Computational Science 2

http://www.tu-chemnitz.de/physik/THUS/lehre/CSM_SS13.php

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Seminar
Exercises

Exercise 3 (25.4.2013):

The ant in the labyrinth

from ***An Introduction to Computer Simulation Methods***,
Chapter 13, Problem 13.8

a) For $p = 1$, the ants walk on a perfect lattice, and hence, $\langle R^2(t)\rangle = 2dDt$. Suppose that an ant does a random walk on a spanning cluster with $p > p_c$ on a square lattice. Assume that $\langle R^2(t)\rangle \to 4D_s(p)t$ for $p > p_c$ and sufficiently long times. We have denoted the diffusion coefficient by D_s because we are considering random walks only on spanning clusters and are not considering walks on the finite clusters that also exist for $p > p_c$. Generate a cluster at $p = 0.7$ using the single cluster growth algorithm (Leath algorithm). Choose the initial position of the ant to be the seed site and modify your program to observe the motion of the ant on the screen. Use $L \geq 101$ and average over at least 100 walkers for t up to 500. Where does the ant spend much of its time? If $\langle R^2(t)\rangle \propto t$, what is $D_s(p)/D(p = 1)$?

b) As in part (a) compute $\langle R^2(t)\rangle$ for $p = 1.0, 0.8, 0.7, 0.65$, and 0.62 with $L = 101$. If time permits, average over several clusters. Make a log-log plot of $\langle R^2(t)\rangle$ versus t. What is the qualitative t-dependence of $\langle R^2(t)\rangle$ for relatively short times? Is $\langle R^2(t)\rangle$ proportional to t for longer times? (Remember that the maximum value of $\langle R^2(t)\rangle$ is bounded by the finite size of the lattice.) If $\langle R^2(t)\rangle \propto t$, estimate $D_s(p)$. Plot $D_s(p)/D(p = 1)$ as a function of p and discuss its qualitative dependence.

c) Compute $\langle R^2(t)\rangle$ for $p = 0.4$ and confirm that for $p < p_c$, the clusters are finite, $\langle R^2(t)\rangle$ is bounded, and diffusion is impossible.

d) Because there is no diffusion for $p < p_c$, we might expect that D_s vanishes as $p \to p_c$ from above, that is, $D_s(p) \sim (p - p_c)^{\mu_s}$ for $p \gtrsim p_c$. Extend your calculations of part (b) to larger L, more walkers (at least 1000) and more values of p near p_c and estimate the dynamical exponent μ_s.

e) At $p = p_c$, we might expect $\langle R^2(t)\rangle$ to exhibit a different type of t-dependence, for example, $\langle R^2(t)\rangle \to t^{2/z}$ for large t. Do you expect the exponent z to be greater or less than two? Do a simulation of $\langle R^2(t)\rangle$ at $p = p_c$ and estimate z. Choose $L \geq 201$ and average over several spanning clusters.

f) The algorithm we have been using corresponds to a blind ant, because the ant chooses from four outcomes even if some of these outcomes are not possible. In contrast, the "myopic" ant can look ahead and see the number q of nearest neighbor occupied sites. The ant then chooses one of the q possible outcomes and thus always takes a step. Redo the simulations in part (b). Does $\langle R^2(t)\rangle$ reach its asymptotic linear dependence on t earlier or later compared to the blind ant?