Mean first-passage time for superdiffusion in a slit pore with sticky boundaries

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This Brief Report examines Levy motion in a slit pore with sticky boundaries, i.e., boundaries that absorb particles for a random amount of time. A set of equations is developed that can explicitly be solved for mean travel distance to a plane for a particle released from the origin and can iteratively be used to compute mean first-passage time (MFPT). Results from the theory compare favorably with Monte Carlo simulations.

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This work is motivated by a desire to develop a theoretical formulation for the mean first-passage time (MFPT) for Levy particles in a slit pore with sticky boundaries. The theoretical results provide design and data processing tools for experimentalists.

Researchers often use a slit pore or a rectangular microchannel to experimentally or numerically study microbial dynamics [1–6]. Many species of microbes divide their time between a motile free swimming phase and a sorbed phase in which they may exist in a biofilm or attach singly to a surface [4,7]. The free swimming cell provides an example of transport that is both nonlinear and random. In a stagnant fluid many microbes exhibit straight runs followed by tumbles (random changes in direction) [7], resembling the typical trace of a Levy flight [8]. Apart from the study of microbial transport, Levy motions have found use in a wide range of physical problems, including turbulent diffusion [9–12], transport in heterogeneous porous media [13,14], stochastic interpolation of aquifer properties [15], scattering of waves [16], and anomalous diffusion in rotating flows [17], to name a few.

The transition density for increments in a Levy motion is given by an α-stable distribution [18], α lies in (0,2], with time-dependent parameters. When $\alpha=2$, the distribution is Gaussian and a classical Brownian motion results. Gaussian distributions and symmetric α-stable distributions look very similar except that the latter is characterized by a heavier tail. The heavy tail ensures that Levy motions are superdiffusive.

We conceptualize an infinite slit pore filled with fluid being driven by a pressure gradient in the x direction and thus the velocity profile in the y direction normal to the walls is parabolic (Poiseuille flow). The initial distribution of Levy particles is Dirac midway between the walls. The objective is to compute the MFPT to a plane located a given distance downstream from the source. Particle transport within this flow field is modeled as a symmetric α_f-stable Levy motion with drift subject to sticky boundaries. The parameters that define the Levy motion are α_f which governs the thickness of the tail of the density and is often called the characteristic exponent, and σ_f which sets the width of the distribution and is often known as the scaling factor. Both parameters can be obtained experimentally from the finite-size Lyapunov exponent [19,20]. Upon collision with the pore walls, particle attachment occurs. Sticking times can vary from infinity (irreversible sorption) to zero (instantaneous release). The local sorption time is modeled as the absolute value of an α_w-stable distribution with parameters α_w and σ_w. This is an extension of the model of Bonilla and Cushman [5] for Brownian motion with sticky boundaries, whose local time was also governed by an α-stable distribution. In passing, we point out that the α-stable Levy motion is renormalizable and hence upscalable to complex porous media [21].

The nonlocal character of the fractional advection-diffusion equation (the Fokker-Planck equation for an α-stable Levy process) makes formulating realistic boundary conditions in an Eulerian domain difficult. Indeed, most of the literature available on theoretical evaluation of first-passage times takes into account simple boundary conditions where complete adsorption or reflection occurs in a one-dimensional finite or semi-infinite domain [22–30]. Formulas have been derived to compute the mean number of times a site is visited during Levy flights [29] and the average time spent by Levy flights on an interval with absorbing barriers [26,27]. The solutions proposed for the transition density for Levy motion in bounded domains vary from purely analytical [23–25] to semianalytic, wherein a modified fractional advection-diffusion equation was derived and solved using a finite difference technique [30].

For the simplistic case of transport by Levy diffusion without drift, it is obvious that at any moment snapshots of the particle concentration will be symmetric about both the x and y axis provided the source is midway between the walls. The mean travel distance (MTD) in the x direction after a fixed number of steps is zero because the number of particles taking forward jumps is on average equal to the number of particles taking backward jumps of the same magnitude. In fact, the MTD will not be altered even if one integrates the distribution along the x axis after every step and puts the resultant mass back onto the vertical line passing through the centroid of the distribution. The particles are independent and hence making them converge on a line after every step will not affect their motion in the subsequent steps. For the purpose of computing the MTD, the two-dimensional (2D) distribution can therefore be transformed to a 1D distribution in the y direction. This conceptualization remains valid even when there is drift because the velocity does not change in the x direction. To compute the MTD in the presence of parabolic drift, one can simply multiply the velocity at the current y coordinate by the corresponding density at that location and use that to calculate the incremental displacement after each time step. The MTD after N steps can be computed by adding all incremental displacements.

Gitterman [23] derived a 1D (transverse direction in our model) density in the presence of adsorbing walls,

$$G(y,n;\chi) = \frac{1}{b}\sum_{k=1}^{\infty} \sin\left[\frac{k\pi}{2b}(\chi)\right]\sin\left[\frac{k\pi}{2b}(y)\right] \times \exp\left[-D\left(\frac{k\pi}{2b}\right)^{\alpha_f} n\Delta t\right], \quad (1)$$

where χ is the location of input in the transverse direction, n is the number of steps a particle has taken up to time t, Δt is the time interval separating successive steps, $2b$ is the distance between absorbing barriers, and $D = \sigma^{\alpha}/|\Delta t \cos(\alpha\pi/2)|$ is the diffusion coefficient for symmetric Levy flights. The parameters α and σ are the characteristic exponent and scaling factor associated with the underlying symmetric α-stable Levy process. It should be noted that the value of the diffusion coefficient, D, is modified when a 2D problem is converted to a 1D problem. The direction of displacement vectors is uniformly distributed on a unit circle. The value of the y component of the mean unit vector in all four quadrants is $\cos(\pi/4)$. Hence the value of the scaling parameter σ_f should be modified by a factor of $\cos(\pi/4)$ so that only the component of displacement vector in the y direction enters the computation of the probability density function in Eq. (1).

The above paragraph pertains to the absorbing boundary case. To develop a framework for the sticky boundary, we first concentrate on the instantaneous absorption and release case (i.e., $\sigma_w \to 0$). For this case, Eq. (1) can be applied to find the density function along the transverse direction of a pore as long as the particle is not released back into the same pore. To account for all particles released back into the system, and at the same time benefit from the form of Eq. (1), we visualize an infinite number of identical pores stacked upon each other. Each slit pore has the same parabolic drift. Particles originating from a point source located on the midplane of the central pore (call it pore No. 1) diffuse symmetrically to reach either the top or the bottom wall (boundary). The particles are absorbed and instantaneously released, but the releases are made in the next adjacent pore upwards for the top wall, and the next adjacent pore downwards for the bottom wall. These two pores take all particles released from pore No. 1, and together they are labeled pore No. 2. The top wall of the upper pore and the bottom wall of the lower pore would release particles into the next adjacent upward and downward pores (labeled pore No. 3). Relying on the symmetry of the problem, we allow particles exiting the bottom wall of an upper pore to be instantaneously released into the next pore adjacent to its lower counterpart, and vice versa for particles exiting the top wall of the lower pore. It should be noted that in the event of a particle getting absorbed at one of the walls, its release into the adjacent pore is counted as the next step and not a continuation of the previous step. The process continues in this fashion for an infinite number of pores, thus ensuring mass conservation. However, unlike the central pore (pore No. 1) for which the source is located on midplane, the location of sources (χ) as a result of first release in pore No. 2 and beyond is no longer fixed but has an α-stable distribution with a stability index of α_f and a scaling factor of $\sigma_f \cos(\pi/4)$. Therefore, except in pore No. 1, a particle has a finite probability of release from any point in between the top and the bottom wall. Because of finite widths of pores, a normalized α-stable distribution is used to distribute particles between the two walls. Since an α-stable distribution has heavy tails, the normalization may significantly alter the shape of the distribution when the width ($2b$) of the pore is small. Henceforth we assume a large b/σ_f.

The probability density function in the ith pore, as a result of the mass released from a neighboring pore at mth step, can be written as

$$G^i(y,n;m) = \int_0^{2b} G(y,n;\chi)\delta^i(\chi,m)d\chi = \int_0^{2b} \frac{\delta^i}{b}\sum_{k=1}^{\infty} \sin\left[\frac{k\pi}{2b}(\chi)\right]\sin\left[\frac{k\pi}{2b}(y)\right] \times \exp\left[-D\left(\frac{k\pi}{2b}\right)^{\alpha_f} n\Delta t\right]d\chi, \quad (2)$$

for all $n \geqslant m \geqslant i$. Recall the earliest that a particle can appear in the ith pore is after $i-1$ steps. The term δ^i, which is a function of χ and m, is a measure of the distribution of the fraction of particles entering the ith pore at the mth step. It can be found by multiplying the differential releases from the previous pore by the normalized α-stable distribution,

$$\delta^i(\chi,m) = f_{\alpha_f}(\chi)R^{i-1}, \quad (3)$$

where

$$R^{i-1}(m) = \nabla\int_0^{2b}\left[\sum_{l=i-1}^{m} G^{i-1}(y,m;l)\right]dy, \quad (4)$$

R^{i-1} is interpreted as the mass injected into the ith pore at the mth step.

Any algorithm to implement the above set of equations begins in the central pore with $\delta^1(\chi,m)$ given by a Dirac input at $\chi=b$. Thus the probability density function in the central pore is readily known for all points in space and time by a straightforward application of Eq. (1). The chain of computations progressively moves towards the next neighbors by using Eqs. (4), (3), and (2) (in that order), and then summing the values obtained from Eq. (2) to find probability density functions in the individual pores,

$$G^i(y,n) = \sum_{m=i}^{n} G^i(y,n;m). \quad (5)$$

The total probability density function can be found by summing Eq. (5) over all pores,

$$G(y,n) = \sum_{i=1}^{\infty} G^i(y,n). \quad (6)$$

Several plots of solutions of Eq. (6) are shown in Fig. 1. Particles diffuse symmetrically after starting as a Dirac input from the midpoint between the walls. As time progresses, particles accumulate near the walls. The density profiles be-

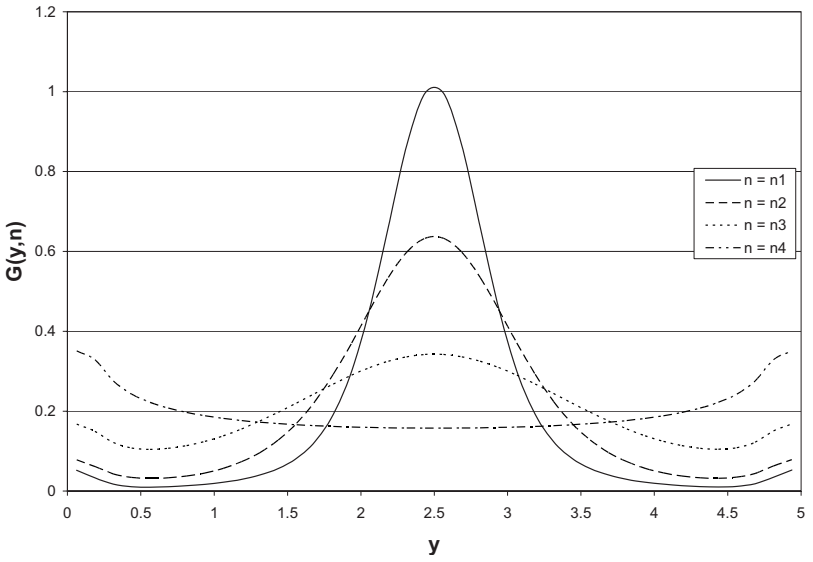

FIG. 1. Typical plots of $G(y,n)$ obtained by solving Eq. (6) for four different values of number of steps (n). Curves with higher values in the middle correspond to relative smaller values of n, i.e., $n1<n2<n3<n4$.

come stationary with typically thicker ends and thinner middle portions.

The MTD $\bar{L}$ can be envisaged as the sum of incremental displacements in the x direction after each time step. It can be found by superimposing the velocity field onto $G(y,n)$. After N steps,

$$\bar{L} = \sum_{n=1}^{N} \int_{y=0}^{2b} G(y,n)v(y)dy. \tag{7}$$

Equations (2)–(7) thus provide an explicit way to compute the MTD when the net amount of time (number of steps, N) is known. It is important to reiterate here that as of yet, the generalized sticky boundary condition has not been included in the analysis. The mean first passage time may be obtained from the MTD to a plane by inversion and a standard iterative scheme can be employed for this purpose. The value of N can be found iteratively given the MTD is specified for the plume centroid. The distance traveled by the centroid is the same as the distance between the point source and the passage plane. By multiplying N by Δt, the MFPT can be found when boundaries are instantaneously releasing particles back into the system.

To this point, $G(y,n)$ is not a function of boundary stickiness. That is, after n steps, the transverse density profile will always conform to Eq. (6) irrespective of the degree of stickiness, although the time it requires for n steps to occur will change as a function of the stickiness. Stickiness introduces larger time intervals between successive steps, and this random time is tied to the probability of hit (collision) between a particle and the pore walls. Parashar and Cushman [31] developed an expression for the average number of hits between source and the passage plane by neglecting the first hit that occurs when particles originating on the midplane reach one of the boundaries for the first time. However, if total number of steps (N) is not too large, one may include the steps required for first hit via the passage time equation in Gitterman [23],

$$N_{sf} = \frac{4}{\pi D \Delta t}\left(\frac{2b}{\pi}\right)^{\alpha_f} \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m+1)^{1+\alpha_f}}. \tag{8}$$

A modified formula for the average number of hits during N steps of Levy process can be written as

$$N_{hit} = 1 + \frac{N - N_{sf}}{N_s + 1}, \tag{9}$$

where N_S is given as [31]

$$N_S = \frac{2^{1+\alpha_f/2}\Gamma\left(\frac{1}{2}+\frac{\alpha_f}{4}\right)\Gamma(-1/2)}{\alpha_f\sqrt{\pi}\Gamma(-\alpha_f/4)}\left(\frac{2b}{\sigma_f}\right)^{\alpha_f/2}. \tag{10}$$

The denominator in Eq. (9) displaces a particle by a single step before computing the number of steps needed to reach a boundary. It is also assumed here that the expected value of the ratio between the total number of steps and the steps needed for a particle to reach one of the walls is the same as the ratio between their respective expected values, which is of course an approximation. When boundaries are sticky and the waiting time is modeled as the modulus of an α_w-stable distribution with scaling factor σ_w, the net retardation $\Re$ introduced is computed by taking the product of N_{hit} and the expected value of the α_w-stable distribution,

$$\Re = N_{hit}\frac{2\Gamma(1-1/\alpha_w)\sigma_w}{\pi}. \tag{11}$$

After N steps, the average total amount of time a particle stays in the system is given by the sum of $\Re$ and $N\Delta t$. Having found N iteratively using Eqs. (2)–(7), the nondimensional MFPT $\bar{T}$ can be found,

$$\bar{T} = \frac{v_{av}(\Re + N\Delta t)}{\bar{L}}, \tag{12}$$

where v_{av} is the average velocity

$$v_{av} = \left(\frac{-\nabla p}{3\mu}\right)b^2, \tag{13}$$

and ∇p and μ are the longitudinal pressure gradient and the dynamic viscosity of the fluid.

We compare the nondimensional MFPT [Eq. (12)] with

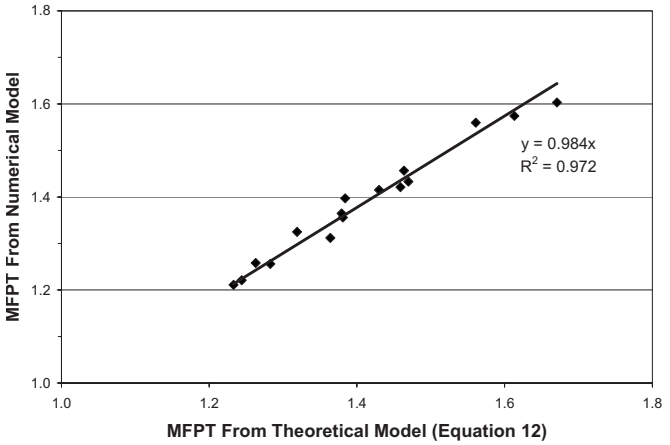

FIG. 2. Comparison of the theoretical [solution of Eq. (12)] vs numerical model (solution of stochastic differential equation) for the MFPT for 16 data sets.

the values obtained by implementing the Monte Carlo method of Parashar and Cushman [31]. The numerical model is based on the Lagrangian perspective, that is, a stochastic Levy driven ordinary differential equation with parabolic drift is solved within the confines of a slit pore with sticky boundaries.

Results obtained for the MFPT from Eq. (12) and the Monte Carlo simulation for several data sets are plotted in Fig. 2. The combinations of parameters were chosen to allow for a broad range (1.2 to 1.7) in MFPT results. For the ideal case of zero sorption, the MFPT approaches 1. The numerical and the theoretical results are consistent. The small differences between the two approaches do not follow any recognizable trend. Possible sources of errors include (a) the assumption of a large b over σ_f ratio; (b) introduction of a normalized α-stable distribution in the theoretical model; (c) coarse resolution when performing numerical integration; (d) rounding and truncation errors in the Monte Carlo simulation; and (f) limited computational resources to carry out long-term simulations for a large number of particles in the Monte Carlo framework.

To summarize, a theory for the MFPT of a Levy motion in a slit pore with sticky boundaries was developed. The theory is based on extending the solution for an absorbing boundary condition to an infinite number of parallel pores that mimic the sticky boundary condition. Equations (2)–(7) can be solved for the number of steps N required to travel a given distance from a source. Using N to find the average number of hits a particle experiences between the source and the passage plane, and by computing the expected value of waiting time for sorbed particles on pore walls, Eq. (12) was used to obtain the nondimensional MFPT. The results obtained from the theory compare favorably to those obtained from a Monte Carlo simulation which is far more computer intensive.

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