

BIASED RANDOM WALKS, PARTIAL DIFFERENTIAL EQUATIONS AND UPDATE SCHEMES

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Abstract

There is much interest within the mathematical biology and statistical physics community in converting stochastic agent-based models for random walkers into a partial differential equation description for the average agent density. Here a collection of noninteracting biased random walkers on a one-dimensional lattice is considered. The usual master equation approach requires that two continuum limits, involving three parameters, namely step length, time step and the random walk bias, approach zero in a specific way. We are interested in the case where the two limits are not consistent. New results are obtained using a Fokker–Planck equation and the results are highly dependent on the simulation update schemes. The theoretical results are confirmed with examples. These findings provide insight into the importance of updating schemes to an accurate macroscopic description of stochastic local movement rules in agent-based models when the lattice spacing represents a physical object such as cell diameter.

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1. Introduction

Lattice-based random walks conducted by noninteracting and interacting agents are used to simulate many processes in the physical and biological sciences. Recently there has been much interest in converting stochastic agent-based models of local movement into a partial differential equation (PDE) description for the average agent density or occupancy as a continuous function using various mean-field treatments [1, 7, 17, 18, 22, 23, 26, 27]. A common approach is to consider the change of occupancy at each lattice site over discrete time steps or in continuous time, in terms of a master equation. Appropriate continuum limits are then taken. For unbiased random walkers (a symmetric random walk process), there is only one limit that is needed. However, for biased random walkers (an asymmetric random walk process),

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there are two limits which need to be made consistent. The only way to do this is to make an assumption about the size of the random walk bias [6, 10].

We are interested in the case in which the two limits are not consistent. New results are obtained for random walkers on a one-dimensional lattice using an alternative approach in terms of a Fokker–Planck equation. Simulation results for noninteracting agents moving on lattices are dependent on the simulation update schemes. We compare the effect of two common updating schemes on the expected evolution of a collection of noninteracting agents. For discrete-time processes, there are several ways of progressing m random walkers from one time n to the next. The updating of the m agents can be done synchronously or asynchronously to obtain the state of the system at time $n + 1$. When we refer to the updating of an individual agent, we refer to allowing that agent to hop left, hop right, or not move, depending on the associated hopping probabilities. The choice of updating schemes affects the simulation results.

Two update schemes are considered: the synchronous update scheme, and the most common type of asynchronous updating, namely the random sequential update scheme. Consider a system of m agents. In the synchronous update (SU) scheme, at each discrete time step all m agents within the system are updated at the same time, and therefore only once each time step. This scheme is associated with the classic discrete-time random walk, as each agent is conducting a discrete-time random walk independent of the other agents. In the random sequential update (RSU) scheme, at each time step, m sequential independent random choices of an agent are made, and each agent is immediately updated upon selection [5]. Of course, sometimes a particular agent will be selected for updating more than once, or not at all, in a given time step. However, on average, the number of times a given agent is chosen per time step will be unity. The RSU scheme is the discrete-time analogue of a continuous time process [20]. It is commonly used in many biological contexts where no more than one random walker can occupy a site (called an exclusion process) [7, 9, 14].

Since the choice of updating scheme affects simulation outcomes, the average behaviour of the system and the associated PDEs are expected to be different for the SU and RSU schemes. We explore these issues in the context of a general biased random walk, where the left and right hopping probabilities may depend on the location of agents and time. Two PDE descriptions are obtained through the Fokker–Planck formalism.

2. Noninteracting random walkers

Consider an infinite one-dimensional lattice with lattice spacing Δ . Let $i \in \mathbb{Z}$ denote the number of the lattice site, so that the position of an agent at site i is given by $x = i\Delta$. Let $n \in \mathbb{N}$ denote the n th time step and τ the duration of each time step, so that $t = n\tau$. Nonconstant time steps can be utilised and are discussed in Section 6.

Consider a fixed number of agents on the lattice. When chosen, the agents can move distance Δ (a single lattice site, left or right) in time step τ , according to hopping probabilities. The agent movements are independent of each other. This means that the number of agents of any particular lattice site is unconstrained.

Let $p_n^L(i)$ and $p_n^R(i)$ denote the left and right hopping probabilities for an agent at site i into the nearest neighbour sites ($i - 1$ or $i + 1$, respectively). Hence, $p_n^L(i)$ ($p_n^R(i)$) is the probability that an agent (selected to be updated) will move left (right) a distance Δ within time τ , given that the agent is at site i at the n th time step. These probabilities may be dependent on both the agent's current site i and on the time step n at which the update occurs. For simple random walks these probabilities are typically constant and sum to unity. Here we allow more generality and provide examples later. We note that allowing for generality with respect to the time step for hopping probabilities is uncommon for discrete-time random walks, especially when attempting to derive an approximating PDE. One of our examples provides a natural demonstration of a time-dependent random walk, and how a PDE can be derived which gives an accurate approximation of the random walk.

The motility parameter $p_n^L(i) + p_n^R(i)$ is the probability that an agent (selected to be updated) will move a distance Δ within time τ , given that the agent is at site i at the n th time step. For example, in cell migration simulations, a lattice spacing Δ typically represents a cell diameter [9, 14]. If $p_n^L(i) + p_n^R(i) = 1$ then, on average, the cell/agent is certain to move (one lattice space) each time step. Without loss of generality, it is usual to perform dimensionless simulations setting $\Delta = \tau = 1$ [3, 4, 18].

To describe the evolution of agents, we consider the expected occupancy of a site. Define the random variable $\gamma_n(i)$ to be the number of agents on site i at the n th time step. The expected occupancy of a site i at time step n is denoted by

$$C_n(i) = \mathbb{E}[\gamma_n(i)].$$

We are interested in the evolution of $C_n(i)$. To this end, we transform to continuous variables according to $i \mapsto x/\Delta$, $n \mapsto t/\tau$ and $C_n(i) \mapsto C(x, t)$. In addition, the hopping probabilities transform as $p_n^L(i) \mapsto p^L(x, t)$ and $p_n^R(i) \mapsto p^R(x, t)$. We develop a PDE for the average occupancy $C(x, t)$ which approximates $C_n(i)$ for given Δ and τ . This setup is highly versatile, and can be used to approximate random walkers updating with either the SU or RSU schemes.

3. Discrete-time master equation approach

The usual method for producing a PDE describing the movement of agents in a discrete-time process is the discrete-time master equation approach [8, 15, 18, 22, 23]. The change in the expected occupancy $C_n(i)$ at each site i from time step n to time step $n + 1$ can be expressed as

$$C_{n+1}(i) - C_n(i) = p_n^L(i+1)C_n(i+1) + p_n^R(i-1)C_n(i-1) - [p_n^L(i) + p_n^R(i)]C_n(i). \quad (3.1)$$

The first two terms on the right-hand side account for agents moving into site i , while the last term accounts for agents leaving the site. This master equation implicitly assumes that agents move only once (or on average move only once) per time step. Equation (3.1) can be converted into a PDE by taking the continuum limits of the lattice

spacing Δ and the size of the intervals between consecutive time steps τ (assuming them to be constant). Transforming to continuous variables and performing Taylor expansions about x and t , we obtain

$$\begin{aligned} \frac{\partial C}{\partial t} &= -\frac{\Delta}{\tau} [(p^R(x, t) - p^L(x, t))C(x, t)] \\ &\quad + \frac{\Delta^2}{2\tau} \frac{\partial^2}{\partial x^2} [(p^R(x, t) + p^L(x, t))C(x, t)] + O(\Delta^3/\tau, \tau). \end{aligned}$$

Taking the typical limits of $\Delta, \tau \rightarrow 0$, the following advection–diffusion PDE is obtained:

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} [V(x, t)C(x, t)] + \frac{1}{2} \frac{\partial^2}{\partial x^2} [D(x, t)C(x, t)], \quad (3.2)$$

where

$$V(x, t) = \lim_{\Delta, \tau \rightarrow 0} \frac{\Delta}{\tau} (p^R(x, t) - p^L(x, t)), \quad (3.3)$$

$$D(x, t) = \lim_{\Delta, \tau \rightarrow 0} \frac{\Delta^2}{\tau} (p^R(x, t) + p^L(x, t)). \quad (3.4)$$

For the above limits to formally exist, we require the expression $p^R(x, t) - p^L(x, t)$ to be $O(\Delta)$ [6, 10].

We are interested in whether the PDE (3.2) provides a good approximation to averaged noninteracting random walk simulation data. The coefficients in (3.2) are obtained by a limiting process $\Delta, \tau \rightarrow 0$ and require $p^R - p^L = O(\Delta)$ for consistency, whereas simulation data typically has $\Delta = \tau = 1$ as discussed, while the bias parameter may be $p^R - p^L = O(1)$. To this end, we introduce a different approach.

4. The Fokker–Planck equation

The Fokker–Planck equation is a PDE that describes the evolution of the transition density function for some diffusion process $\{X(t)\}_{t \geq 0}$ with time [12, 24, 25]. In addition, it describes the evolution of a continuous concentration of independent stochastically evolving particles from some initial condition, where each particle evolves according to the diffusion $\{X(t)\}_{t \geq 0}$ [2, 12]. The concentration of these particles, $C(x, t)$, evolves as

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} [\mu(x, t)C(x, t)] + \frac{\partial^2}{\partial x^2} \left[\frac{1}{2} \sigma^2(x, t)C(x, t) \right], \quad (4.1)$$

where $\mu(x, t)$ and $\sigma^2(x, t)$ are termed the infinitesimal mean and infinitesimal variance, respectively, of the stochastic process $X(t)$, defined by

$$\mu(x, t) = \lim_{h \rightarrow 0} \frac{1}{h} \mathbb{E}[X(t+h) - X(t) \mid X(t) = x], \quad (4.2)$$

$$\sigma^2(x, t) = \lim_{h \rightarrow 0} \frac{1}{h} \mathbb{E}[(X(t+h) - X(t))^2 \mid X(t) = x]. \quad (4.3)$$

The functions μ and σ^2 are often called the drift coefficient and diffusivity coefficient, respectively [12, 24].

It is well known that diffusion processes often prove to be accurate approximations of discrete processes. Karlin and Taylor [12] outline means of determining when discrete processes are accurately approximated by diffusions, and provide examples of such processes, such as the Wright–Fisher process. Here we utilise diffusion processes to approximate the expected evolution of a collection of random walkers.

5. The Fokker–Planck equation and random walks

Let the discrete stochastic process $\{X_n^{(\Delta)}\}_{n \geq 0}$ give the continuum position of an individual agent conducting a random walk with hopping probabilities given by $p_n^L(i)$ and $p_n^R(i)$, using the SU scheme. As such, $X_n^{(\Delta)} = \Delta X_n$, where X_n is the lattice site occupied by the agent at the n th time step. Following a similar approach to Karlin and Taylor [12], we determine a diffusion that approximates the interpolated process $\{X^{(\Delta)}(t)\}_{t \geq 0}$, where $X^{(\Delta)}(t) = X_{\lfloor t/\tau \rfloor}^{(\Delta)}$, with τ the time step length (this can be generalized to nonconstant time steps).

This is achieved by deriving expressions analogous to equations (4.2)–(4.3) by using the mean and second moment of the displacement of the random walker over one time step. These expressions are then substituted into the Fokker–Planck equation to produce a PDE that gives an approximation for the expected evolution of a collection of noninteracting random walkers (using the SU scheme). Specifically, we express μ and σ^2 as follows:

$$\begin{aligned} \mu &= \frac{1}{\tau} \mathbb{E}[X_{n+1}^{(\Delta)} - X_n^{(\Delta)} \mid X_n^{(\Delta)} = \Delta i] = V_{\Delta, \tau} \mathbb{E}[X_{n+1} - X_n \mid X_n = i] \\ &= V_{\Delta, \tau} (p_n^R(i) - p_n^L(i)), \end{aligned} \quad (5.1)$$

$$\begin{aligned} \sigma^2 &= \frac{1}{\tau} \mathbb{E}[(X_{n+1}^{(\Delta)} - X_n^{(\Delta)})^2 \mid X_n^{(\Delta)} = \Delta i] = D_{\Delta, \tau} \mathbb{E}[(X_{n+1} - X_n)^2 \mid X_n = i] \\ &= D_{\Delta, \tau} (p_n^R(i) + p_n^L(i)), \end{aligned} \quad (5.2)$$

where

$$V_{\Delta, \tau} = \frac{\Delta}{\tau}, \quad D_{\Delta, \tau} = \frac{\Delta^2}{\tau}. \quad (5.3)$$

As for the discrete-time master equation approach, we move to continuous variables x and t and continuous functions $p^R(x, t)$ and $p^L(x, t)$. The Fokker–Planck formalism requires us to take the limits as $\Delta \rightarrow 0$ and $\tau \rightarrow 0$. This gives

$$\mu(x, t) = \lim_{\Delta, \tau \rightarrow 0} V_{\Delta, \tau} (p^R(x, t) - p^L(x, t)), \quad (5.4)$$

$$\sigma^2(x, t) = \lim_{\Delta, \tau \rightarrow 0} D_{\Delta, \tau} (p^R(x, t) + p^L(x, t)). \quad (5.5)$$

Note that substituting equations (5.4)–(5.5) into the Fokker–Planck equation (4.1) gives the same PDE derived via the discrete-time master equation approach,

equation (3.2). Again, for the above limits to formally exist, we require the expression $p^R(x, t) - p^L(x, t)$ to be $O(\Delta)$.

The Fokker–Planck approach and the discrete-time master equation approach focus on a discrete process approaching a continuous process via the limits $\Delta, \tau \rightarrow 0$. However, in the discrete simulation, agents perform random moves to the nearest neighbour sites with spacing Δ at discrete time steps τ . Much current research focuses on deriving PDEs that provide an accurate approximation of the evolution of expected site occupancy for random walks, typically for $\Delta = 1$ and $\tau = 1$ [8, 15, 18, 22, 23], and where the bias $p^R(x, t) - p^L(x, t)$ may be $O(1)$. We ask: does equation (3.2) give the best PDE in these situations? As highlighted by Hywood and Landman [11], this does not appear to be the case. In the following arguments we outline a potentially more useful PDE for these particular circumstances.

The issue is not with the expression used for the infinitesimal mean, but with the expression used for the infinitesimal variance. Kimura [13], in considering the evolution of a gene frequency Z_n within a population, determined that when using the Fokker–Planck equation it was more natural to use the variance of $Z_{n+1} - Z_n$ rather than the second moment as is normally the case for the Fokker–Planck equation. Lange [16] also alluded to this approach to approximating discrete processes. The idea holds true for deriving PDEs to describe the evolution of the expected site occupancy for random walkers on a lattice. We continue by outlining why this is the case.

Firstly we note that for a diffusion process $\{X(t)\}_{t \geq 0}$,

$$\begin{aligned} \text{Var}(X(t+h) - X(t) \mid X(t) = x) \\ = \mathbb{E}[(X(t+h) - X(t))^2 \mid X(t) = x] - (\mathbb{E}[X(t+h) - X(t) \mid X(t) = x])^2, \end{aligned}$$

and since $(\mathbb{E}[X(t+h) - X(t) \mid X(t) = x])^2 = o(h)$ for a diffusion process, we must have

$$\begin{aligned} \lim_{h \rightarrow 0} \frac{1}{h} \text{Var}(X(t+h) - X(t) \mid X(t) = x) &= \lim_{h \rightarrow 0} \frac{1}{h} \mathbb{E}[(X(t+h) - X(t))^2 \mid X(t) = x] \\ &= \sigma^2(x, t). \end{aligned} \tag{5.6}$$

If we want the diffusion $X(t)$ to approximate the interpolated discrete process $X_{\lfloor t/\tau \rfloor}^{(\Delta)}$, with small time steps τ , we want

$$\text{Var}(X(t+\tau) - X(t) \mid X(t) = x) \approx \text{Var}(X_{n+1}^{(\Delta)} - X_n^{(\Delta)} \mid X_n^{(\Delta)} = \Delta i).$$

This suggests that

$$\sigma^2(x, t) \approx \frac{1}{\tau} \text{Var}(X_{n+1}^{(\Delta)} - X_n^{(\Delta)} \mid X_n^{(\Delta)} = \Delta i).$$

However, the equivalence demonstrated in equation (5.6) will not necessarily hold when considering the analogous expressions for discrete processes such as the random walks considered here. Let us consider a set of random walkers which update with the

SU scheme. It is easy to see that

$$\begin{aligned}\mathbb{E}[X_{n+1}^{(\Delta)} - X_n^{(\Delta)} | X_n^{(\Delta)} = \Delta i] &= \Delta(p_n^R(i) - p_n^L(i)), \\ \mathbb{E}[(X_{n+1}^{(\Delta)} - X_n^{(\Delta)})^2 | X_n^{(\Delta)} = \Delta i] &= \Delta^2(p_n^R(i) + p_n^L(i)).\end{aligned}$$

If, as previously stated, we have $p_n^R(i) - p_n^L(i) = O(\Delta)$, then $(\mathbb{E}[X_{n+1}^{(\Delta)} - X_n^{(\Delta)} | X_n^{(\Delta)} = \Delta i])^2$ is of smaller order than $\mathbb{E}[(X_{n+1}^{(\Delta)} - X_n^{(\Delta)})^2 | X_n^{(\Delta)} = \Delta i]$. So in this case, for small Δ we have $\text{Var}(X_{n+1}^{(\Delta)} - X_n^{(\Delta)} | X_n^{(\Delta)} = \Delta i) \approx \mathbb{E}[(X_{n+1}^{(\Delta)} - X_n^{(\Delta)})^2 | X_n^{(\Delta)} = \Delta i]$. In this circumstance, it would be natural to set σ^2 as in equation (5.2), which when converting to continuous variables and functions gives equation (5.5).

However, if $p_n^R(i) - p_n^L(i) = O(1)$ then $(\mathbb{E}[X_{n+1}^{(\Delta)} - X_n^{(\Delta)} | X_n^{(\Delta)} = \Delta i])^2$ is instead the same order as $\mathbb{E}[(X_{n+1}^{(\Delta)} - X_n^{(\Delta)})^2 | X_n^{(\Delta)} = \Delta i]$. Then, even for small Δ , the approximation $\text{Var}(X_{n+1}^{(\Delta)} - X_n^{(\Delta)} | X_n^{(\Delta)} = \Delta i) \approx \mathbb{E}[(X_{n+1}^{(\Delta)} - X_n^{(\Delta)})^2 | X_n^{(\Delta)} = \Delta i]$ does not necessarily hold. We suggest that in these circumstances it is more natural to use μ as in equation (5.1) and replace equation (5.2) with

$$\sigma^2 = \frac{1}{\tau} \text{Var}(X_{n+1}^{(\Delta)} - X_n^{(\Delta)} | X_n^{(\Delta)} = \Delta i) = D_{\Delta, \tau} \text{Var}(X_{n+1} - X_n | X_n = i), \quad (5.7)$$

with $V_{\Delta, \tau}$ and $D_{\Delta, \tau}$ defined as in (5.3). Moving to continuous variables and functions we get the following expressions:

$$\mu_{\text{SU}}(x, t) = V_{\Delta, \tau}(p^R(x, t) - p^L(x, t)), \quad (5.8)$$

$$\sigma_{\text{SU}}^2(x, t) = D_{\Delta, \tau}(p^R(x, t) + p^L(x, t) - (p^R(x, t) - p^L(x, t))^2), \quad (5.9)$$

where the subscript SU indicates that the random walk updates using the SU scheme.

We note that equations (5.8)–(5.9) do not contain the limits $\Delta, \tau \rightarrow 0$. The examples in Section 6 demonstrate that substitution of the expressions in equations (5.8)–(5.9) into the Fokker–Planck equation (4.1) gives extremely accurate approximations of the expected evolution of collections of discrete random walkers. It should be noted that our arguments still require that Δ and τ are not too large, compared to unity, and that in fact the equations that are produced improve in accuracy as Δ and τ decrease.

The above reasoning also holds when considering the RSU scheme. An identical approach of analysing the expectation and variance of the displacement of individual random walkers can be used to produce expressions for equations (5.1) and (5.7), which, when substituted into the Fokker–Planck equation, give a PDE that is very accurate at approximating the expected evolution of a collection of random walkers updating using the RSU scheme. When moving to continuous variables and functions for the RSU scheme, equations (5.1) and (5.7) become

$$\mu_{\text{RSU}}(x, t) = V_{\Delta, \tau}(p^R(x, t) - p^L(x, t)), \quad (5.10)$$

$$\sigma_{\text{RSU}}^2(x, t) = D_{\Delta, \tau}(p^R(x, t) + p^L(x, t)), \quad (5.11)$$

where the subscript RSU indicates that the random walk updates using the RSU scheme. The proofs of how the expressions in equations (5.8)–(5.9) and equations (5.10)–(5.11) are produced are provided in [Appendix A](#).

When comparing the infinitesimal mean and variance for the SU and RSU schemes in equations (5.8)–(5.9) and equations (5.10)–(5.11), several interesting properties are apparent. Both schemes have the same drift coefficient: it is of course nonzero only when the process is biased. In contrast, the diffusive term may differ between the two schemes. For a biased process, the infinitesimal variance for the RSU scheme is (always) larger than for the SU scheme. This makes sense since in the RSU scheme there is a chance that the leading agent is chosen to move more than once during a single time step. This can potentially cause a larger spread of the agent population for a given simulation. This capacity for a larger spread of agents implies that an approximating diffusion for the RSU scheme would have a larger infinitesimal variance. Indeed, these properties will be observed in the examples provided. For a symmetric process, $\mu(x, t) \equiv 0$ and the diffusive terms are identical for both update schemes, namely $\sigma^2(x, t) = D_{\Delta, \tau}(p^R(x, t) + p^L(x, t))$. Therefore, for a symmetric process, the average behaviour of the stochastic process is independent of the type of update scheme. We next compare simulation data and solutions to the Fokker–Planck equations for different update schemes.

It is important to appreciate the difference between these two cases and the well-known result obtained with the discrete-time master equation approach. The Fokker–Planck approach using the RSU scheme produces the same PDE as the discrete-time master equation approach if the strict limits for V and D in (3.3)–(3.4) are replaced by (5.10)–(5.11). Furthermore, when $p^R(x, t) - p^L(x, t) = O(\Delta)$ as $\Delta \rightarrow 0$, as is strictly required in the continuum limit for the master equation approach, $\sigma_{\text{SU}}^2(x, t) = \sigma_{\text{RSU}}^2(x, t)$. However, our interest arises for the case when agents are moving on a lattice where $\Delta = O(1)$. We show through examples that there can be large discrepancies between the two variances given by (5.9) and (5.11).

6. Examples

Data from averaged simulations are compared with solutions of equation (4.1). Each lattice site between $M_l \leq x \leq M_r$ (for some chosen M_l and M_r) is initially occupied by a single agent, while the remaining lattice sites are empty. Simulations are performed and averaged over a number of simulations. The PDEs are solved using Matlab's *pdepe*.

Our first example of a biased random walk has constant left and right hopping probabilities p^L and p^R . [Figure 1](#) shows expected site occupancy $C(x, t)$ profiles in space at different times. The average simulation results are well approximated by the solution to the PDE for both the SU and RSU cases. In particular, we observe that the RSU scheme is slightly more spread out (albeit difficult to see here, but easily apparent in [Figures 2 and 3](#)), but the solution to the Fokker–Planck equation approximates well the leading edges of the simulation results. The (blue) simulation

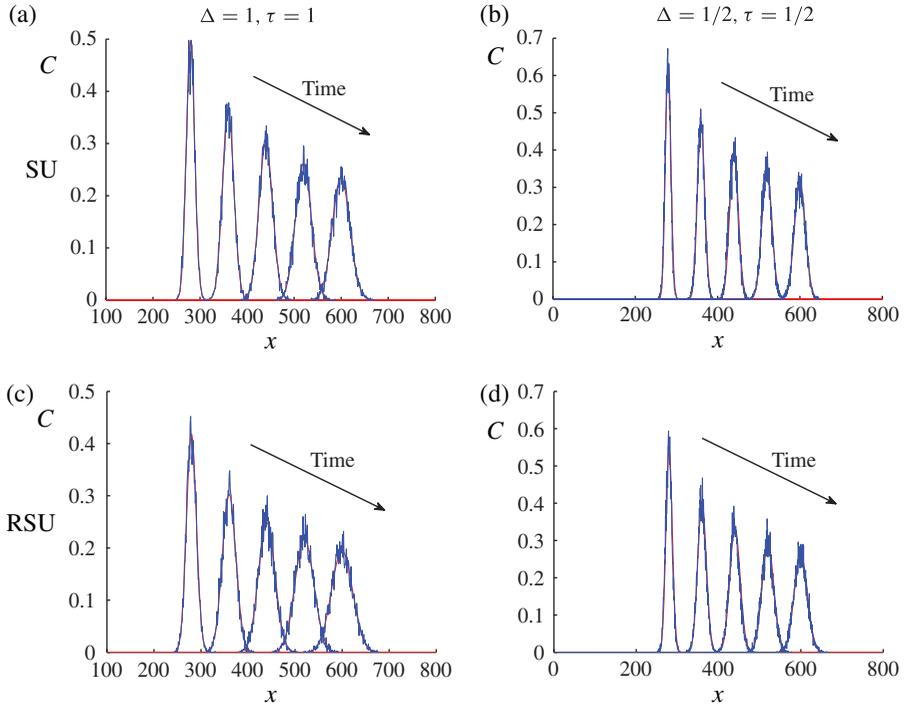


FIGURE 1. Expected occupancy $C(x, t)$ versus position x at different times t using the SU scheme (top row) and RSU scheme (bottom row). Simulation results averaged over 500 realisations (blue curve) and PDE solution profiles (equation (4.1) with equations (5.8)–(5.9) and equation (4.1) with equations (5.10)–(5.11) for SU and RSU schemes) (red curve) for $t = 200, 400, 600, 800, 1000$. Here $p^R = 0.45$ and $p^L = 0.05$. The initial distribution of agents has all sites with $195 \leq x \leq 205$ completely occupied. In (a,c) $\Delta = 1$ and $\tau = 1$. In (b,d) $\Delta = 1/2$ and $\tau = 1/2$. Note the different vertical and horizontal axis scales. (Colour available online.)

results have oscillations, because they are averaged over a relatively small number of individual realisations. If the number of realisations increases, the oscillations decrease in amplitude.

The next examples arise from a reinterpretation of a discrete model for a growing biological tissue [3, 4, 11]. They demonstrate the robustness of the Fokker–Planck approach for the case where the hopping probabilities depend on both space and time. They also provide a simple means of introducing time dependence into random walks and how this time dependence can be incorporated into approximating PDEs.

Let $L(t)$ be some specified increasing continuous function. This defines a lattice site number $N(t) = \lfloor L(t)/\Delta \rfloor$. If n is the number of time steps that have occurred, then the transformation $n \mapsto N(t) - N(0)$ is made when moving to the continuous framework. For ease of notation we write $M(t) = N(t) - N(0)$. We consider a collection of random walkers that initially can only occupy lattice sites i such that $0 < i < N(0)$. Let the

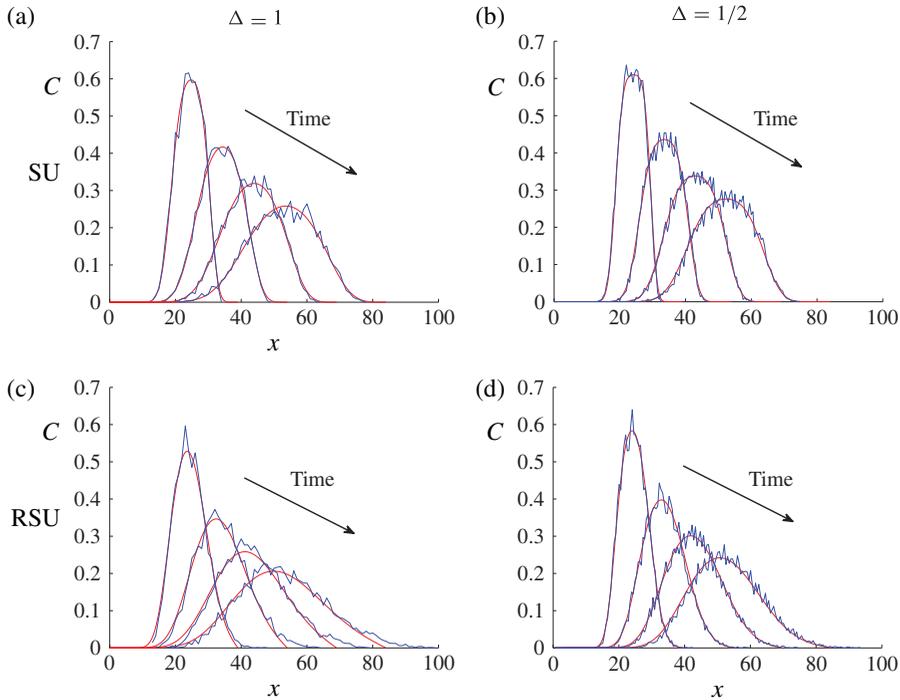


FIGURE 2. Expected occupancy $C(x, t)$ versus position x at different times t using the SU scheme (top row) and RSU scheme (bottom row). Simulation results averaged over 1000 realisations (blue curve) and PDE solution profiles (equation (4.1) with equations (5.8)–(5.9) and equation (4.1) with equations (5.10)–(5.11) for SU and RSU schemes) (red curve) for $t = 15, 30, 45, 60$. The hopping probabilities are given by (6.1) with $L(t) = 24 + t$. The initial distribution of agents has all sites with $12 \leq x \leq 18$ completely occupied. In (a,c) $\Delta = 1$. In (b,d) $\Delta = 1/2$. Here the time step interval is a constant, namely $\tau = \Delta$. (Colour available online.)

hopping probabilities be

$$p_n^L(i) = 0, \quad p_n^R(i) = \min\{i/(N(0) + n), 1\}. \quad (6.1)$$

This is an example of a totally asymmetric random walk.

Now, rather than have τ being a fixed constant, we allow τ to change with the number of steps. Let T_j be the time at which the j th time step occurs. Then $T_j = \min\{t : M(t) = j\}$. Now let τ_j be the value of the time interval between the j th and $(j + 1)$ th time steps, that is, $\tau_j = T_{j+1} - T_j$. From the definitions of $M(t)$ and τ_j , it is clear that $\tau_{M(t)}$ gives the time step length that includes the time with value t .

It is worth noting that the time step interval $\tau_{M(t)}$ is dependent on $L(t)$ and Δ . Furthermore, as $\Delta \rightarrow 0$, we also have $\tau_{M(t)} \rightarrow 0$ for all t . Therefore, while the length of each time step may vary (for example, decrease as time increases), the potential number of moves remains equal to the number of agents m in the system.

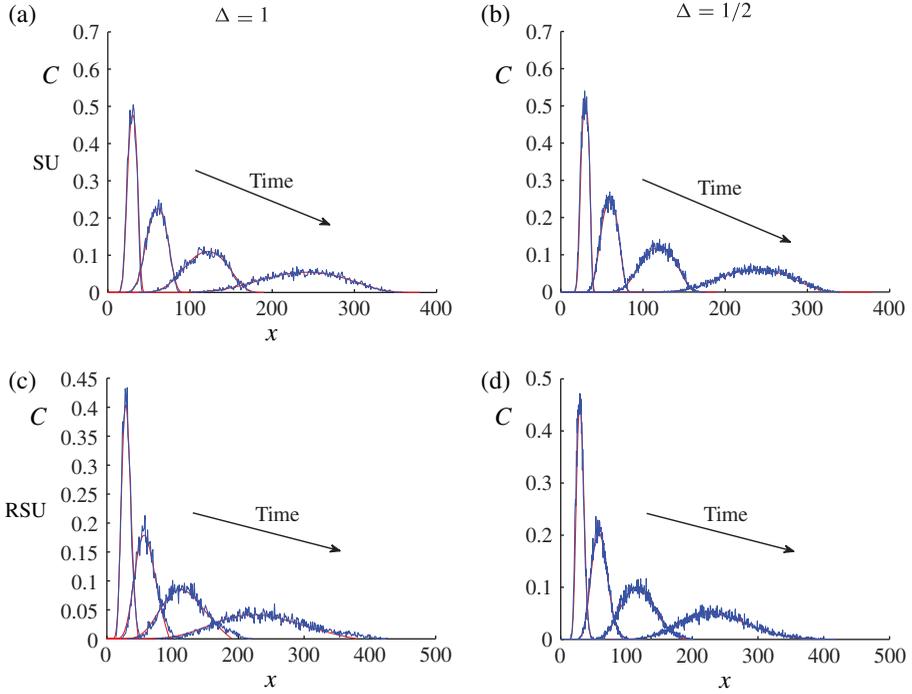


FIGURE 3. Expected occupancy $C(x, t)$ versus position x at different times t using the SU scheme (top row) and RSU scheme (bottom row). Simulation results averaged over 1000 realisations (blue curve) and PDE solution profiles (equation (4.1) with equations (5.8)–(5.9) and equation (4.1) with equations (5.10)–(5.11) for SU and RSU schemes) (red curve) for $t = 1, 2, 3, 4$. The hopping probabilities are given by (6.1) with $L(t) = 24e^{0.69t}$. The initial distribution of agents has all sites with $12 \leq x \leq 18$ completely occupied. In (a,c) $\Delta = 1$. In (b,d) $\Delta = 1/2$. Here the time step interval decreases as t increases. Note the different vertical and horizontal axis scales. (Colour available online.)

For this example, for small enough Δ , the coefficients in (5.3) can be rewritten as the approximations [11]

$$V_{\Delta, \tau} = \frac{\Delta}{\tau_{M(t)}} \approx L'(t), \quad D_{\Delta, \tau} = \frac{\Delta^2}{\tau_{M(t)}} \approx L'(t)\Delta, \quad (6.2)$$

where $L'(t)$ is the time derivative of $L(t)$. Moving to the continuous variables x and t and using the approximation $\Delta N(t) \approx L(t)$ together with (6.2), the drift and diffusivity terms in the Fokker–Planck formulation (equations (5.8)–(5.11)) can be expressed as

$$\begin{aligned} \mu_{\text{SU}}(x, t) &= L'(t) \frac{x}{L(t)}, & \sigma_{\text{SU}}^2(x, t) &= \Delta L'(t) \frac{x}{L(t)} \left(1 - \frac{x}{L(t)}\right), \\ \mu_{\text{RSU}}(x, t) &= L'(t) \frac{x}{L(t)}, & \sigma_{\text{RSU}}^2(x, t) &= \Delta L'(t) \frac{x}{L(t)}, \end{aligned}$$

for the SU and RSU schemes, respectively.

We consider two choices of the function $L(t)$, linear and exponential, and two values of Δ , illustrated in Figures 2 and 3, respectively. The PDE solutions approximate the averaged simulation results very well. In these two figures, it is easy to see that, as expected, the spread of agents is larger for the RSU case at each time. It is most apparent for the last illustrated time.

Relatively large values of Δ (values 1/2, 1) have been used in these examples. With smaller values, the accuracy of the PDE description is even greater. Of course, as Δ is decreased to zero, the diffusive terms become negligible and the PDE is a pure convective equation, as expected. However, for spatially dependent probabilities the convective component contributes two terms through the product rule, namely a transport term and a kinetic (dilution) term. This occurs because the tracked mass in the growing tissue is conserved.

7. Conclusions

We compare the usual discrete-time master equation approach with an alternative framework for establishing an approximating PDE description for a population of biased random walkers. The Fokker–Planck approach is used to derive PDEs to approximate simulation data where either a synchronous or an asynchronous update scheme is implemented. The PDEs are different if the random walk is biased (asymmetric). For unbiased (symmetric) random walks, the update scheme does not influence the average behaviour and the PDEs are identical. By contrast, the discrete-time master equation approach produces the PDE appropriate only to the RSU scheme, and overestimates the diffusivity if the SU scheme is used. The accuracy of the PDE descriptions has been demonstrated with several examples. While only walks on a one-dimensional lattice have been considered here, this approach can be extended to higher dimensions.

This work highlights the influence of updating schemes when using stochastic random walkers in real world applications. In order to deduce population-level behaviour, the appropriate PDE description is affected by the type of simulation updating scheme, as well as by the local probabilistic movement rules. These considerations are important to the expanding field of agent-based models, applied to traffic flow, pedestrian flow and biological cell migration. In particular, this study reconciles the discrepancy between two different continuum representations of a discretely growing lattice used in modelling biological tissue growth, where the lattice spacing represents cell diameter [3, 11].

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Appendix A. Proofs of equations (5.8)–(5.11)

Let m be the number of agents in the system. For ease we simplify the notation introduced in Section 5 and define $\Delta Y_n(i)$ to be the random variable for the displacement of an agent over one time step, where i denotes the lattice site number and n denotes the n th time step.

A.1. SU scheme Each agent is given the opportunity to move exactly once per time step, so each will be updated exactly once at each time step. Then $\mathbb{P}(Y_n(i) = 1) = p_n^R(i)$, $\mathbb{P}(Y_n(i) = -1) = p_n^L(i)$ and $\mathbb{P}(Y_n(i) = 0) = 1 - p_n^L(i) - p_n^R(i)$. Transforming to continuous variables in the usual way, it is easy to verify that

$$\begin{aligned}\mathbb{E}[\Delta Y(x, t)] &= \Delta[p^R(x, t) - p^L(x, t)], \\ \mathbb{E}[(\Delta Y(x, t))^2] &= \Delta^2[p^R(x, t) + p^L(x, t)], \\ \text{Var}(\Delta Y(x, t)) &= \Delta^2[(p^R(x, t) + p^L(x, t)) - (p^R(x, t) - p^L(x, t))^2].\end{aligned}$$

Thus, for sufficiently small Δ and τ , the coefficients in the Fokker–Planck equation are given by

$$\begin{aligned}\mu(x, t) &= \frac{1}{\tau} \mathbb{E}[\Delta Y(x, t)] = V_{\Delta, \tau}(p^R(x, t) - p^L(x, t)), \\ \sigma^2(x, t) &= \frac{1}{\tau} \text{Var}(\Delta Y(x, t)) = D_{\Delta, \tau}[(p^R(x, t) + p^L(x, t)) - (p^R(x, t) - p^L(x, t))^2],\end{aligned}$$

where $V_{\Delta, \tau}$ and $D_{\Delta, \tau}$ are given by (5.3).

A.2. RSU scheme Now m random choices of agents are given an opportunity to move at each time step. Therefore, any particular agent may be updated more than once, or not at all, at some time steps. We write $Y_n(i) = \sum_{k=0}^Z J_k(i, n)$, where: (i) Z is a random variable giving the number of times that the considered agent is selected to update, so that $Z \stackrel{d}{=} \text{Binomial}(m, 1/m)$; and (ii) $J_k(i, n) = -1, 0, 1$ are the random variables indicating the displacement of the agent at the k th update.

Since $J_k(i, n)$ may be dependent on position, the random variables $J_k(i, n)$ may not be independent. Specifically, we have the following conditional distribution for $J_k(i, n)$:

$$\begin{aligned}\mathbb{P}(J_k(i, n) = 1 \mid J_1(i, n), J_2(i, n), \dots, J_{k-1}(i, n)) &= p_n^R(i + J_1(i, n) + J_2(i, n) + \dots + J_{k-1}(i, n)), \\ \mathbb{P}(J_k(i, n) = -1 \mid J_1(i, n), J_2(i, n), \dots, J_{k-1}(i, n)) &= p_n^L(i + J_1(i, n) + J_2(i, n) + \dots + J_{k-1}(i, n)), \\ \mathbb{P}(J_k(i, n) = 0 \mid J_1(i, n), J_2(i, n), \dots, J_{k-1}(i, n)) &= 1 - p_n^L(i + J_1(i, n) + J_2(i, n) + \dots + J_{k-1}(i, n)) \\ &\quad - p_n^R(i + J_1(i, n) + J_2(i, n) + \dots + J_{k-1}(i, n)).\end{aligned}$$

Transforming to continuous variables in the usual way, we determine the moments of $\Delta Y(x, t)$ using expressions for $\mathbb{E}[J_k(x, t)]$ and $\text{Var}(J_k(x, t))$. From the conditional distribution of $J_k(i, t)$,

$$\begin{aligned}\mathbb{E}[J_k(i, n)] &= \mathbb{E}[\mathbb{E}[J_k(i, n) \mid J_1(i, n), J_2(i, n), \dots, J_{k-1}(i, n)]] \\ &= \mathbb{E}[p_n^R(i + J_1(i, n) + J_2(i, n) + \dots + J_{k-1}(i, n))] \\ &\quad - \mathbb{E}[p_n^L(i + J_1(i, n) + J_2(i, n) + \dots + J_{k-1}(i, n))].\end{aligned}\quad (\text{A.1})$$

This expression cannot be simplified for general hopping probabilities. However, moving to continuous variables, equation (A.1) can be written as

$$\begin{aligned}\mathbb{E}[J_k(x, t)] &= \mathbb{E}[p^R(x + \Delta J_1(x, t) + \Delta J_2(x, t) + \dots + \Delta J_{k-1}(x, t), t)] \\ &\quad - \mathbb{E}[p^L(x + \Delta J_1(x, t) + \Delta J_2(x, t) + \dots + \Delta J_{k-1}(x, t), t)],\end{aligned}$$

and, similarly,

$$\begin{aligned}\mathbb{E}[J_k(x, t)^2] &= \mathbb{E}[p^R(x + \Delta J_1(x, t) + \Delta J_2(x, t) + \dots + \Delta J_{k-1}(x, t), t)] \\ &\quad + \mathbb{E}[p^L(x + \Delta J_1(x, t) + \Delta J_2(x, t) + \dots + \Delta J_{k-1}(x, t), t)].\end{aligned}$$

Using the dominated convergence theorem [19], with the natural assumption of continuity for $p^R(x, t)$ and $p^L(x, t)$, it can be shown that

$$\lim_{\Delta \rightarrow 0} \mathbb{E}[J_k(x, t)] = p^R(x, t) - p^L(x, t), \quad \lim_{\Delta \rightarrow 0} \mathbb{E}[J_k(x, t)^2] = p^R(x, t) + p^L(x, t). \quad (\text{A.2})$$

Therefore,

$$\lim_{\Delta \rightarrow 0} \text{Var}(J_k(x, t)) = p^R(x, t) + p^L(x, t) - (p^R(x, t) - p^L(x, t))^2. \quad (\text{A.3})$$

The number of agents m is required to be large in order for the RSU scheme to approximate a continuous time process [20]. Consider an initial condition in which the lattice sites within $M_l \leq x \leq M_r$ are occupied by agents. As Δ decreases, the number of lattice sites falling inside these segments increases, and thus the number of agents in the system will also increase. Thus $m \rightarrow \infty$ is equivalent to taking $\Delta \rightarrow 0$.

Using the limits (A.2)–(A.3) and the fact that $Z \rightarrow Z^* = \text{Poisson}(1)$ as $m \rightarrow \infty$ (or equivalently as $\Delta \rightarrow 0$), we deduce [21] that

$$\begin{aligned}\lim_{\Delta \rightarrow 0} \mathbb{E}[Y(x, t)] &= \lim_{\Delta \rightarrow 0} \mathbb{E}\left[\mathbb{E}\left[\sum_{k=0}^Z J_k(x, t) \mid Z\right]\right] \\ &= \lim_{\Delta \rightarrow 0} \mathbb{E}\left[\sum_{k=0}^Z \mathbb{E}[J_k(x, t)]\right] = p^R(x, t) - p^L(x, t).\end{aligned}$$

Using the law of total variance, we write

$$\lim_{\Delta \rightarrow 0} \text{Var}(Y(x, t)) = \lim_{\Delta \rightarrow 0} \mathbb{E}[\text{Var}(Y(x, t) \mid Z)] + \lim_{\Delta \rightarrow 0} \text{Var}(\mathbb{E}[Y(x, t) \mid Z]). \quad (\text{A.4})$$

Using the law of iterated expectation, the first term on the right side of equation (A.4) becomes

$$\begin{aligned} \lim_{\Delta \rightarrow 0} \mathbb{E}[\text{Var}(Y(x, t) | Z)] &= \lim_{\Delta \rightarrow 0} \mathbb{E}\left[\text{Var}\left(\sum_{k=1}^Z J_k(x, t) \mid Z\right)\right] \\ &= \lim_{\Delta \rightarrow 0} \mathbb{E}\left[\sum_{k=1}^Z \text{Var}(J_k(x, t))\right] \\ &= p^R(x, t) + p^L(x, t) - (p^R(x, t) - p^L(x, t))^2. \end{aligned} \quad (\text{A.5})$$

Similarly, the second term on the right side of equation (A.4) can be written as

$$\lim_{\Delta \rightarrow 0} \text{Var}(\mathbb{E}[Y(x, t) | Z]) = \lim_{\Delta \rightarrow 0} \text{Var}\left(\sum_{k=1}^Z \mathbb{E}[J_k(x, t)]\right) = (p^R(x, t) - p^L(x, t))^2. \quad (\text{A.6})$$

Combining (A.5) and (A.6) in (A.4) gives

$$\lim_{\Delta \rightarrow 0} \text{Var}(Y(x, t)) = p^R(x, t) + p^L(x, t).$$

Thus, for sufficiently small Δ and τ , the coefficients in the Fokker–Planck equation are given by

$$\begin{aligned} \mu(x, t) &= \frac{1}{\tau} \mathbb{E}[\Delta Y(x, t)] = V_{\Delta, \tau}(p^R(x, t) - p^L(x, t)), \\ \sigma^2(x, t) &= \frac{1}{\tau} \text{Var}(\Delta Y(x, t)) = D_{\Delta, \tau}(p^R(x, t) + p^L(x, t)), \end{aligned}$$

where $V_{\Delta, \tau}$ and $D_{\Delta, \tau}$ are given by (5.3).

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