

Computational Science 2

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Seminar Exercises

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Exercise 5 (09.05.2017):

Diffusion limited aggregation

from *An Introduction to Computer Simulation Methods*,
Chapter 13, Problem 13.9

- a) **DLAApp** generates diffusion limited aggregation clusters on a square lattice. Each walker begins at a random site on a launching circle of radius $r = R_{\max} + 2$, where $R_{\max}$ is the maximum distance of any particle in the cluster from the origin. To save computer time, we remove a walker that reaches a distance $2R_{\max}$ from the seed site and place a new walker at random on the circle of radius r . If the clusters appear to be fractals, make a visual estimate of the fractal dimension. Choose a lattice of linear dimension $L \geq 61$. Modify **DLAApp** by color coding the sites in the cluster according to their time of arrival, for example, color the first group of sites white, the next group blue, the next group red, and the last group green. Which parts of the cluster grow faster? Do any of the late arriving green particles reach the center?
- b) At $t = 0$ the four perimeter (growth) sites on the square lattice each have a probability $p_i = \frac{1}{4}$ of becoming part of the cluster. At $t = 1$, the cluster has mass two and six perimeter sites. Identify the perimeter sites and convince yourself that their growth probabilities are not the same. Do a Monte Carlo simulation and verify that two perimeter sites have growth probabilities $p = \frac{2}{9}$ and the other four have $p = \frac{5}{36}$.
- c) **DLAApp** generates clusters inefficiently, because most of the CPU time is spent while the random walker is wandering far from the perimeter sites of the cluster. There are several ways of making your program more efficient. One way is to let the walker take bigger steps the further it is from the cluster. For example, if the walker is a distance $R > R_{\max}$, a step of length greater than or equal to $R - R_{\max} - 1$ may be permitted if this distance is greater than one lattice unit. If the walker is very close to the cluster, the step length is one lattice unit. Make this modification to class **DLA** and estimate the fractal dimension of diffusion limited clusters generated on a square lattice by computing $M(r)$, the number of sites in the cluster within a radius r centered at the seed site. Because very large clusters are needed to accurately estimate the fractal dimension, you will obtain only approximate results.