PHY566 Group Project #1 (version B)

Due Date: March 23rd, 10:00am via Sakai

Random Walk, Diffusion and Mixing

1. **2D Random Walk:** [10 points]
   write a program to simulate a random walker in 2 dimensions, taking steps of unit length in $\pm x$ or $\pm y$ direction on a discrete square lattice.

   a) plot $\langle x_n \rangle$ and $\langle (x_n)^2 \rangle$ up to $n = 100$ by averaging over at least 10^4 different walks for each $n > 3$.

   b) show that the motion is diffusive, i.e. that the mean square distance from the starting point $\langle r^2 \rangle \propto t$ (with t being the time, i.e. $t \sim n$) and determine the value of the diffusion constant (a simple "eyeball" fit to your numerical data is sufficient).

2. **Diffusion Equation:** [10 points]

   a) show analytically that the spatial expectation value $\langle x(t)^2 \rangle$ of the 1D Normal Distribution,

   $$\rho(x,t) = \frac{1}{\sqrt{2\pi\sigma(t)^2}} \exp\left(-\frac{x^2}{2\sigma(t)^2}\right) \quad , \tag{1}$$

   equals $\sigma(t)^2$.

   b) write a program to solve the 1D diffusion equation using the finite difference form with a diffusion constant $D = 2$. Start from an initial density profile that is sharply peaked around $x = 0$, but extends over a few grid sites (box profile). Verify (using a fit) that at later times the numerically calculated density profile corresponds to a Normal Distribution with $\sigma(t) = \sqrt{2Dt}$ (i.e. perform a fit for 5 different time snapshots over which significant changes of the distribution are visible).

3. **Mixing of two Gases:**
   Use the techniques and insights gained previously to write a program to simulate the mixing of two gases in 2D in a rectangular enclosure:

   a) Set up a 2D grid in `xy` space with dimensions `120 x 80`. Fully populate the left third of the grid with a gas of species "A" and the right third of the grid with a gas of species "B". The center third of the grid remains empty. Pick a random location on the grid, and have the gas particle move at random one position up/down/left/right. If the selected position is occupied, reject the move and pick another particle (you may optimize the algorithm by only picking from occupied sites). Repeat for a large number of iterations. [10 points]

   b) Plot the linear population densities $n_A(x)$ and $n_B(x)$ after select time-intervals. Also plot a few sample configurations of the grid at various time-steps. [10 points]

   c) average the densities over 100 trials for added accuracy and replot the densities [10 points]

Your homework submission should consist of:

- a public Github account, containing the code and revision history for all codes developed in this project. You need to invite the instructor (Github account: `sabass`) to become a member of your repository.

- a document outlining the problem, detailing your solution and discussion of your results - the document should include the requested figures. The document should be in pdf format

- the source code of your program should be downloadable from the Github account - do not submit the code via Sakai, but provide a link to your repository in your document.

- a group presentation to be given in class