Computational Science 1

`http://www.tu-chemnitz.de/physik/THUS/de/lehre/CSM_WS1819.php`

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Seminar
Exercises

Exercise 7 (4.12.2018):

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

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

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:

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

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

$$D = \frac{1}{2d}\lim_{N\to\infty}\frac{\langle R^2\rangle}{N}, \tag{3}$$

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?