

Computational Science 1

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Seminar Exercises

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Exercise 6 (9.12.2014):

A random walk in two dimensions

from *An Introduction to Computer Simulation Methods*,
Chapter 7, Problem 7.8

- a) Consider a collection of walkers initially at the origin of a square lattice. At each unit of time, each of the walkers moves at random with equal probability in one of the four possible directions. Create a drawable class, **Walker2D**, which contains the positions of M walkers moving in two dimensions and draws their location, and modify **WalkerApp**. Unlike **WalkerApp**, this new class need not specify the maximum number of steps. Instead the number of walkers should be specified.
- b) Run your application with the number of walkers $M > 1000$ and allow the walkers to take at least 500 steps. If each walker represents a bee, what is the qualitative nature of the shape of the swarm of bees? Describe the qualitative nature of the surface of the swarm as a function of the number of steps, N . Is the surface jagged or smooth?
- c) Compute the quantities $\langle x \rangle, \langle y \rangle, \langle (\Delta x)^2 \rangle$, and $\langle (\Delta y)^2 \rangle$ as a function of N . The average is over the M walkers. Also compute the mean square displacement $\langle R^2 \rangle$ given by

$$\langle R^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 + \langle y^2 \rangle - \langle y \rangle^2 = \langle (\Delta x)^2 \rangle + \langle (\Delta y)^2 \rangle \quad (1)$$

What is the dependence of each quantity on N ?

- d) Estimate $\langle R^2 \rangle$ for $N = 8, 16, 32$, and 64 by averaging over a large number of walkers for each value of N . Assume that $R = \sqrt{\langle R^2 \rangle}$ has the asymptotic N dependence:

$$R \sim N^\nu, \quad (N \gg 1) \quad (2)$$

and estimate the exponent ν from a log-log plot of $\langle R^2 \rangle$ versus N . The exponent ν is related to how a random walk fills space. If $\nu \approx 1/2$, estimate the magnitude of the self-diffusion coefficient D from the relation $\langle R^2 \rangle = 4DN$. Note that in general, the diffusion coefficient D is given by

$$D = \frac{1}{2d} \lim_{N \rightarrow \infty} \frac{\langle R^2 \rangle}{N}, \quad (3)$$

where d is the dimension of space.

- e) Plot the number of lattice points (flowers) that have been visited by the swarm in dependence on the number of steps N . Does this number fulfill a scaling relation analogous to Eq. (2)? If yes, what is the value of ν ?