PHYS 481 Assignment 7: Diffusion

Due: Friday Nov 29 at 23:00

AI policy for this assignment: no use of generative AI tools.

Question 1 [5 pts]

A 10 cm long box is filled with CO_2 at room temperature and atmospheric pressure. The middle portion of the box from 4 to 6 cm is sealed off from the rest of the box, and a trace amount of N_2 is injected into the middle section until the N_2 density reaches 10^{10} N_2 molecules per cubic cm. The resulting mean free path of the N_2 molecules is 67 nm and their average speed is 480 m/s. Using a random walk with Gaussian steps, simulate what happens when the barriers at 4 and 6 cm are removed. You may either assume that particles that hit the walls at 0 and 10 cm are reflected off the walls (so that a particle that steps to -0.01 cm is re-introduced to the box at 0.01 cm) or you may use periodic boundaries (so that a particle that steps to -0.01 cm returns at 9.99 cm).

Create a movie of the density of N_2 molecules as a function of position (i.e. a histogram, in units of cm^{-3}) as they diffuse throughout the box over a period of 30 seconds.

[**HINT:** Start developing your code with a small number of particles N (perhaps a few hundred) and then increase it when you think your code works. A good target for N would be about about 100,000. A good target for the number of timesteps is about 50 steps; use that information and the information in the question to determine the expected width of the Gaussian random walk step.]

Question 2 [5 pts]

Repeat question 1 using an explicit Euler numerical solution of the Fokker-Planck equation. Use about 100 spatial points and a small enough timestep that the method is stable. Use either periodic boundary conditions or Neumann conditions with d/dx=0.

Question 3 [2 pts]

Compare the final N_2 density at t=30 seconds from questions 1 and 2 by combining the final histogram from question 1 and the final plot from question 2 .

Questions 1 and 2 result in animations, but Gradescope does not display animations in Jupyter notebooks. Please submit to Gradescope as follows:

1. Save your animations as GIFs.
2. Make sure your ipynb notebook is less than 1 MB. (If not, remove any inline animations.)
3. Combine your 2 GIFS and your ipynb notebook into a single .zip file.
4. Submit the zip file to Gradescope.

Rubric

Each question results in a plot or animation and uses the same 8-point rubric as on previous assignments. An example of a “minor error” in the 1-pt categories is if the code is commented, but not clearly, or the plot is missing a unit on one axis.

Code	**Commenting**: Clear and concise comments explaining the code.	1 pt	0: Missing or major error. 0.5: Minor error. 1: Correct.
	Logical Structure: Code is logically organized into functions and modules.	1 pt	
	Readability: Code is well-formatted with consistent and easily understood naming conventions.	1 pt	
Plot(s)	**Clarity**: Plot is clear and easy to understand.	1 pt	
	Labels and Units: Proper labels and units are included on all axes.	1 pt	
	Correctness: Plot shows the expected outcome of the question.	3 pts	0: Plot is missing or entirely incorrect. 1: Plot shows evidence of major conceptual errors. 2: Plot shows evidence of minor errors in the analysis. 3: Correct answer.