BP205 Molecular Dynamics of the Cell
Problem Set 3
Due February 3rd in class

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1. Simulating a 1-dimensional reaction diffusion system.

Consider a 1-dimensional line of cells. All cells in the line are capable of producing some small molecule. The rate at which they do so is determined by the local concentration of this small molecule, which we'll represent as the de-dimensionalized concentration C, according to

$$\frac{dC}{dt} = \frac{C^3}{.5^3 + C^3} \qquad \text{(eq.1)}$$

a. First, calculate the Peclet number related to the cell's ability to interact with the small molecule – assume a cell size of 1 µm, a cell speed of 30 µm/sec (if the cells were in motion), and a diffusion constant of $2*10^2$ µm^2/sec. Are diffusive or convective forces primarily responsible for cell-small molecule interactions?

Now, produce a MATLAB simulation of the system – represent the line of cells as a vector with length 50, with a single value at each point representing the concentration of C at that point. We'll use de-dimensionalized units for all variables and constants in the system. In addition to the reaction described in equation 1, there is also constant degradation of the small molecule, which occurs at a rate proportional to C with constant 1. Finally, diffusion occurs with de-dimensionalized D = 100.

b. First, set C=0 initially at all points. Simulate the system using one of MATLAB's ode solvers until C reaches constant value at all positions (we'll call this "steady state"). What does the final distribution of C look like?

c. Now, set C at all points = 1 initially and simulate until C no longer changes. What does the final distribution of C look like?

Next, we'll simulate an external stimulus.

d. Set the initial C at all points except for nodes 20-30 equal to the value that was reached at steady state in part c. Now set the initial concentration at nodes 20-30 equal to the value that was reached at steady state in part b. What does the final distribution of C look like?

e. Now, set the diffusion constant equal to 10 units. With the same initial conditions as in part d, simulate the system – what final state does the system reach?

f. Finally – test a range of values of D between 10 and 100 and report the final state of the system for each value. Does the final state transition gradually between its two extremes observed in b and c, or is there an abrupt transition for some value of D? If an abrupt transition occurs – around what value of D does it happen?

2. Life at low Reynold's number

a. When swimming through water, how slowly would you have to move to have Reynold's number equal to that of *E. coli* swimming through water?

b. How large would you have to be to achieve *E. coli*'s Reynold's number? (assume that you move at a normal human swimming speed)

c. How dense would the water have to be for you to achieve *E. coli* Reynold's number? (assuming that you are human sized swimming at normal human speed)