Experiment 2.2: DLA, a microscopic growth model

Introduction

Under certain conditions surprisingly complicated structures can grow in nature as, for example, snowflakes. This is quite astonishing since the physics behind the growth process itself is rather simple: starting from some nucleus the snowflake gains size due to the fact that additional water molecules from the adjacent air get attached to the growing snowflake. Since attached molecules stick to the snowflake the air surrounding the snowflake will have a lower density of water molecules left and new molecules have to approach the snowflake from outside this surrounding region just by a random motion, a diffusion process. Hence, the process is controlled by a diffusion equation for the density of particles (water molecules).

Figure 1: Picture of a snowflake from http://www.its.caltech.edu/∼atomic

This kind of growth is called dendritic growth and one of the most important models for the study of dendritic growth is the DLA (**d**iffusion **l**imited **a**ggregation) model [1]. The DLA model simplifies the growth process to its two most important basic features, namely, (i) the random motion of particles reflecting a diffusion process and, (ii) the fact that these particles attach to a cluster the size of which grows with the number of attached particles. The growth is then proportional to the incoming flux of particles.

The DLA model is not only useful for the investigation of diffusion and the growth process itself. Instead, the resulting grown cluster has also interesting features since it contributes to the understanding of fractality.

The size of common geometrical objects (physically measured as mass, area, volume...) scales with their typical length scale (diameter, length,...) to the power of the dimension of the object. Hence, the relevant exponent is an integer, for real physical objects usually 1, 2, or 3.. For example, the area A of a circle with radius r is $A = \pi r^2 \sim r^d$. Here the dimension d is 2 since a circle is a two-dimensional object. For a generalised spherical object in d dimensions its volume V is $V \sim r^d$. In contrast to this, fractals are objects with a surprising geometrical property where the size of the objects scales with its length scale to some non-integer exponent.

The concept of fractality is important for the understanding of many different kinds of physical objects [2] and it is related to the concept of self-similarity, where each smaller part of the object, properly enlarged, is similar to the whole object. Inspecting the figure above you will indeed find that the snowflake is self-similar.

Objectives

- Write a code for the simulation of the DLA model in two dimensions on the square lattice.
- Graphically represent the grown DLA cluster.
- Calculate the fractal dimension from the data during the growth process.

Experiment: the DLA model

- **General aspects and initial condition**

  Consider a square lattice with $L \times L$ lattice sites (a two-dimensional array of integers) which can be either occupied or empty (0 or 1). Initially, the lattice is empty apart from the centre of the lattice where an initial nucleus is placed, i. e., this site is occupied (set to 1) and counts as initial cluster of size $S = 1$.

- **Motion of the particles and cluster growth**

  Then a particle is started randomly moving in the lattice. The starting point is a random position on a circle around the nucleus with radius r_s. From here a random motion of the particle is simulated, i. e., with the help of random numbers the particle moves to one of the four adjacent positions. If the distance to the nucleus grows too much, say, the distance to the centre becomes larger than some cut-off radius r_o the particle is lost and a new one is started.

  If the particles eventually touches the nucleus (is one of the nearest neighbours of the cluster) it stays at this position, i. e., this site is occupied from now on. The cluster size S is now 2 and the next particle is started.

  Since the cluster grows during this procedure, the radius r_s where the particles start has to be readjusted, such that it is always larger the maximum distance r_c of any particle in the cluster to the centre of the lattice.

Note that r_c has to be determined all the time while r_s and r_o have to be readjusted. The efficiency of the simulation will depend on how you do this. Of course, all these quantities have to fit into the system and the simulation must end when this condition is no longer fulfilled.

- **Graphical representation and determination of the fractal dimension**

  For a graphical representation you can simply store the coordinates, (x, y), of the cluster (the occupied sites) at the end of the simulation. A standard graphics program will then draw the cluster. Discuss the following points: Why does this structure arise and not a more or less circular cluster? Where does the symmetry come from?

  For the evaluation of the fractal dimension one has to calculate the size of the cluster, S, and the mean radius, R, (radius of gyration),

$$R = \sqrt{\frac{1}{S}\sum_{i=1}^{S} \underline{r}_i^2}, \tag{1}$$

  where $\underline{r}_i$ is the distance of the particle i to the centre of the cluster (lattice). Calculating $S(R)$ during the growth of the cluster one can determine the fractal dimension D_f assuming that the relation

$$S \sim R^{D_f} \tag{2}$$

  holds for larger cluster sizes S. Try lattice sizes with L of the order of 500 which will lead to cluster sizes of the order of some 10000. What does the number you obtain for D_f tell you and what would one naively expect?

References

[1] T. A. Witten and L. M. Sander, Phys. Rev. Lett. **47**, 1400 (1981)

[2] J. Feder, *Fractals*, Plenum Press, New York (1988)