1. In class, we discussed the diffusion equation and also a bit about Boltzmann statistics. In this problem, we will explore diffusion in the presence of an external field.

We saw in class that the mass current $J_z$ of diffusing particles is given in terms of the diffusion constant $D$ and local density $n(z,t)$ as

$$J_z = -D \frac{\partial n}{\partial z}$$

(in one dimension). Consider now an external field acting so that the diffusing particles feel an external force with $z$-component $F_z = -\frac{dU}{dz}$, where $U(z)$ is the potential energy of a particle at $z$. If the force $F_z = F_0$ (i.e. a constant force independent of $z$), then the potential energy is (up to a constant) $U(z) = -F_0 z$.

With this added force, the mass current is taken to be

$$J_z = -D \frac{\partial u}{\partial z} + n \mu F_0$$

where $\mu$ is the mobility.

a) Consider the case where $J_z = 0$ (i.e. equilibrium). Recall first that in equilibrium, based on our discussion of Boltzmann statistics, that at temperature $T$ we have $n(z) = n_0 e^{-U(z)/k_B T}$. Next, show that there is a relationship between $\mu$ and $D$,

$$\mu = \frac{D}{k_B T}$$

b) Use the continuity equation $\frac{\partial n}{\partial t} + \frac{\partial J_z}{\partial z} = 0$ to obtain the one-dimensional Smoluchowski equation,

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial z^2} - \frac{DF_0}{k_B T} \frac{\partial n}{\partial z}$$

which can be used to model the response of a fluid to external fields including the approach to equilibrium.

2. Write a code to perform a random walk in three dimensions. Run the code for many iterations, corresponding to a large ensemble of trajectories. Determine in both
cases $\langle r^2 \rangle$ as a function of time. Make a log-log plot of your results, and determine from a linear fit to the data, as described in class, the exponents $\nu$. Verify that for $\langle r^2 \rangle \sim t^{2\nu}$ you obtain $\nu = 1/2$ for your random walk.

3. The Hamiltonian $H_\Omega$ for a two-dimensional spin system is given by

$$H_\Omega = -\frac{1}{2}J \sum_{i=1}^{N} \sum_{j=1}^{N} S_{ij} \left( S_{i+1,j} + S_{i-1,j} + S_{i,j+1} + S_{i,j-1} \right)$$  \hspace{1cm} (1)

We can also consider adding an applied external field $H$ which adds a term to the Hamiltonian $-H \sum_{j=1}^{N} S_j$. A more shorthand way to write this is

$$H_\Omega = -J \sum_{(ij)} S_i S_j - H \sum_{i} S_i$$  \hspace{1cm} (2)

where the summation is over nearest neighbor spins and $H$ is an externally applied field.

Show that the heat capacity, $C = \frac{\partial (H_\text{meta})}{\partial T}$ can be found from the fluctuations in equilibrium,

$$C = \frac{1}{k_B T^2} \left[ \langle H_\text{meta}^2 \rangle - \langle H_\text{meta} \rangle^2 \right]$$

and also show that the susceptibility $\chi = \frac{\partial M}{\partial H}$ can be found from the equilibrium fluctuations in the magnetization $M$,

$$\chi = \frac{1}{k_B T} \left[ \langle M^2 \rangle - \langle M \rangle^2 \right]$$

4. Write a code to explore the thermodynamics of the Ising model on a square lattice in two dimensions using Metropolis Monte Carlo. Use periodic boundary conditions so that spins on the edge of your square interact with spins on the opposite edge. Write a subroutine “cluster” to compute the local energy of spin at site $i,j$ with its nearest neighbors. Now here is the Monte-Carlo algorithm which samples random states with probability in accord with the partition function:

0. Begin with a random array of spins.
1. Compute the energy $E_1$ of the current spin state.
2. Choose a spin on the lattice at random and flip its spin state.
3. Recompute the energy $E_2$ of the new spin state.
4. Determine the energy difference $\Delta = E_1 - E_2$.

5. If $\Delta \leq 0$, accept the current step in the ensemble. Save the current spins and energy and return to 1.

6. If $\Delta > 0$, draw a random number between 0 and 1.

7. If the random number is less than $\exp\left(-\frac{\Delta}{k_BT}\right)$, accept the current step into the ensemble and save the current spins and energy. Return to 1.

8. If the random number is greater than or equal to $\exp\left(-\frac{\Delta}{k_BT}\right)$, then reject the current step. Reset the spins to what they were before the spin was flipped in step 2. Return to step 1.

Evolve a lattice of $100 \times 100$ spins. The exact result for the transition temperature found by Onsager is $k_BT_c = \frac{2J}{\log(1+\sqrt{2})} \approx 2.2692J$. To determine the transition temperature and other quantities, write your code in terms of the dimensionless parameter $K = \frac{J}{k_BT}$, and explore the region from $K = 0.3$ to $K = 0.5$. Perform your simulation at 50 uniformly distributed values of $K$ in this range. Each time you change the coupling constant $K$, retain the spins from previous value of $K$. This provides a good guess for the spin configuration.

Make a plot of energy vs. Monte-Carlo iteration. You will find that the system will equilibrate after a certain amount of time. This will give you an idea of how much time is required to equilibrate to each new value of $K$. After the system is equilibrated, accumulate statistics for the magnetization $M$ and also the fluctuations required to compute the heat capacity and susceptibility. Create plots of the magnetization $M$, heat capacity $C$, and susceptibility $\chi$ as a function of $\frac{1}{K}$. The transition should be quite close to the Onsager result $1/K = 2.2692$.

A good reference for this problem is "Lectures on Phase Transitions and the Renormalization Group" by Nigel Goldenfeld.