PHYS639, Spring16, Problem 6

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1. A particle is moving in a random direction in 3D with a constant step-size. Plot the distance from the origin as a function of time (number of steps). Do this for a large number of particles and plot the average displacement from the origin as a function of time. When averaged over many trajectories we expect r^2 to be proportional to time. Compute the constant of proportionality – *the diffusion coefficient*.

2. Do exactly the same as before but now imagine that the particles are in a "stream" directed in positive x direction. Make the probability of jumping at an angle θ with the x axis proportional to $\cos(\theta)$.

3. Simulate the *Sugar cube in a cup of coffee* problem. Take a square of a unit size and place large number of points in the middle of this square inside a smaller square of size 0.1. At each time step make every particle move in random direction with a fixed step size. You should observe the sugar cube "diffuse" in the cup. Make sure the particles don't get out of the cup by either bouncing them back or imposing periodic boundary conditions, where if a particle crosses one wall it reenters from the opposite side. Divide your cup into a regular grid and compute the entropy of the system as a function of time using

$$S = -\sum_i P_i \ln P_i,$$

where the sum is over all cells and P_i is the number of sugar particles in the i^{th} cell.

Deliverables

For all four cases above, plot the following:

1. For problems (1) and (2), plot average r^2 as a function of time. Compute the diffusion coefficient.

2. For problem (3), plot few snapshots of your simulation.

3. For problem (3), plot entropy as a function of time. Choose your step size small enough so that the diffusion is reasonably slow.