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Simplified calculation of diffusivity for a lattice-based random walk with a single obstacle

Matthew J. Simpson [a,*], Michael J. Plank [b,c]

[a] School of Mathematical Sciences, Queensland University of Technology, Brisbane, Australia
[b] School of Mathematics and Statistics, University of Canterbury, Christchurch 8140, New Zealand
[c] Te Pūnaha Matatini, a New Zealand Centre of Research Excellence, New Zealand

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ABSTRACT

Motion of cells in living tissues is hindered by obstacles, which may be stationary or may also move. We present a simplified method to calculate the exact Fickian diffusivity for a tracer particle in a random walk with one obstacle.

In vivo cell motion involves crowding effects that can be modelled using lattice-based random walks [1–5]. Stationary obstacles have a major impact on the transport of tracer particles [6–8]. Mercier and Slater introduced an exact method to calculate the reduced Fickian diffusivity of a tracer particle on a lattice with stationary obstacles [9,10]. The method has several applications [11–18]. Here we present a simplified approach for performing these calculations for a single agent and single obstacle, paying particular attention to the differences between the case where the obstacle is stationary from the case where the obstacle is motile.

Consider an unbiased random walk for two agents – a tracer agent and an obstacle with a given motility – on a lattice with periodic boundaries. The agents are initially placed randomly, and agent i attempts to undergo a nearest neighbour according to an independent Poisson process of rate P_i $(i = 1, 2)$. Motility events that would place an agent on an occupied site are aborted. Simulations (Supplementary Material) are used to record the horizontal component of the tracer agent's squared displacement, $x^2(t)$, and the Fickian diffusivity, $\overline{D}$, of the tracer can be estimated by examining the long-time behaviour of the mean squared displacement, $\langle x^2(t)\rangle$ (Supplementary Material). Fig. 1(a) shows that $\overline{D}/D_0 \approx 0.81$ when the obstacle is stationary, and $\overline{D}/D_0 \approx 0.84$ when the obstacle is motile, where D_0 is the diffusivity in the absence of the obstacle.

We describe the model as a continuous-time Markov process [19,20] $\{X(t) \in S : t \geqslant 0\}$ with $n = M - 1$ states, where M is the number of lattice sites. These states correspond to the relative displacement of the tagged agent (agent 1) from the obstacle (agent 2). For example, on a 3×3 lattice, $n = 8$, as shown in Fig. 1(b). Any transition can be achieved by the movement of agent 1 in a particular direction, or by the movement of agent 2 in the opposite direction. The probability $p_i(t)$ of being in state i at time t satisfies $\mathrm{d}\mathbf{p}/\mathrm{d}t = \mathbf{p}Q$ [19], where $\mathbf{p}(t) = (p_1(t), \ldots, p_n(t))$, and Q is the transition matrix with elements $q_{ij} = \lim_{\delta t \to 0}[P(X(t+\delta t) = j \mid X(t) = i)]/\delta t$ if $i \neq j$, and $q_{ij} = -\sum_{k \neq i} q_{ik}$ if $i = j$.

The diffusivity of agent 1, D, is given by the Nernst-Einstein equation [9,10], $D/D_0 = \lim_{\epsilon \to 0}(\mu(\epsilon)/\mu_0)$, where $\mu(\epsilon)$ is the mobility of agent 1 in the presence of a directional bias of strength ϵ, and $\mu_0 = P_1/2$ is the mobility of agent 1 in the presence of the same bias without obstacles [9,10]. The Nernst-Einstein equation applies to the diffusivity of agent 1 in the x and y directions separately. However, for a square lattice, these diffusivities are equal for our model, so we just deal with the x direction. A horizontal bias of strength ϵ means that agent 1 moves to the right/left with probabilities $(1 \pm \epsilon)/4$, and up/down with probability $1/4$ each. The movement of agent 2 is unbiased.

Transition rates are calculated including a horizontal bias, ϵ. If $i \to j$ corresponds to agent 1 moving to the right then $q_{ij} = P_1(1+\epsilon)/4 + P_2/4$. If $i \to j$ corresponds to agent 1 moving to

* Corresponding author.
E-mail address: matthew.simpson@qut.edu.au (M.J. Simpson).

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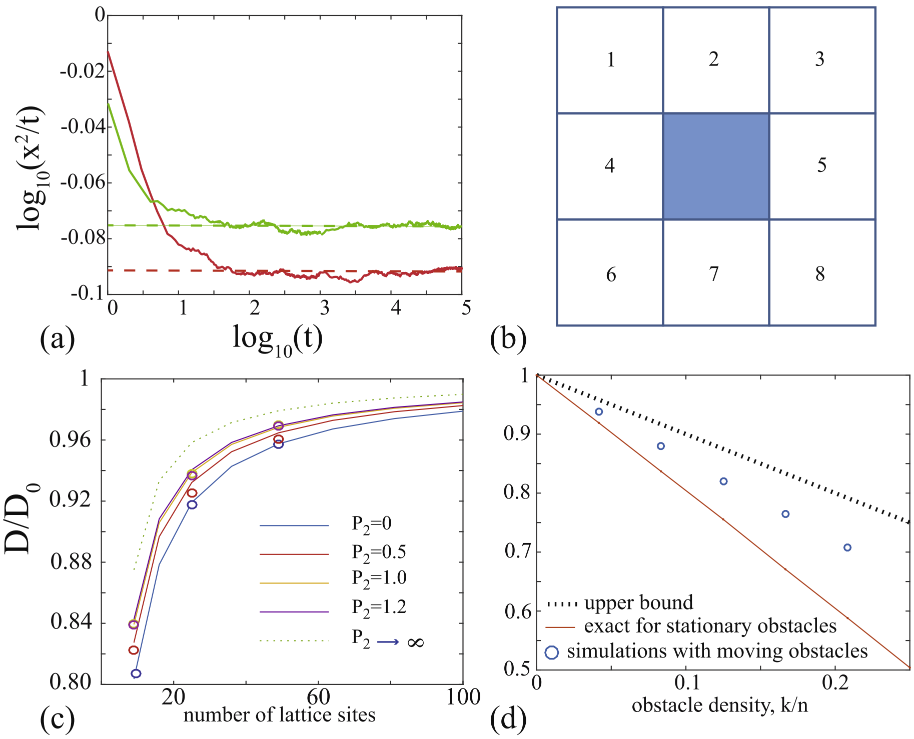

Fig. 1. (a) Stochastic simulation data on a 3×3 lattice for a tracer agent with a stationary (red, $P_1 = 1, P_2 = 0$) and moving (green, $P_1 = P_2 = 1$) obstacle. (b) State space for the Markov process in the 3×3 case showing the $n = 8$ states and the prohibited state (blue). (c) D/D_0 as a function of the number of lattice sites and P_2, exact (solid) and stochastic (circles) results. (d) D/D_0 as a function of obstacle density on a 5×5 lattice: simulations of moving obstacles with $P_2 = 1$ (circles), exact method for stationary obstacles, averaged over 10^5 random obstacle configurations (red line), and upper bound (black line). (For interpretation of the references to colour in this figure caption, the reader is referred to the web version of this article.)

the left then $q_{ij} = P_1(1-\epsilon)/4 + P_2/4$. If $i \to j$ corresponds to agent 1 moving up/down then $q_{ij} = (P_1 + P_2)/4$. All other transition rates are zero. By a suitable choice of timescale, we set $P_1 = 1$, and P_2 represents the movement rate of agent 2 relative to that of agent 1. An example showing the structure of Q is given in Supplementary Material.

The mobility is $\mu(\epsilon) = \mathbf{v} \cdot \mathbf{p}/\epsilon$, where $\mathbf{p}$ is the stationary distribution obtained by solving $\mathbf{p}Q = \mathbf{0}$, and $\mathbf{v}$ is a vector containing the drift velocity in each state. The drift velocity is $\epsilon/2$ in all states, except the two states in which the agent and obstacle are horizontally adjacent (states 4 and 5 in Fig. 1(b)). The drift velocity is $-(1-\epsilon)/4$ in state 4 and $(1+\epsilon)/4$ in state 5 (Supplementary Material). For arbitrary n, we denote these as states as l and r, for *left* and *right*. We simplify the problem by expressing Q, $\mathbf{p}$ and $\mathbf{v}$ as ϵ-independent and ϵ-dependent components [11,13], i.e. $Q = Q_0 + \epsilon Q_\epsilon$, leading to $D/D_0 = 2(\mathbf{v}_\epsilon . \mathbf{p}_0 + \mathbf{v}_0 . \mathbf{p}_\epsilon)$ for agent 1. In the unbiased case, the stationary distribution is uniform, $\mathbf{p}_0 = (1/n)[1, \ldots, 1]$, and the drift velocity $\mathbf{v}_0$ is zero for all states, except states r and l where $\mathbf{v}_0$ is $\pm 1/4$. The ϵ-dependent component $\mathbf{v}_\epsilon$ is 1/2 for all states, except states r and l where $\mathbf{v}_\epsilon$ is 1/4 (Supplementary Material). Calculating the two scalar products gives:

$$D/D_0 = (1 - 1/n) + (p_{\epsilon,r} - p_{\epsilon,l})/2, \tag{1}$$

where $\mathbf{p}_\epsilon$ is found by solving the linear system $\mathbf{p}_\epsilon Q_0 = -\mathbf{p}_0 Q_\epsilon$. To satisfy the constraint $\sum_{i=1}^{n} p_i = 1$, one column of Q must be replaced by a column of 1's. The two terms in parenthesis on the right in Eq. (1) provide a meaningful physical interpretation: $1 - 1/n$ is the proportion of unoccupied sites. Because agent 1 is biased to the right, agent 1 is more likely to be located to the left of agent 2, hence $p_{\epsilon,r} < p_{\epsilon,l}$, and $1 - 1/n$, is an upper bound for D/D_0.

Results in Fig. 1(c) show D/D_0 for agent 1. For this model D/D_0 increases with n and P_2, with good agreement between the exact and stochastic calculations. Fig. 1(c) confirms that D/D_0 approaches $1 - 1/n$, as P_2 increases. When P_2 is small, the stationary distribution is close to that for a stationary obstacle. In this case, the biased movement of agent 1 means it is more likely to be located to the left of agent 2 than to the right of agent 2, making the second term in Eq. (1) relatively large and negative. However, when P_2 is large, agent 2 moves very frequently. Because the movement of agent 2 is unbiased, its movements act to return the process towards a uniform distribution. Hence, agent 1 is almost equally likely to be located left or right of agent 2, and $p_{\epsilon,r} \approx p_{\epsilon,l}$.

While Eq. (1) applies for a single obstacle, the upper bound for D/D_0 extends to $1 - k/n$ in the case of k obstacles moving on a lattice with $n + 1$ sites [18]. If there are k obstacles on a lattice with $n + 1$ sites, $1 - k/n$ is an upper bound for D/D_0. To illustrate, we perform simulations with k obstacles, all moving at rate $P_2 = 1$, on a 5×5 lattice. Fig. 1(d) shows that D/D_0 for the tagged agent falls between D/D_0 for the same number of stationary obstacles and the upper bound. This is consistent with our observation that D/D_0 increases with P_2, and approaches $1 - k/n$ as P_2 is sufficiently large.

In summary, we present a simplified exact method to calculate the Fickian diffusivity of a tagged agent undergoing a random walk in the presence of an obstacle. The simplification relies on formulating the random walk as a Markov process [20] whose state space represents the relative displacement between the agent and obstacle. While it is standard to represent a random walk as a Markov process [20], our approach provides physical insight by reformulating the approach of Mercier and Slater [9,10] as a Markov process and taking advantage of the state space simplification when there is a single agent and a single obstacle. In principle, our approach applies to systems with arbitrary many obstacles, but is only tractable for one obstacle. Nevertheless, the structure of Eq. (1) provides physical insight into the role of obstacle motility since the exact result interpolates between the case where the obstacle is stationary and the upper bound when the obstacle moves sufficiently fast. Our results relate to previous observations about lattice-free models of Brownian motion [21]. The diffusivity of a tagged agent moving on a lattice increases with the movement rate of the obstacles, which is consistent with results from a lattice-free description [5,22]. When an infinitesimally small particle diffuses in a lattice-free model, the effect of the obstacles vanishes in the limit where their movement rate becomes arbitrarily large [22]. However, in a lattice-based model, the tagged agent always has a finite size, equal to one lattice spacing. In this case, our results show that obstacles always reduce the tagged agent diffusivity even in the limit $P_2 \to \infty$.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.rinp.2017.08.063.

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