Homework 05:

A1. **Exact solution to the diffusion equation**

Eq. 4.20 in the book is the diffusion equation for a one-dimensional universe (or a case in our universe where the other two dimensions are restricted, like food coloring spreading in a thin pipette of water). The full solution of this equation is a function of both space and time. It describes how the evolution of a particular concentration profile changes over time. One can imagine many different starting configurations and different boundary conditions as well.

The easiest set of boundary conditions and initial conditions can be realized by a very long, very narrow tube of water with just the smallest drop of food coloring placed in the center of the tube. Because the tube is very long, we'll just pretend like the domain of our problem is $-\infty < x < +\infty$. We'll approximate the drop of food coloring as a very narrow Gaussian, centered at the origin:

$$c(x,t) = \frac{N}{\sqrt{4\pi Dt}} \exp\left(\frac{-x^2}{4Dt}\right)$$

Where N is the total number of particles and D is the diffusion constant.

- Does this solution have the right units? Is the argument to the exponential dimensionless as it should be?
- If you integrate this function over space, what should you get? Does it work?
- If you've had a partial differential equations class (like PHSCS 318 or MATH 334), you could easily find the family of functions that form the general solution to this equation by using the method of separation of variables. Instead of going to the trouble though, I've just shown you the answer. Show that the Gaussian given above is indeed a solution to the diffusion equation (Eq. 4.20).
- Make a plot of this solution as both a function of time and position. In other words, make some sort of a surface plot where one axis is x, one axis is t, and the third axis is the density, $c(x,t)$.

A2. **Are walkers just as good?**

Now we'll solve the problem of A1 again, but without any math. We'll just put a bunch of walkers in the middle of our domain and see what happens. So this amounts to writing a small program again. You can play with the one I wrote (posted on the website) but it would be better if you wrote your own. Do what you can afford. I'll give you two strategies for doing it.

Strategy 1: Represent your domain by an array with, say, 100 slots. This array will store the number of walkers at each position. Each slot corresponds to a particular x value and the number in the slot is the number of walkers. The beginning configuration will be, say, 10000 walkers in slot 50 and the same in slot 51, zeros in all the other slots. (It's better to start with two bins full, rather than one. To see this, try it with only 1 occupied bin.)

Caveat: This is an easy way to approach the problem, but it's not quite the same as the problem described in A1—this formulation of the problem doesn't let the walkers go to all the way to $+\infty$ or $-\infty$ because we've fixed the number of position bins. I think it's close enough for what we're trying to learn though. I found it harder to program than strategy 2. (It's more efficient though.)

Strategy 2: Make an array where each slot, i, represents the position position of the i-th walker. Set the beginning value for each walker to zero and randomly add $+1$ or -1 to each position. (Better to start 1/2 the walkers at zero and 1/2 the walkers at 1. Do you see why when you run your program?) Do this many, many times. Plot the evolution as a *histogram* of positions.

- Whichever way you do it (strategy 1 or strategy 2), you'll get essentially the same result. Does your simulation solution look much like the solution to A1? Whatever differences there are, how can you make them smaller?

- Make a plot, like you did for A1, that shows $c(x, t)$ as a a surface plot or some other plot that shows the same information.

A3. **Entropy in diffusion problems** Let's continue with a problem based on our physical situation of a narrow tube of water with a small drop of food coloring placed in the center.

- What happens after waiting a long time?
- If you plotted the entropy of the system as a function of time, what do you think it would look like? Sketch your guess before going on.
- We can calculate the entropy of the system, at a specific time, by summing over the positions bins:

$$S = -\sum_{\text{bins}} \frac{N_i}{N} \ln\left(\frac{N_i}{N}\right)$$

  where N_i is the number of particles in the i-th bin and N is the total number of particles in the simulation.

  Modify your program (if necessary) from Problem A2 so that the walkers are restricted to a finite interval. (Walkers that try to step out of bounds just stay put on the edge.) Then use the equation above to calculate the entropy as a function of step number. Convince yourself and me that the entropy tells us something useful about the evolution of the system. Attach your code and plots.