Continuous-time random walks on bounded domains

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A useful perspective to take when studying anomalous diffusion processes is that of a continuous-time random walk and its associated generalized master equation. We derive the generalized master equations for continuous-time random walks that are restricted to a bounded domain and compare numerical solutions with kernel-density estimates of the probability-density function computed from simulations. The numerical solution of the generalized master equation represents a powerful tool in the study of continuous-time random walks on bounded domains.

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I. INTRODUCTION

Anomalous diffusion processes have been observed in many applications; for example, contaminant flow in groundwater [1], dynamic motions in proteins [2], turbulence in fluids [3], and dynamics of financial markets [4] have all been verified experimentally to exhibit characteristics of anomalous diffusion; see Ref. [5] for a review. A diffusion process is termed anomalous when the mean square displacement satisfies

$$\langle X^2(t)\rangle = \int_{\mathbb{R}} x^2 v(x,t)\,\mathrm{d}x \sim t^{\gamma}, \quad \gamma \neq 1, \tag{1}$$

unlike normal diffusion, where $\gamma = 1$. In (1), v is the probability-density function of the random variable $X(t)$, which is the displacement of a diffusing particle at time t. When $0 < \gamma < 1$, such a process is subdiffusive, while $\gamma > 1$ indicates a superdiffusive process. A thorough survey of theoretical considerations for anomalous diffusion processes can be found in Ref. [6].

One common perspective to take when studying anomalous diffusion processes is that of a continuous-time random walk (CTRW) and its associated generalized master equation [6,7]. As discussed in Refs. [6,8,9], this perspective is especially useful when the diffusion process lacks finite characteristic scales, e.g., mean square displacement of a particle or the mean wait-time between collisions. Though the relationship between a CTRW in free space and anomalous diffusion processes has been well studied, the same cannot be said for the subsequent relationship on bounded domains. Of the existing research, much is concerned with graphs and lattices, and comparatively little work exists on the generalized master equations for CTRWs on general bounded domains. Recent efforts, namely, Ref. [8], however, have made advances to remedy this by investigating certain Markovian CTRWs with absorbing and reflecting boundary conditions. The analysis in Ref. [8] is limited in relying on special cases so that explicit, closed-form, solutions to the generalized master equations can be found for simple one-dimensional domains. This analysis becomes difficult when the Markovian assumption is removed, the domains in two and three dimensions are not simple, and the step density is not suitably chosen; e.g., it is approximated from data.

There is also a well-known relationship between the generalized master equations for CTRWs in free space and fractional diffusion equations. For bounded domains, considerably more research exists for fractional diffusion than for integro-differential equations, such as the aforementioned generalized master equations. For instance, Ref. [10] gives a probabilistic interpretation of the Lévy-Feller fractional diffusion equation with absorbing boundaries, where the fraction of the Laplacian is restricted to $\alpha \in (1,2)$; i.e., the cases $\gamma \geqslant 2$ in Eq. (1) are not considered. Other work, e.g., Ref. [11], considers fractional diffusion equations on bounded domains with reflecting boundaries. However, even for fractional diffusion, there is little notion of general boundary conditions outside specialized domains, e.g., rectangles and parallelepipeds in two and three dimensions, respectively.

In this paper, we derive the generalized master equations for both Markovian and non-Markovian continuous-time bounded random walks (CTBRWs) with either absorbing or insulated boundaries. An insulated boundary restricts the random walker from taking a step past the boundary; e.g., a special case of insulated boundaries is the reflective behavior described in Ref. [8].

Boundary conditions such as these appear naturally when a diffusion process is restricted to a bounded domain, e.g., contaminant flow in an underground aquifer. The boundary conditions for a random walker induce volume constraints on the solution of the generalized master equation, and the resulting equations are then studied via a variational formulation and conforming finite-element method described in Refs. [12,13]. This computational approach allows for the study of a wide class of problems on nontrivial bounded domains in two and three dimensions, a capability currently unavailable.

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TABLE I. Pseudocode for simulating a CTBRW.

Absorbing boundaries	Insulated boundaries

$a_0 = 0$
simulate $x_0 \sim u_0(x)$
for k from 1 to T
  simulate $t_k \sim \omega(t)$
  $a_k = a_{k-1} + t_k$
  simulate $s_k \sim \phi(s)$
  $x_k = x_{k-1} + s_k$
  if $x_k \notin (0,1)$
    break
  end
end
	$a_0 = 0$
	simulate $x_0 \sim u_0(x)$
	for k from 1 to T
	  simulate $t_k \sim \omega(t)$
	  $a_k = a_{k-1} + t_k$
	  simulate $s_k \sim \phi(s)$
	  $x_k = x_{k-1} + s_k$
	  if $x_k \notin (0,1)$
	    $x_k = x_{k-1}$
	  end
	end

We demonstrate that the numerical solutions to the generalized master equations agree with kernel-density estimates of the solution from CTBRW simulations. This renders the aforementioned finite-element formulation a powerful tool in studying CTBRWs as models of anomalous diffusion because computationally intensive CTBRW simulations may be avoided.

II. CTRW IN A BOUNDED DOMAIN

We consider separable CTRWs; i.e., wait times are independent of the choice of step. The wait-time density is denoted with ω and the step density with $J(y,x)$; i.e., $J(y,x)$ is the probability density of taking a step from y to x and, consequently, $\int_{\mathbb{R}} J(y,x)\,\mathrm{d}x = 1$. Note, however, that $\int_{\mathbb{R}} J(y,x)\,\mathrm{d}y \neq 1$ in general. It is well known (see, e.g., Refs. [4,6,14]) that the probability-density function of the CTRW, $u(x,t)$, satisfies the generalized master equation

$$u_t(x,t) = \int_0^t \Lambda(t-t') L_{\mathbb{R}}^J u(x,t')\,\mathrm{d}t', \tag{2}$$

where the Laplace transform of the memory kernel Λ is

$$\widehat{\Lambda}(\zeta) = \frac{\zeta\widehat{\omega}(\zeta)}{1-\widehat{\omega}(\zeta)},$$

and we have introduced the operator

$$L_I^f u(x,t) := \int_I [u(y,t)f(y,x) - u(x,t)f(x,y)]\,\mathrm{d}y.$$

The analogous operator to $L_I^f u(x,t)$ for a CTRW on a lattice has been studied previously; see, e.g., Ref. [15].

For this paper, we consider two choices of Λ in (2):

$$\Lambda(t-t') = \frac{1}{2\tau}\delta(t-t'), \tag{3a}$$

$$\Lambda(t-t') = \frac{1}{\tau^2}\exp\left(-\frac{t-t'}{\tau/2}\right), \tag{3b}$$

which are tantamount to specifying that wait times are distributed as

$$\mathrm{Exp}(2\tau), \quad \text{i.e., } \omega(t) = \frac{1}{2\tau}\exp\left(-\frac{t}{2\tau}\right), \tag{4a}$$

$$\mathrm{Gamma}\,(2,\tau), \quad \text{i.e., } \omega(t) = \frac{t}{\tau^2}\exp\left(-\frac{t}{\tau}\right), \tag{4b}$$

respectively, both of which imply finite mean wait times. In fact, (4a) and (4b) imply that the underlying CTRWs are compound Poisson and renewal reward processes, respectively. With (3), (2) reduces to

$$u_t(x,t) = \frac{1}{2\tau} L_{\mathbb{R}}^J u(x,t), \tag{5a}$$

$$u_t(x,t) + \frac{\tau}{2}u_{tt}(x,t) = \frac{1}{2\tau} L_{\mathbb{R}}^J u(x,t). \tag{5b}$$

Since the mean wait time is finite, (5a) and (5b) are models for either normal diffusion or anomalous superdiffusion, depending on whether $\int_{\mathbb{R}} (x-y)^2 J(y,x)\,\mathrm{d}x$ is finite or infinite, respectively. By selecting a heavy-tailed wait-time density, we may obtain models for subdiffusion, normal diffusion, or superdiffusion, depending now upon the interplay between the characteristic step-length variance and characteristic mean wait time. We refer the reader to Ref. [6] for further information.

Boundary conditions for CTBRWs manifest themselves in the definition of the step density $J(y,x)$ and are now described. We let ϕ be a symmetric probability density that should be interpreted as the step density in the absence of boundary conditions.

We first describe the behavior of fully absorbing boundaries. Once a random walker reaches, or steps beyond, the boundary $\partial\Omega$, it is banned from Ω for all future time. This description gives the step density

$$J(y,x) = \begin{cases} \phi(x-y), & y \in \Omega, \\ \delta(x-y), & y \notin \Omega, \end{cases} \tag{6}$$

so that a random walker may step from $y \in \Omega$ to $x \in \mathbb{R}$ via the radial density $\phi(x-y)$.

It is convenient then to set $u(x,t) = 0$ for $x \notin \Omega$, and inserting (6) into (2) gives

$$\begin{cases} u_t(x,t) = \int_0^t \Lambda(t-t') L_{\mathbb{R}}^{\phi} u(x,t')\,\mathrm{d}t', & x \in \Omega, \\ u(x,t) = 0, & x \notin \Omega, \end{cases}$$

and, thus,

$$u_t(x,t) = \frac{1}{2\tau} L_{\mathbb{R}}^{\phi} u(x,t), \quad x \in \Omega, \tag{7a}$$

$$u_t(x,t) + \frac{\tau}{2}u_{tt}(x,t) = \frac{1}{2\tau} L_{\mathbb{R}}^{\phi} u(x,t), \quad x \in \Omega. \tag{7b}$$

Equation (7a) was studied in the context of a Markovian CTRW in Ref. [8], and (7b) belongs to a non-Markovian CTRW.

The case of fully insulated boundaries restricts a random walker from reaching, or stepping beyond, $\partial\Omega$. One interpretation of this description gives rise to

$$J(y,x) = \chi_\Omega(x)\phi(x-y) + \delta(x-y)\int_{\mathbb{R}\setminus\Omega} \phi(z-y)\,\mathrm{d}z, \quad y \in \Omega. \tag{8}$$

The step density (8) states that a random walker may step from $y \in \Omega$ to $x \in \Omega$ via the radial density $\phi(x-y)$. Further, there is a nonzero probability, $\int_{\mathbb{R}\setminus\Omega} \phi(z-y)\,\mathrm{d}z$, of the walker at $y \in \Omega$ not taking a step. Together, these guarantee that the random walker remains in Ω for all time, and, consequently, defining $J(y,x)$ for $y \notin \Omega$ in (8) is not required.

Insertion of (8) into (2) gives

$$u_t(x,t) = \int_0^t \Lambda(t-t') L_\Omega^\phi u(x,t')\,\mathrm{d}t', \quad x \in \Omega,$$

and, thus,

$$u_t(x,t) = \frac{1}{2\tau} L_\Omega^\phi u(x,t), \quad x \in \Omega, \tag{9a}$$

$$u_t(x,t) + \frac{\tau}{2} u_{tt}(x,t) = \frac{1}{2\tau} L_\Omega^\phi u(x,t), \quad x \in \Omega. \tag{9b}$$

Now, we relate Eqs. (7) and (9) to nonlocal boundary value problems that have been postulated and studied in various different settings [8,12,13,16,17]. A nonlocal boundary value problem augments (5) by constraining the solution on a nonzero volume, generalizing the notion of classical boundary conditions to that of a volume constraint. Such volume constraints need not be relegated to the exterior of Ω. We specify an initial density $u_0(x)$ on Ω, satisfying $u_0 \geqslant 0$ and $\int_\Omega u_0(x)\,\mathrm{d}x = 1$.

The nonlocal Dirichlet boundary value problems are

$$\begin{cases} u_t(x,t) = \frac{1}{2\tau} L_{\mathbb{R}}^\phi u(x,t), & x \in \Omega, \\ u(x,t) = 0, & x \notin \Omega, \\ u(x,0) = u_0(x), & x \in \Omega, \end{cases} \tag{10a}$$

and

$$\begin{cases} u_t(x,t) + \frac{\tau}{2} u_{tt}(x,t) = \frac{1}{2\tau} L_{\mathbb{R}}^\phi u(x,t), & x \in \Omega, \\ u(x,t) = 0, & x \notin \Omega, \\ u(x,0) = u_0(x), & x \in \Omega, \\ u_t(x,0) = 0, & x \in \Omega. \end{cases} \tag{10b}$$

The nonlocal Dirichlet boundary condition constrains u for $x \notin \Omega$, analogous to the classical Dirichlet boundary condition that does so at the points on the boundary.

The nonlocal Neumann boundary value problems are

$$\begin{cases} u_t(x,t) = \frac{1}{2\tau} L_\Omega^\phi u(x,t), & x \in \Omega, \\ u(x,0) = u_0(x), & x \in \Omega, \end{cases} \tag{11a}$$

and

$$\begin{cases} u_t(x,t) + \frac{\tau}{2} u_{tt}(x,t) = \frac{1}{2\tau} L_\Omega^\phi u(x,t), & x \in \Omega, \\ u(x,0) = u_0(x), & x \in \Omega, \\ u_t(x,0) = 0, & x \in \Omega. \end{cases} \tag{11b}$$

The integrals in (11), in contrast to those in (10), are over Ω rather than all of $\mathbb{R}$. This implies a constraint on diffusion so that it occurs strictly inside Ω; i.e., density neither enters nor exits Ω, which is analogous to the classical Neumann boundary condition.

In summary, the descriptions of the boundary conditions for the CTBRW determine J in (2) so that (2) reduces to an appropriate nonlocal boundary value problem in (10) or (11). Evidently, these nonlocal boundary value problems describe the time evolution of the probability density of the state of the corresponding CTBRW. The analysis in Refs. [12,13] allows us to analyze (10) and (11) via a variational formulation and conforming finite-element method, so extending the class of problems computationally tractable.

We simulate N random walkers, and a kernel-density estimate of u at various points in time is computed. This kernel-density estimate is compared to the finite-element solution of the associated nonlocal boundary value problem. We select ϕ to be a Lévy stable density with stability index α, characterized via

$$\phi(s) = \mathcal{F}^{-1}\{\exp(-\varepsilon^\alpha |\xi|^\alpha)\}(s) \tag{12}$$

and choose $\alpha = 3/2$ and $\varepsilon = 0.25$. For simulations with absorbing boundaries, we use $u_0(x) = 2x$, and for insulated boundaries, $u_0(x) = \frac{\pi}{2}\sin(\pi x)$. These choices of u_0, in consideration of the respective boundary conditions, were opportune and have no effect on our conclusions.

A walker begins at a random location $x_0 \in (0,1)$ according to the initial density $u_0(x)$. For each k, a wait time t_k is generated from ω, and the arrival time $a_k = a_{k-1} + t_k$ is recorded. A step s_k is generated from ϕ, the new location $x_k = x_{k-1} + s_k$ is recorded, and then boundary conditions are imposed. For instance, if $x_k \notin (0,1)$ for the case of absorbing boundary conditions, the random walk is stopped. In the case of insulated boundary conditions, if $x_k \notin (0,1)$, we set $x_k = x_{k-1}$; i.e., the walker waits at the current position. Again, this treatment of an insulated boundary differs from the reflective behavior in Ref. [8] and is merely one approach for treating insulated boundaries. Deciding on the appropriate treatment is application specific and depends largely on the mechanism driving the CTBRW. Note that the position of the random walker is known for all time; e.g., the walker is at position x_k for the time interval $[a_k, a_{k+1})$. A summary of the algorithm for simulating a CTBRW is given in Table I.

Data from the CTBRW simulations are used to estimate the density $u(x,t)$. Let $p_i(t)$ denote the ith random walker's

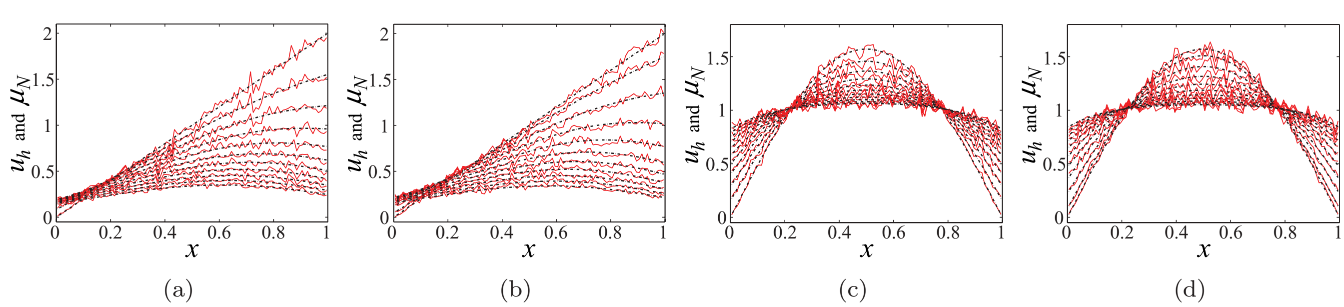

FIG. 1. (Color online) Panels (a)–(d) show kernel-density estimates of the CTBRW simulations (solid lines) on $\Omega = (0,1)$ with $N = 8 \times 10^4$ and numerical solutions (dashed lines) of the nonlocal boundary value problems (10a)–(11b), respectively. The horizontal axis is x and the vertical axis is the value of the density. The ten curves represent ten different values of $t \in [0,0.5]$.

position at time t and partition $\Omega = (0,1)$ into n subintervals Ω_i. Then define the kernel-density estimate:

$$\mu_N(x,t) := \sum_{k=1}^{n} \chi_{\Omega_k}(x)\left\{\frac{1}{Nh}\sum_{i=1}^{N}\chi_{\Omega_k}(p_i(t))\right\}. \qquad (13)$$

Though results exist that give the "optimal" bandwidth, i.e., h, so as not to oversmooth or undersmooth the data, it is convenient in this case to pick h to be the mesh size induced by the finite-element discretization. We denote the numerical solutions to (10) and (11) with u_h.

We present simulation results for $N = 8 \times 10^4$ random walkers with $h = 0.01$ and $t \in [0,0.5]$. To produce a, visually, more pleasing comparison between u_h and μ_N, the kernel-density estimate in (13) is plotted as a continuous piecewise linear function by connecting the heights of μ_N at each of the midpoints of the subintervals Ω_i. Figure 1 shows results of the CTBRW simulations on $(0,1)$.

III. CONCLUSIONS

The results in Sec. II corroborate that the nonlocal boundary value problems in (10) and (11) are indeed the generalized master equations for a CTBRW with appropriate boundary conditions. Consequently, a rapid means of investigating statistics of the CTBRW, e.g., exit times, exists via finding numerical solutions to generalized master equations and thus renders the recently developed variational formulation and numerical methods powerful tools. Without this capability, estimating such statistics requires simulations of the CTBRW, a computationally demanding task.

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