

Trading Places: Agent exchange in diffusion processes

Adriana Zanca

Supervisors: Professor Kerry Landman and Professor Barry Hughes
The University of Melbourne

February 2014

In recent years, motivated largely by questions in developmental biology and tissue engineering [1], there has been considerable interest in systems of interacting, randomly-moving agents, including exclusion processes and more subtle inter-agent interacting systems. The purpose of this project is to investigate interacting agent systems in which agents occupying adjacent positions on a lattice are able to exchange positions (further to simple exclusion) [1]. A previous area of research was the effect of simple exclusion on multiple species systems [2]. This paper studies the effect of position exchanges on multiple species agent systems and compares these effects with the simple exclusion multiple species results. The project involves simulations, as well as mean-field based continuum approximations leading to partial differential equations [3].

1 Introduction

A square lattice is populated by random walkers, who will be referred to as ‘agents’ from now on, with a concentration C . These agents are able to be referred to as random walkers because they move in a sequence of random steps within the lattice [4]. This is a discrete-space, discrete-time agent-based model. An interacting agent system is one in which the behaviour of a single agent, or group of agents, has an effect on another agent, or group of agents [5,6]. Previously, interacting agent systems involving simple exclusion have been explored [2, 5, 7, 8, 13]. In simple exclusion processes, for any position on the lattice, no more than one agent can be occupying that particular

position at any time [2,5]. If another agent attempts to move into an occupied position, the move is aborted (see Figure 1). Here, a one-dimensional problem is considered, where agents have two possible directions of movement: left and right. The agents in the system are directed by unbiased movement, defining the simple exclusion process as symmetric [2,7]. Define P to be the probability of an agent being able to attempt to move, in this case there is probability $P/2$ of moving left and probability $P/2$ of moving right. Defining P allows control over the level of activity of the agents. In all simulations in this paper, P is defined to be 1 (maximum level of activity), in order to highlight the different properties of each of the systems. Agent-based systems allow the observer to track the movement of individual agents by tagging, or labelling, a particular agent as well as the movement of the population as a whole [2, 5, 7, 9, 10].

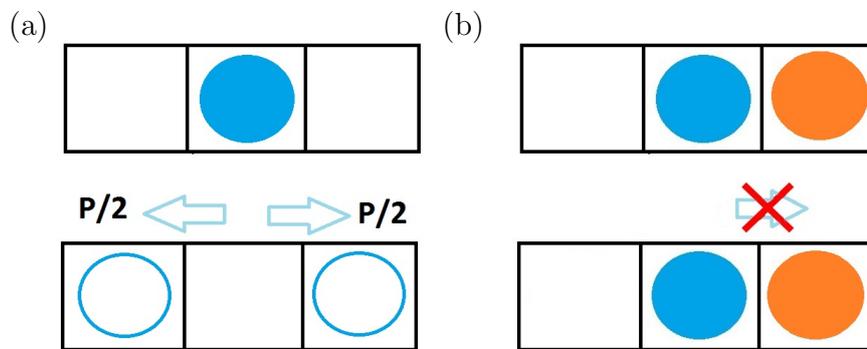


Figure 1: Simple exclusion: (a) The blue agent in the middle position has equal chance of moving left or right. Either direction results in a successful move. (b) If the blue agent in the middle attempts to move right, the move is aborted due to the orange agent in its way.

An alternative to simple exclusion is to consider an interacting agent systems where agent exchange is permitted to occur [1]. As in the simple exclusion case, agents are distributed on a one-dimensional lattice and permitted to randomly walk, with P being the probability that an agent is allowed an attempt to move. However, now if an agent attempts to move into an occupied position, the agent has probability β of exchanging positions with its neighbour, as opposed to having an aborted move (see Figure 2). Biological motivation of this type of process has been explored previously [1]. In both the simple exclusion and agent exchange cases, agents are only permitted to attempt to move one lattice space at a time. Step sizes greater than one are not considered, and hence the moves performed in these systems have local consequences.

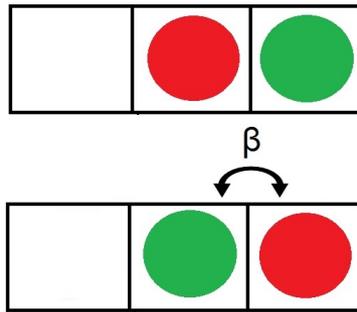


Figure 2: Trading places: if the red agent attempts to move to the right, it has probability β of swapping with the green agent.

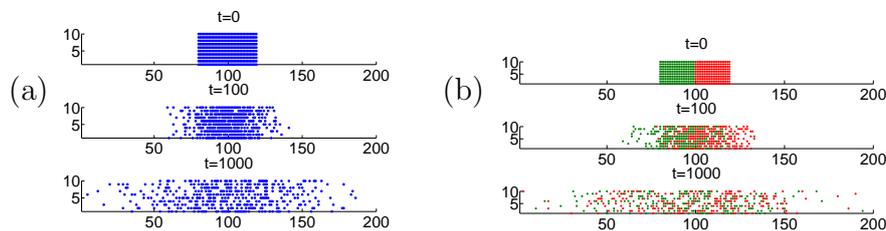


Figure 3: $\beta = 1.0$ (all swapping moves accepted) (a) Ten independent one-dimensional lattices populated by a single species of agents. (b) Ten independent one-dimensional lattices occupied by R and G species.

Due to the nature of swapping, it is desirable to consider the behaviour of subpopulations [1, 2, 5, 11, 13], or different species, not only single species systems. A single species of agents, C , can be defined as one where all agents behave in the same way (in this case either by simple exclusion or by exchanging positions with other agents) and are marked with the same ‘colour’ (as can be seen in Figure 3, above). Multi-species are defined as two groups who, like single species defined previously, all behave in the same fashion, however, are marked with different colours: red, R , and green, G . The R and G groups are subpopulations of the total population, C , such that $R + G = C$.

From average column occupancy statements, partial differential equations (PDEs) describing the movement of populations and subpopulations can be obtained [1–3, 12]. Independence of occupancy of neighbouring sites is assumed in this study and is crucial to the conservation of mass arguments in the average column occupancy statements used to derive the PDEs describing the movement of populations. If independence was

not assumed, correlation terms would need to be considered. Previously, it has been shown that correlation terms cancel for simple exclusion processes [3]. However, this may not be so for processes involving agent exchange. The presence of correlation terms would be clear in the case that the PDE solution showed significant difference to the simulation column averages. As the fit for the PDE solution compared to simulation was quite good, the independence assumption is suitable for the purposes of this paper.

Microscale properties of interacting agent systems are of considerable interest. Global population models for agent exchange in biological processes have been investigated [1]. To investigate microscale properties, a single agent is tagged in a system of agents (as opposed to subpopulations, where numerous agents are tagged and assigned a species). The location of the tagged agent is monitored and characteristics, such as the agent's net displacement and sum of squares displacement, are noted. Consideration of microscale behaviour is given in this paper.

2 Single Species

2.1 Derivation of Partial Differential Equations

Consider a one-dimensional lattice (all results given in this paper can be generalised to higher dimensions, however, the focus of this paper will be on one-dimensional cases). Let Δ be the lattice spacing and τ be a time increment. In order to describe the movement of a population, the change in occupancy at site $i \in \mathbb{Z}$ between time t and $t + \tau$ must first be considered. Average column occupancy statements arise by conservation of mass arguments (in these systems, the number of agents in the system is constant) [7]. For simple exclusion, it has been shown that the change in occupancy can be given by the master equation [7]:

$$C_i(t + \tau) - C_i(t) = \frac{P}{2} \{ [1 - C_i(t)]C_{i-1}(t) + [1 - C_i(t)]C_{i+1}(t) - [1 - C_{i-1}(t)]C_i(t) - [1 - C_{i+1}(t)]C_i(t) \}. \quad (1)$$

$C_i(t)$ in equation (1) represents site i being occupied at time t , and hence $[1 - C_i(t)]$ represents site i being vacant at time t . The $P/2$ term represents the equal chance of and agent moving left or right. In the braces on the right of equation (1) are terms representing the possibilities of movement into and out of site i by an agent. Those terms, from left to right, represent an agent at site $i - 1$ moving in to a vacant site

at site i , an agent at site $i + 1$ moving in to a vacant site at site i , an agent at site i moving out to a vacant site at $i - 1$ and an agent at site i moving out to a vacant site at $i + 1$. The positive terms symbolise moves that would increase the occupancy at site i and the negative terms symbolise moves that would decrease the occupancy at site i . As the lattice considered is one-dimensional, C_i is equal to 1 or 0 (exclusively) at any time. Since $0 \leq C_i \leq 1$, equation (1) can be interpreted as a probability statement.

Equation (1) must be converted from a discrete to a continuous statement. In order to make this conversion, let $x = i\Delta$ and $t = k\tau$. Thus the discrete term $C_i(t)$ becomes the continuous variable, $C(x, t)$ (further, $C_{i-1}(t)$ becomes $C(x - \Delta, t)$ and $C_{i+1}(t)$ becomes $C(x + \Delta, t)$). Taking Taylor series expansions, keeping terms up to order $\mathcal{O}(\Delta^2)$, gives:

$$C_{i+1}(t) = C(x, t) + \Delta \frac{\partial C(x, t)}{\partial x} + \frac{\Delta^2}{2} \frac{\partial^2 C(x, t)}{\partial x^2} + \mathcal{O}(\Delta^3), \quad (2)$$

and

$$C_{i-1}(t) = C(x, t) - \Delta \frac{\partial C(x, t)}{\partial x} + \frac{\Delta^2}{2} \frac{\partial^2 C(x, t)}{\partial x^2} + \mathcal{O}(\Delta^3). \quad (3)$$

Making the appropriate substitutions, as described above in equations (2) and (3), into equation (1) and simplifying terms yields:

$$C_i(t + \tau) - C_i(t) = \frac{P\Delta^2}{2} \frac{\partial^2 C(x, t)}{\partial x^2}. \quad (4)$$

Dividing equation (4) by τ , taking the limit as $\Delta, \tau \rightarrow 0$ jointly and holding Δ^2/τ constant gives the PDE describing the movement for a population of agents in a simple exclusion process [7] ($C(x, t)$ will now be written as C for brevity):

$$\frac{\partial C}{\partial t} = D_0 \frac{\partial^2 C}{\partial x^2}, \quad (5)$$

where

$$D_0 = \frac{P}{2} \lim_{\Delta^2, \tau \rightarrow 0} \frac{\Delta^2}{\tau}. \quad (6)$$

Equation (5) is a linear diffusion equation. It is a parabolic PDE equivalent to the one-dimensional case of the heat equation. The form of this equation is critical to the success of its solution matching simulation results, as discussed in section 4, below.

2.2 Incorporating Agent Exchange

The master equation for agent exchange processes has the same terms as simple exclusion, to incorporate movement, as well as additional terms to include swapping, highlighted in red font in equation (7), below:

$$C_i(t + \tau) - C_i(t) = \frac{P}{2} \{ [1 - C_i(t)]C_{i-1}(t) + [1 - C_i(t)]C_{i+1}(t) - [1 - C_{i-1}(t)]C_i(t) - [1 - C_{i+1}(t)]C_i(t) + \beta [C_{i-1}C_i(t) + C_{i+1}(t)C_i(t) - C_i(t)C_{i-1}(t) - C_i(t)C_{i+1}(t)] \}. \quad (7)$$

β represents the probability of a successful swapping move. The terms in the larger, red, square bracket from left to right represent an agent at site $i - 1$ swapping with an agent at site i , an agent at site $i + 1$ swapping with an agent at site i , an agent at site i swapping with an agent at site $i - 1$ and an agent at site i swapping with an agent at site $i + 1$. Note that these terms cancel out, and therefore, including swapping in the single species case does not alter the master equation, irrespective of the value of β . Hence, the PDE describing the movement of a single species of agents in an agent exchange process is the same as that for a single species simple exclusion process, the diffusion equation (5).

3 Multiple Species

3.1 Simple Exclusion

In the situation that there are two species in the system, R and G , each species will have a PDE describing the movement of the sub-population. For the simple exclusion case, the master equation governing the movement of the R species is given by:

$$R_i(t + \tau) - R_i(t) = \frac{P}{2} \{ [1 - R_i(t) - G_i(t)]R_{i-1}(t) + [1 - R_i(t) - G_i(t)]R_{i+1}(t) - [1 - R_{i-1}(t) - G_{i-1}(t)]R_i(t) - [1 - R_{i+1}(t) - G_{i+1}(t)]R_i(t) \}. \quad (8)$$

From left to right, the terms in the braces on the right of equation (8) represent an R agent at site $i - 1$ moving in to a vacant site at site i , an R agent at site $i + 1$ moving in to a vacant site at site i , an R agent at site i moving out to a vacant site at site $i - 1$ and an R agent at site i moving into a vacant site at site $i + 1$. Note that adding the R and G species equates to a single population, as described previously,

$R + G = C$. Using the same process as was described in section 2.1, it is found that the PDE describing the movement of the R species [5] is:

$$\frac{\partial R}{\partial t} = D_0 \frac{\partial}{\partial x} \left\{ (1 - R - G) \frac{\partial R}{\partial x} + R \frac{\partial}{\partial x} (R + G) \right\}. \quad (9)$$

D_0 is defined as in equation (6). The PDE for the G species can be obtained by exchanging R 's and G 's in equation (9) (since both subpopulations have the same behaviour here). Equation (9), the equation governing the movement of subpopulations, has key differences to the diffusion equation describing the movement of a single population, equation (5). Equation (9) is not a parabolic PDE, it is an advection-diffusion, or convection, equation with hyperbolic terms. The presence of hyperbolic terms is of great importance in section 4. Summing the PDEs of the R and G species appropriately produces equation (5). This is to be expected, as $R + G = C$.

3.2 Agent exchange

Including exchanging moves, the master equation for the R species has the same terms to account for movement as in (8), with additional terms for swap moves, written in red font in equation (10), below:

$$\begin{aligned} R_i(t + \tau) - R_i(t) = & \frac{P}{2} \{ [1 - R_i(t) - G_i(t)] R_{i-1}(t) + [1 - R_i(t) - G_i(t)] R_{i+1}(t) \\ & - [1 - R_{i-1}(t) - G_{i-1}(t)] R_i(t) - [1 - R_{i+1}(t) - G_{i+1}(t)] R_i(t) \\ & + \beta [G_i(t) R_{i-1}(t) + G_i(t) R_{i+1}(t) - R_i(t) G_{i-1}(t) - R_i(t) G_{i+1}(t)] \}. \end{aligned} \quad (10)$$

β is the probability of a successful swap (the same for each subpopulation). $\beta = 0$ represents the simple exclusion case and $\beta = 1$ represents all swapping moves being successful. From left to right, the terms in the larger red square bracket of equation (10) symbolise an R agent at site $i - 1$ swapping with a G agent at site i , an R agent at site $i + 1$ swapping with a G agent at site i , an R agent at site i swapping with a G agent at site $i - 1$ and an R agent at site i swapping with a G agent at site $i + 1$. Using the techniques as described in section 2.1, the PDE describing the movement of the population of R agents in a process including agent exchange is:

$$\frac{\partial R}{\partial t} = D_0 \frac{\partial}{\partial x} \left\{ (1 - R - G) \frac{\partial R}{\partial x} + R \frac{\partial}{\partial x} (R + G) + \beta \left(G \frac{\partial R}{\partial x} - R \frac{\partial G}{\partial x} \right) \right\}. \quad (11)$$

Again, D_0 is as defined in equation (6) and the advection-diffusion equation describing the movement of the G population is obtained by exchanging R 's for G 's and vice versa. Summing the advection-diffusion equations for R and G species does result in the diffusion equation for a single species, equation (5).

In the case that $\beta = 1$, the PDE describing the movement of the R population is:

$$\frac{\partial R}{\partial t} = D_0 \frac{\partial^2 R}{\partial x^2}. \quad (12)$$

Equation (12) is a diffusion equation with no advection terms. $\beta = 1$ is the only value of β that produces a diffusion equation with no advection terms in a subpopulation - this result is particularly important when comparing PDE solutions with simulation results. Note that equation (12) is the same as equation (4), exchanging C 's for R 's. This signifies that when all swapping moves are accepted, a subpopulation of swapping agents will behave in the same way as a single population of agents in an exclusion process.

4 Simulation

To gain insight into the processes involved in agent exchange and simple exclusion, simulations were conducted using the numerical computing environment, MATLAB. Agents were selected to move by *random sequential update* [5]. Random sequential update is a process whereby an agent is chosen at random and is given the opportunity to move. The agent moves with probability P . Irrespective of whether or not a move was successful, another agent is selected at random, independently of the previous selection. The independence of selections results in some agents being chosen to move many times and others not at all. On average, agents will be chosen once per time step. Define N to be the number of agents in a system. In any one time step, N independent selections are made.

Simulation results required several (ten [example shown in Figure 3, section 1] or twenty for block initial conditions and 100 or 200 for mirrored triangle initial conditions) independent rows of one-dimensional simulations to be run simultaneously, with a variety of different initial conditions tested (see Figures 4, 5, 6, 7 and 8). Block initial conditions are those in which a certain number of columns, all grouped together all have a uniform initial concentration, for example the columns $80 \leq x \leq 120$ all having an initial concentration of $C = 0.2$. Mirrored triangle initial conditions require one

subpopulation to have an initial concentration of a certain level at a starting column and concentration decreases linearly for all subsequent columns, for example, the concentration of a red species being governed by the equation, $C = 0.2 - (0.0125)(x - 80)$. The term ‘mirrored’ refers to the fact that the other subpopulation (the green species) will have the same initial condition in reverse, instead of having the initial concentration $C = 0.2 - (0.0125) * (x - 80)$, (red species) the green species initial concentration will be governed by $C = (0.0125)(x - 80)$, this can be seen in Figure 8. The different number of repeats for the different initial conditions in Figures 4, 5, 6, 7 and 8 reflect the differing complexity and computing time for different initial conditions.

Column averages for every column were taken and plotted at times indicated in the figures. PDE solutions were calculated using an in-built PDE solver and plotted on the same graphs as the simulation results. Zero-flux boundary conditions were implemented (thus, simulation times were restricted so as not to let agents reach the boundaries of the lattice they are occupying). Figures 4, 5, 6, 7 and 8 (shown below), compare the PDE solution with simulation column averages over many simulation runs. Ideally, the PDE solution would match the simulations. For the single species cases (shown in the first columns of Figures 4, 5, 6, 7 and 8), the PDE solution matches the simulations results very well. This is because the PDE governing the movement of a single species (the same for both simple exclusion and agent exchange cases) is the one-dimensional heat equation (only parabolic differential terms are present). The in-built PDE solver can solve the heat equation with a high level of accuracy. However, the equations governing the movement of subpopulations also contain advection (hyperbolic) terms that the in-built solver cannot solve as well as pure diffusion. To combat these effects, a number of different initial conditions were trailed. Different initial boundaries and lower initial concentration of agents produced a better match between simulation and PDE solutions (as seen when comparing Figure 4 and 5 with Figures 5, 6 and 7).

The solution to the simple exclusion PDE ($\beta = 0$) in the multiple species case is known to fit simulation results well up to high initial densities, from previous papers [2, 5] (the simulations in referenced papers were completed using different programs). Figures 6 and 7 have particularly small values for initial concentration ($C = 0.01$), for values of C above 0.2, the PDE solutions given by the in-built solver do not match simulations well. The issue regarding initial concentration remains to be resolved. The solution is programming a PDE solver that can solve advection-diffusion equations to greater degree of accuracy and allow more control over parameters. A user-

programmed solver would result in the simulation results and PDE solutions matching better than the results seen in Figure 4 and 5 and at higher densities than those shown in Figures 6, 7 and 8.

The only value of β for which comparisons between simulation results for subpopulations and PDE solutions are particularly poor are when $\beta = 0$. However, the PDE solution not matching subpopulation simulations for the simple exclusion case does not make results for other values of β invalid. The PDE solution matches the simulation results better for non-zero values of β because advection terms have a smaller contribution for these values. As discussed in section 3, $\beta = 1$ gives a diffusion equation with no advection terms, and accordingly, the comparison between simulations and PDE solutions when $\beta = 1$ produces a close fit. Developing one's own PDE solver would confirm the accuracy of the fit shown in Figures 4, 5, 6, 7 and 8 for non-zero values of β . Note that independence of occupancy of sites could also contribute to a poor fit between PDE solutions and simulation results. It is known that there is independence of average column occupancy for $\beta = 0$ [5, 7], thus this assumption cannot account for the poor fit for that particular value. On the other hand, the fair match for other values of β show that the independence of occupancy of sites assumption is acceptable for those cases.

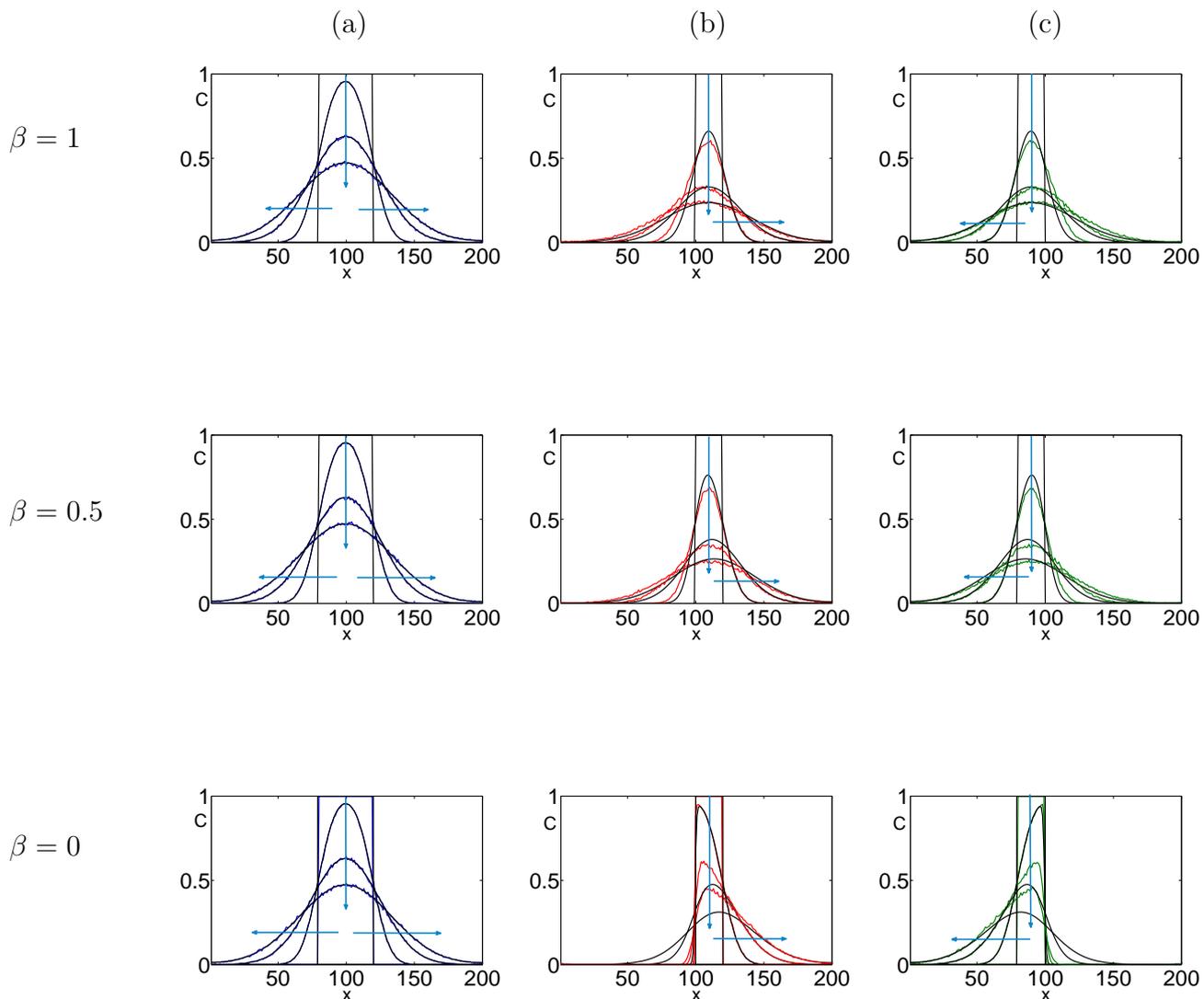


Figure 4: Block initial conditions: G fully occupies $80 \leq x \leq 99$, R fully occupies $100 \leq x \leq 119$, $t = 0, 100, 500, 1000$, averaged over 500 repeats. PDE solutions displayed in thick black line. Arrows indicate increasing time. (a) Sum of the R and G sub-populations (equivalent to observing a total population), simulations displayed in blue, thinner line. (b) R species, simulations displayed in red, thinner line. (c) G species, simulations displayed in green, thinner line. (Increasing the value of β increases the spread of the agents.)

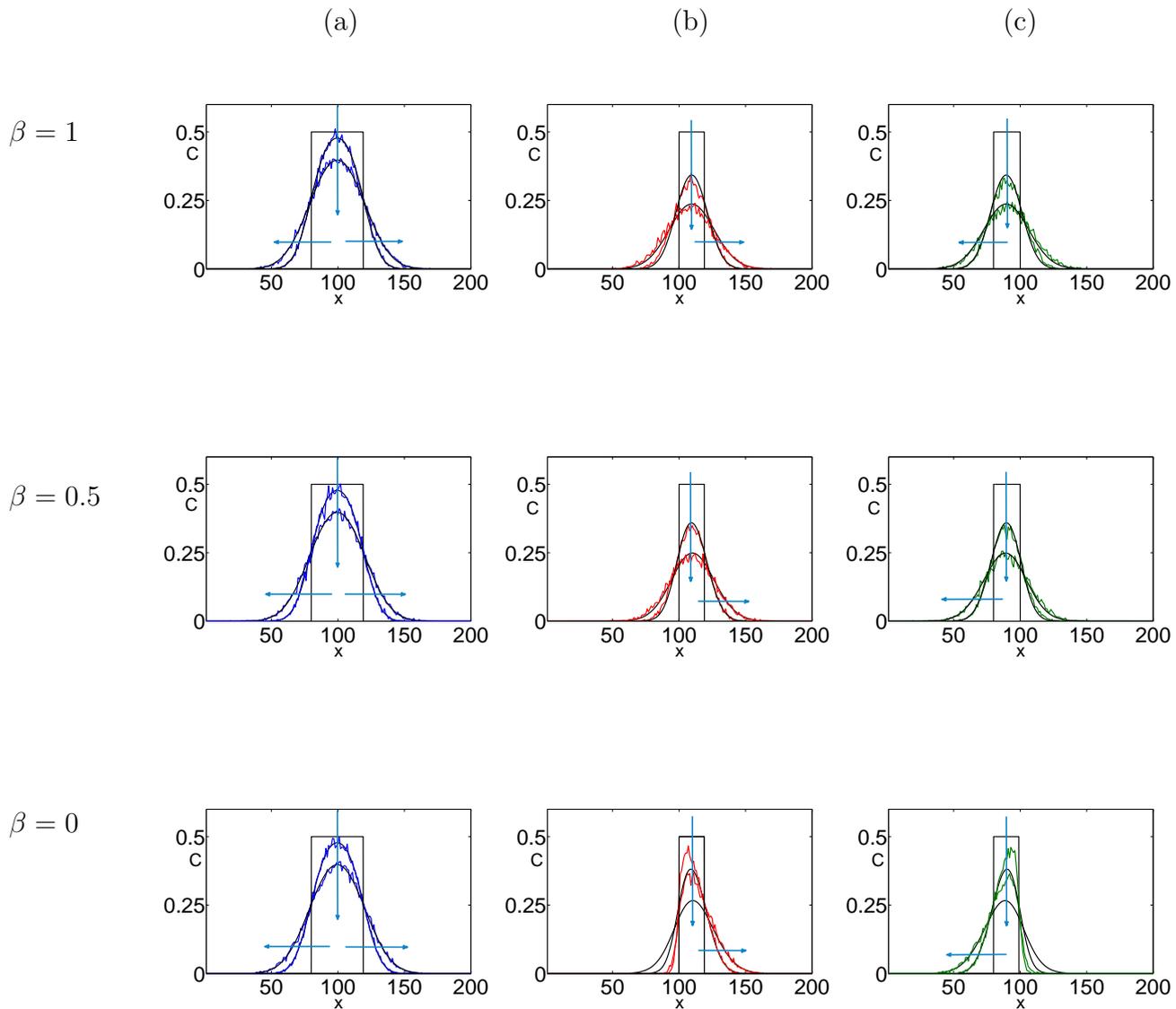


Figure 5: Block initial conditions: G occupies $80 \leq x \leq 99$ with concentration 0.5, R occupies $100 \leq x \leq 119$ with concentration 0.5. $t = 0, 100, 250$, averaged over 100 repeats. PDE solutions displayed in thick black line. Arrows indicate increasing time. (a) Sum of the R and G sub-populations (equivalent to observing a total population), simulations displayed in blue, thinner line. (b) R species, simulations displayed in red, thinner line. (c) G species, simulations displayed in green, thinner line.

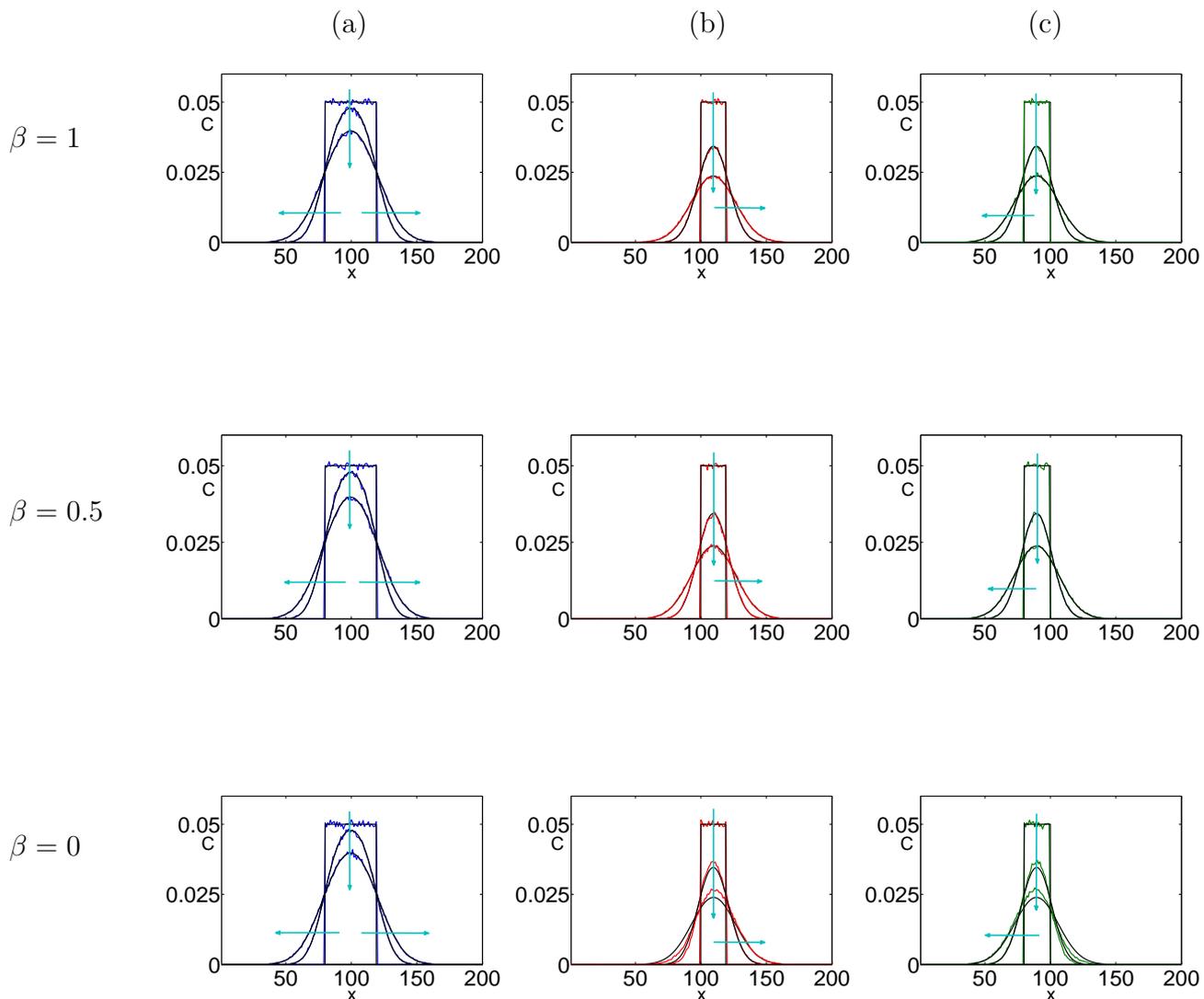


Figure 6: Block initial conditions: G occupies $80 \leq x \leq 99$ with concentration 0.05, R occupies $100 \leq x \leq 119$ with concentration 0.05. $t = 0, 100, 300, 500$, averaged over 10000 repeats. PDE solutions displayed in thick black line. Arrows indicate increasing time. (a) Sum of the R and G sub-populations (equivalent to observing a total population), simulations displayed in blue, thinner line. (b) R species, simulations displayed in red, thinner line. (c) G species, simulations displayed in green, thinner line.

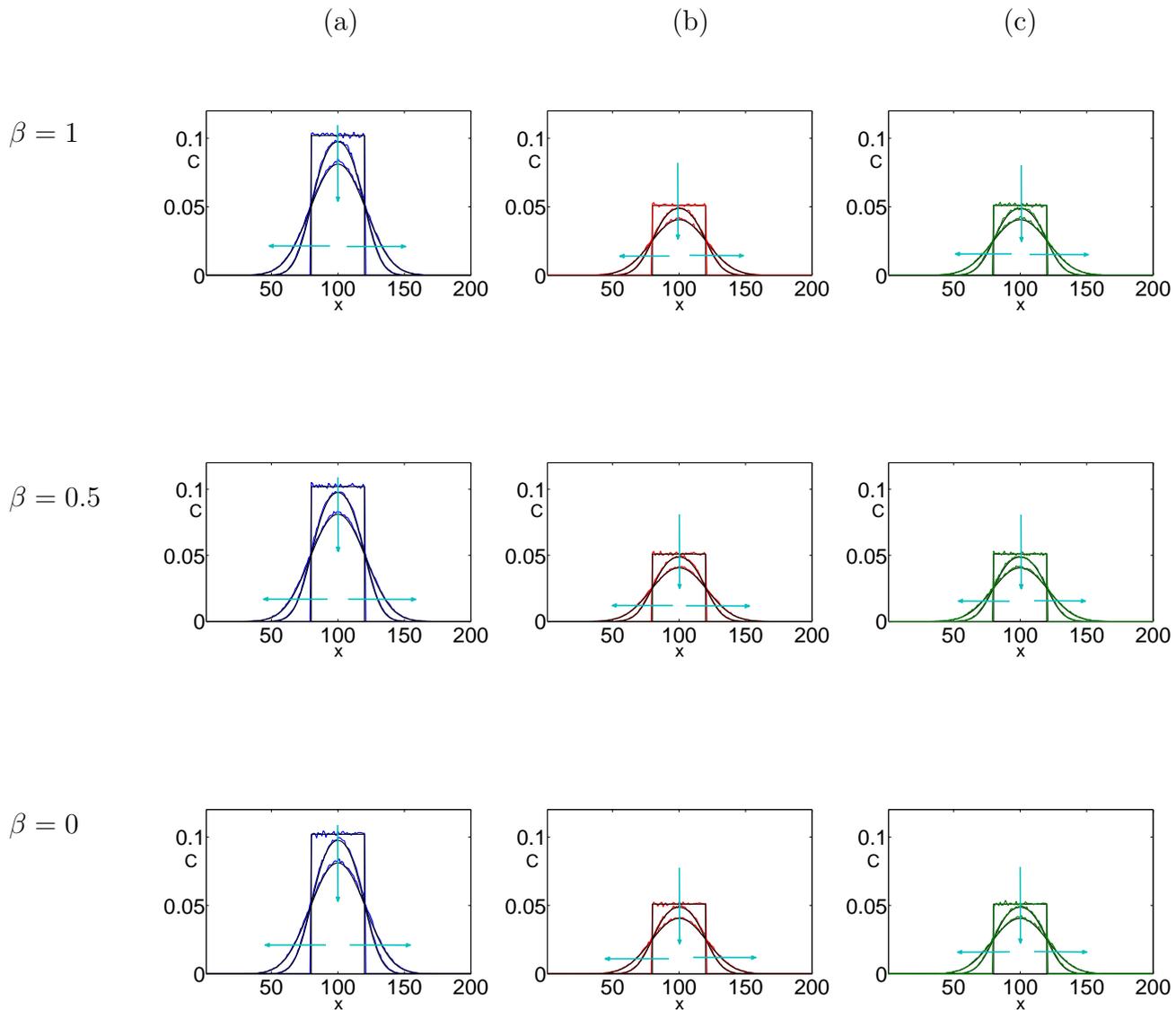


Figure 7: Mixed initial conditions: G and R occupies $80 \leq x \leq 120$ with concentration 0.1, $t = 0, 100, 300, 500$, averaged over 10000 repeats. PDE solutions displayed in thick black line. Arrows indicate increasing time. (a) Sum of the R and G sub-populations (equivalent to observing a total population), simulations displayed in blue, thinner line. (b) R species, simulations displayed in red, thinner line. (c) G species, simulations displayed in green, thinner line.

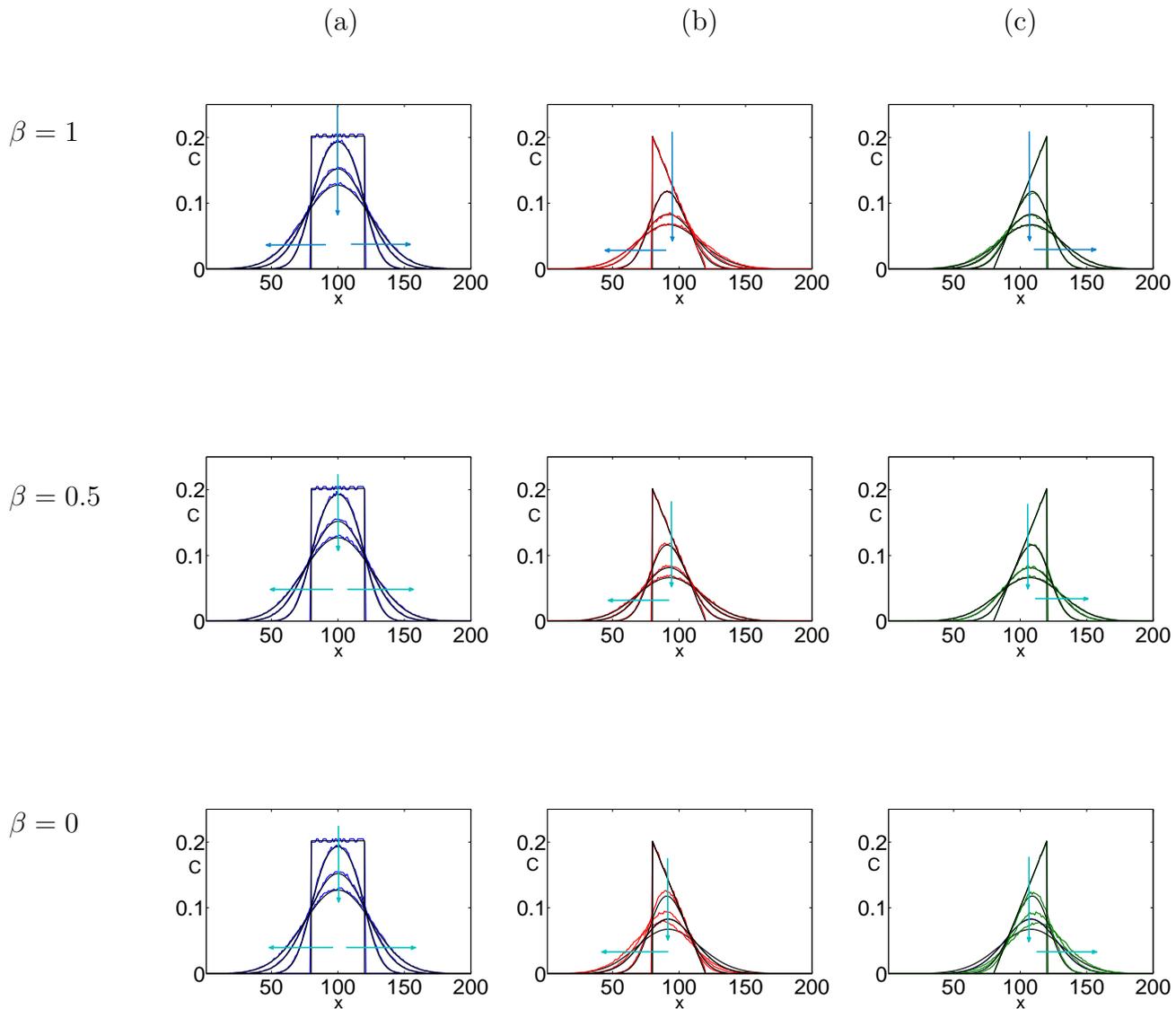


Figure 8: Initial conditions: Mirrored triangle (described above), $t = 0, 100, 300, 500$, averaged over 250 repeats. PDE solutions displayed in thick black line. Arrows indicate increasing time. (a) Sum of the R and G sub-populations (equivalent to observing a total population), simulations displayed in blue, thinner line. (b) R species, simulations displayed in red, thinner line. (c) G species, simulations displayed in green, thinner line.

5 Including Bias

5.1 Single Species

Consider equation (1), the master equation for a symmetric simple exclusion process. Equation (1) can be generalised to incorporate bias in movement. Processes with bias are no longer symmetric, they are asymmetric [2, 7]. In order to include bias, hence converting equation (1) into its appropriate asymmetric form, the master equation must include extra components to account for the weighting in the direction of moves. The master equation for a single species simple exclusion process with bias on a one-dimensional lattice, equation (1) transformed [7], is:

$$C_i(t + \tau) - C_i(t) = \frac{P}{2} \{ \color{blue}{(1 + \rho)} [1 - C_i(t)] C_{i-1}(t) + \color{blue}{(1 - \rho)} [1 - C_i(t)] C_{i+1}(t) \\ - \color{blue}{(1 - \rho)} [1 - C_{i-1}(t)] C_i(t) - \color{blue}{(1 + \rho)} [1 - C_{i+1}(t)] C_i(t) \}, \quad (13)$$

where the terms in blue are the terms added to equation (1) representing bias. $-1 \leq \rho \leq 1$ determines the weighting of the bias. Negative values of ρ signify bias to the left and positive values of ρ signify bias to the right. $\rho = 0$ states that there is no bias (as in the systems mentioned in previous sections) [7]. Using the same technique as described in section 2.1, the PDE describing the movement of the total population [7] is:

$$\frac{\partial C}{\partial t} = D_0 \frac{\partial^2 C}{\partial x^2} - V_0 \frac{\partial}{\partial x} (C[1 - C]), \quad (14)$$

where D_0 is defined as in equation (6) and V_0 is defined as:

$$V_0 = P\rho \lim_{\Delta, \tau \rightarrow 0} \frac{\Delta}{\tau}. \quad (15)$$

Agent exchange involves two agents (rather than one, as in a simple exclusion move). This results in agent exchange being an inherently symmetric problem. Bias cannot be introduced into swap moves as defined in this paper, since in a swap move, one of the agents must move to the left and the other must move to the right, with respect to their initial position, and all agents have the same probability of swapping. It follows that for a single species, the master equation and resulting PDE governing the movement of a population of agents allowed to perform agent exchange moves is the same as that for simple exclusion bias case, equations (13) and (14).

5.2 Multi-Species

Considering multi-species, a difference exists between the simple exclusion and agent exchange processes. The bias analogue of equation (8), simple exclusion multi-species, is given by:

$$R_i(t+\tau) - R_i(t) = \frac{P}{2} \{ (1 + \rho)[1 - R_i(t) - G_i(t)]R_{i-1}(t) + (1 - \rho)[1 - R_i(t) - G_i(t)]R_{i+1}(t) - (1 - \rho)[1 - R_{i-1}(t) - G_{i-1}(t)]R_i(t) - (1 + \rho)[1 - R_{i+1}(t) - G_{i+1}(t)]R_i(t) \}, \quad (16)$$

where ρ has the same definition as previously and blue font indicates a term introduced into equation (8) to incorporate bias. The PDE [2,5] resulting from this master equation is:

$$\frac{\partial R}{\partial t} = D_0 \frac{\partial}{\partial x} \left\{ R \frac{\partial G}{\partial x} - [-1 + G] \frac{\partial R}{\partial x} \right\} - V_0 \frac{\partial}{\partial x} \{ R[1 - G - R] \}. \quad (17)$$

D_0 is defined as in equation (6) and V_0 defined by equation (15). As previously, exchanging R s for G s and vice versa results in the PDE for the G species and adding the PDEs for both species gives the single species PDE, equation (16). The bias analogue of equation (10) is:

$$R_i(t+\tau) - R_i(t) = \frac{P}{2} \{ (1 + \rho)[1 - R_i(t) - G_i(t)]R_{i-1}(t) + (1 - \rho)[1 - R_i(t) - G_i(t)]R_{i+1}(t) - (1 - \rho)[1 - R_{i-1}(t) - G_{i-1}(t)]R_i(t) - (1 + \rho)[1 - R_{i+1}(t) - G_{i+1}(t)]R_i(t) + \beta[G_i(t)R_{i-1}(t) + G_i(t)R_{i+1}(t) - G_{i-1}(t)R_i(t) - G_{i+1}(t)R_i(t)] \}. \quad (18)$$

Leading to the PDE (by the process described in section 2.1):

$$\frac{\partial R}{\partial t} = D_0 \frac{\partial}{\partial x} \left\{ [1 - \beta]R \frac{\partial G}{\partial x} + [1 + (-1 + \beta)G] \frac{\partial R}{\partial x} \right\} - V \frac{\partial}{\partial x} \{ R[1 - G - R] \} \quad (19)$$

$$= D_0 \frac{\partial}{\partial x} \left\{ R \frac{\partial G}{\partial x} - [-1 + G] \frac{\partial R}{\partial x} + \beta \left[G \frac{\partial R}{\partial x} - R \frac{\partial G}{\partial x} \right] \right\} - V_0 \frac{\partial}{\partial x} \{ R[1 - G - R] \} \quad (20)$$

Note that ρ does not appear in terms that involve β , reflecting the lack of bias in agent exchange moves.

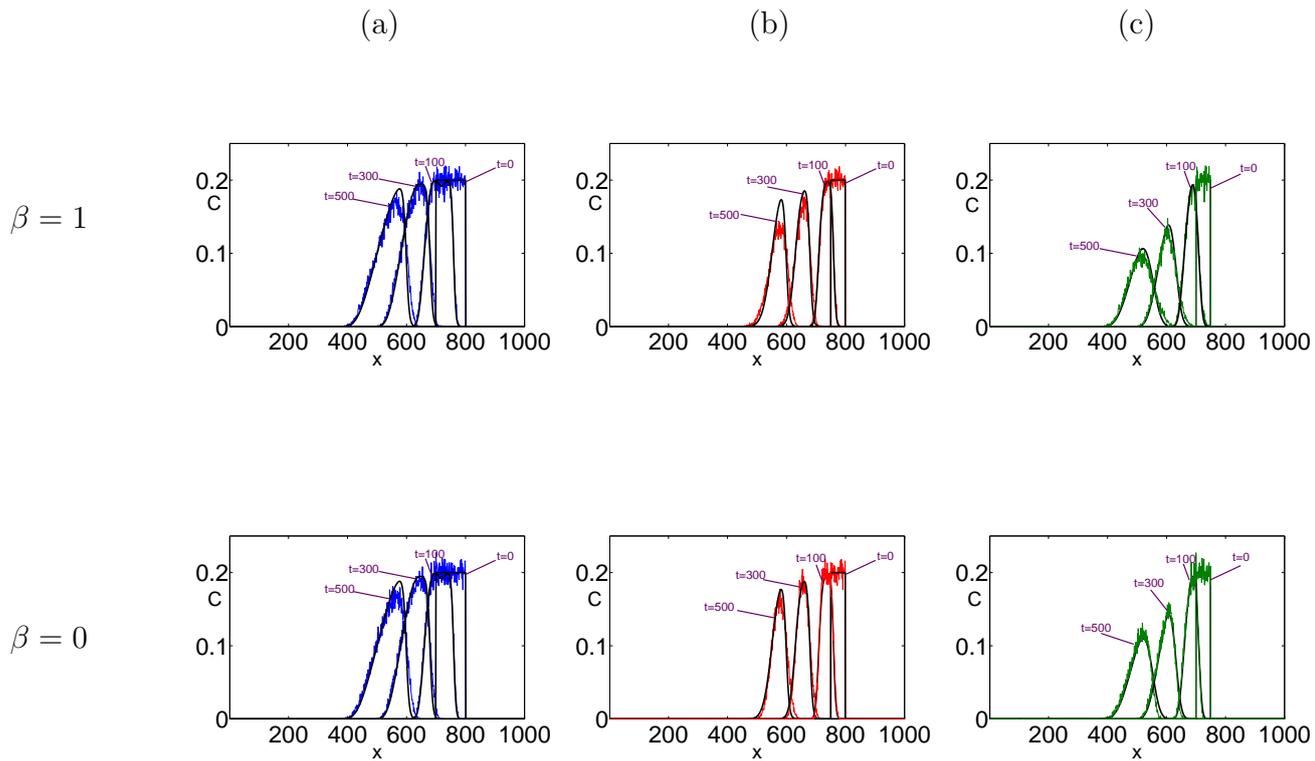


Figure 9: Block initial conditions: G occupies $700 \leq x \leq 749$ with initial concentration 0.2 and R occupies $750 \leq x \leq 799$ with initial concentration 0.2. $t = 0, 100, 300, 500$, averaged over 200 repeats. $\rho = -0.5$ (left bias). PDE solutions displayed in thick black line. (a) Sum of the R and G sub-populations (equivalent to observing a total population), simulations displayed in blue, thinner line. (b) R species, simulations displayed in red, thinner line. (c) G species, simulations displayed in green, thinner line.

6 Microscale Models

Thus far, the movement of populations have been considered. Another area of interest is the movement of individual agents in the system. As previously, the system will involve agents who all move in the same manner, with the same probability of movement and agent exchange for every agent. Again the symmetric, unbiased case is considered ($\rho = 0$). The one-dimensional lattice is randomly populated, with agent concentration in the lattice denoted by C . From this system, an agent is selected at random and ‘tagged’. Tagging allows the observer to identify where the individual tagged agent is at any time. The net displacement and sum of squares displacement for the agent for different values of β are considered. Net displacement is calculated by [7]:

$$X_t - X_0 = \sum_{k=1}^t (X_k - X_{k-1}). \quad (21)$$

X_t denotes the position of the tagged agent at time t . In order to study statistical fluctuations, the sum of squares displacement is also investigated. This is given by [7]:

$$S_t = \sum_{k=1}^t (X_k - X_{k-1})^2. \quad (22)$$

It is known that in a simple exclusion process ($\beta = 0$), the sum of squares displacement is density dependent and given by [5, 7]:

$$S_t \approx P(1 - C), \quad (23)$$

where C is the concentration of agents in the system. When $C = 1$ (full occupancy of the lattice) and $\beta = 0$ (no swapping moves), $S_t = 0$; no individual agent is able to move. This is shown in Figure 10(a), where simulation results are compared with the line $S_t = P(1 - C)$.

Empirical results suggest that for $0 \leq \beta \leq 1$, the movement of an individual agent can be described by:

$$S_t \approx P\{(1 - C) + 2\beta C\}. \quad (24)$$

These results can be seen in Figure 10. The factor of two in front of the βC term arises due to there being two agents moving per swapping move. Thus, an agent does not need to be selected to move in order to change position on the lattice. If a neighbouring site is occupied, an agent may move positions by swapping without being

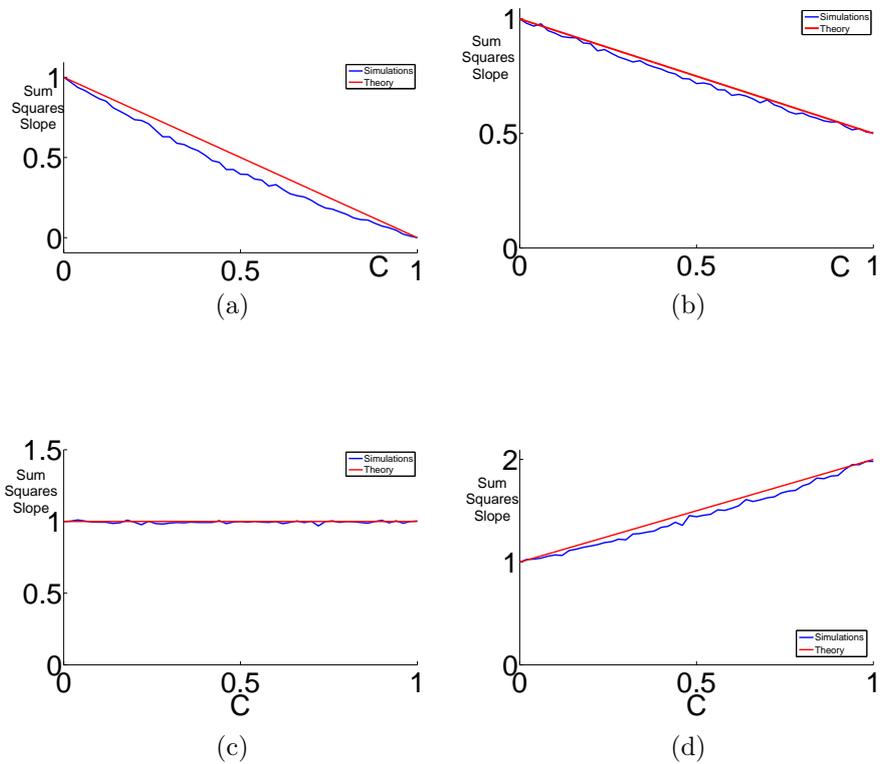


Figure 10: Sum of squares slope (shown in blue) compared with its expected value (shown in red). Averaged over 100 repeats. $t = 500$. (a) $\beta = 0.0$ (b) $\beta = 0.25$ (c) $\beta = 0.5$ (d) $\beta = 1.0$

the random agent selected to move. If only half of the swapping moves are accepted, on average, all agents will still swap once per time step in a crowded lattice. S_t is a time-dependent parameter, simulation results show the slope of S_t , where the slope of the curve is independent of time. That a successful agent exchange move always involves two agents and is a symmetric process has a large influence on the behaviour of individuals within the population.

7 Conclusion

Insight has been gained into agent exchange systems on a macroscale and microscale level. It has been found that including agent exchange in a simple exclusion process does not have any effect on the movement of the total population. However, when considering subpopulations and the movement of individual agents, agent exchange has a dramatic effect. For a finite one-dimensional lattice fully occupied, with agents obeying simple exclusion, colouring the left half of the population red and the right half green, observations at any time would show the same result - there is no movement. On the other hand, if agents are permitted to swap places, there is a lot of movement and the red and green become evenly mixed over time. If all swapping moves are accepted, then the sub-populations behave in the same manner as a single population of simple exclusion agents. On the microscale, introducing agent exchange allows much greater movement of individual agents. Future work would involve developing a PDE solver that can solve advection-diffusion equations with greater accuracy, resulting in PDE solutions matching simulations more closely and examining correlation between occupancy of lattice sites for agent exchange processes.

The moves in this paper have had local consequences as each step size for moving and swapping is equal to one. To generalise swapping and simple exclusion moves to any step size, $d \in \mathbb{N}$, would have a profound effect on the PDEs governing the movement of populations, as well as individuals within the population. It would be expected that when $d > 1$ the populations would spread much more quickly than the case considered here, where $d = 1$.

Though it has been shown that agent exchange is a symmetric process involving two agents, breaking a population into smaller populations (say three or four subpopulations) and giving different weights to successful swaps would produce new and interesting results (in this paper, the same weighting has been given to each subpopulation). Allowing more than one agent to occupy a lattice site could also potentially be of interest. A number of different unexplored rules could be trialled, each with differing applications. For future research, the possibilities are endless.

Acknowledgements

I wish to thank my supervisors, Professor Kerry Landman and Professor Barry Hughes for their support, guidance and patience throughout the duration of my project. Further, I wish to thank AMSI and The University of Melbourne for allowing me to undertake this research over the summer. Finally, I wish to thank everyone who has contributed to my project by discussing mathematics and various other topics with me; particularly, other AMSI scholars and masters students at The University of Melbourne, as well as those who have proof-read this paper.

References

- [1] Painter, KJ 2009, 'Continuous Models for Cell Migration in Tissues and Applications to Cell Sorting via Differential Chemotaxis', *Bulletin of Mathematical Biology*, vol. 71, pp. 1117-1147.
- [2] Simpson, MJ, Landman, KA & Hughes, BD 2009, 'Multi-species simple exclusion processes', *Physica A*, vol. 388, pp.399-406.
- [3] Penington, CJ, Hughes, BD & Landman, KA 2011, 'Building macroscale models from microscale probabilistic models: a general probabilistic approach for nonlinear diffusion and multi-species phenomena', *Physical Review E*, vol. 84, 041120.
- [4] Hughes, B.D 1995, *Random Walks and Random Environments*, Vol. 1, Oxford University Press.
- [5] Landman, KA & Fernando, AE 2011, 'Myopic random walkers and exclusion processes: Single and multispecies', *Physica A*, vol. 390, pp. 3742-3753.
- [6] Janssen, MA & Ostrom, E 2006, 'Empirically Based, Agent-based models', *Ecology and Society*, vol. 11, iss. 2, art. 37.
- [7] Simpson, MJ, Landman, KA & Hughes, BD 2009, 'Diffusing Populations: Ghosts or Folks?', *Australasian J Eng Education*, vol. 15, pp.59-67.
- [8] Chowdhury, D, Schadschneider, A & Nishinari, K 2005, 'Physics of transport and traffic phenomena in biology: from molecular motora and cells to organisms', *Physics of Life Reviews*, vol. 2, iss. 4, pp318-352.

- [9] Simpson, MJ, Landman, KA & Hughes, BD 2009, 'Distinguishing between Directed and Undirected Cell Motility within an Invading Cell Population', *Bulletin of Mathematical Biology*, vol. 71, pp. 781-799.
- [10] Simpson, MJ, Landman, KA & Hughes, BD 2009, 'Pathlines in exclusion processes', *Physical Review E*, vol. 79, 031920.
- [11] Fanelli, D & McKane, AJ 2010, 'Diffusion in a crowded environment', *Physical Review E*, vol. 82, 021113.
- [12] Simpson, MJ, Merrifield, A, Landman, KA & Hughes, BD 2007, 'Simulating invasion with cellular automata: Connecting cell-scale and population-scale properties', *Physical Review E*, vol. 76, 021928.
- [13] Brzank, A & Schutz, GM 2007, 'Phase transition in the two-component symmetric exclusion process with open boundaries', *Journal of Statistical Mechanics: Theory and Experiment*, P08028.