Modeling Diffusion

We have seen how to model a random walk in 1D and the code `random_walk_2D.m` produces a random walk in 2D: at each time step, a random distance and direction is selected. In both cases, the average distance from starting point increases as the square root of time. When we run many trials of such random walk processes and look at parameters such as the average and variance across trials of the distances traveled or positions reached, we are studying the distribution of results. We can instead model how the distribution itself changes. This is similar to measuring how the concentration profile of a particular chemical species changes with time, without producing an individual trajectory for each and every molecule. In general, a model of how a probability distribution changes with time is known as a Master Equation. For the particular case of diffusion of a chemical species, this becomes the Diffusion Equation.

Diffusion in 1D

The diffusion equation relates the change in time of concentration at one point to the concentrations nearby. In 1D molecules can move in the direction of $+x$ or $-x$ with equal probability. If we assume the average distance molecules move is $dx$ in time $dt$ then the number that arrive at a position $x$ is equal to that leave the position $x-dx$ and move in a positive direction plus the number that leave $x+dx$ and move in a negative direction. We assume all those previously at position $x$ have moved away to both $x+dx$ and $x-dx$ in equal proportion. Thus, denoting the total concentration at position $x$ at time $t$ by $C(x,t)$ we have: $C(x,t+dt) = C(x,t)(1-f) + \frac{f}{2} [C(x-dx,t) + C(x+dx,t)]$.

Therefore: \[
\frac{dC(x,t)}{dt} = \frac{C(x,t+dt) - C(x,t)}{dt} = \frac{f}{2dt} [C(x-dx,t) + C(x+dx,t) - 2C(x,t)]
\]

or $\frac{dC}{dt} = D \frac{d^2C}{dx^2}$ where $D$ is the diffusion constant with units of distance-squared per unit time.

When we model this on the computer, we can just use the top line of the equations to update the quantities at one position depending on the surrounding values. The final differential equation is the diffusion equation that can be solved analytically for a number of initial conditions. The code `diffuse1D.m` implements this diffusion.

Diffusion in 2D

In more than one dimension, we can produce a model by calculating the values of concentration at a grid of points separated by intervals of $dx$ and $dy$ so that the change in concentration at a position is due to the flow of molecules in the +/- y direction as well as +/- x. Since there are 4 directions that can be reached, we have: $C(x,t+dt) = C(x,t)(1-f) + \frac{f}{4} [C(x-dx,y,t) + C(x+dx,y,t) + C(x,y-dy,t) + C(x,y+dy,t)]$. 