Assessment 3 – Final project – Option 4

General comments

The objective of the final project is to test your ability to use all the features of C we have studied within the module and to apply those to an area of physics or mathematics. Remember that you must produce code in agreement with the general expectations detailed in the introduction to the module (code structure, indentation, commenting, sensible variable names, etc.).

Your final submission should include your code (one .c file) and your report (one .pdf file). The report should include appropriate references and figures, and should be up to six pages in length. Half the total marks will be awarded for the code and half for the report.

Instructions

1. Write a program that simulates the random walk of a particle in one, two and three dimensions. The code must:

a) Perform a random walk on a one-dimensional lattice (of spacing Δx) for time T. At each time step (of size Δt), the particle randomly moves either forwards in x by distance Δx (with probability p), backwards by distance Δx (with probability p) or stays still (with probability $1-2p$). Choose $p = D\Delta t/(\Delta x)^2$ where D is the diffusion constant.

b) Extend the above to the two-dimensional case where now, at each time step, the particle independently moves in both the x and y directions (in each case with the same probabilities as above). Further, extend to the three-dimensional case.

c) For the two- and three-dimensional cases, extend your simulation to a self-avoiding random walk where the particle cannot visit the same lattice point more than once.

d) Provide some way to visualise the simulation output (using Python, gnuplot or another plotting program). **[50 marks]**

2. Within your report, explain the approach you took and how your code works. This should include the memory requirements of your code, how the runtime might be decreased if needed, the limitations of your approach, and ways that your code might be improved in future. **[20 marks]**

3. Use your code (rather than analytical methods) to explore the following questions. In each case, within the report, write up your findings and results (along with suitable plots and discussion) and explain how you used your program to address the question.

a) For a one-dimensional random walk, how does the average (over millions of runs) final squared-position $\langle x^2 \rangle$ depend on the simulation time T and the diffusion constant D? How does this change for the average final absolute-position $\langle |x| \rangle$? What is the functional form that relates $\langle x^2 \rangle$ to T and D, and $\langle |x| \rangle$ to T and D?

b) How do the above results change for two- and three-dimensional random walks? What about for self-avoiding random walks?

c) What happens for a non-symmetric random walk where the probability of moving in one direction is different to that to move in the opposite direction? **[30 marks]**