

## Problem Set 2

1. **Percolation.** Write a computer program to simulate percolation clusters on a square site lattice (two-dimensional array) using the Leath algorithm (discussed in Lecture 3 notes and handouts).

- (a) Imagine flipping fair coins ( $p = 1/2$ ) and arranging them in a square lattice configuration, as shown in lecture. In the limit of an infinitely large “random-coin lattice”, what is the probability  $R_\infty(1/2)$  of having an infinite connected path of “heads” from a given site? To answer this question, use your program to estimate  $R_L(p)$ , the probability that a cluster “spans” from the origin to to a large circle of radius  $L$ :

$$R_L(p) = \frac{\text{number of spanning clusters observed}}{\text{total number of clusters grown}}.$$

Do this for several large values of  $L$  (e.g. 10, 100, 1000,...) and try to extrapolate to  $L = \infty$ .

- (b) Using the largest value of  $L$  considered in (a), compute estimates of  $R_L(p)$  for different values of  $p$  ranging from 0 to 1, and plot  $R_L$  versus  $p$ . From these results, calculate an estimate of the critical point  $p_c^*$  as the value where  $R_L(p_c^*) = 1/2$ . How accurate is your estimate? <sup>1</sup>
- (c) Pick  $p = p_c^*$ , the critical point determined in (b), and a large radius  $L$ . Grow  $N \gg 1$  spanning clusters (ignoring those which do not span), and plot  $\log M(r)$  versus  $\log r$  for  $1 \leq r \leq L$ , where  $M(r)$  is the expected mass inside a circle of radius  $r$ ,

$$M(r) = \frac{\text{total number of occupied sites from all } N \text{ clusters inside a radius } r}{N}$$

Repeat for  $p = 0.65 > p_c$ , and show your results on the same plot. Comment on the difference with the critical case<sup>2</sup>

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<sup>1</sup>Extra credit: To determine  $p_c$  more precisely, you can try repeating this calculation for different values of  $L$  and extrapolating to  $L = \infty$  using the theoretical formula,  $\log p_c^*(L) \sim -(1/\nu) \log L$ . How many digits can you determine for  $p_c$ ? What is  $\nu$ ?

<sup>2</sup>Extra credit: Repeat for several values of  $p$  above  $p_c$ . For each set of data,  $M(r)$ , estimate the correlation length  $\xi(p)$  as the size  $r$  where the scaling of the mass changes from  $M \propto L^{D_f}$  to  $M \propto L^d$  (where  $d = 2$ ). Can you choose  $\xi(p)$  to collapse the data onto a single universal curve,  $\log(M/\xi^{D_f})$  versus  $\log(r/\xi)$ ?

2. **Diffusion (Random Walks)**. Write a program to simulate a random walk on the square lattice starting from the origin: At each time step  $n = 1, 2, 3, \dots, N$  the walker moves to one of the four neighboring sites with equal probability<sup>3</sup>.

- (a) Repeat the random walk  $M$  times, and measure the root-mean-square distance from the origin after  $n$  steps,  $n = 1, 2, \dots, N$ :

$$\sigma_n = \sqrt{\frac{1}{M} \sum_{i=1}^M (\text{position } r_i \text{ of } i\text{th walker after } n \text{ steps})^2}$$

Plot  $\log \sigma_n$  versus  $\log n$  to measure the exponent  $\nu$  defined by  $\sigma_n \propto n^\nu$  (from the slope). Also calculate (or derive) the prefactor  $A$  in the exact result,  $\sigma_n = An^\nu$ .

- (b) Calculate the probability density  $P_N(r)$  of the final radial distance from the origin  $r$  after  $N$  steps by making a histogram:

$$P_N(r) = \frac{\text{number of walkers ending between } r \text{ and } r + \delta r}{M \cdot \delta r}$$

where  $\delta r$  is some appropriate bin size, which makes your distribution look smooth. Plot your data for  $P_N(r)$  compared with the asymptotic result,

$$\Phi_N(r) \sim \frac{2r}{N} e^{-r^2/N}$$

which is valid as  $N \rightarrow \infty$  for  $r = O(\sqrt{N})$  according to the Central Limit Theorem<sup>4</sup>. To see the gaussian shape, also compare  $P_N(r)/(2\pi r)$  with  $\Phi_N(r)/(2\pi r)$ , which accounts for the number of points  $2\pi r \delta r$  in a shell of width  $\delta r$  and radius  $r$ .

- (c) Calculate the distribution  $P(\eta)$  of the fraction of time  $\eta$  spent by a single walker “to the right” of the starting point at the origin ( $x > 0$ ) during an  $N$  step walk,

$$\eta_i = \frac{\text{number of steps that the } i\text{th walker spends in the region } x > 0}{N}.$$

i.e. simulate  $i = 1, \dots, M$  walkers through  $N$  steps each, and compute a histogram:

$$P(\eta) = \frac{\text{number of walkers with } \eta_i \text{ between } \eta \text{ and } \eta + \delta \eta}{M \cdot \delta \eta}$$

using some reasonable bin width  $\delta \eta$  in the interval  $0 \leq \eta \leq 1$ . Comment on the shape of the distribution. Is it anything like what you expected?

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<sup>3</sup>Extra Credit: Make a picture of a large “cluster” of points visited by a random walker on the square lattice. Try to calculate the fractal dimension  $D_f$  of this set using the methods of problem 1. Is it really a fractal ( $D_f < d = 2$ )?

<sup>4</sup>Extra credit: Plot  $P_N(r)/\Phi_N(r)$  to more precisely determine the extent of the “central region” beyond which the approximation fails, which is often much wider than predicted by the CLT. Repeat for different values of  $N$  and try to determine how the edge of the central region scales (as  $N^a$  for some  $a \geq 1/2$ ).

3. **Diffusion-Limited Aggregation.** Write a program to simulate DLA growth from a point on the square lattice: Release random walkers from a random point on a large circle centered at the origin, and let each one go until it sticks (with probability one) adjacent to a boundary site on the growing cluster. To speed up the computation, you can remove a walker that wanders outside the circle and start a new one. You can also try starting with a fairly small circle, and letting it get bigger to stay ahead of the growth. However, a circle which is too close to the growing tips (e.g. such that the distance between outer branches is comparable to the distance to the circle) will somewhat affect the morphology of resulting DLA cluster.

Try to measure the fractal dimension of the clusters. Make pictures of typical DLA clusters, and compare with pictures of clusters from percolation (problem 1) and random walk paths (problem 2).

### **A Few Project Ideas:**

1. Study random walks and/or DLA on percolation clusters to model diffusion and growth in a disordered substrate.
2. Study how changing the rules for “sticking” to a growing DLA cluster affects its fractal dimension and other details of its morphology. This can make the model more realistic for situations like electrodeposition or the growth of bacterial colonies.
3. Study percolation in a microstructure, i.e. restrict the percolation problem is to a subset of the original lattice. Interesting examples could include cutting ellipsoidal holes out of the lattice, and studying connectivity of the holes to an outer boundary of the lattice (to model conduction pathways in a lithium rechargeable battery electrode) or cutting out subcritical percolation clusters (to model conduction pathways in a multicomponent metal-insulator alloy).
4. Study reaction-diffusion problems, where walkers either die or give birth to new walkers whenever they meet. This can be done on a simple lattice or on a percolation cluster (to model a random environment).
5. Study the distributions of the spanning cluster masses and minimum chemical distances in three dimensions and compare with the analytical predictions of the “Stochastic Renormalization Group” (recently proposed by MZB).
6. Study random-walk models for granular drainage (including the “Spot Model” recently proposed by MZB) and apply such models to describe the flow of radioactive balls in the MIT pebble-bed nuclear reactor.