Supplementary material to accompany: Incorporating pushing in exclusion process models of cell migration

Christian A. Yates*

Department of Mathematical Sciences, University of Bath,
Claverton Down, Bath, BA2 7AY, UK

Andrew Parker and Ruth E. Baker

Wolfson Centre for Mathematical Biology,
Mathematical Institute, University of Oxford,
Andrew Wiles Building, Woodstock Road, Oxford, OX2 6GG, UK

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* Corresponding Author: c.yates@bath.ac.uk; Website: http://people.bath.ac.uk/cy386/
I. PUSHING PROBABILITY MASTER EQUATIONS

A. PME for adjacent pushing

Here we present the PME for type II adjacent pushing, noting that type I adjacent pushing can be derived similarly (as described below). Each potential push is explicitly dependent on the occupancy of five sites. Firstly, if site \((i, j)\) is occupied, we enumerate the ways it can become unoccupied: either the agent in site \((i, j)\) can move in any unoccupied direction with probability \(\frac{P^m}{4}\), or it could move into an occupied site and subsequently push that agent into an unoccupied neighbour. The terms after the first factor of \(Q^m\) in the following PME enumerate the case where the pushed-agent has three unoccupied neighbours, see Fig. 4 (a) of the main text. The second factor of \(Q^m\) corresponds to two of the neighbours of the pushed-agent being unoccupied, see Fig. 4 (b) of the main text. Terms multiplied by the third factor of \(Q^m\) describe the case where only one neighbour of the pushed cell is unoccupied, see Fig. 4 (c) of the main text.

The terms following the second factor of \(P^m\), on page 5, describe how an unoccupied site at \((i, j)\) may become occupied due to an unprompted move by an agent in an adjacent site, or by an agent in its adjacent cite being pushed in the appropriate direction by agents in its immediate neighbourhood. The first \(Q^m\) describes a push where each neighbour of site \((i, j)\) is surrounded by occupied sites. The second \(Q^m\) is where each neighbour of \((i, j)\) has two occupied sites. The final \(Q^m\) is where each neighbour of \((i, j)\) has just one occupied site (the site which is instigating the push).

\[
C_{n+1}(i, j) - C_n(i, j) =
\]

\[-\frac{P^m}{4}N_{tn}(i, j) \left( (1 - C_n(i - 1, j)) + (1 - C_n(i, j - 1)) + 
(1 - C_n(i, j + 1)) + (1 - C_n(i + 1, j)) + Q^m \left( (1 - C_n(i - 2, j))(1 - C_n(i - 1, j - 1))C_n(i - 1, j)(1 - C_n(i - 1, j + 1)) + 
C_n(i, j + 1)(1 - C_n(i, j + 2))(1 - C_n(i + 1, j + 1))(1 - C_n(i - 1, j + 1)) + 
(1 - C_n(i - 1, j - 1))(1 - C_n(i, j - 2))C_n(i, j - 1)(1 - C_n(i + 1, j - 1)) + 
\right) \right)
\]
\[
(1 - C_n(i + 1, j - 1))C_n(i + 1, j)(1 - C_n(i + 1, j + 1))(1 - C_n(i + 2, j)) + 
Q^n \left( C_n(i - 1, j)(C_n(i - 2, j)(1 - C_n(i - 1, j - 1))(1 - C_n(i - 1, j + 1)) + 
(1 - C_n(i - 2, j))C_n(i - 1, j - 1)(1 - C_n(i - 1, j + 1)) + 
(1 - C_n(i - 2, j))(1 - C_n(i - 1, j - 1))C_n(i - 1, j + 1) + 
C_n(i, j - 1)(C_n(i - 1, j - 1)(1 - C_n(i, j - 2))(1 - C_n(i + 1, j - 1)) + 
(1 - C_n(i - 1, j - 1))C_n(i, j - 2)(1 - C_n(i + 1, j - 1)) + 
(1 - C_n(i - 1, j - 1))(1 - C_n(i, j - 2))C_n(i + 1, j - 1) + 
C_n(i, j + 1)(C_n(i - 1, j + 1)(1 - C_n(i, j + 2))(1 - C_n(i + 1, j + 1)) + 
(1 - C_n(i - 1, j + 1))C_n(i, j + 2)(1 - C_n(i + 1, j + 1)) + 
(1 - C_n(i - 1, j + 1))(1 - C_n(i, j + 2))C_n(i + 1, j + 1) + 
C_n(i + 1, j)(C_n(i + 1, j - 1)(1 - C_n(i + 1, j + 1))(1 - C_n(i, j - 2)) + 
(1 - C_n(i + 1, j - 1))C_n(i, j - 1)(1 - C_n(i + 1, j + 1)) + 
(1 - C_n(i + 1, j - 1))(1 - C_n(i, j - 2))C_n(i + 1, j - 1) + 
C_n(i, j + 1)(C_n(i - 1, j + 1)(1 - C_n(i, j + 2))(1 - C_n(i + 1, j + 1)) + 
(1 - C_n(i - 1, j + 1))C_n(i, j + 2)(1 - C_n(i + 1, j + 1)) + 
(1 - C_n(i - 1, j + 1))(1 - C_n(i, j + 2))C_n(i + 1, j + 1) + 
\right) + 
\]
\[
C_n(i + 1, j - 1)(1 - C_n(i + 1, j + 1))C_n(i + 2, j) + (1 - C_n(i + 1, j - 1))C_n(i + 1, j + 1)C_n(i + 2, j)\]

\[
\frac{P_m}{4}(1 - C_n(i, j))\left(C_n(i - 1, j) + C_n(i, j - 1) + C_n(i, j + 1) + C_n(i + 1, j)\right) +
\]

\[
\frac{Q_m}{3}\left(C_n(i - 2, j)C_n(i - 1, j - 1)C_n(i - 1, j)C_n(i - 1, j + 1) + C_n(i, j + 1)C_n(i, j + 2)C_n(i + 1, j + 1)C_n(i - 1, j + 1) + C_n(i, j - 1)C_n(i - 1, j - 1)C_n(i, j - 2)C_n(i, j - 1) + (1 - C_n(i - 1, j - 1))C_n(i, j - 2)(1 - C_n(i + 1, j - 1)) + (1 - C_n(i - 1, j - 1))(1 - C_n(i, j - 2))C_n(i + 1, j - 1) + C_n(i, j + 1)(1 - C_n(i - 1, j + 1))(1 - C_n(i, j + 2))(1 - C_n(i + 1, j + 1)) + (1 - C_n(i - 1, j + 1))C_n(i, j + 2)(1 - C_n(i + 1, j + 1)) + (1 - C_n(i - 1, j + 1))(1 - C_n(i, j + 2))C_n(i + 1, j + 1) + C_n(i + 1, j)(1 - C_n(i + 1, j + 1))(1 - C_n(i + 1, j + 1)) + (1 - C_n(i + 1, j - 1))C_n(i + 1, j + 1)(1 - C_n(i + 1, j + 1)) + (1 - C_n(i + 1, j - 1))C_n(i + 1, j + 1))\right) +
\]

\[
3Q_m\left(C_n(i - 1, j)C_n(i - 2, j)C_n(i - 1, j - 1)(1 - C_n(i - 1, j + 1)) + C_n(i - 2, j)(1 - C_n(i - 1, j - 1))C_n(i - 1, j + 1) + (1 - C_n(i - 2, j))C_n(i - 1, j - 1)C_n(i - 1, j + 1) +
\]

4
\[
C_n(i, j - 1)C_n(i - 1, j - 1)C_n(i, j - 2)(1 - C_n(i + 1, j - 1)) + \\
C_n(i - 1, j - 1)(1 - C_n(i, j - 2))C_n(i + 1, j - 1) + \\
(1 - C_n(i - 1, j - 1))C_n(i, j - 2)C_n(i + 1, j - 1) + \\
C_n(i, j + 1)(C_n(i - 1, j + 1)C_n(i, j + 2)(1 - C_n(i + 1, j + 1)) + \\
C_n(i - 1, j + 1)(1 - C_n(i, j + 2))C_n(i + 1, j + 1) + \\
(1 - C_n(i - 1, j + 1))C_n(i, j + 2)C_n(i + 1, j + 1) + \\
C_n(i + 1, j)(C_n(i + 1, j - 1)C_n(i + 1, j + 1)(1 - C_n(i + 2, j)) + \\
C_n(i + 1, j - 1)(1 - C_n(i + 1, j + 1))C_n(i + 2, j) + \\
(1 - C_n(i + 1, j - 1))C_n(i + 1, j + 1)C_n(i + 2, j))
\]

The above assumes that an agent that has been pushed, will decide where to move based on how many unoccupied sites are around it, so if a push is possible, it will occur.

We can also consider the case of type I adjacent pushing. In this case, the probability of a push occurring changes in the PME above. The second and fifth factors of \(Q^m\), describing a push by a site into a neighbour with two other unoccupied neighbours, are reduced to \(2Q^m/3\). Similarly, when only one of those neighbours are unoccupied, as with the third and sixth \(Q^m\), we reduce the probability by a factor of 3 to \(Q^m/3\).

B. Pushing multiple agents in a line

Here we present the PME for cells which are allowed to push up to \(K\) other agents in a straight line in a chosen direction.

\[
C_{n+1}(i, j) - C_n(i, j) = -\frac{P^m}{4} C_n(i, j) \left[ (1 - C_n(i + 1, j)) + (1 - C_n(i - 1, j)) \right. \\
+ (1 - C_n(i, j + 1)) + (1 - C_n(i, j - 1)) \\
+ \left. \sum_{k=1}^{K} Q^m_k \left[ (1 - C_n(i + k + 1, j)) \prod_{m=1}^{k} C_n(i + m, j) \right. \right]
\]
\[+ (1 - C_n(i - k - 1, j)) \prod_{m=1}^{k} C_n(i - m, j)\]
\[+ (1 - C_n(i, j + k + 1)) \prod_{m=1}^{k} C_n(i, j + m)\]
\[+ (1 - C_n(i, j - k - 1)) \prod_{m=1}^{k} C_n(i, j - m)\}\]
\[+ \frac{P_m}{4} (1 - C_n(i, j)) \left[ C_n(i + 1, j) + C_n(i - 1, j)\right]\]
\[+ C_n(i, j + 1) + C_n(i, j - 1)\]
\[+ \sum_{k=1}^{K} Q_m \left\{ \prod_{m=1}^{k+1} C_n(i + m, j) + \prod_{m=1}^{k+1} C_n(i - m, j)\right\}\]
\[+ \prod_{m=1}^{k+1} C_n(i, j + m) + \prod_{m=1}^{k+1} C_n(i, j - m)\}. \quad (2)\]

II. COMPARISON BETWEEN DIFFERENT VALUES OF \(K\) FOR THE PUSHING OF MULTIPLE AGENTS IN A LINE

Fig. 1 displays the evolution of the histogram distance error (HDE) between the ILM and the PLM for the model in which agents can push multiple other agents in a line. The comparison is carried out for a range of values of \(K = 0, 1, 2, 3, 4\), the number of cells a pushing cell can move out of the way. The model with no pushing \((K = 0)\) is, as expected, the most accurate. The disparity between the ILM and PLM increases as the value of \(K\) increases.

III. COMPARISON BETWEEN DIFFERENT VALUES OF \(Q^m\)

In Fig. 2 we compare the evolution of the HDE between the ILM and the PLM for a range of values of \(Q^m = 0, 0.1, 0.5, 1\), the probability of a successful push. The model with no pushing is, as expected, the most accurate. Accuracy decreases as the value of \(Q^m\) increases, as expected.
FIG. 1. The evolution of the HDE over the time period $t \in [0, 200]$ for the multiple agent pushing model with varying $K$. Model and simulation parameters and descriptions are as in the main text with $Q_m^k = 0.5$ for $k = 1 \ldots K$. Line descriptions are as in the legend. The scenario with the best correspondence between the ILM and PLM is simple diffusion ($K = 0$, solid red line). The quality of the correspondence between the ILM and PLM decreases as $K$ increases. $K = 0$ corresponds to no pushing and $K = 1$ to the basic pushing case.

FIG. 2. The evolution of the HDE over the time period $t \in [0, 200]$ for the basic pushing model with varying $Q^m$. Model and simulation parameters and descriptions are as in the main text. Line descriptions are as in the legend. The scenario with the best correspondence between the ILM and PLM is simple diffusion ($Q^m = 0$, solid red line). The quality of the correspondence between the ILM and PLM decreases as $Q^m$ increases.