

Random Walk/Diffusion Summary

Write up a summary of your random walk/diffusion programs. Include the following sections:

[1.] Introduction: containing general information about random walks. For example: What is a random walk, and how does it differ from steady motion in the same direction? What does Pascal's triangle have to do with random walks? What might cause a molecule in a cell or in the air to move randomly? What role does temperature play?

[2.] Description of Program: for a set of random walks looking for a target molecule in a two dimensional cell with walls. For example: What is its structure? How do the loops work? What does it read in/print out? How do is the walker confined? How does it know if it reached the target? Include a copy of the program.

[3.] Figure showing a sample walk: Use xmgrace to make a plot of your walk. Try to make the figure appealing visually, eg by displaying the wall positions and also the position of the target molecule. Export it as postscript and include it in your report. Use 'convert' to change to other formats (pdf, jpg, gif) if you like.

[4.] Description of an 'Energy Landscape' Program: for a random walker at temperature T that receives an energetic kick at every step with probability P . What is the basic algorithm? How does it differ from a simple random walk in a flat landscape? Include a copy of the program.

[5.] Systematic study of the walker performance: Show results for different energy landscapes. Some examples are:

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 (This is a flat energy landscape which does not change from site to site)

0 1 0 1 0 1 0 1 0 1 0 1 ... (Generate this using energy[i]=i%2)

0 1 2 0 1 2 0 1 2 0 1 2 ... (Generate using energy[i]=i%3)

0 0 1 0 0 1 0 0 1 0 0 1 (Find a way to generate this also)

[6.] Effect of Temperature: How is the walker's motion affected by different temperatures $T = 0.5, 1, 2, 4, 8, 16$? To answer this question you might want to find the fraction of walkers that go left and the fraction that go right and the average number of steps before the walker exits the region.

[7.] Effect of Kicking Probability: How is the walker's motion affected by different kicking probabilities $P = 0, 0.1, 0.2, 0.5, 0.8, 0.9, 1.0$? To answer this question you might want to find the fraction of walkers that go left and the fraction that go right and the average number of steps before the walker exits the region.

[8.] Role of Temperature: Does T speed up or slow down the walkers? For $P = 0$, make a plot of (i) average number of steps (ii) fraction of walkers that go left as a function of temperature T for various cases. What conclusions can you draw? Include the plot in your summary.

[9.] Energy Landscape Symmetry: Examine the different energy landscape by plotting energy[i] vs i for i between 0 to 30. Identify which landscapes have left-right symmetry and which do not. Include the plot in your summary.

[10.] Role of P and T : in breaking the left-right symmetry. In which cases, do the walkers preferentially walk one way. Plot: (i) Fraction of walkers that go left as a function of P for fixed $T=1$, (ii) Fraction of walkers that go left as a function of T for fixed $P=0.1$, for different energy landscapes. Include the plot in your summary.

If you like, you can choose to include an analysis of one of the following additional sections/problems:

[11.] Effect of Cell Morphology: Consider cells which are not square, that is, with $X_{\text{size}} \neq Y_{\text{size}}$. Figure out whether it is easier or harder for the molecules to find each other. In answering this question, you might want to compare the probability of a walker finding a target at $(x_0, y_0) = (3, 4)$ for several cells with the same area but different aspect ratios, for example $X_{\text{size}} = 12, Y_{\text{size}} = 12$ versus $X_{\text{size}} = 16, Y_{\text{size}} = 9$ versus $X_{\text{size}} = 24, Y_{\text{size}} = 6$. Which type of cell would evolution prefer if the question of diffusing molecules locating each other were the most important issue?

[12.] Continuous Random Walk: Write a program to do a random walk in a cell where the walker is not confined to a lattice, eg by allowing steps of arbitrary length in arbitrary directions. Make a plot of one of the resulting walks.