Description of Electronic Supplementary Material for 'From a discrete model of chemotaxis with volume-filling to a generalised Patlak-Keller-Segel model' published on Proceedings of the Royal Society A

Federica Bubba   Tommaso Lorenzi   Fiona R. Macfarlane

Online Resource 1

Video to support Figure 2 in the paper. Comparison between the simulation results for the discrete model (solid lines) and numerical solutions of the generalised PKS model (dotted lines). The left panel displays the cell density (blue lines) and the right panel display the concentration of chemoattractant (red lines). The results from the discrete model correspond to the average over five realisations of the underlying biased random walk. The cell density and the concentration of chemoattractant resulting from each realisation are plotted in pale blue and magenta, respectively, to demonstrate the robustness of the results obtained. A complete description of the set-up of numerical simulations and the numerical methods employed is given in Appendix B.

Online Resource 2

Video to support Figure 4 in the paper. Comparison between the simulation results for the discrete model (solid lines) and numerical solutions of the generalised PKS model (dotted lines). The top panels display the cell density (blue lines) and the bottom panels display the concentration of chemoattractant (red lines). The three sets of panels refer to different values of the parameter η in the discrete model - *i.e.* **a.** $\eta = 0.9801$, **b.** $\eta = 4.9005$, **c.** $\eta = 294.03$ - which correspond to different values of the parameter χ in the continuum model. The results from the discrete model correspond to the average over five realisations of the underlying biased random walk. The cell density and the concentration of chemoattractant resulting from each realisation are plotted in pale blue and magenta, respectively, to demonstrate the robustness of the results obtained. A complete description of the set-up of numerical simulations and the numerical methods employed is given in Appendix B.

Online Resource 3

Video to support Figure 5 in the paper. Comparison between the simulation results for the discrete model (solid lines) and numerical solutions of the generalised PKS model (dotted lines). The top panels display the cell density (blue lines) and the bottom panels display the concentration of chemoattractant (red lines) for different values of the size of the cell population, that is, different values of the parameter B in (3.17) – *i.e.* **a.** $B = 0.25$, **b.** $B = 1$, **c.** $B = 5$. The results from the discrete model correspond to the average over five realisations of the underlying biased random walk. The cell density and the concentration of chemoattractant resulting from each realisation are plotted in pale blue and magenta, respectively, to demonstrate the robustness of the results obtained. A complete description of the set-up of numerical simulations and the numerical methods employed is given in Appendix B.

Online Resource 4

Video to support Figure 7 in the paper. Comparison between numerical solutions of the generalised PKS model, numerical solutions of the classical PKS model, and the simulation results for the corresponding discrete models. The solid, blue lines and the solid, red lines highlight the cell density and the concentration of chemoattractant of the discrete model with volume-filling effects. On the other hand, the solid, green lines and the solid, yellow lines highlight the cell density and the concentration of chemoattractant of the discrete model with without volume-filling effects. The dotted lines highlight the numerical solutions of the corresponding PKS models. Different panels refer to different values of the parameter $u_{\max}$ - *i.e.* **a.** $u_{\max} = 2 \times 10^6$, **b.** $u_{\max} = 2 \times 10^7$, **c.** $u_{\max} = 2 \times 10^9$. The results from the discrete model with volume-filling effects correspond to the average over thirty realisations of the underlying biased random walk, while the results from the discrete model without volume-filling effects correspond to the average over ten realisations. The cell density and the concentration of chemoattractant resulting from each realisation are plotted in paler colours to demonstrate the robustness of the results obtained. A complete description of the set-up of numerical simulations and the numerical methods employed is given in Appendix B.

Online Resource 5

Video to support Figure 9 in the paper. Comparison between the simulation results for the discrete model (solid lines) and numerical solutions of the generalised PKS model (dotted lines). The top panels display the cell density (blue lines) and the bottom panels display the concentration of chemoattractant (red lines) for progressively smaller cell numbers and critical cell densities, that is, progressively lower values of the parameter A^0 in (3.18) – *i.e.* **a.** $A^0 = 10^5$, **b.** $A^0 = 10^4$, **c.** $A^0 = 10^3$, **d.** $A^0 = 10^2$. The results from the discrete model correspond to the average over five realisations of the underlying biased random walk. The cell density and the concentration of chemoattractant resulting from each realisation are plotted in pale blue and magenta, respectively. A complete description of the set-up of numerical simulations and the numerical methods employed is given in Appendix B.

Online Resource 6

Appendices of the paper:

Appendix A. Formal derivation of the generalised PKS model (1.2)-(1.4);

Appendix B. Details of numerical simulations in 1D;

Appendix C. Details of numerical simulations in 2D.

Online Resource 7

Matlab codes for 1D and 2D numerical simulations.