Computer Sciences for Physics and Chemistry – Homework

This exercise is about the modeling of the diffusion of particles in physics or chemistry. It is composed of two parts, one simulating the diffusion in one dimension and one in a plane.

First part
Diffusion in 1 dimension: the drunk walker

Let us consider a drunk walker that moves along in a street (considered as a straight line). At each step, he has a probability p to move forward and $1 - p$ to move backward.

1. Write a function that calculates the final position of the walker as a function of the parameter p and the number of steps N.
2. What is the expected final position for $p = 0.5$? Check your guess by running your function 100 times for 1000 steps.
3. Represent the result as a histogram. Calculate the standard deviation σ_{1000} and demonstrate that the distribution you obtained is a Gaussian.
4. Do the same for 20, 50, 100 and 200 steps. Fit the standard deviation σ_N as a function of the number of steps N with appropriate mathematical law.
5. Now $p = 0.75$. What is the expected final position as a function of the number of time steps N. Check your assumption.

Second part
Diffusion in 2 dimensions: diffusion of a dye in water

In this part, we will simulate the diffusion of a dye drop in a water puddle. The water puddle is represented by a lattice of 20 lines and 20 columns. At the initial time step, box of the lattice is empty, except the four at the center which contains 100 particles of dye. At each time step, each molecule moves according to the following rules :
(i)   the molecule has a probability p to stay in its box,
(ii) if the molecule moves, it moves one box and all possible moving directions are equiprobable (e.g. $0.25 \cdot (1 - p)$ to go up, down, left or right if the particle is in the center of the lattice, $0.33 \cdot (1 - p)$ to go up, down or left if the particle in is a top-right box of a row, or $0.5 \cdot (1 - p)$ to go down or right if the particle is in the upper left corner box), and
(iii) the molecule can not go out of the lattice.

1. Write a function that computes the final position of each molecule walker as a function of the parameter p and the number of steps N.
2. Fix $p = 0.2$. Represent the positions of the molecules in a scattered plot **after 5, 10, 20 and 50 time steps**.

In physics or chemistry, we define the notion of entropy to quantify the neatness of a system. For a discrete system, the entropy is calculated like this

$$S = -k_B \cdot \sum_i P_i \cdot ln(P_i)$$

Where $k_B = 1.38e^{-23}$ is the Boltzmann constant and P_i is the average ratio of particles in the box i (number of particle in the box i divided by the total number of particle

3. Run **25 computations with $N = 50$** time steps and calculate the average value of P_i for each box. Then, computes the entropy for $N = 50$.
4. Do the same for $N = 5$, $N = 10$, $N = 20$ **and** $N = 50$. Plot $S(N)$ and find a mathematical function that fits the variation of entropy with respect to the number of time steps $S(N)$

Recommandations for the Report

Write a report that contains, for both part of the exercise, the four following parts:
- A description of the scripts you developed.
- A discussion on the rationale of the functions and modules you used.
- A description of the way you tested and verify that your functions work.
- Your results for each question as well as an analysis of these results.
- A discussion on results and comparison with theory or your expectations.

The report should not exceed 6 pages and have to be submitted on Moodle as a single PDF file.

Important Notice
This is an individual work. Everyone has to develop their own code and write their own reports. Submitted reports will be analyzed by anti-plagiarism software and similarities between several reports will be sanctioned.