transform [33] with a sampling time scale of Δt, identifying $t=n\,\Delta t$.

The passage from discrete time to continuous time using the star transform can be seen by considering the discrete convolution $H(n)$ defined by

$$H(n)=\sum_{m=0}^{n}K(m-n)G(m), \tag{35}$$

where $G(n)$ is an arbitrary discrete function. The star transform of this convolution gives

$$\hat{H}^{\star}(s|\Delta t)=\hat{K}^{\star}(s|\Delta t)\hat{G}^{\star}(s|\Delta t), \tag{36}$$

and the inverse Laplace transform with respect to the variable s yields

$$H(t|\Delta t)=\int_0^t K\big(t-t'\bigm|\Delta t\big)G\big(t'\bigm|\Delta t\big)dt'. \tag{37}$$

Applying this process to the discrete time GME, Eq. (32), gives the corresponding continuous time GME in the limit of $\Delta t\to 0$.

$$\begin{aligned} \lim_{\Delta t\to 0} X(x_i,t)-X(x_i,t-\Delta t) = {} & \lim_{\Delta t\to 0}\int_0^t \frac{K(t-t'|\Delta t)}{2}\big(X\big(x_{i-1},t'\bigm|\Delta t\big)+X\big(x_{i+1},t'\bigm|\Delta t\big)-2X\big(x_i,t'\bigm|\Delta t\big)\big)dt' \\ & -\int_0^t \frac{K(t-t'|\Delta t)}{2}\big(f(x_{i+1},t)X\big(x_{i+1},t'\bigm|\Delta t\big)-f(x_{i-1},t)X\big(x_{i-1},t'\bigm|\Delta t\big)\big)dt'. \end{aligned}$$

Dividing both sides of this equation by Δt then gives

$$\begin{aligned} \frac{dX(x_i,t)}{dt} = {} & \lim_{\Delta t\to 0}\int_0^t \frac{K(t-t'|\Delta t)}{2\Delta t}\big(X\big(x_{i-1},t'\bigm|\Delta t\big)+X\big(x_{i+1},t'\bigm|\Delta t\big)-2X\big(x_i,t'\bigm|\Delta t\big)\big)dt' \\ & -\int_0^t \frac{K(t-t'|\Delta t)}{2\Delta t}\big(f(x_{i+1},t)X\big(x_{i+1},t'\bigm|\Delta t\big)-f(x_{i-1},t)X\big(x_{i-1},t'\bigm|\Delta t\big)\big)dt'. \end{aligned} \tag{38}$$

We can introduce a length scale, through an arbitrary lattice spacing Δx, by setting $x_i=x$ and $x_{i+1}=x+\Delta x$. Multiplying the RHS of Eq. (38) by $\frac{\Delta x^2}{\Delta x^2}$ and taking the limit as $\Delta x\to 0$ gives the governing equation for the diffusion limit as a generalised Fokker–Planck equation,

Please cite this article in press as: C.N. Angstmann et al., A discrete time random walk model for anomalous diffusion, J. Comput. Phys. (2014), http://dx.doi.org/10.1016/j.jcp.2014.08.003

$$\frac{\partial X(x,t)}{\partial t} = \lim_{\Delta x\to 0,\Delta t\to 0} \frac{\Delta x^2}{2\Delta t} \int_0^t K\big(t-t' \mid \Delta t\big)\left(\frac{\partial^2 X(x,t')}{\partial x^2} - 2\beta \frac{\partial F(x,t)X(x,t')}{\partial x}\right)dt', \tag{39}$$

where the force,

$$F(x,t) = \lim_{\Delta x\to 0} \frac{(p_r(x+\Delta x,t|x) - p_\ell(x-\Delta x,t|x))}{\beta\Delta x} \tag{40}$$

$$= \lim_{\Delta x\to 0} \frac{f_{\Delta x}(x,t)}{\beta\Delta x}. \tag{41}$$

2.2. Memoryless waiting time

If the probability of jumping at any step is independent of the number of steps that the particle has waited we will refer to the probability of jumping as being memoryless. In the case of continuous time this property is only shown by the exponential waiting time density. In discrete time, if r is the probability of the particle jumping in any step, then for a memoryless process the probability of jumping on the nth step after arrival is

$$\psi(n) = r(1-r)^{n-1} \tag{42}$$

for $n > 0$ and zero otherwise. The survival probability is then given by

$$\Phi(n) = (1-r)^n. \tag{43}$$

The Z transform of this waiting time density, Eq. (42), is given by

$$\hat{\psi}(z) = \sum_{n=1}^{\infty} r(1-r)^{(n-1)} z^{-n}, \tag{44}$$

$$= \frac{r}{r+z-1}. \tag{45}$$

Similarly the Z transform of the survival probability function is

$$\hat{\Phi}(z) = \frac{z}{r+z-1}. \tag{46}$$

The Z transform of the memory kernel is then obtained from Eq. (27), yielding

$$\hat{K}(z) = \frac{r}{z}, \tag{47}$$

and the inverse Z transform then yields

$$K(n) = r\delta_{n,1}, \tag{48}$$

where δ is the Kronecker delta function.

We now substitute the memory kernel, Eq. (48), into the generalised master equation, Eq. (32), to obtain

$$X(x_i,n) = r\, p_r(x_i,n|x_{i-1})X(x_{i-1},n-1) + r\, p_\ell(x_i,n|x_{i+1})X(x_{i+1},n-1) + (1-r)X(x_i,n-1). \tag{49}$$

This is the master equation for DTRWs with memoryless waiting time densities and space- and time-dependent forcing.

2.2.1. Diffusion limit of the memoryless GME

The star transform, Eq. (34), of the memory kernel, Eq. (48), is given by

$$\hat{K}^\star(s|\Delta t) = re^{-s\Delta t}, \tag{50}$$

and the inverse Laplace transform with respect to the variable s yields

$$K(t|\Delta t) = r\delta(t-\Delta t). \tag{51}$$

Substituting this into the generalised Fokker–Planck equation, Eq. (39), and taking a Taylor series expansion about t for terms involving $X(x, t-\Delta t)$, then gives,

$$\frac{\partial X(x,t)}{\partial t} = D\left(\frac{\partial^2 X(x,t)}{\partial x^2} - 2\beta \frac{\partial F(x,t)X(x,t)}{\partial x}\right), \tag{52}$$

where

$$D = \lim_{\Delta x\to 0,\Delta t\to 0} \frac{r\Delta x^2}{2\Delta t}. \tag{53}$$

This is the standard Fokker–Plank equation for diffusion in an external space- and time-dependent force field $F(x,t)$.

Please cite this article in press as: C.N. Angstmann et al., A discrete time random walk model for anomalous diffusion, J. Comput. Phys. (2014), http://dx.doi.org/10.1016/j.jcp.2014.08.003

2.3. Power-law Sibuya waiting time

If the waiting time distribution has a finite first moment then the walk will behave asymptotically like the memoryless case. By considering a heavy tailed waiting time distribution this will no longer be the case and the process will asymptotically follow a fractional governing equation. For tractability, here we consider the Sibuya distribution [35] for the waiting time distribution,

$$\psi(n) = (-1)^{n+1}\frac{\Gamma(\alpha+1)}{\Gamma(n+1)\Gamma(\alpha-n+1)}, \tag{54}$$

for $0<\alpha<1$ and $n>0$. The Sibuya distribution is the waiting time distribution for a particle that has a probability $\frac{\alpha}{n}$ of jumping after waiting n steps. The probability of a zero length wait is zero, and hence $\psi(0)=0$. It is interesting to note that this distribution is the negative of the coefficients of the Grünwald–Letnikov fractional derivative of order α. The Grünwald–Letnikov fractional derivative involving a discrete sum is formally equivalent to the Riemann–Liouville fractional derivative involving an integral [3] and it has been widely used to replace Riemann–Liouville fractional derivatives in numerical methods [36]. The survival probability function corresponding to the Sibuya waiting time distribution is given by,

$$\Phi(n) = \frac{(-1)^n\Gamma(\alpha)}{\Gamma(n+1)\Gamma(\alpha-n)}. \tag{55}$$

After taking the Z transforms,

$$\hat{\psi}(z) = 1-\left(1-z^{-1}\right)^{\alpha} \tag{56}$$

and

$$\hat{\Phi}(z) = \left(1-z^{-1}\right)^{\alpha-1} \tag{57}$$

we arrive at the Z transform of memory kernel

$$\hat{K}(z) = \left(1-z^{-1}\right)^{1-\alpha} - \left(1-z^{-1}\right). \tag{58}$$

The Z transform can be inverted to give

$$K(n) = \frac{\Gamma(n-1+\alpha)}{\Gamma(\alpha-1)\Gamma(n+1)} + \delta_{n,1}. \tag{59}$$

Note that this can be defined recursively for $n\geq 3$ by

$$K(n) = \frac{n+\alpha-2}{n}K(n-1). \tag{60}$$

Again it is interesting to note that $K(n)-\delta_{n,1}$ are the coefficients of the Grünwald–Letnikov fractional derivative of order $1-\alpha$.

We now substitute the memory kernel into the GME, Eq. (29), to arrive at the GME for DTRWs with the Sibuya heavy tailed waiting time density and space- and time-dependent forcing,

$$\begin{aligned} X(x_i,n) = {} & p_r(x_i,n|x_{i-1})\left(\sum_{m=0}^{n-1}\frac{\Gamma(n-m-1+\alpha)}{\Gamma(\alpha-1)\Gamma(n-m+1)}X(x_{i-1},m) + X(x_{i-1},n-1)\right) \\ & + p_\ell(x_i,n|x_{i+1})\left(\sum_{m=0}^{n-1}\frac{\Gamma(n-m-1+\alpha)}{\Gamma(\alpha-1)\Gamma(n-m+1)}X(x_{i+1},m) + X(x_{i+1},n-1)\right) \\ & - \sum_{m=0}^{n-1}\frac{\Gamma(n-m-1+\alpha)}{\Gamma(\alpha-1)\Gamma(n-m+1)}X(x_i,m). \end{aligned} \tag{61}$$

2.4. Diffusion limit of Sibuya GME

The star transform of the Sibuya memory kernel is

$$\hat{K}^{\star}(s|\Delta t) = \left(1-e^{-s\Delta t}\right)^{1-\alpha} - \left(1-e^{-s\Delta t}\right). \tag{62}$$

Taking the power series expansion of the exponential, $e^{-s\Delta t}$, and retaining the lowest order term in Δt we have

$$\hat{K}^{\star}(s|\Delta t) \sim (s\Delta t)^{1-\alpha}. \tag{63}$$

Please cite this article in press as: C.N. Angstmann et al., A discrete time random walk model for anomalous diffusion, J. Comput. Phys. (2014), http://dx.doi.org/10.1016/j.jcp.2014.08.003

The inverse Laplace transform with respect to s yields

$$K(t|\Delta t)=\lim_{\Delta t\to 0}\frac{\Delta t}{\Delta t^{\alpha}}\mathcal{L}^{-1}\{s^{1-\alpha}\}(t)+\mathcal{O}(\Delta t). \tag{64}$$

This can be substituted into the generalised Fokker–Planck equation, Eq. (39), giving

$$\frac{\partial X(x,t)}{\partial t}=D_{\alpha}\int_{0}^{t}\mathcal{L}^{-1}\{s^{1-\alpha}\}(t-t')\left(\frac{\partial^2 X(x,t')}{\partial x^2}-2\beta\frac{\partial F(x,t)X(x,t')}{\partial x}\right)dt', \tag{65}$$

where

$$D_{\alpha}=\lim_{\Delta x\to 0,\Delta t\to 0}\frac{\Delta x^2}{2\Delta t^{\alpha}}. \tag{66}$$

The integral on the RHS of Eq. (65) is a convolution so that we can take the Laplace transform to obtain

$$s\hat{X}(x,s)-X(x,0)=D_{\alpha}\left(s^{1-\alpha}\left(\frac{\partial^2\hat{X}(x,s)}{\partial x^2}-2\beta\frac{\partial F(x,t)\hat{X}(x,s)}{\partial x}\right)\right),$$

and then we take the inverse Laplace transform, with the identification,

$$\mathcal{L}^{-1}\{s^{1-\alpha}\hat{X}(x,s)\}={}_0D_t^{1-\alpha}X(x,t)$$

to arrive at

$$\frac{\partial X(x,t)}{\partial t}=D_{\alpha}\left(\frac{\partial^2}{\partial x^2}\left({}_0D_t^{1-\alpha}X(x,t)\right)-2\beta\frac{\partial}{\partial x}\left(F(x,t){}_0D_t^{1-\alpha}X(x,t)\right)\right). \tag{67}$$

3. Numerical scheme

Given that the GME for the DTRW with Sibuya distributed waiting times, Eq. (61), approaches the fractional Fokker–Planck equation, Eq. (67), in the limit of small lattice spacing, Δx, and small time step, Δt, the solution of the GME can be used as an approximation to the solution of the FFPE. Thus the GME for the DTRW provides an explicit numerical scheme that will converge to the FFPE in the appropriate limit, as described below.

The fractional Fokker–Planck equation is given by

$$\frac{\partial\rho(x,t)}{\partial t}=D_{\alpha}\left(\frac{\partial^2}{\partial x^2}\left(D_t^{1-\alpha}\left(\rho(x,t)\right)\right)-2\beta\frac{\partial}{\partial x}\left(F(x,t)D_t^{1-\alpha}\left(\rho(x,t)\right)\right)\right), \tag{68}$$

where D_{α} and α are parameters and $F(x,t)$ is an external space- and time-dependent force. In our numerical method we approximate the solution to the FFPE, Eq. (68), with the solution of the GME for DTRWs, Eq. (61), through the identification

$$\rho(x,t)\approx X(i,n), \tag{69}$$

where $i=\lfloor x/\Delta x\rfloor$ and $n=\lfloor t/\Delta t\rfloor$.

It remains to match the parameters, D_{α} and $F(x,t)$, from the FFPE with the appropriate parameters in the GME. The diffusion coefficient from the FFPE sets the ratio of the space and length scales through the relation,

$$D_{\alpha}=\frac{\Delta x^2}{2\Delta t^{\alpha}}. \tag{70}$$

Treating Δx as the free parameter in this ratio we identify

$$\Delta t=\left(\frac{\Delta x^2}{2D_{\alpha}}\right)^{\frac{1}{\alpha}}. \tag{71}$$

This leaves only a relationship between the force function from the FFPE, $F(x,t)$, and the bias function from the GME, $f(x,t)$. Consistent with the derivation of the FFPE from CTRWs we introduce Boltzmann weights [5] for the bias probabilities as follows:

$$p_r(x_{i+1},n|x_i)=\frac{\exp[-\beta V(x_{i+1},t)]}{\exp[-\beta V(x_{i-1},t)]+\exp[-\beta V(x_{i+1},t)]} \tag{72}$$

where

$$F(x,t)=-\frac{\partial V(x,t)}{\partial x}. \tag{73}$$

Please cite this article in press as: C.N. Angstmann et al., A discrete time random walk model for anomalous diffusion, J. Comput. Phys. (2014), http://dx.doi.org/10.1016/j.jcp.2014.08.003

It is straightforward to show that

$$\lim_{\Delta x \to 0} p_r(x_{i+1}, n|x_i) = \lim_{\Delta x \to 0} \frac{1}{2}\big(1 + \beta \Delta x F(x_i, t)\big), \tag{74}$$

is consistent with Eq. (30) and Eq. (40). A similar relation holds for $p_\ell(x_{i-1}, n|x_i)$.

3.1. Boundary conditions

Boundary conditions are imposed on the problem in a standard manner. For example, on a finite domain, $x \in [0, L]$, where $L = k\Delta x$ and $t = n\Delta t$, we have boundary conditions as follows:

Dirichlet: If

$$\rho(0, t) = b_1(t) \tag{75}$$

and

$$\rho(L, t) = b_2(t), \tag{76}$$

then

$$X(0, n) = b_1(n) \tag{77}$$

and

$$X(k, n) = b_2(n). \tag{78}$$

Zero-Flux: If

$$\left.\frac{\partial \rho(x, t)}{\partial x}\right|_{x=0} - 2\beta F(0, t)\rho(0, t) = 0 \tag{79}$$

and

$$\left.\frac{\partial \rho(x, t)}{\partial x}\right|_{x=L} - 2\beta F(L, t)\rho(L, t) = 0, \tag{80}$$

then we have

$$X(-1, n) = \frac{p_\ell(x_{-1}, n|x_0) X(0, n)}{p_r(x_0, n|x_{-1})} \tag{81}$$

and

$$X(k+1, n) = \frac{p_\ell(x_{k+1}, n|x_k) X(0, n)}{p_r(x_k, n|x_{k+1})} \tag{82}$$

3.2. Initial conditions

For the initial condition

$$\rho(x, 0) = g(x), \tag{83}$$

where $g(x)$ is bounded, we simply sample $g(x)$ via

$$X(i, 0) = g(i\Delta x). \tag{84}$$

However, if

$$\rho(x, 0) = \delta\big(x - x^*\big) \tag{85}$$

we take

$$X(i, 0) = \frac{\delta_{x,x^*}}{\Delta x} \tag{86}$$

such that

$$\int_{-\infty}^{\infty} \rho(x, 0)dx = \lim_{\Delta x \to 0} \sum_{\forall x_i} X(x_i, 0)\Delta x. \tag{87}$$

3.3. Implementation

Here we summarise the details necessary to implement the DTRW, presented in pseudo code in Algorithm 1. Calling the function "DTRW" will return the $N \times 2L$ sized array of values for X, where L parameterises the size of the spatial grid, and we solve for N times steps. Note that the algorithm determines N according to Eq. (71), which uses the provided spatial resolution Δx and final simulation time T.

We note the other crucial input arguments include the anomalous exponent, α, the diffusion coefficient, D_α, along with jump probabilities p_ℓ and p_r (though note that we may simply use $p_\ell = 1 - p_r$), which may be dependent on x_i and t and may be calculated from a potential using Eq. (72).

Algorithm 1 Discrete time random walk with Sibuya waiting time.

function CalculateSibuyaKernel(N, α)
  $K_0 \leftarrow 0$
  $K_1 \leftarrow \alpha$
  $K_2 \leftarrow \alpha(1-\alpha)/2$
  for $i \leftarrow 3$ to N **do**
    $K_i \leftarrow \frac{i+\alpha-2}{n} K_{i-1}$
  return K
function DTRW(T, α, D_α, Δx, L, p_ℓ, p_r)
  $\Delta t \leftarrow (\frac{\Delta x^2}{2D_\alpha})^{1/\alpha}$
  $N \leftarrow T/\Delta t$
  $K \leftarrow$ CalculateSibuyaKernel(N, α)
  $X(x_i, 0) \leftarrow$ Initial conditions
  for $n \leftarrow 1$ to N **do**
    for $x_i \leftarrow x_{-L}$ to x_L **do**
      $i(x_i, n) \leftarrow 0$
      for $m \leftarrow 0$ to n **do**
        $i(x_i, n) \leftarrow i(x_i, n) + K(n-m) \times X(x_i, m)$
    for $x_i \leftarrow x_{-L}$ to x_L **do**
      $X(x_i, n) \leftarrow X(x_i, n-1) + p_\ell(x_{i+1}, n) \times i(x_{i+1}, n) + p_r(x_{i-1}, n) \times i(x_{i-1}, n) - i(x_i, n)$
  return X

4. Examples

4.1. Example 1: $F(x,t) = 0$ with zero-flux boundary conditions

We begin with the example of anomalous diffusion on a line subject to zero-flux boundary conditions. In this case the fractional Fokker–Planck equation simplifies to the standard fractional diffusion equation,

$$\frac{\partial \rho(x,t)}{\partial t} = D_\alpha D_t^{1-\alpha} \frac{\partial^2 \rho(x,t)}{\partial x^2}, \tag{88}$$

subject to the boundary conditions,

$$\left.\frac{\partial \rho(x,t)}{\partial x}\right|_{x=0} = 0, \tag{89}$$

and

$$\left.\frac{\partial \rho(x,t)}{\partial x}\right|_{x=1} = 0. \tag{90}$$

Initially the particle is taken to be at $x = 1/2$, i.e.,

$$\rho(x,0) = \delta\left(x - \frac{1}{2}\right). \tag{91}$$

We take the parameters $D_\alpha = 1$, and $\alpha = 4/5$.

The analytical solution can be found by subordinating the solution to the standard diffusion equation given the same boundary and initial conditions [1,37]. It is straightforward to show, using separation of variables, that the solution to the standard diffusion equation,

$$\frac{\partial \chi(x,t)}{\partial t} = \frac{\partial^2 \chi(x,t)}{\partial x^2}, \tag{92}$$

with boundary conditions and initial conditions given above, is of the form,

Please cite this article in press as: C.N. Angstmann et al., A discrete time random walk model for anomalous diffusion, J. Comput. Phys. (2014), http://dx.doi.org/10.1016/j.jcp.2014.08.003

$$\chi(x,t) = 1 + \sum_{n=1}^{\infty} (-1)^n 2 \exp\left(-(2n\pi)^2 t\right) \cos[2n\pi x]. \tag{93}$$

This can be subordinated by an inverse alpha stable subordinator, $T(t,\tau)$ to find the solution to the fractional diffusion equation [1,37],

$$\rho(x,t) = \int_0^{\infty} \chi(x,\tau) T(t,\tau) d\tau. \tag{94}$$

As the subordination of the exponential function, $\exp(-ct)$, is a Mittag–Leffler, $E_\alpha(-ct^\alpha)$, function [38]. This yields

$$\rho(x,t) = 1 + \sum_{n=1}^{\infty} (-1)^n 2 E_\alpha\left(-(2n\pi)^2 t^\alpha\right) \cos[2n\pi x] \tag{95}$$

as the infinite series solution to the fractional diffusion equation, subject to the boundary conditions and initial condition given above.

To implement the numerical scheme for this problem we choose $k+1$ to be the number of equally spaced points in the interval $[0,1]$. Then $\Delta x = L/k$. Using Eq. (71) we set a value for Δt given $D_\alpha = 1$, and $\alpha = 4/5$. As there is no force term the bias function $f(x,t)$ is zero. Hence the GME that must be solved can be simplified to the following difference equation:

$$X(i,n) = X(i,n-1) + \sum_{m=0}^{n-1} K(m-n)\left(X(i-1,m) + X(i+1,m) - X(i,m)\right) \tag{96}$$

with $K(n)$ given by Eq. (59), and $\alpha = 4/5$. The boundary conditions, consistent with Eq. (81), and Eq. (82), are

$$X(-1,n) = X(0,n), \tag{97}$$

$$X(k+1,n) = X(k,n). \tag{98}$$

The initial condition consistent with Eq. (86) is

$$X(i,0) = \frac{\delta_{i,\lfloor \frac{k}{2} \rfloor}}{\Delta x}. \tag{99}$$

Finally the solution to the fractional diffusion equation can then be approximated by

$$\rho(x,t) = X(i,n) \tag{100}$$

with $x = i\Delta x$ and $t = n\Delta t$.

We present results for a range of Δx and compare them to the analytical solution in Fig. 1. Within the same figure we also show measures of convergence between the numerical scheme $X_{\Delta x}(x,t)$ and the analytical solution $\rho(x,t)$ for $t > 0$. The measures of convergence that we have investigated are the L^∞ norm of the absolute difference,

$$\left\| X_{\Delta x}(x,t) - \rho(x,t) \right\|_\infty \tag{101}$$

and the L^∞ norm of the relative difference,

$$\left\| \frac{X_{\Delta x}(x,t) - \rho(x,t)}{\rho(x,t)} \right\|_\infty. \tag{102}$$

The latter can also measure convergence in the case of unbounded solutions.

4.2. Example 2: $F(x) = 1$ with time varying boundary conditions

Following Example 1 in [25], we consider the following fractional Fokker–Planck equation

$$\frac{\partial \rho(x,t)}{\partial t} = \frac{\partial^2}{\partial x^2}\left(D_t^{1-\alpha}\left(\rho(x,t)\right)\right) - \frac{\partial}{\partial x}\left(D_t^{1-\alpha}\left(\rho(x,t)\right)\right) \tag{103}$$

with the anomalous exponent $\alpha = \frac{4}{5}$, and subject to the time-dependent boundary conditions

$$\rho(0,t) = \frac{-3t^{0.8}}{\Gamma[1.8]} - \frac{2t^{1.6}}{\Gamma[2.6]}, \tag{104}$$

$$\rho(1,t) = \frac{-t^{0.8}}{\Gamma[1.8]} - \frac{2t^{1.6}}{\Gamma[2.6]}, \tag{105}$$

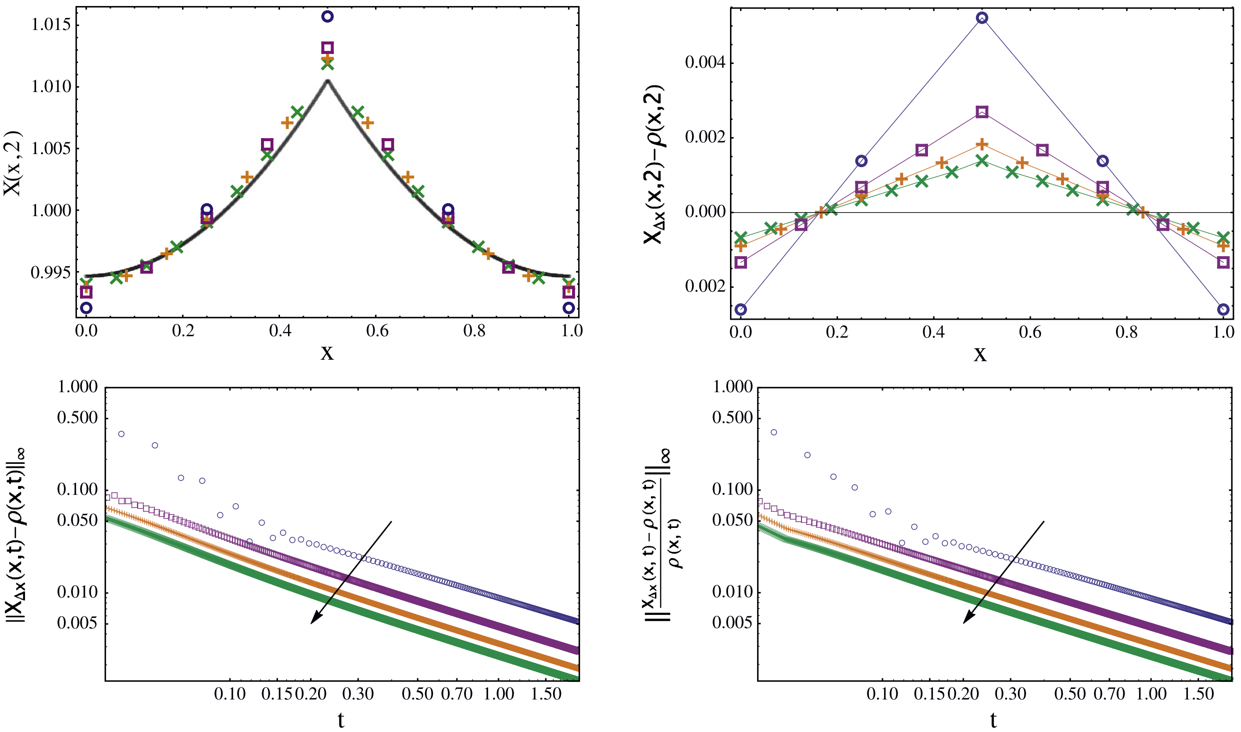

Fig. 1. Convergence of numerical solution for Example 1. Numerical solutions are shown for different values of Δx with $\Delta x = \frac{1}{4}$ (Blue ◯), $\frac{1}{8}$ (Purple ☐), $\frac{1}{12}$ (Orange +) and $\frac{1}{16}$ (Green ×). $\Delta t = 0.42045\Delta x^{10/4}$. The arrow denotes decreasing Δx. *Top Left*—Plot of numerical and analytical (solid curve) solutions at $t = 2$. *Top Right*—Difference between each numerical solution and the analytical solution at $t = 2$. *Bottom Left*—The L^∞ norm of the absolute difference between the numerical simulation and the analytical solution. *Bottom Right*—The L^∞ norm of the relative difference between the numerical simulation and the analytical solution. Note that the bottom plots are on a log–log scale.

and initial condition

$$\rho(x,0) = x(1-x). \tag{106}$$

As shown in [25], this has the solution

$$\rho(x,t) = x(1-x) + (2x-3)\frac{t^{0.8}}{\Gamma[1.8]} - \frac{2t^{1.6}}{\Gamma[2.6]}. \tag{107}$$

This example provides an interesting test case for the numerical method presented here as the solution is negative and hence cannot be interpreted as probability density of a random walk.

To implement the numerical scheme we set the number of points in the interval $[0,1]$ to be $(k+1)$. Then $\Delta x = 1/k$ and Δt is found from Eq. (71). From the given FFPE it can be seen that the force is constant in both space and time, $F(x,t) = -1$, so we may define a potential,

$$V(x,t) = x. \tag{108}$$

From Eq. (72) and taking $\beta = \frac{1}{2}$, the probability of jumping right is in this case independent of time and space,

$$p_r = \frac{\exp(-\frac{1}{2}\Delta x)}{\exp(-\frac{1}{2}\Delta x) + \exp(\frac{1}{2}\Delta x)}. \tag{109}$$

The GME in this case is given by

$$X(i,n) = X(i,n-1) + \sum_{m=0}^{n-1} K(m-n)\big(p_r X(i-1,m) + (1-p_r)X(i+1,m) - X(i,m)\big), \tag{110}$$

with $K(n)$ from Eq. (59). The boundary conditions consistent with Eq. (77) and Eq. (78) are

$$X(0,n) = \frac{-3(n\Delta t)^{0.8}}{\Gamma[1.8]} - \frac{2(n\Delta t)^{1.6}}{\Gamma[2.6]}, \tag{111}$$

$$X(1,n) = \frac{-(n\Delta t)^{0.8}}{\Gamma[1.8]} - \frac{2(n\Delta t)^{1.6}}{\Gamma[2.6]}, \tag{112}$$

Please cite this article in press as: C.N. Angstmann et al., A discrete time random walk model for anomalous diffusion, J. Comput. Phys. (2014), http://dx.doi.org/10.1016/j.jcp.2014.08.003

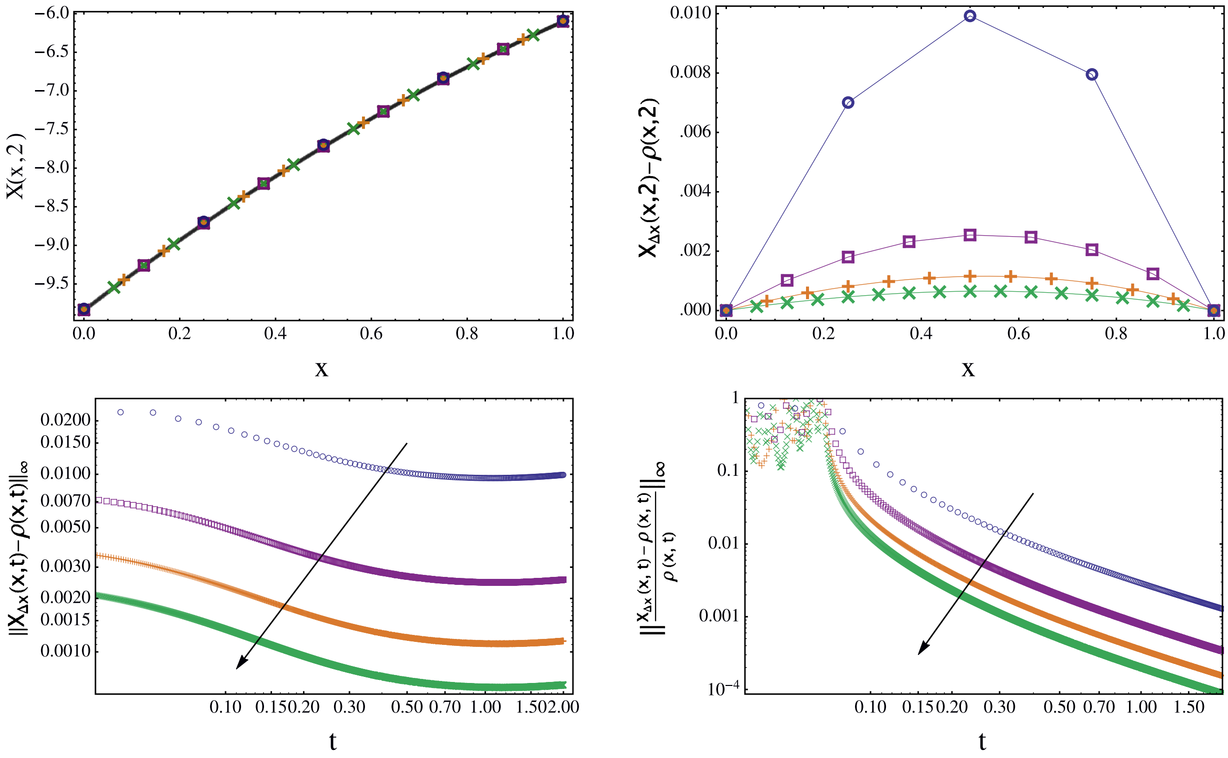

Fig. 2. Convergence of numerical solution for Example 2. Numerical solutions are shown for different values of Δx with $\Delta x = \frac{1}{4}$ (Blue ◯), $\frac{1}{8}$ (Purple □), $\frac{1}{12}$ (Orange +) and $\frac{1}{16}$ (Green ×). $\Delta t = 0.42045\Delta x^{10/4}$. The arrow denotes decreasing Δx. *Top Left*—Plot of numerical and analytical (solid curve) solutions at $t = 2$. *Top Right*—Difference between each numerical solution and the analytical solution at $t = 2$. *Bottom Left*—The L^∞ norm of the absolute difference between the numerical simulation and the analytical solution. *Bottom Right*—The L^∞ norm of the relative difference between the numerical simulation and the analytical solution.

and the initial condition is

$$X(i,0) = i\Delta x(1 - i\Delta x). \tag{113}$$

Finally the solution can then be approximated by

$$\rho(x,t) = X(i,n) \tag{114}$$

with $x = i\Delta x$ and $t = n\Delta t$.

Different measures of convergence are shown in Fig. 2. The numerical solution of the GME, Eq. (61), approaches the analytic solution as the parameter Δx is decreased.

4.3. Example 3: $F(x) = -\frac{1}{x+1}$ with time varying boundary conditions

Following Example 2 in [25], we consider the behaviour on the interval [0, 1] of the fractional Fokker–Planck equation

$$\frac{\partial \rho(x,t)}{\partial t} = \frac{\partial^2}{\partial x^2}\left(D_t^{1-\alpha}\left(\rho(x,t)\right)\right) + \frac{\partial}{\partial x}\left(\frac{1}{x+1}D_t^{1-\alpha}\left(\rho(x,t)\right)\right). \tag{115}$$

In this example we take $\alpha = \frac{4}{5}$. The boundary conditions are given by

$$\rho(0,t) = 1 + \frac{8t^{0.8}}{\Gamma[1.8]}, \tag{116}$$

and

$$\rho(1,t) = 8 + \frac{16t^{0.8}}{\Gamma[1.8]}. \tag{117}$$

The initial condition is taken to be

$$\rho(x,0) = (x+1)^3. \tag{118}$$

The exact solution is given by [25]

$$\rho(x,t) = (x+1)^3 + 8(x+1)\frac{t^{0.8}}{\Gamma[1.8]}. \tag{119}$$

Similarly to the previous example, we set the number of points in the interval $[0,1]$ to be $k+1$. Then $\Delta x = 1/k$ and Δt is found from Eq. (71). The potential in this example is

$$V(x,t) = \ln(x+1). \tag{120}$$

As in the previous case, we use Eq. (72) with $\beta = \frac{1}{2}$ to obtain the probability of jumping right, which, in this case is independent of time but dependent on space,

$$p_r(x) = \frac{\exp(-\frac{1}{2}\ln(x+\Delta x+1))}{\exp(-\frac{1}{2}\ln(x+\Delta x+1)) + \exp(-\frac{1}{2}\ln(x-\Delta x+1))} \tag{121}$$

The GME in this case is given by

$$X(i,n) = X(i,n-1) + \sum_{m=0}^{n-1} K(m-n)\big(p_r(i-1)X(i-1,m) + \big(1-p_r(i+1)\big)X(i+1,m) - X(i,m)\big), \tag{122}$$

where $K(n)$ is the memory kernel given in Eq. (59). The boundary conditions are given by

$$X(0,n) = 1 + \frac{8(n\Delta t)^{0.8}}{\Gamma[1.8]}, \tag{123}$$

$$X(1,n) = 8 + \frac{16(n\Delta t)^{0.8}}{\Gamma[1.8]}, \tag{124}$$

and the initial condition is

$$X(i,0) = (i\Delta x + 1)^3. \tag{125}$$

In an identical manner to the previous two cases the solution can then be approximated by

$$\rho(x,t) = X(i,n) \tag{126}$$

with $x = i\Delta x$ and $t = n\Delta t$.

The convergence of the numerical solution to the analytical solution, with decreasing Δx, is shown in Fig. 3.

4.4. Example 4: $F(x) = -2\pi\sin(2\pi x)$ on a periodic domain

The effects of fractional diffusion for a particle moving in a spatially periodic potential has been considered in [39]. By simulating an ensemble of particles undergoing a CTRW the authors showed that the time evolution of the PDF has qualitative differences for small α values, compared to standard diffusion $\alpha = 1$. To investigate this example we take an array of delta functions that is commensurate with the period of the potential as the initial condition. The solution of the infinite domain problem can then be considered in a single unit cell with periodic boundary conditions. In this example we consider a spatially periodic potential

$$V(x,t) = \cos(2\pi x). \tag{127}$$

The fractional Fokker–Planck equation for this example is given by

$$\frac{\partial\rho(x,t)}{\partial t} = \frac{\partial^2}{\partial x^2}\big(D_t^{1-\alpha}\big(\rho(x,t)\big)\big) + \frac{\partial}{\partial x}\big(2\pi\sin(2\pi x)D_t^{1-\alpha}\big(\rho(x,t)\big)\big), \tag{128}$$

with periodic boundary conditions

$$\rho(0,t) = \rho(1,t), \tag{129}$$

and the initial condition

$$\rho(x,0) = \delta(x-0) + \delta(x-1). \tag{130}$$

As in the previous examples, we set the number of points in the interval $[0,1]$ to be $k+1$. Then $\Delta x = 1/k$ and Δt is found from Eq. (71). Once again we use Eq. (72) with $\beta = \frac{1}{2}$ to obtain the probability of jumping right, which again, is independent of time but dependent on space,

$$p_r(x) = \frac{\exp(-\frac{1}{2}\cos(2\pi(x+\Delta x)))}{\exp(-\frac{1}{2}\cos(2\pi(x+\Delta x))) + \exp(-\frac{1}{2}\cos(2\pi(x-\Delta x)))}. \tag{131}$$

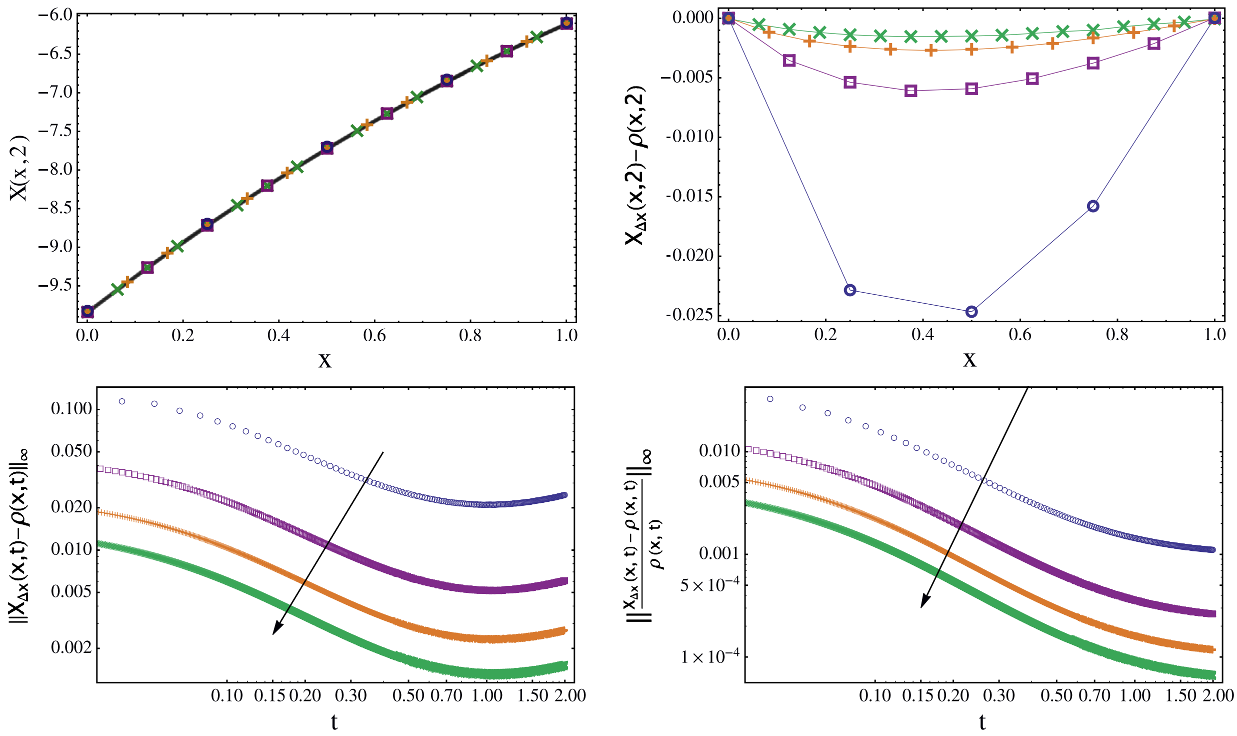

Fig. 3. Convergence of numerical solution for Example 3. Numerical solutions are shown for different values of Δx with $\Delta x = \frac{1}{4}$ (Blue ◯), $\frac{1}{8}$ (Purple □), $\frac{1}{12}$ (Orange +) and $\frac{1}{16}$ (Green ×). $\Delta t = 0.42045\Delta x^{10/4}$. The arrow denotes decreasing Δx. *Top Left*—Plot of numerical and analytical (solid curve) solutions at $t = 2$. *Top Right*—Difference between each numerical solution and the analytical solution at $t = 2$. *Bottom Left*—The L^∞ norm of the absolute difference between the numerical simulation and the analytical solution. *Bottom Right*—The L^∞ norm of the relative difference between the numerical simulation and the analytical solution.

The GME is then given by

$$X(i,n) = X(i,n-1) + \sum_{m=0}^{n-1} K(m-n)\big(p_r(i-1)X(i-1,m) + \big(1-p_r(i+1)\big)X(i+1,m) - X(i,m)\big), \tag{132}$$

where $K(n)$ is the memory kernel given in Eq. (59). The boundary condition is

$$X(0,n) = X(1,n), \tag{133}$$

and the initial condition is

$$X(i,0) = \frac{(\delta_{i,1} + \delta_{i,k+1})}{\Delta x}. \tag{134}$$

The time evolution of the solution to the GME is shown in Fig. 4 for two different values of α. For $\alpha = 0.45$ we see the eventual peak in the density arises from the centre, whereas for $\alpha = 0.9$ the peak is formed from the coalescing of two separate peaks. This behaviour is in qualitative agreement with the results shown in Fig. 5 of [39].

5. Summary

In this paper we have introduced a discrete time random walk model for anomalous subdiffusion in an external space- and time-dependent force field. We have derived the generalised master equations for this model and we show that in the diffusion limit this limits to the fractional Fokker–Planck equation for subdiffusion with space- and time-dependent forcing. We then show how the discrete time random walk model can be used to provide an explicit numerical method for solving fractional Fokker–Planck equations. In future work we plan to extend our numerical method to fractional reaction diffusion equations.

Acknowledgements

This work was supported by the Australian Commonwealth Government (ARC DP140101193).

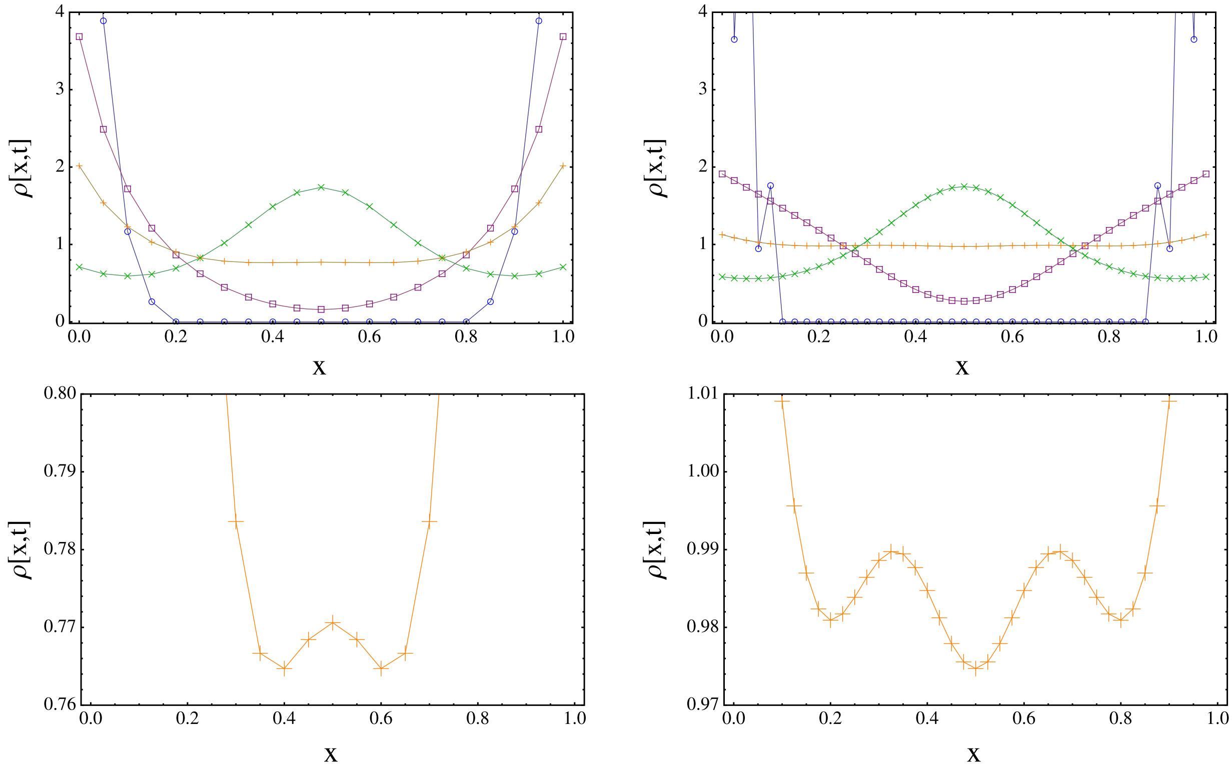

Fig. 4. Numerical solution of Example 4. Numerical solutions are shown for different values of α. *Top Left*—Here $\alpha = \frac{9}{20}$, $\Delta x = 0.05$, and $\Delta t = 3.53744 \times 10^{-7}$. The solution is plotted at four different times, $t = 1.06123 \times 10^{-6}$ (Blue ○), $t = 4.1388 \times 10^{-5}$ (Purple □), $t = 3.17308 \times 10^{-4}$ (Orange +), $t = 1.06113 \times 10^{-2}$ (Green ×). *Top Right*—Here $\alpha = \frac{9}{10}$, $\Delta x = 0.025$, and $\Delta t = 1.27464 \times 10^{-4}$. The solution is plotted at four different times, $t = 5.09858 \times 10^{-4}$ (Blue ○), $t = 9.68729 \times 10^{-3}$ (Purple □), $t = 1.98844 \times 10^{-2}$ (Orange +), $t = 4.53773 \times 10^{-2}$ (Green ×). *Bottom Left*—Here $\alpha = \frac{9}{20}$, $\Delta x = 0.05$, and $\Delta t = 3.53744 \times 10^{-7}$. The solution at $t = 3.17308 \times 10^{-4}$ (Orange +) highlights the emergence of the central peak. *Bottom Right*—Here $\alpha = \frac{9}{10}$, $\Delta x = 0.025$, and $\Delta t = 1.27464 \times 10^{-4}$. The solution at $t = 1.98844 \times 10^{-2}$ (Orange +) highlights the emergence of two of centre peaks that eventually coalesce into the central peak.

References

[1] R. Metzler, J. Klafter, The random walk's guide to anomalous diffusion: a fractional dynamics approach, Phys. Rep. 339 (2000) 1–77.
[2] E. Montroll, G. Weiss, Random walks on lattices II, J. Math. Phys. 6 (1965) 167.
[3] K. Oldham, J. Spanier, The Fractional Calculus, Academic Press, 1974.
[4] R. Metzler, E. Barkai, J. Klafter, Anomalous diffusion and relaxation close to thermal equilibrium: a fractional Fokker–Planck equation approach, Phys. Rev. Lett. 82 (18) (1999) 3563.
[5] E. Barkai, R. Metzler, J. Klafter, From continuous time random walks to the fractional Fokker–Planck equation, Phys. Rev. E 61 (1) (2000) 132.
[6] M.M. Meerschaert, D.A. Benson, H.-P. Scheffler, B. Baeumer, Stochastic solution of space–time fractional diffusion equations, Phys. Rev. E 65 (4) (2002) 041103.
[7] I.M. Sokolov, J. Klafter, Field-induced dispersion in subdiffusion, Phys. Rev. Lett. 97 (14) (2006) 140602.
[8] B.I. Henry, T.A.M. Langlands, S.L. Wearne, Anomalous diffusion with linear reaction dynamics: from continuous time random walks to fractional reaction–diffusion equations, Phys. Rev. E 74 (3) (2006) 031116.
[9] S. Fedotov, Non-Markovian random walks and nonlinear reactions: subdiffusion and propagating fronts, Phys. Rev. E 81 (1) (2010) 011117.
[10] B.I. Henry, T.A.M. Langlands, P. Straka, Fractional Fokker–Planck equations for subdiffusion with space- and time-dependent forces, Phys. Rev. Lett. 105 (17) (2010) 170602.
[11] T.A.M. Langlands, B.I. Henry, S.L. Wearne, Fractional cable equation models for anomalous electrodiffusion in nerve cells: finite domain solutions, SIAM J. Appl. Math. 71 (4) (2011) 1168–1203.
[12] C.N. Angstmann, I.C. Donnelly, B.I. Henry, Continuous time random walks with reactions, forcing, and trapping, Math. Model. Nat. Phenom. 8 (2) (2013) 17–27.
[13] D.S. Banks, C. Fradin, Anomalous diffusion of proteins due to molecular crowding, Biophys. J. 89 (5) (2005) 2960–2971.
[14] F. Santamaria, S. Wils, E. De Schutter, G.J. Augustine, Anomalous diffusion in Purkinje cell dendrites caused by spines, Neuron 52 (4) (2006) 635–648.
[15] N. Malchus, M. Weiss, Elucidating anomalous protein diffusion in living cells with fluorescence correlation spectroscopy—facts and pitfalls, J. Fluoresc. 20 (2010) 19–26.
[16] F. Santamaria, S. Wils, E. De Schutter, G.J. Augustine, The diffusional properties of dendrites depend on the density of dendritic spines, Eur. J. Neurosci. 34 (4) (2011) 561–568.
[17] J.H. Jeon, V. Tejedor, S. Burov, E. Barkai, C. Selhuber-Unkel, K. Berg-Sørensen, L. Oddershede, R. Metzler, In vivo anomalous diffusion and weak ergodicity breaking of lipid granules, Phys. Rev. Lett. 106 (4) (2011) 48103.
[18] B.M. Regner, D. Vučinić, C. Domnisoru, T.M. Bartol, M.W. Hetzer, D.M. Tartakovsky, T.J. Sejnowski, Anomalous diffusion of single particles in cytoplasm, Biophys. J. 104 (8) (2013) 1652–1660.

Please cite this article in press as: C.N. Angstmann et al., A discrete time random walk model for anomalous diffusion, J. Comput. Phys. (2014), http://dx.doi.org/10.1016/j.jcp.2014.08.003

[19] S.B. Yuste, L. Acedo, An explicit finite difference method and a new von Neumann-type stability analysis for fractional diffusion equations, SIAM J. Numer. Anal. 42 (5) (2005) 1862–1874.
[20] T.A.M. Langlands, B.I. Henry, The accuracy and stability of an implicit solution method for the fractional diffusion equation, J. Comput. Phys. 20 (2) (2005) 719–736.
[21] S.B. Yuste, Weighted average finite difference methods for fractional diffusion equations, J. Comput. Phys. 216 (1) (2006) 264–274.
[22] C. Tadjeran, M.M. Meerschaert, H.-P. Scheffler, A second-order accurate numerical approximation for the fractional diffusion equation, J. Comput. Phys. 213 (1) (2006) 205–213.
[23] W. Deng, Numerical algorithm for the time fractional Fokker–Planck equation, J. Comput. Phys. 227 (2) (2007) 1510–1522.
[24] C.-M. Chen, F. Liu, I. Turner, V. Anh, A Fourier method for the fractional diffusion equation describing sub-diffusion, J. Comput. Phys. 227 (2) (2007) 886–897.
[25] S. Chen, F. Liu, P. Zhuang, V. Anh, Finite difference approximations for the fractional Fokker–Planck equation, Appl. Math. Model. 33 (1) (2009) 256–273.
[26] X. Li, C. Xu, A space–time spectral method for the time fractional diffusion equation, SIAM J. Numer. Anal. 47 (3) (2009) 2108–2131.
[27] W. McLean, K. Mustapha, Convergence analysis of a discontinuous Galerkin method for a sub-diffusion equation, Numer. Algorithms 52 (2009) 69–88.
[28] I. Podlubny, T. Skovranek, B.M.V. Jara, I. Petras, V. Verbitsky, Y. Chen, Matrix approach to discrete fractional calculus III: non-equidistant grids, variable step length and distributed orders, Philos. Trans. R. Soc. A 371 (1990) (2013) 20120153.
[29] C. Piret, E. Hanert, A radial basis functions method for fractional diffusion equations, J. Comput. Phys. 238 (2013) 71–81.
[30] M.S.V.M. Kenkre, E.W. Montroll, Generalized master equations for continuous-time random walks, J. Stat. Phys. 9 (1973) 45–50.
[31] R. Gorenflo, F. Mainardi, D. Moretti, P. Paradisi, Time fractional diffusion: a discrete random walk approach, Nonlinear Dyn. 29 (2002) 129–143.
[32] R. Gorenflo, A. Vivoli, F. Mainardi, Discrete and continuous random walk models for space–time fractional diffusion, J. Math. Sci. 132 (5) (2006) 614–628.
[33] A.V. Oppenheim, R.W. Schafer, J.R. Buck, et al., Discrete-Time Signal Processing, vol. 2, Prentice-Hall, Englewood Cliffs, 1989.
[34] C.N. Angstmann, B.I. Henry, Continuous time random walks that alter environmental transport properties, Phys. Rev. E 84 (2011) 061146.
[35] M. Sibuya, Generalized hypergeometric, digamma and trigamma distributions, Ann. Inst. Stat. Math. 3 (1979) 373–390.
[36] I. Podlubny, Fractional Differential Equations, Mathematics in Science and Engineering, vol. 198, Academic Press, 1998.
[37] I.M. Sokolov, Thermodynamics and fractional Fokker–Planck equations, Phys. Rev. E 63 (5) (2001) 056111.
[38] N. Bingham, Limit theorems for occupation times of Markov processes, Probab. Theory Relat. Fields 17 (1) (1971) 1–22.
[39] E. Heinsalu, M. Patriarca, I. Goychuk, P. Hanggi, Fractional diffusion in periodic potentials, J. Phys. Condens. Matter 19 (6) (2007) 065114.