

Mathematical Biology 5120-S14: Problem Set 1

Due Tuesday February 18 at beginning of class.

After trying the problems yourself, I encourage you to talk to each other about how to solve them. If you cannot work a problem out, don't leave it — be sure to come and ask for help.

1. Particles can move because of other reasons than diffusion. Suppose particles with number density $N(x, t)$ are suspended in a fluid which is moving with velocity $u(x, t)$ and that the particles move with the fluid ($u(x, t) > 0$ means motion to the right).
 - a) What is the flux function $J(x, t)$ in this situation (assume the particles do not also diffuse)?
 - b) What is the partial differential equation (PDE) satisfied by the function $N(x, t)$?
 - c) What are the flux function and PDE in the case that the particles move both because they are carried by the fluid and because they diffuse?
2. Suppose particles move just by diffusion.
 - a) Suppose that a number N_0 particles are injected at $x = 0$ at time $t = 0$, and another N_1 particles are injected at the origin at time $t = t_1 > 0$. Write down the function $N(x, t)$ that gives the number density of particles at location x at time t . (Hint: The PDE is linear so you can add solutions. Also note that you will have different formulas for $0 < t < t_1$ and for $t_1 < t$). Let $t_1 = 1$, and use Maple or some other graphics program to plot the solution at $x = 1$ as a function of time for diffusion coefficients $D = 10^{-3}$ and $D = 10^{-6}$. Comment on the concentration plots you obtain.
 - b) Now assume instead that particles are injected at rate r per unit time starting at time $t = 0$ (so $r dt$ particles are injected in a short time dt). Write down the function $N(x, t)$ as an integral involving the Gaussian solution for diffusion we obtained in class.
3. For this problem, you will use MATLAB to simulate the random walk process discussed in class. Set $\Delta x = 0.1$, $\tau = 0.01$, $M = 100$, and $N = 1000$. At time $t = 0$, start with N particles at location $x = 0$. In each of M timesteps of size τ , move each of the N particles, according to the rule: Particle j moves left with probability p_l and right with probability p_r . Keep track of the location of the N

particles. After M steps, plot a histogram of the particle positions normalized by the total number of particles N . Also plot the exact probability distribution for the particle locations at time $t = M \cdot \tau$, as derived in class, and plot the Gaussian approximation to the probability distribution derived in class. Do the simulation again with $N = 4000$ particles, and make the same plots. Do it a third time with $N = 16000$ particles. Comment on how the histograms compare with the exact probability distribution as N gets larger. For each simulation also compute the furthest distance a particle has moved, compute the mean position of a particle, and compute the root-mean-squared distance of the particles from their starting location. How to the mean position and root-mean-squared distance compare with the exact results derived in class?

Note that this problem has a two-fold purpose. One is to give you some increased understanding of the random walk process. The second is to give you experience in using MATLAB to carry out simulations.

4. This problem has to do with buffered and facilitated diffusion. Assume that the diffusion coefficient of oxygen is $D_{oxy} = 1.2(10)^{-5}$ cm²/sec and that of myoglobin is $D_{myo} = 4.4(10)^{-7}$ cm²/sec.
 - a) Calculate the effective diffusion coefficient of oxygen in a solution containing $1.2(10)^{-5}$ moles/cm³ myoglobin. Assume that the rate constants for the uptake of oxygen by myoglobin are $k_+ = 1.4(10)^{10}$ cm³/(mole sec) and $k_- = 11$ /sec.
 - b) Carbon dioxide inside cells can also bind to myoglobin and this can augment CO₂ transport. Find the maximal enhancement of diffusive transport of carbon dioxide via binding with myoglobin. Use $D_{CO_2} = 1.92(10)^{-5}$ cm²/sec, $k_+ = 2.0(10)^8$ cm³/(mole sec) and $k_- = 1.7(10)^{-2}$ /sec. Compare the amount of facilitation of carbon dioxide transport with that of oxygen at similar concentrations.

Be sure to show all details on each problem for full credit