Computational Science 1

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Seminar Exercises

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Exercise 7 (7.12.2017):

The two-dimensional self-avoiding walk and the Rosenbluth and Rosenbluth algorithm

from ***An Introduction to Computer Simulation Methods***,
Chapter 7, Problem 7.28-29

Consider the self-avoiding walk on the square lattice. Choose an arbitrary site as the origin and assume that the first step is “up”. The walks generated by the three other possible initial directions only differ by a rotation of the whole lattice and do not have to be considered explicitly. The second step can be in three rather than four possible directions because of the constraint that the walk cannot return to the origin. To obtain unbiased results, we generate a random number to choose one of the three directions. Successive steps are generated in the same way. If the next step does lead to a self-intersection, the walk must be terminated to keep the statistics unbiased. In this case we must start a new walk at the origin.

a) Write a program that implements this algorithm and record the fraction $f(N)$ of successful attempts at constructing polymer chains with N total monomers. Represent the lattice as a array so that you can record the sites that already have been visited. What is the qualitative dependence of $f(N)$ on N? What is the maximum value of N that you can reasonably consider?

b) Determine the mean square end-to-end distance $\langle R_N^2 \rangle$ for values of N that you can reasonably consider with this sampling method.

c) The described method becomes very inefficient for long chains, that is, the fraction of successful attempts decreases exponentially. To overcome this attrition, implement the Rosenbluth and Rosenbluth enrichment method in which each walk of N steps is associated with a weighting function $w(N)$. The desired unbiased value of $\langle R^2 \rangle$ is obtained by weighting R_i^2, the value of R^2 obtained in the ith trial, by the value of $w_i(N)$, the weight found for this trial. Hence we write

$$\langle R^2 \rangle = \frac{\sum_i w_i(N) R_i^2}{\sum_i w_i(N)} \tag{1}$$

where the sum is over all trials. Compute $\langle R^2 \rangle$ for $N = 4$, 8, 16, and 32. Estimate the exponent ν from a log-log plot of $\langle R^2 \rangle$ versus N. Can you distinguish your estimate for ν from its random walk value $\nu = 1/2$.