Computational Physics
Physics 410 2014W
Assignment 6
Due: Friday, November 28, 2014 11PM

In this assignment you will be solving the diffusion equation:

$$\frac{\partial P}{dt} = D\frac{\partial^2 P}{\partial x^2}$$

for the probability distribution of particles $P(x,t)$ in a 1D gas confined to a circle of length $L = 100$ (or if you prefer a line segment with periodic boundary conditions) using two different methods. Assume that the particles are initially distributed at time $t = 0$ as a normalized Gaussian

$$P(x,0) = \frac{1}{\sqrt{2\pi\sigma_0^2}} e^{-\frac{(x-\bar{x}_0)^2}{2\sigma_0^2}}$$

centred at $\bar{x}(0) = \bar{x}_0 = 33$ with standard deviation $\sigma(0) = \sigma_0 = 5$.

1. FTCS Method

Solve this diffusion equation using the Forward-Time-Centered-Space (FTCS) method with $D = 0.25$, a grid spacing $a = 1$, and time steps of size $h = 1$. Plot the resulting solution at times $t = (2, 10, 100, 1000, 10000)$ (on the same plot). Plot the mean $\bar{x}(t)$ and standard deviation $\sigma(t)$ as a function of time and comment on your results. Be sure to implement the periodic boundary conditions (the grid points at $x = 0$ and $x = L$ should be identified with each other in your algorithm).

2. Random Walk Method

Solve this diffusion equation by generating a series of M random walks of each with $T = 10000$ steps. Populate the initial positions of the M random walkers according to the initial Gaussian distribution at $t = 0$. For each time step $t > 0$ randomly move each walker to the left or the right (with equal probability) a length $l = \frac{1}{2}$. Plot the normalized probability distribution of the random walkers at time steps $t = (2, 10, 100, 1000, 10000)$ (on the same plot) for the three cases $M = 10000, 100000, 1000000$. Plot the mean $\bar{x}(t)$ and standard deviation $\sigma(t)$ as a function of time in each case and comment on your results. Plot a selection of 10 random walks $x_j(t)$ as a function of time. What is the effective diffusion constant D of this Monte Carlo simulation?

Compare and contrast your results from Part 1. and Part 2. Discuss how and why each of these methods arrive at a solution. Discuss how you might implement a space and time-dependent diffusion parameter $D(x,t)$ in each case. Which method is preferable (and why) if modelling diffusion in a high-dimensional space (say $d = 10$ rather than $d = 1$)?