Homework 1: Due Feb. 5, 2015

1. A quantitative understanding of diffusion was given by Einstein in his theory of Brownian motion. He showed that if a spherical solute molecule is large compared to the solvent molecule, then

$$D = \frac{kT}{6\pi\mu a}, \tag{1}$$

where $k = \frac{R}{N_A}$ is Boltzmann's constant, N_A is Avogadro's number, T is the absolute temperature of the solution, μ is the coefficient of viscosity for the solute, and a is the radius of the solute molecule. The molecular weight of a spherical molecule is

$$M = \frac{4}{3}\pi a^3 \rho, \tag{2}$$

where ρ is the molecular density, so that in terms of molecular weight,

$$D = \frac{kT}{3\mu}\left(\frac{\rho}{6\pi^2 M}\right)^{1/3}. \tag{3}$$

The density of most large protein molecules is nearly constant (about $1.3 - 1.4$ g/cm^3), so that $DM^{1/3}$ is nearly the same for spherical molecules at a fixed temperature.

Table 1: Molecular weight and diffusion coefficients of some biochemical substances in dilute aqueous solution.

Substance	Molecular Weight	D(cm^2/s)
hydrogen	1	4.5×10^{-5}
oxygen	32	2.1×10^{-5}
carbon dioxide	48	1.92×10^{-5}
glucose	192	6.60×10^{-6}
insulin	5,734	2.10×10^{-6}
Cytochrome c	13,370	1.14×10^{-6}
Myoglobin	16,900	5.1×10^{-7}
Serum albumin	66,500	6.03×10^{-7}
hemoglobin	64,500	6.9×10^{-7}
Catalase	247,500	4.1×10^{-7}
Urease	482,700	3.46×10^{-7}
Fibrinogen	330,000	1.97×10^{-7}
Myosin	524,800	1.05×10^{-7}
Tobacco mosaic virus	40,590,000	5.3×10^{-8}

Determine how well the relationship $D \sim M^{-1/3}$ holds for the substances listed in Table 1 by plotting D and M on a log-log plot.

2. Suppose a particle moves to the right with probability α and to the left with probability β and stays put with probability $1 - \alpha - \beta$ in some fixed increment of time.

(a) Following arguments given in class, formulate this as a discrete random walk process and determine the limiting partial differential equation.

(b) Simulate this process on a grid of 101 points starting with a particle at the middle. From your simulation estimate the expected exit time (each step takes one unit of time) and the splitting probabilities as a function of α, taking $\alpha + \beta = 1$.

3. (a) Determine the expected time for a diffusing particle of oxygen or hemoglobin to escape from a domain of radius R (or length $2R$ in one dimension) starting at the center of the domain, for a 1-, 2-, or 3- dimensional domain. Determine these times for domains with radii 10^{-4}, 10^{-2}, and 10 cm.

   (b) Perform a stochastic simulation experiment for the previous problem in 1 dimension. Start with a particle at the origin and allow it to diffuse until it hits a boundary at distance $x = \pm R$ and record the time of the first hit. Do this for many such particles and plot the distribution of times, and check to see if the mean of this distribution agrees with what you calculated in the previous exercise. Do this experiment for hemoglobin and oxygen as in the previous problem.

4. Segel, Chet and Henis (1977) used

$$D = \frac{\pi N^2}{4C_0^2 A^2 T}, \tag{4}$$

to estimate the diffusion coefficient for bacteria. With the external concentration C_0 at $7 \times 10^7 \text{ml}^{-1}$, at times $t = 2$, 5, 10, 12.5, 15, and 20 minutes, they counted N of 1,800, 3,700, 4,800, 5,500, 6,700, and 8,000 bacteria, respectively, in a capillary of length 32 mm with 1 μl total capacity. In addition, with external concentrations C_0 of 2.5, 4.6, 5.0, and 12.0 $\times 10^7$ bacteria per milliliter, counts of 1,350, 2,300, 3,400, and 6,200 were found at $t = 10$ minutes. Estimate D.