Computational Science 1

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Seminar
Exercises

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Exercise 7 (6.12.2012):

Diffusion controlled chemical reaction in one dimension

from ***An Introduction to Computer Simulation Methods***,
Chapter 7, Problem 7.33

Simulate the reaction $A+A \to 0$. Assume that N particles do a random walk on a one-dimensional lattice of length L with periodic boundary conditions. Every particle moves once in one unit of time. We study the concentration $A = N/L$ of particles. Especially we are interested in the long time behavior when A becomes small. Begin with all sites occupied, $A(t = 0) = 1$.

a) Make a log-log plot of the quantity $A(t)^{-1} - A(0)^{-1}$ versus the time t. The times should be separated by exponential intervals so that your data is equally spaced on a logarithmic plot. Does your log-log plot yield a straight line for long times? If so, calculate its slope. Is the mean-field approximation for $A(t)$ valid in one dimension? You can obtain crude results for small lattices of order $L = 100$ and times of order $t = 10^2$. To obtain results to within 10%, you will need lattices of order $L = 10^4$ and times of order $t = 2^{13}$.

b) More insight into the origin of the time dependence of $A(t)$ can be gained from the behavior of the quantity $P(r, t)$, the probability that the nearest neighbor distance is r at time t. The nearest neighbor distance of a given particle is defined as the minimum distance between it and any of the other particles. The distribution of these distances changes dramatically as the reaction proceeds, and this change can give information about the reaction mechanism. Place the particles at random on a one-dimensional lattice and verify that the most probable nearest neighbor distance is $r = 1$ (one lattice constant) for all concentrations. (This result is true in any dimension.) Then verify that the distribution of nearest neighbor distances on a one-dimensional lattice is given by

$$P(r, t = 0) = 2Ae^{-2A(r-1)}. \tag{1}$$

Is this form properly normalized? Start with $A(t = 0) = 0.1$ and find $P(r, t)$ for $t = 10, 100$, and 1000. Average over all particles. How does $P(r, t)$ change as the reaction proceeds? Does it retain the same form as the concentration decreases?

c) Compute the quantity $D(t)$, the number of distinct sites visited by an individual walker. How does the time dependence of $D(t)$ compare to the computed time dependence of $A(t)^{-1} - 1$?