When push comes to shove: exclusion processes with nonlocal consequences

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1 Abstract

An alternative motility mechanism to simple exclusion is formulated, in which agents are granted more freedom to move under the compromise that interactions are no longer necessarily local. We call this mechanism the 'shoving' process. A nonlinear diffusion equation is derived using mean-field based continuum approximations. PDEs are also derived for interacting subpopulations under this new mechanism and for a subpopulation obeying simple exclusion that interacts with a subpopulation obeying exclusion by shoving. Numerical solutions of the PDEs are compared to simulation results for both the single and multi-species process.

2 Introduction

2.1 Exclusion processes

Stochastic agent-based models are useful for modelling complex phenomena such as cell motility (Sander & Deisboeck, 2002) and traffic flow (Schadschneider, 2002). One can use them to extract information on a microscopic level about the behaviour of individual agents through tagging and calculations based on such, or on a macroscopic level by considering the average behaviour of the collective. A random walk model (Hughes, 1995) consists of agents moving in a sequence of random steps. For example, on a one-dimensional lattice with spacing Δ, an agent at site i will attempt to move to one of two target sites $i + \Delta$ or $i - \Delta$ at each time step.

Lattice-based random walk models of interacting agents where each site can be occupied by at most one agent are called *exclusion processes* (Liggett, 1999). These models will
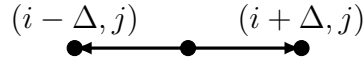
$$(i - \Delta, j) \qquad (i + \Delta, j)$$

Figure 1: The possible target sites for an agent at site i.

serve as the focus for this project, and have continuous analogues in the form of a partial differential equation (PDE)

2.2 Random Walks and Diffusion

It is well-known that (symmetric) exclusion processes give rise to PDEs of the form

$$\frac{\partial C}{\partial t} = D_0 \frac{\partial}{\partial x} \left[\mathcal{D}(C) \frac{\partial C}{\partial x} \right], \tag{1}$$

where $C(x, t)$ describes the average concentration, D_0 is the diffusivity constant and $\mathcal{D}$ is typically a polynomial (Simpson et al, 2009a). We illustrate how one can derive a PDE from from exclusion processes, using simple exclusion as an example (Simpson et al, 2009b).

Under a *symmetric simple exclusion process*, each agent has a probability P of attempting a move and can move left or right with equal chance. The process is called 'symmetric' due to the absence of bias in movement by agents. Since agents can only step to adjacent sites, performing simple random walks, the exclusion process is 'simple'.

By considering the average occupancy of sites over time, we can use conservation of mass arguments to develop a partial differential equation. Let $C_i(t)$ denote the average occupancy of an agent at site i at time t. The rules imposed by simple exclusion mean $0 \leq C_i(t) \leq 1$. We say that an agent is at site i after k time steps if $x = i\Delta$ at time $t = k\tau$, where Δ is the lattice spacing and τ is a time increment. We also assume that the average occupancy of sites are independent. This allows us to derive the change in average occupancy using intuitive, probabilistic arguments. The change in average occupancy between times $t + \tau$ and t, sometimes called the *master equation*, is then given by

$$\begin{aligned} C_i(t + \tau) - C_i(t) = &\frac{P}{2} C_{i-1}(t) \left[1 - C_i(t) \right] + \frac{P}{2} C_{i+1}(t) \left[1 - C_i(t) \right] \\ &- \frac{P}{2} C_i(t) \left[1 - C_{i-1}(t) \right] - \frac{P}{2} C_i(t) \left[1 - C_{i+1}(t) \right] \end{aligned} \tag{2}$$

One can interpret $C_i(t)$ as the probability that an agent is occupying site i at time t and thus $1 - C_i(t)$ is the probability that site i is free at time t. The first two terms on the right
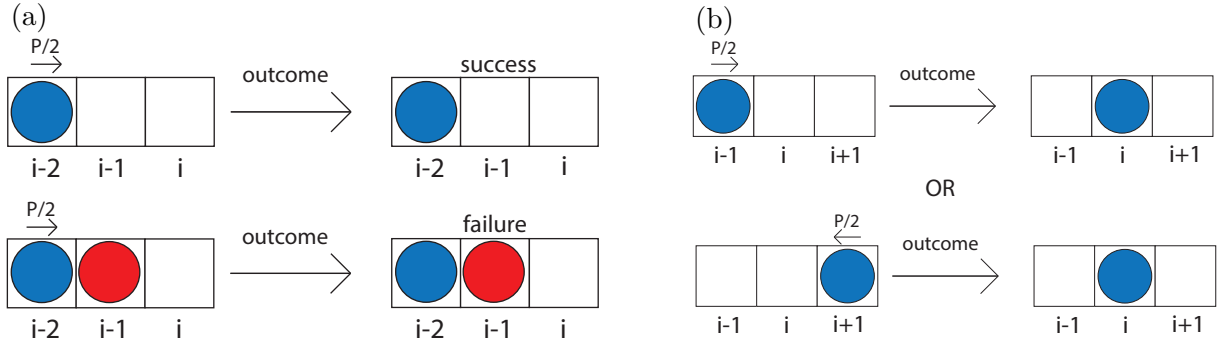
Figure 2: Moves for agents under simple exclusion. (a) Possible outcomes for an agent moving right from site $i - 2$. In the bottom image, the red agent in site $i - 1$ prevents the blue agent in site $i - 2$ from moving, and so the move is aborted. (b) Possible increases in average occupancy at site i.

hand side of (2) describe increases in occupancy and are illustrated by figure 2(b). The first term describes an agent in site $i - 1$ moving to the right, provided that site i is free. Similarly, the second term describes an agent in site $i + 1$ moving to the left, provided that site i is free. The third term describes an agent moving to the left from site i, provided that site $i - 1$ is unoccupied, decreasing the occupancy. The fourth term describes an agent moving to the right from site i, provided that site $i + 1$ is unoccupied, decreasing the occupancy. Taking the second order Taylor expansion of each term, keeping terms up to $O(\Delta^2)$, and dividing both sides by τ, we obtain

$$\frac{C(x, t + \tau) - C(x, t)}{\tau} = \frac{P\Delta^2}{2\tau} \frac{\partial^2 C}{\partial x^2} \tag{3}$$

Taking the limits $\Delta \to 0$, $\tau \to 0$ while keeping Δ^2/τ constant,

$$\frac{\partial C}{\partial t} = D_0 \frac{\partial^2 C}{\partial x^2}, \tag{4}$$

where

$$D_0 = \lim_{\Delta, \tau \to 0} \left(\frac{P\Delta^2}{2\tau} \right). \tag{5}$$

This is clearly a special case of (4), with $\mathcal{D}(C) \equiv 1$ being a (constant) polynomial, and so (4) describes linear diffusion. The linearity of the PDE reflects the symmetric nature of the exclusion process. For *asymmetric simple exclusion processes*, where agents can move with bias, the resulting PDE is a nonlinear advection-diffusion equation (Simpson et al, 2009b).

2.3 Multi-species exclusion processes

In the previous section we assumed that the agents were all of the same species. It is often of relevance and interest to consider the population of agents as a system of interacting subpopulations. Previous research (Simpson et al, 2009a) has shown that interacting subpopulations under simple exclusion can be described by a system of advection-diffusion equations, revealing new insights into the process. For illuminative purposes, we consider a system made up of two subpopulations – red agents and green agents – that interact under simple exclusion and how this leads to a system of coupled PDEs. We again only consider agents moving under symmetric simple exclusion.

Let $R_i(t)$ and $G_i(t)$ denote the average occupancies of red and green agents respectively at site i at time t. Let $C_i(t) = R_i(t) + G_i(t)$ denote the average occupancy of the total population. We use the same formalism as before to give a continuum approximation of the process to $R_i(t)$ and $G_i(t)$. Since both red and green agents interact under the exact same process, we only need to consider the change in mass for one species and use symmetry arguments to deduce the change for the other species. Consider the change in average occupancy for red agents, without loss of generality. The change in average occupancy between times $t + \tau$ and t is

$$
\begin{aligned}
R_i(t+\tau) - R_i(t) &= \frac{P}{2} R_{i-1}(t) \left[1 - R_i(t) - G_i(t)\right] + \frac{P}{2} R_{i+1}(t) \left[1 - R_i(t) - G_i(t)\right] \\
&\quad - \frac{P}{2} R_i(t) \left[1 - R_{i-1}(t) - G_{i-1}(t)\right] - \frac{P}{2} R_i(t) \left[1 - R_{i+1}(t) - G_{i+1}(t)\right]
\end{aligned}
\tag{6}
$$

This equation is analogous to (2) in that we still require target sites to be completely free, hence the use of $1 - R_i - G_i$. The probability $1 - R_i$ is *not* the probability that site i is free, but the probability that there is *no red agent* at site i – there may be a green agent occupying the site. Taking the second-order Taylor expansion of each term, keeping terms up to $O(\Delta^2)$, while dividing by τ we obtain, with appropriate manipulation,

$$
\frac{R_i(t+\tau) - R_i(t)}{\tau} = \frac{P\Delta^2}{2\tau} \frac{\partial}{\partial x} \left[(1 - R - G) \frac{\partial R}{\partial x} + R \frac{\partial(R+G)}{\partial x} \right]
\tag{7}
$$

Taking the limits $\Delta \to 0$, $\tau \to 0$, while keeping Δ^2/τ constant

$$
\frac{\partial R}{\partial t} = D_0 \frac{\partial}{\partial x} \left[(1 - R - G) \frac{\partial R}{\partial x} + R \frac{\partial(R+G)}{\partial x} \right],
\tag{8}
$$

Similarly, for green agents

$$
\frac{\partial G}{\partial t} = D_0 \frac{\partial}{\partial x} \left[(1 - R - G) \frac{\partial G}{\partial x} + G \frac{\partial(R+G)}{\partial x} \right],
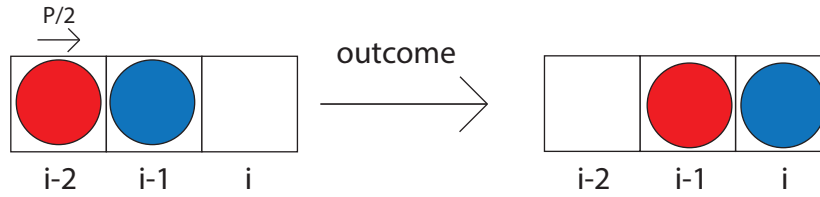\tag{9}
$$

Figure 3: The red agent moves right into site $i-1$, shoving the blue agent in site $i-1$ to site i.

where D_0 is defined by (5) for both (8) and (9). We can see that both PDEs describe linear advection-diffusion equations. Adding the two PDEs and substituting $C = R + G$ returns the PDE for single species simple exclusion, as described by (4).

3   Alternative motility mechanism

One key characteristic of simple exclusion is the possibility of aborted moves. As the concentration of agents increases, the number of aborted moves will increase. We seek to avoid this by developing a new exclusion process known as *shoving*. This is motivated by the nature of cells and other similar crowd-like situations, where simple exclusion may not be such a realistic model. Under the shoving exclusion process, each agent has a probability P of attempting a move and can move either left or right with equal probability. Like simple exclusion, if an agent attempts to move to an unoccupied site, it will do so. However, if the target site is occupied, the moving agent will 'shove' the agent occupying the target site in the same direction as the moving agent. That is, the agents do not swap places, but shift across in the 'forward' direction, as highlighted by figure 3.

To ensure the certain success of attempted moves, we say that shoves are always successful. In other words, if each agent attempting to move to an occupied site has a probability P_s of shoving the occupant of the target site, then we set $P_s = 1$. This means that interactions between agents are no longer restricted to agents that are adjacent to each other. As a result, the nature of the diffusion change significantly, as we will see. We consider three different processes: single species shoving, multi-species shoving and mixed exclusion, which we call 'bullies and weaklings', and derive one-dimensional partial differential equations for each of these processes. It should be noted that although we derive one-dimensional PDEs for simplicity, the results can naturally be extended for general n-dimensional processes, with appropriate replacement of spatial partial derivatives with ∇ and dividing (5) by n. This assumes that shoving in higher dimensions still takes place in the same line of motion.
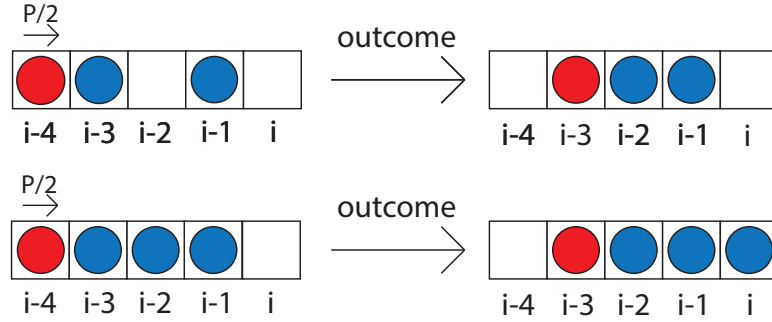
Figure 4: In the top image, the agent moving right from $i - 4$ will not increase the average occupancy for i because site $i - 2$ is unoccupied. In the bottom image, the agent in $i - 4$ will increase the average occupancy for i because all sites from $i - 4$ to $i - 1$ are occupied. The agents causing the shove are coloured in red.

4 Continuum modelling

4.1 Single species motility

Consider one population of agents that are all the same type and can either shove or be shoved. We assume that the process takes place on an infinite one-dimensional lattice with spacing Δ. The infinite domain is to avoid any issues of agents being shoved past the boundaries and to guarantee the success of attempted moves. Denote the average occupancy of a site i at time t by $C_i(t)$, where $i \in \mathbb{Z}$. Again, we use a mean-field assumption and say that the average occupancy of sites is independent. We say that an agent is at site i after k time increments if $x = i\Delta$ at $t = k\tau$, where τ is one time increment. The change in average occupancy between times t and $t + \tau$ of site i is given by

$$
\begin{aligned}
C_i(t + \tau) - C_i(t) = {} & \frac{P}{2}(1 - C_i(t)) \sum_{k=1}^{\infty} \prod_{l=1}^{k} C_{i-l}(t) + \frac{P}{2}(1 - C_i(t)) \sum_{k=1}^{\infty} \prod_{l=1}^{k} C_{i+l}(t) \\
& - \frac{P}{2}C_i(t) - \frac{P}{2}C_i(t)
\end{aligned}
\tag{10}
$$

Each term in the first summation denotes an agent k spots to the left of site i causing an increase in average occupancy by shoving if and only if all the sites from $i-1$ to $i-k$ are occupied, provided site i is unoccupied. This is illustrated in figure 4. Similar reasoning is given for the second summation, for agents k sites to the right moving to the left. The third and fourth terms denote an agent in site i leaving by moving to the left or right. For convenience in deriving the partial differential equation, we consider the first n terms in

each of the summations. The master equation then becomes

$$C_i(t + \tau) - C_i(t) = \frac{P}{2}(1 - C_i(t)) \sum_{k=1}^{n} \prod_{l=1}^{k} C_{i-l}(t) + \frac{P}{2}(1 - C_i(t)) \sum_{k=1}^{n} \prod_{l=1}^{k} C_{i+l}(t)$$
$$- \frac{P}{2} C_i(t) - \frac{P}{2} C_i(t) \tag{11}$$

Expanding out the right hand side and rearranging, keeping terms up to $O(C^n)$ and writing C_i for brevity

$$C_i(t + \tau) - C_i(t) = \frac{P}{2} \bigg(C_{i-1} - 2C_i + C_{i+1}$$
$$+ C_{i-1}C_{i-2} - C_iC_{i-1} + C_{i+1}C_{i+2} - C_iC_{i+1}$$
$$+ \cdots$$
$$+ \prod_{l=1}^{n} C_{i-l} - \prod_{l=0}^{n} C_{i-l+1} + \prod_{l=1}^{n} C_{i+l} - \prod_{l=0}^{n} C_{i+l-1} \bigg) \tag{12}$$

Taking the Taylor expansion up to $O(\Delta^2)$ and dividing by τ, we obtain

$$\frac{C_i(t + \tau) - C_i(t)}{\tau} = \frac{P\Delta^2}{2\tau} \left[\frac{\partial^2 C}{\partial x^2} + 4\left(\frac{\partial C}{\partial x}\right)^2 + 4C\frac{\partial^2 C}{\partial x^2} + \cdots \right.$$
$$\left. + n^2(n-1)C^{n-2}\left(\frac{\partial C}{\partial x}\right)^2 + n^2 C^{n-1}\frac{\partial^2 C}{\partial x^2} \right]$$
$$= \frac{P\Delta^2}{2\tau} \left[\frac{\partial^2 C}{\partial x^2} + \frac{\partial}{\partial x}\left(2^2 C\frac{\partial C}{\partial x}\right) + \cdots + \frac{\partial}{\partial x}\left(n^2 C^{n-1}\frac{\partial C}{\partial x}\right) \right]$$
$$= \frac{P\Delta^2}{2\tau} \frac{\partial}{\partial x}\left(\sum_{k=1}^{n} k^2 C^{k-1}\frac{\partial C}{\partial x} \right) \tag{13}$$

Taking the limits $\Delta \to 0$, $\tau \to 0$ and $n \to \infty$ while keeping Δ^2/τ constant, we obtain the PDE

$$\frac{\partial C}{\partial t} = D_0 \frac{\partial}{\partial x} \left[\frac{1+C}{(1-C)^3} \frac{\partial C}{\partial x} \right], \tag{14}$$

where D_0 is defined as in (5). Here $\mathcal{D}(C) \equiv \dfrac{1+C}{(1-C)^3}$, which is not a polynomial but a rational function with singularity at $C = 1$. This is reflective of the fact that interactions

between agents are no longer local on the lattice and therefore are complex than under simple exclusion. As $C \to 1$, i.e. the process approaches full density, the diffusion coefficient $\mathcal{D}$ diverges to infinity. Intuitively, this is because at higher densities, each agent is shoved more by other agents and so diffusion is enhanced. To further understand this process, we will now consider a population consisting of interacting subpopulations of agents.

4.2   Multi-species motility

Previous research (Simpson et al, 2009a) has shown that for interacting subpopulations following simple exclusion, the resulting PDEs reveal more subtle interactions than the single species process. Namely, there is convection involved as well as diffusion. Therefore, we seek a derivation of PDEs for multi-species shoving under similar motivation.

Consider a population of agents that is divided into red agents and green agents. Both subpopulations interact under the same shoving process and each agent can shove or be shoved by either species of agents. Denote the average occupancies of red and green agents $R_i(t)$ and $G_i(t)$ respectively. Since there is no difference in the motility between red or green agents, it is enough to derive the PDE for one subpopulation and deduce the other by symmetry. We say that an agent is at site i after k time steps if $x = i\Delta$ at time $t = k\tau$, where τ is a time increment and Δ is the lattice spacing of an infinite one-dimensional lattice, as previously defined. Without loss of generality, we consider the change in average occupancy for red agents. This is given by

$$
\begin{aligned}
R_i(t+\tau) - R_i(t) &= \frac{P}{2}(1-R_i)R_{i-1}\left(1 + \sum_{k=2}^{\infty}\prod_{l=2}^{k} C_{i-l}\right) + \frac{P}{2}(1-R_i)R_{i+1}\left(1 + \sum_{k=2}^{\infty}\prod_{l=2}^{k} C_{i+l}\right) \\
&\quad - \frac{P}{2}R_i G_{i-1}\left(1 + \sum_{k=2}^{\infty}\prod_{l=2}^{k} C_{i-l}\right) - \frac{P}{2}R_i G_{i+1}\left(1 + \sum_{k=2}^{\infty}\prod_{l=2}^{k} C_{i+l}\right) \\
&\quad - \frac{P}{2}R_i - \frac{P}{2}R_i.
\end{aligned}
\tag{15}
$$

We have written $R_i(t) = R_i$, $G_i(t) = G_i$, and $C_i(t) = C_i = R_i + G_i$ for brevity. Each term in the first summation of (15) describes an agent at site $i - k$ shoving in the right direction, which causes an increase *only if* sites $i - k$ to $i - 2$ are occupied - the species does not matter, hence the use of C_i - provided there is a *red* agent in site $i - 1$ and no red agent in site i (note that this does not necessarily mean site i is empty). Similar reasoning is given for the second summation, describing agents k sites to the right moving left. Each term of the third summation describe an agent k sites to the left shoving in the right direction, causing a decrease *only if* all sites up to $i - 1$ are occupied *and* a *green* agent

is occupying site $i-1$. Similar reasoning is given for the fourth summation, describing agents k sites to the right moving left . The 1 in each of the brackets is to account for agents in sites $i-1$ and $i+1$ moving on their own to site i.

Again, we consider only the first n terms and take the limit to infinity at the end. Thus the equation becomes

$$
R_i(t+\tau) - R_i(t) = \frac{P}{2}\left[(1-R_i)R_{i-1}\left(1+\sum_{k=2}^{n}\prod_{l=2}^{k}C_{i-l}\right) + (1-R_i)R_{i+1}\left(1+\sum_{k=2}^{n}\prod_{l=2}^{k}C_{i+l}\right)\right.
$$
$$
\left. - R_iG_{i-1}\left(1+\sum_{k=2}^{n}\prod_{l=2}^{k}C_{i-l}\right) - R_iG_{i+1}\left(1+\sum_{k=2}^{n}\prod_{l=2}^{k}C_{i+l}\right) - 2R_i\right]
$$
(16)

Expanding and keeping up to $O(R^n)$

$$
R_i(t+\tau) - R_i(t) = \frac{P}{2}\left(R_{i-1} - 2R_i - R_{i+1}\right.
$$
$$
+ R_{i-1}C_{i-2} - R_iR_{i-1} + R_{i+1}C_{i+2} - R_iR_{i+1} - R_iG_{i-1} - R_iG_{i+1}
$$
$$
+ \cdots
$$
$$
+ R_{i-1}\prod_{l=2}^{n}C_{i-l} - R_iR_{i-1}\prod_{l=3}^{n}C_{i-l+1} + R_{i+1}\prod_{l=2}^{n}C_{i+l}
$$
$$
\left. - R_iR_{i+1}\prod_{l=3}^{n}C_{i+l-1} - R_iG_{i-1}\prod_{l=3}^{n}C_{i-l+1} - R_iG_{i+1}\prod_{l=3}^{n}C_{i+l-1}\right)
$$
(17)

$$
= \frac{P}{2}\left(R_{i-1} - 2R_i - R_{i+1}\right.
$$
$$
+ R_{i-1}C_{i-2} - R_iC_{i-1} + R_{i+1}C_{i+2} - R_iC_{i+1}
$$
$$
+ \cdots
$$
$$
\left. + R_{i-1}\prod_{l=2}^{n}C_{i-l} - R_i\prod_{l=2}^{n}C_{i-l+1} + R_{i+1}\prod_{l=2}^{n}C_{i+l} - R_i\prod_{l=2}^{n}C_{i+l-1}\right)
$$
(18)

In (18) we factorise terms and make use of the relation $C_i = R_i + G_i$ again. Taking the Taylor expansion up to $O(\Delta^2)$ and dividing by τ, we obtain

$$
\frac{R_i(t+\tau) - R_i(t)}{\tau} = \frac{P\Delta^2}{2\tau}\frac{\partial}{\partial x}\left[\frac{\partial R}{\partial x} + C\frac{\partial R}{\partial x} + 3R\frac{\partial C}{\partial x} + C^2\frac{\partial R}{\partial x} + 8RC\frac{\partial C}{\partial x} + C^3\frac{\partial R}{\partial x}\right.
$$

$$+ 15RC^2\frac{\partial C}{\partial x} + \cdots + C^{n-1}\frac{\partial R}{\partial x} + R(n^2 - 1)C^{n-2}\frac{\partial C}{\partial x}\Bigg] \qquad (19)$$

$$= \frac{P\Delta^2}{2\tau}\frac{\partial}{\partial x}\left[\sum_{k=1}^{n} C^{k-1}\frac{\partial R}{\partial x} + R\sum_{k=2}^{n}(k^2 - 1)C^{k-2}\mathbf{1}_{\{n\geq 2\}}\frac{\partial C}{\partial x}\right], \qquad (20)$$

where $\mathbf{1}$ is the indicator function. Taking $\Delta \to 0$, $\tau \to 0$ and $n \to \infty$ while keeping Δ^2/τ constant,

$$\frac{\partial R}{\partial t} = D_0\frac{\partial}{\partial x}\left[\frac{1}{1-C}\frac{\partial R}{\partial x} + R\frac{(3-C)}{(1-C)^3}\frac{\partial C}{\partial x}\right] \qquad (21)$$

$$= D_0\frac{\partial}{\partial x}\left[\frac{1}{1-R-G}\frac{\partial R}{\partial x} + R\frac{(3-R-G)}{(1-R-G)^3}\frac{\partial(R+G)}{\partial x}\right], \qquad (22)$$

where D_0 is given by (5). Therefore, by symmetry,

$$\frac{\partial G}{\partial t} = D_0\frac{\partial}{\partial x}\left[\frac{1}{1-C}\frac{\partial G}{\partial x} + G\frac{(3-C)}{(1-C)^3}\frac{\partial C}{\partial x}\right] \qquad (23)$$

$$= D_0\frac{\partial}{\partial x}\left[\frac{1}{1-R-G}\frac{\partial G}{\partial x} + G\frac{(3-R-G)}{(1-R-G)^3}\frac{\partial(R+G)}{\partial x}\right]. \qquad (24)$$

Adding (21) and (23) gives the single species PDE, as specified by (14). Equations (22) and (24) describe a set of coupled nonlinear advection-diffusion equations, as do (21) and (23). For $C = R + G \ll 1$, the diffusion coefficient $\dfrac{1}{1-C}$ dominates, but for $C \approx 1$, the convection coefficient $\dfrac{(3-C)}{(1-C)^3}\dfrac{\partial C}{\partial x}$ dominates for (21) and (23). This highlights the subtlety of the shoving process that is revealed in considering interacting subpopulations that follow the exclusion process.

In considering interacting subpopulations under this motility mechanism, the process of deriving the PDEs is straightforward since every subpopulation follows the same process. We now ask what happens when two subpopulations that operate under different mechanisms interact with each other. Namely, what happens when a subpopulation that obeys simple exclusion interacts with a subpopulation that obeys the shoving process. We call this the *bullies and weaklings* model.

4.3 Mixed motility: bullies and weaklings

Consider a population that is again made up of red agents and green agents. The red agents obey the shoving process and can shove both red and green agents. We call this

subpopulation the 'bullies'. The green agents obey simple exclusion and cannot move if a site is occupied, regardless of species. We call them 'weaklings'. Adopting the same formalism as the previous section, the change in average occupancy for the bullies (red agents) between times $t + \tau$ and t is given by

$$
\begin{aligned}
R_i(t + \tau) - R_i(t) = {} & \frac{P}{2} R_{i-1}(t) \left[1 - R_i(t)\right] \left[1 + R_{i-2}(t) + \sum_{k=3}^{\infty} R_{i-k}(t) \prod_{l=2}^{k-1} C_{i-l}(t)\right] \\
& + \frac{P}{2} R_{i+1}(t) \left[1 - R_i(t)\right] \left[1 + R_{i+2}(t) + \sum_{k=3}^{\infty} R_{i+k}(t) \prod_{l=2}^{k-1} C_{i+l}(t)\right] \\
& - \frac{P}{2} G_{i-1}(t) R_i(t) \left[R_{i-2}(t) + \sum_{k=3}^{\infty} R_{i-k}(t) \prod_{l=2}^{k-1} C_{i-l}(t)\right] \\
& - \frac{P}{2} G_{i+1}(t) R_i(t) \left[R_{i+2}(t) + \sum_{k=3}^{\infty} R_{i+k}(t) \prod_{l=2}^{k-1} C_{i+l}(t)\right] \\
& - \frac{P}{2} R_i(t) - \frac{P}{2} R_i(t).
\end{aligned} \tag{25}
$$

The first term of the right hand side of (25) describes agents k sites to the left of site i moving to the right, increasing the average occupancy by shoving *if and only if* a red agent is occupying sites $i - k$ and $i - 1$ with all sites in between being occupied, provided there is no red agent in site i. Similar reasoning is given for the second term. The third term of the right hand site of (25) describes agents k sites to the left of site i moving to the right, decreasing the average occupancy by shoving *if and only if* a red agent is occupying site $i - k$, a green agent is occupying site $i - 1$ with all sites in between being occupied, provided a red agent is in site i. Similar reasoning is given for the fourth term. The fifth and sixth terms describe a red agent in site i moving left and right, decreasing the average occupancy.

Considering the first n terms of each sum, expanding and rearranging by the degrees of terms, keeping terms up to $O(C^n)$

$$
\begin{aligned}
R_i(t + \tau) - R_i(t) = \frac{P}{2} \Big(& R_{i+1} - 2R_i + R_{i-1} \\
& + R_{i-1}R_{i-2} - R_i R_{i-1} + R_{i+1}R_{i+2} - R_i R_{i+1} \\
& + R_{i-1}C_{i-2}R_{i-3} - R_i R_{i-1}R_{i-2} + R_{i+1}C_{i+2}R_{i+3} \\
& - R_i R_{i+1}R_{i+2} - R_i G_{i-1}R_{i-2} - R_i G_{i+1}R_{i+2} \\
& + \cdots
\end{aligned}
$$

$$
\begin{aligned}
&+ R_{i-1}R_{i-n}\prod_{l=3}^{n}C_{i-l+1} - R_iR_{i-1}R_{i-n+1}\prod_{l=4}^{n}C_{i-l+2} \\
&+ R_{i+1}R_{i+n}\prod_{l=3}^{n}C_{i+l-1} - R_iR_{i+1}R_{i+n-1}\prod_{l=4}^{n}C_{i+l-2} \\
&\left. - R_iG_{i-1}R_{i-n+1}\prod_{l=4}^{n}C_{i-l+2} - R_iG_{i+1}R_{i+n-1}\prod_{l=4}^{n}C_{i+l-2} \right) \quad (26) \\
&= \frac{P}{2}\left(R_{i+1} - 2R_i + R_{i-1} \right. \\
&\quad + R_{i-1}R_{i-2} - R_iR_{i-1} + R_{i+1}R_{i+2} - R_iR_{i+1} \\
&\quad + R_{i-1}C_{i-2}R_{i-3} - R_iC_{i-1}R_{i-2} \\
&\quad + R_{i+1}C_{i+2}R_{i+3} - R_iC_{i+1}R_{i+2} \\
&\quad + \cdots \\
&\quad + R_{i-1}R_{i-n}\prod_{l=3}^{n}C_{i-l+1} - R_iR_{i-n+1}\prod_{l=3}^{n}C_{i-l+2} \\
&\quad \left. + R_{i+1}R_{i+n}\prod_{l=3}^{n}C_{i+l-1} - R_iR_{i+n-1}\prod_{l=3}^{n}C_{i+l-2} \right). \quad (27)
\end{aligned}
$$

In (27), we have used the relation $C_i = R_i + G_i$, as we did for (18). Taking the second-order Taylor expansion of each term, retaining terms up to $O(\Delta^2)$, while dividing by τ, the master equation becomes

$$
\begin{aligned}
\frac{R_i(t+\tau) - R_i(t)}{\tau} =& \frac{P\Delta^2}{2\tau}\frac{\partial}{\partial x}\left[\frac{\partial R}{\partial x} + 4R\frac{\partial R}{\partial x} + 6RC\frac{\partial R}{\partial x} + 3R^2\frac{\partial C}{\partial x} + 8RC^2\frac{\partial R}{\partial x} \right. \\
&\left. + 8R^2C\frac{\partial C}{\partial x} + \cdots + 2nRC^{n-2}\frac{\partial R}{\partial x} + n(n-2)R^2C^{n-3}\frac{\partial C}{\partial x} \right] \quad (28) \\
=& \frac{P\Delta^2}{2\tau}\frac{\partial}{\partial x}\left[\left(1 + R\sum_{k=2}^{n}2kC^{k-2}\mathbf{1}_{\{n\geq 2\}} \right)\frac{\partial R}{\partial x} \right. \\
&\left. + R^2\sum_{k=3}^{n}k(k-2)C^{k-3}\mathbf{1}_{\{n\geq 3\}}\frac{\partial C}{\partial x} \right]. \quad (29)
\end{aligned}
$$

Taking the limits $\Delta \to 0$, $\tau \to 0$ and $n \to \infty$ while keeping Δ^2/τ constant,

$$
\frac{\partial R}{\partial t} = D_0\frac{\partial}{\partial x}\left\{ \left[1 + \frac{2R(2-C)}{(1-C)^2} \right]\frac{\partial R}{\partial x} + R\left[\frac{R(3-C)}{(1-C)^3}\frac{\partial C}{\partial x} \right] \right\} \quad (30)
$$

$$= D_0 \frac{\partial}{\partial x} \left\{ \left[1 + \frac{2R(2 - R - G)}{(1 - R - G)^2} \right] \frac{\partial R}{\partial x} + R \left[\frac{R(3 - R - G)}{(1 - R - G)^3} \frac{\partial (R + G)}{\partial x} \right] \right\}. \qquad (31)$$

D_0 is again given by (5). The governing PDE for bullies describes a nonlinear advection-diffusion equation, with behaviour not unlike PDEs (21) and (23). This is not a surprise as the bullies subpopulation is mostly unaffected by the behaviour of the weaklings.

We can take a different approach to deriving the PDE for the weaklings. For weaklings, we can split up the change in average occupancy into the change in average occupancy due to simple exclusion, and the change in average occupancy due to shoving. The change in average occupancy between times $t + \tau$ and t due to simple exclusion is given by

$$G_i(t + \tau) - G_i(t) = \frac{P}{2} G_{i-1}(t) \left[1 - R_i(t) - G_i(t) \right] + \frac{P}{2} G_{i+1}(t) \left[1 - R_i(t) - G_i(t) \right]$$
$$- \frac{P}{2} G_i(t) \left[1 - G_{i-1}(t) - R_{i-1}(t) \right] - \frac{P}{2} G_i(t) \left[1 - G_{i+1}(t) - R_{i+1}(t) \right].$$
$$(32)$$

Recognising that this is (6) for green agents, G, the resulting PDE is therefore (9). The main task is then to derive the PDE from the change in average occupancy due to shoving. This is given by

$$G_i(t + \tau) - G_i(t) = \frac{P}{2} G_{i-1}(t) \left[1 - G_i(t) \right] \left[R_{i-2}(t) + \sum_{k=3}^{\infty} R_{i-k}(t) \prod_{l=2}^{k-1} C_{i-l}(t) \right]$$
$$+ \frac{P}{2} G_{i+1}(t) \left[R_{i+2}(t) + \sum_{k=3}^{\infty} R_{i+k}(t) \prod_{l=2}^{k-1} C_{i+l}(t) \right]$$
$$- \frac{P}{2} R_{i-1}(t) G_i(t) \left[1 + R_{i-2}(t) + \sum_{k=3}^{\infty} R_{i-k}(t) \prod_{l=2}^{k-1} C_{i-l}(t) \right]$$
$$- \frac{P}{2} R_{i+1}(t) G_i(t) \left[1 + R_{i+2}(t) + \sum_{k=3}^{\infty} R_{i+k}(t) \prod_{l=2}^{k-1} C_{i+l}(t) \right]. \qquad (33)$$

Truncating the sums, expanding and rearranging while retaining terms up to $O(C^n)$

$$G_i(t + \tau) - G_i(t) = \frac{P}{2} \Big(G_{i-1} R_{i-2} + G_{i+1} R_{i+2} - G_i R_{i-1} - G_i R_{i+1}$$
$$+ G_{i-1} C_{i-2} R_{i-3} - G_i G_{i-1} R_{i-2} + G_{i+1} C_{i+2} R_{i+3}$$
$$- G_i G_{i+1} R_{i+2} - G_i R_{i-1} R_{i-2} - G_i R_{i+1} R_{i+2}$$

$$+\cdots$$

$$+ G_{i-1}R_{i-n}\prod_{l=2}^{n}C_{i-l+1} - G_iG_{i-1}R_{i-n+1}\prod_{l=4}^{n}C_{i-l+2}$$

$$+ G_{i+1}R_{i+n}\prod_{l=2}^{n}C_{i+l-1} - G_iG_{i+1}R_{i+n-1}\prod_{l=4}^{n}C_{i+l-2}$$

$$- G_iR_{i-1}R_{i-n+1}\prod_{l=4}^{n}C_{i-l+2} - G_iR_{i+1}R_{i+n-1}\prod_{l=4}^{n}C_{i+l-2}\Bigg) \qquad (34)$$

$$= \frac{P}{2}\Bigg(G_{i-1}R_{i-2} + G_{i+1}R_{i+2} - G_iR_{i-1} - G_iR_{i+1}$$

$$+ G_{i-1}C_{i-2}R_{i-3} - G_iC_{i-1}R_{i-2} + G_{i+1}C_{i+2}R_{i+3}$$

$$- G_iC_{i+1}R_{i+2}$$

$$+\cdots$$

$$+ G_{i-1}R_{i-n}\prod_{l=2}^{n}C_{i-l+1} - G_iR_{i-n+1}\prod_{l=3}^{n}C_{i-l+2}$$

$$+ G_{i+1}R_{i+n}\prod_{l=2}^{n}C_{i+l-1} - G_iR_{i_n-1}\prod_{l=3}^{n}C_{i+l-2}\Bigg). \qquad (35)$$

In (35) we simplified the right hand side using $C_i = R_i + G_i$, as done in (18) and (27). Taking the second-order Taylor expansion, retaining terms up to $O(\Delta^2)$, while dividing by τ we obtain

$$\frac{G_i(t+\tau) - G_i(t)}{\tau} = \frac{P\Delta^2}{2\tau}\frac{\partial}{\partial x}\Bigg[R\frac{\partial G}{\partial x} + 3G\frac{\partial R}{\partial x} + RC\frac{\partial G}{\partial x} + 5GC\frac{\partial R}{\partial x} + 3RG\frac{\partial C}{\partial x}$$

$$+ RC^2\frac{\partial G}{\partial x} + 7GC^2\frac{\partial R}{\partial x} + 8RGC\frac{\partial C}{\partial x} + \cdots + RC^{n-2}\frac{\partial G}{\partial x}$$

$$+ (2n-1)GC^{n-2}\frac{\partial R}{\partial x} + n(n-2)RGC^{n-3}\frac{\partial C}{\partial x}\Bigg] \qquad (36)$$

$$= \frac{P\Delta^2}{2\tau}\frac{\partial}{\partial x}\Bigg\{R\sum_{k=2}^{n}C^{k-2}\mathbf{1}_{\{n\geq 2\}}\frac{\partial G}{\partial x} + G\Bigg[\sum_{k=2}^{n}(2k-1)C^{k-2}\mathbf{1}_{\{n\geq 2\}}\frac{\partial R}{\partial x}$$

$$+ R\sum_{k=3}^{n}k(k-2)C^{k-3}\mathbf{1}_{\{n\geq 3\}}\frac{\partial C}{\partial x}\Bigg]\Bigg\}. \qquad (37)$$

Taking the limits $\Delta \to 0$, $n \to \infty$ and $\tau \to 0$ while keeping Δ^2/τ constant,

$$\frac{\partial G}{\partial t} = D_0 \frac{\partial}{\partial x} \left\{ \frac{R}{1-C} \frac{\partial G}{\partial x} + G \left[\frac{3-C}{(1-C)^2} \frac{\partial R}{\partial x} + \frac{R(3-C)}{(1-C)^3} \frac{\partial C}{\partial x} \right] \right\} \tag{38}$$

$$= D_0 \frac{\partial}{\partial x} \left\{ \frac{R}{1-R-G} \frac{\partial G}{\partial x} + G \left[\frac{3-R-G}{(1-R-G)^2} \frac{\partial R}{\partial x} + \frac{R(3-R-G)}{(1-R-G)^3} \frac{\partial (R+G)}{\partial x} \right] \right\}, \tag{39}$$

where D_0 is given by (5). Adding (9) and (39) gives the full governing PDE for the weakling subpopulation

$$\frac{\partial G}{\partial t} = D_0 \frac{\partial}{\partial x} \left\{ \left(1 - R - G + \frac{R}{1-R-G} \right) \frac{\partial G}{\partial x} + G \left[\frac{3-R-G}{(1-R-G)^2} \frac{\partial R}{\partial x} \right. \right.$$
$$\left. \left. + \left(1 + \frac{R(3-R-G)}{(1-R-G)^3} \right) \frac{\partial (R+G)}{\partial x} \right] \right\} \tag{40}$$

$$= D_0 \frac{\partial}{\partial x} \left\{ \left[1 + \frac{R(R+G)}{1-R-G} \right] \frac{\partial G}{\partial x} + G \left[\left(1 + \frac{3-R-G}{(1-R-G)^2} \right) \frac{\partial R}{\partial x} \right. \right.$$
$$\left. \left. + \frac{R(3-R-G)}{(1-R-G)^3} \frac{\partial (R+G)}{\partial x} \right] \right\}. \tag{41}$$

$$= D_0 \frac{\partial}{\partial x} \left\{ \left(1 + \frac{RC}{1-C} \right) \frac{\partial G}{\partial x} + G \left[\left(1 + \frac{3-C}{(1-C)^2} \right) \frac{\partial R}{\partial x} \right. \right.$$
$$\left. \left. + \frac{R(3-C)}{(1-C)^3} \frac{\partial C}{\partial x} \right] \right\}. \tag{42}$$

The PDE governing this subpopulation also represents a nonlinear advection-diffusion equation, albeit with more complex behaviour than the PDE modelling the average behaviour of the bullies. The convection term is composed of contributions from both the bullies subpopulation and the total population. This increased complexity in behaviour is because agents following simple exclusion are far more constrained in motion than agents who follow the shoving process.

5 Simulation & results

Simulations were carried out on a one-dimensional lattice of length 200, with constant unit spacing and constant unit time increments and the probability P of attempting a move
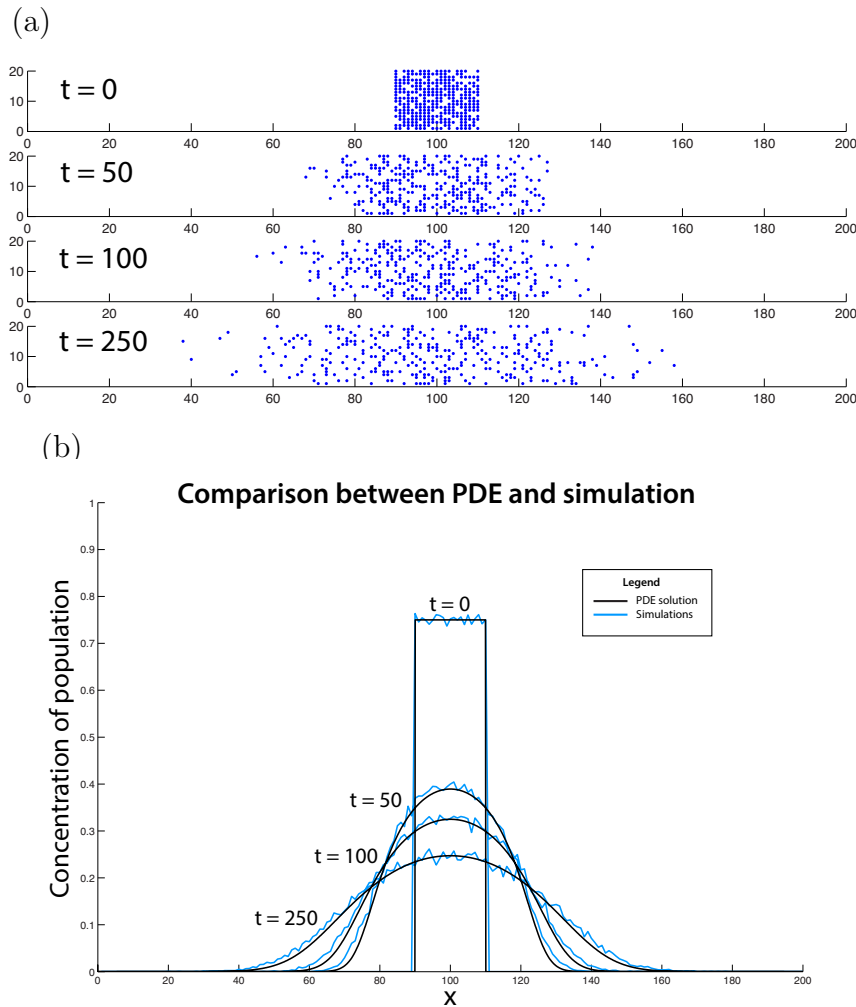
Figure 5: Simulations of the single species process. (a) 20 stacked one-dimensional realisations. (b) Comparisons between average density profiles obtained from 2500 realisations and numerical solutions of the PDE.

always equal to one. The random sequential update method (Chowdhury et al, 2005) was used to simulate motility. That is, if we have N agents occupying the lattice, then we choose N agents at random so that the expected number of moves each agent makes per time step is one. Simulations were stopped before an agent could touch either ends of the lattice to as to simulate an infinite domain. Average density profiles were obtained by averaging over 2500 realisations, so as to compare with numerical solutions for the PDE. Solutions were obtained using the MATLAB routine pdepe.m with Neumann zero-flux boundary conditions.

5.1 Single species motility

For every realisation at $t = 0$, the middle sites $90 \leq x \leq 110$ were filled randomly with the probability of a site being occupied being 0.75. This ensured the average initial density was 0.75. We choose this initial condition because although simulations can be run with uniform density, we cannot solve the PDE with initial density 1, as $C = 1$ is a singularity.

From figure 5(b), we can see that the PDE matches very well with results obtained from the simulations, conforming that the equation obtained analytically correctly describes the process.

5.2 Multi-species motility

At $t = 0$, sites $90 \leq x \leq 100$ were filled with red agents and sites $100 < x \leq 110$ were filled with green agents with the probability that a site is occupied being 0.75. Density profiles were obtained by averaging over 2500 realisations. One thing to note is that red and green agents do not mix if they start unmixed on the lattice in *one dimension*, as shown in figure 6(a). This does not happen in higher dimensions, as agents are able to move around each other.

The discrepancy between the advection-diffusion solutions and the density profiles appears to be quite great: the peaks are consistently undershot and the right tails are consistently overshot, as seen in figures 6(b) and 6(c). Due to this discrepancy, arrows were drawn on figures 6(b) and 6(c) to indicate increasing time, but the figures were captured at the same times as the single species process. Superficial reasons for this discrepancy may be due to incorrect derivations of the PDEs or that density profiles were not averaged over a sufficient number of realisations. However, upon adding the density profiles and solutions for the red and green subpopulations, as done in 6(d), we obtain the density profile and solution for the single species process, with a similarly high degree of accuracy as found for the original single species comparison. This suggests that the inaccuracy of the numerical solutions may lie with the numerical diffusion that is introduced when solving the PDEs on MATLAB. There is a distinct lack of control when using the pdepe.m routine to solve these equations and due to time constraints, it was not possible to write a program to solve the PDEs with more precision.

5.3 Mixed motility

Red (bullies) and green (weaklings) agents were placed on the lattice in the same manner as section 7.2, with density profiles obtained in the same manner as 7.1 and 7.2. In one
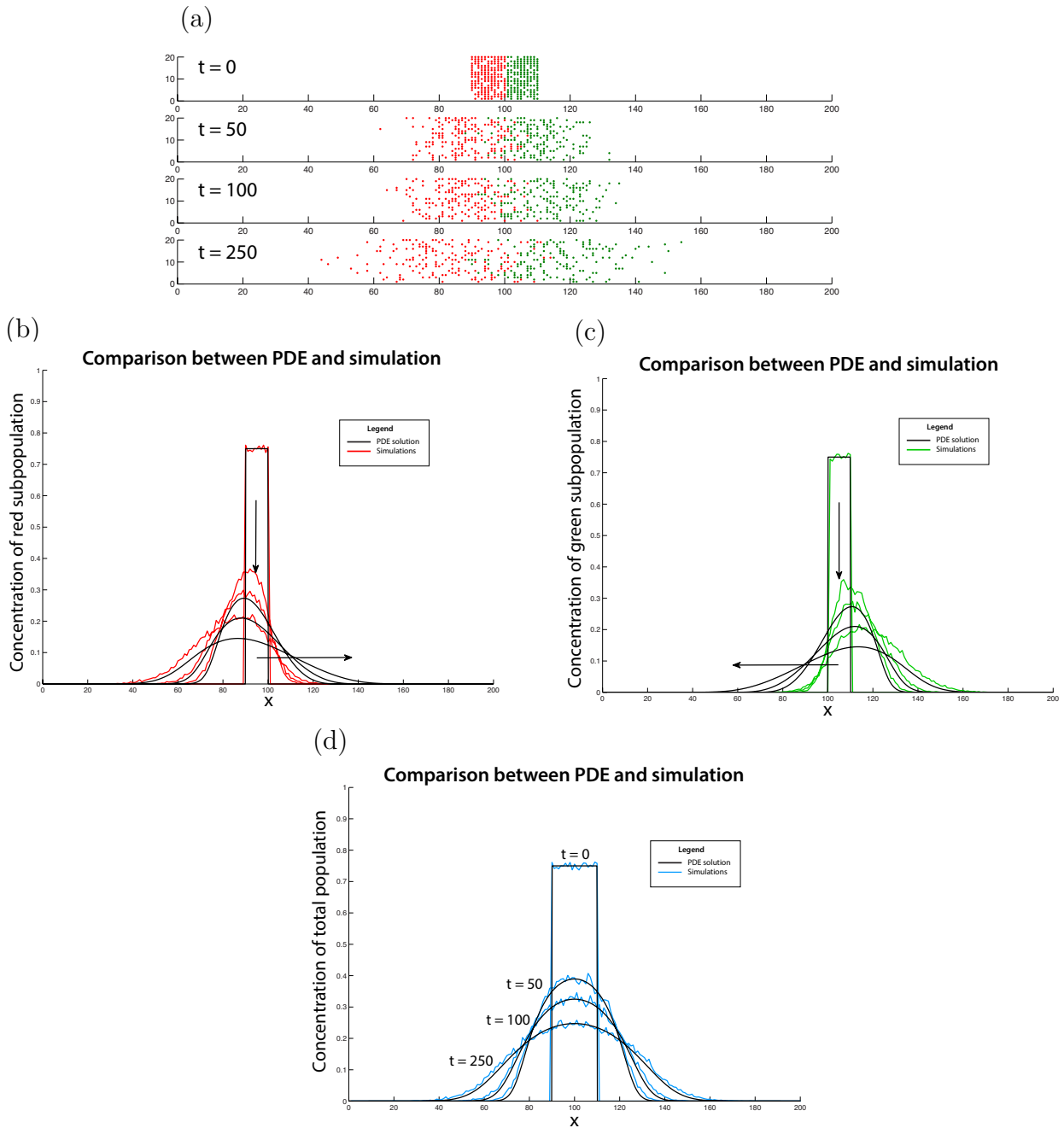
Figure 6: The multi-species process. (a) 20 stacked one-dimensional realisations. (b)-(c) Comparison between simulations and PDEs for red and green agents respectively. (d) The sum of the two subpopulation profiles and solutions.

dimension, mixing still does not occur if agents are placed unmixed on the lattice, since neither type of agents can move past each other. It can be seen in figure 7(a) that the weaklings tend to be clustered together. This is because the bullies can move in any di-
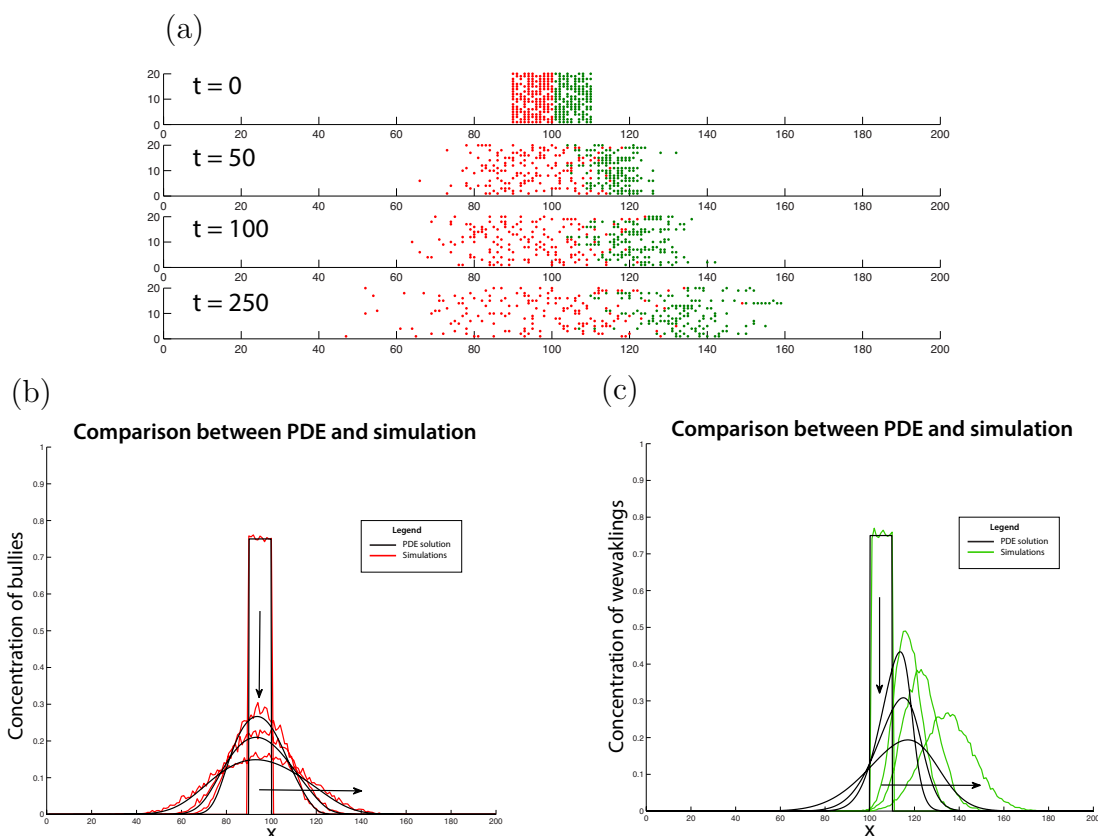
Figure 7: The mixed exclusion process. (a) 20 stacked one-dimensional realisations. (b)-(c) Comparison between simulations and PDEs for bullies and weaklings agents respectively. (d) The sum of the two subpopulation profiles and solutions.

rection, and as some begin to move to the right, the weaklings must also be shoved to the right. However, while some weaklings may have space to move to the left, they will never move past a bully agent, and so the subpopulation will cluster up, while moving on the whole towards the right.

The accuracy of the PDE solutions varies with the two subpopulations. Figure 7(b) shows that the solution of the governing PDE for the bullies subpopulation matches well with the results obtained from simulations – far better than the match between the shoving subpopulations in figures 6(b)-(c). However, there is a greater mismatch between the numerical solutions and the results from simulations for the weaklings subpopulation. The evolution of the peaks and tail ends appears to match the average density profiles, but the PDE wave solution does not propagate as fast as the wave derived from simulations. As there is no single species equivalent of this process, we cannot simply add the two solutions to determine if there is a problem with the analysis or with MATLAB. Previous issues encountered in the previous section and the fact that the general solution shape

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matches simulation results suggest that it is more likely to be the latter.

6   Discussion and conclusions

We have outlined an alternative model to a well-known and oft-used exclusion process and derived a partial differential equation describing this process. Comparisons against simulations have confirmed that this PDE is in fact the continuous analogue of this discrete motility mechanism. We have presented two variations of this process – multi-species processes involving the two exclusion processes outlined in this report – and derived sets of coupled PDEs for these processes. However, further research is required to confirm of these partial differential equations correctly describe these multi-species process. It is believed that the choice of numerical PDE solver plays a part in the discrepancy between the PDE solutions and results from simulations. It is likely that this is the main issue for the process describing two interacting subpopulations under the new mechanism. However, for the process of interacting subpopulations that obey different exclusion rules, it is uncertain if this is the only contribution to the discrepancy between results.

There are a number of areas to explore with this new process for future research. The first that comes to mind is to introduce bias in motion. It has been shown (Simpson et al, 2009b) that an asymmetric simple exclusion process leads to a nonlinear advection-diffusion equation. It would not be unreasonable to suppose the shoving process with bias would produce something similar, which has been confirmed by preliminary analysis. Another possibility would be to consider agents that can shove a distance $d \geq 1$. Preliminary analysis has also been done for this process, but the partial differential equation has not been confirmed to be correct for any value of $d > 1$. The final suggestion of significance would be to introduce the idea of 'weighted' shoves: agents can shove each other, but there is a weight κ of shoving that increases as the number N of agents that have to be shoved increases. This results in shoves of a high number of agents being less successful than shoves of a small number of agents. This weight may be expressed algebraically or exponentially.

7   AMSI experience

The AMSI vacation scholarship provided an excellent forum to gain a deeper insight into the world of academia and research. During the course of the program, I was not only able to put to use a number of skills obtained from my years as an undergraduate student, but also gain and refine other skills that I would not have had the opportunity to improve in

a typical classroom setting. Upon completion of my project, it now seems that research can be motivated by many different factors: previous research, curiosity, problems in nature, etc. Ultimately, the goal of research is, in my opinion, the pursuit of knowledge for knowledge's sake and for knowledge shared – a very admirable and noble pursuit.

The CSIRO Big Day In was an interesting experience. It was enjoyable to meet so many passionate and ambitious students from different universities and to listen to the wide and varied range of interesting talks they presented.

8   Acknowledgments

I would like to extend my sincerest gratitude and thanks to my supervisors, Barry Hughes and Kerry Landman, for their unlimited patience and guidance – in particular, for always prodding me in the right direction when conducting this research. Every meeting and discussion was of significant value and always provided something of insight to take away. I would also like to thank AMSI for granting me the opportunity to conduct this vacation project. For once, I can look back at my summer and say that I was productive with the majority of my time. Finally, I would like to thank the University of Melbourne Department of Mathematics and Statistics for providing such a welcoming and vibrant environment to conduct this vacation scholarship and for allowing me to make liberal use of the faculty tea and coffee with impunity.

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