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# MULTISCALING ANALYSIS OF LARGE-SCALE OFF-LATTICE DLA

Peter OSSADNIK

*Höchstleistungsrechenzentrum, Forschungszentrum Jülich GmbH, Postfach 1913, W-5170 Jülich, Germany*

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An improved algorithm has been used to simulate off-lattice diffusion-limited aggregation (DLA) in two dimensions. This enables us to grow clusters of up to $6 \times 10^6$ particles, which are the largest such clusters made up to now. The density profile in two dimensions is analyzed for the scaling form (multiscaling) $g(r, R) = r^{-d+D(x)}C(x)$ with $x = r/R$, where $R$ is the radius of gyration and $r$ is the distance from the cluster origin. In contrast with previous studies, the dimension $D(x)$ shows no systematic tendency to drop at large values of $x$ but only fluctuates around the global fractal dimension $D = 1.712 \pm 0.003$.

## 1. Introduction

Growth phenomena are very actively studied because of their relevance in many fields. Diffusion-limited aggregation (DLA) [1] is a particularly interesting model which describes phenomena like dielectric breakdown, viscous fingering or electrodeposition. Some of these topics have been summarized, e.g., in refs. [2, 3]. One very interesting question about DLA is the internal structure of the resulting clusters. As is very well known, off-lattice clusters are fractal with an overall fractal dimension $D = 1.715 \pm 0.004$ [4], which is defined through the dependence of the radius of gyration $R_g$ on the cluster mass $M$, i.e. the number of particles, by

$$R_g \propto M^{1/D} . \tag{1}$$

Recently it has been suggested that DLA clusters might have a richer structure which can be described by a multiscaling fractal dimension $D(x)$ that depends continuously on the relative distance $x$ from the cluster origin [5]. In this paper we study the behavior of $D(x)$ for large off-lattice DLA clusters of $10^6$ particles. In section 1 we present a detailed description of an algorithm that produces these large clusters. In section 2 we make some remarks on the

self-similarity of very large scale off-lattice DLA clusters and in section 3 we present the results for the multiscaling dimensions.

## 2. Model and method

The basic process for growing off-lattice DLA clusters is as follows: Initially the cluster or aggregate consists of one single seed particle. Now another particle is launched from "infinity" that may undertake a random walk of fixed step length until it hits the cluster and sticks to it. Afterwards another particle is launched and this process is repeated until a cluster of intended mass is grown. Because of the fixed step length in the random walk and the launching at "infinity" the previously described algorithm is not very efficient.

In all practical DLA algorithms [6, 4] the particles are launched from a randomly chosen position on a finite hypersphere that encloses the cluster. They are stopped if they either hit the cluster or move a large distance away from it. In both cases a new particle is generated at a randomly chosen position on the launching hypersphere. Obviously it is sufficient to have a launching hypersphere that is only slightly larger than the cluster itself.

The major improvement of the algorithm is to modify the step length during the random walk [7, 4]. In the empty regions between the branches of the cluster or far away from it, it is obviously not necessary to have a fixed small step length but rather to allow for longer jumps as long as they do not accidentally cross a branch of the cluster. For that reason it is necessary to find the largest empty region around a given random-walker in order to get a good estimate for the largest possible step length for the next jump.

The idea is essentially to construct maps of the aggregate on different length scales. If the walker wants to take the next step one first consults the coarsest map. If this map indicates that – on this special length scale – the walker is far away from the cluster the jump is executed. Otherwise the next finer map is examined. This process is repeated until a map is found where the jump can be executed or the finest map is reached. In this last map each element contains a list of the precise coordinates of the particles in a small given region to check which one of them, if any, is touched by the walker during the next jump.

After this rough description of the method we now want to present some computational details of the actual implementation of this algorithm. To determine the position of a random-walker we start with a root map consisting of an $N_r^d$-array of pointers, where $N_r$ is the number of lattice sites in one space dimension in the coarsest map. Each array element represents a certain part of size $L_0^d$ of the growth region. If a given pointer contains the special value

"NIL" there are no cluster particles in or near that region. Otherwise it points to a structure of $2^d$ pointers, each of them representing a certain subregion of size $(L_0/2)^d$. On this level again a pointer containing NIL indicates an empty region while a non-NIL entry points to the next finer map. This map structuring is continued to a given depth. In our simulations we used maps of depth six. In the finest level the map elements contain a pointer to a list of coordinates. For the set of particles that should be stored in this list, Tolman and Meakin [4] suggested two possibilities:

(1) All the particles whose centers are in that region.

(2) All the particles that can be contacted by a walker whose center is in that region.

For simulations of large-scale clusters ($\geq 5 \times 10^5$ particles) we found it necessary to implement the first version in order to reduce the memory consumption which was the bottleneck of our simulations.

Another computational parameter with which one can tune the memory and the time consumption is the ratio of the size of the particles to the length scale of the finest map. A small ratio, e.g. 1, leads to fast programs, which need much memory, while a large ratio leads to memory-saving but slow programs. We chose the length scale of the finest map to be four times the size of the particles.

With that implementation we used about 14 Mbytes of memory and about 9 hours of CPU time on a Sun Sparc-station1 to grow a $10^6$ particle cluster. For the simulation of even larger clusters of size $6 \times 10^6$ particles we used a special memory-management strategy in order to reduce the memory consumption. Here we employed the fact that the active growth zone is only a fraction of the whole cluster [8] so that only the coordinates of the recently attached particles are often needed during the simulation while the rest can be stored on disk. In case a walker accidentally travels into the region of the cluster that resides on disk, one has to read the coordinates of the particles back into memory. For the $6 \times 10^6$ particle cluster we kept in (virtual) memory the coordinates of the last $3 \times 10^6$ particles. Here the memory consumption was about 50 Mbytes and the run time was about 6 days. A programme will be published elsewhere and can be obtained from the author.

One interesting feature of our implementation is that for clusters of sizes $10^6$ to $6 \times 10^6$ particles the user CPU time and the memory consumption depend only linearly, or at most with an exponent that is very close to unity, on the cluster size. This is demonstrated in fig. 1. From this data we obtain a power-law behavior where the user CPU time depends with an exponent $\nu_T = 1.047 \pm 0.005$ and the memory consumption depends with an exponent $\nu_m = 0.994 \pm 0.005$ on the cluster size. For very large clusters of $6 \times 10^6$

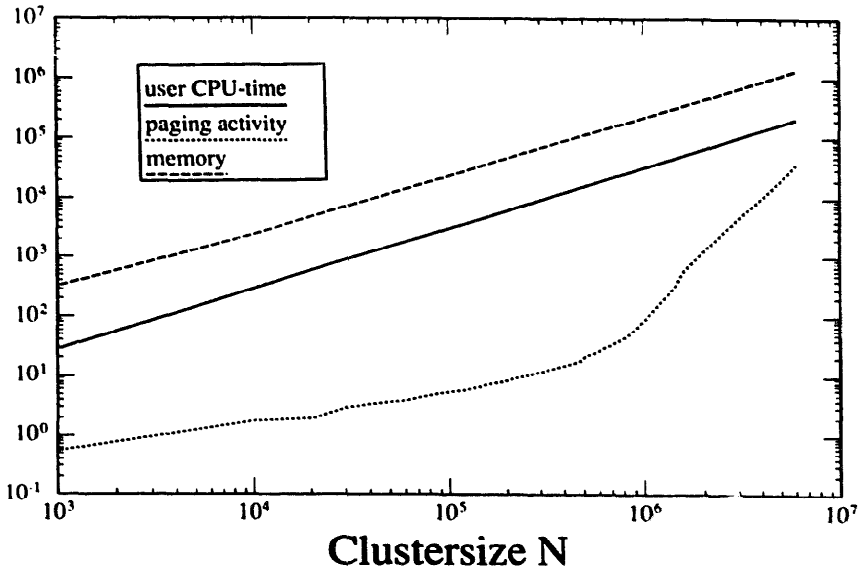


Fig. 1. Size dependence of the user CPU-time, the memory consumption and the paging activity for a $6 \times 10^6$ particle off-lattice DLA cluster.

particles the total run time, i.e. the user and the system CPU time, does no longer depend linearly on the cluster size. This is due to an increased paging activity of the operating system because the main memory of our workstations is only 8 Mbytes which is much less than the actual amount of memory needed for the simulation. This is also demonstrated in fig. 1. Here the paging activity is measured in terms of the system CPU time which is in our case proportional to the disk access time. One clearly sees a crossover behavior at about $10^6$ particles that strongly influences the total run time.

## 3. Statistical self-similarity

Lattice DLA is known to show a slow crossover in the overall shape. While small clusters of only a few thousand particles have a very ramified structure due to strong fluctuations, the shape of large clusters of several million particles is dominated by the structure of the underlying lattice [9]. Large DLA clusters on a square lattice exhibit a starlike overall shape.

Although it might not be expected that also off-lattice DLA clusters exhibit such a crossover behavior in their shape, the asymptotic structure of off-lattice DLA clusters is still quite controversial. Indication exists either for a slow crossover to a fully self-similar structure or for more complex behavior even for infinite sizes. There have been suggestions and numerical evidence in favour of

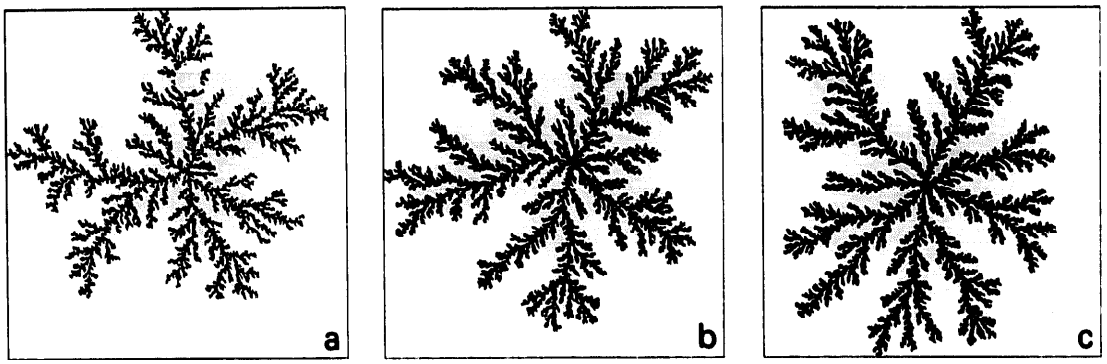


Fig. 2. Comparison of three different off-lattice DLA clusters of sizes differing over three orders of magnitude. (a) $6 \times 10^4$ particles, (b) $6 \times 10^5$ particles and (c) $6 \times 10^6$ particles. All clusters are plotted using the same resolution of 144 dots per inch.

a directed fractal [10], geometrical multifractality [11] or multiscaling [5]. Therefore it should be interesting to investigate if there is some special cluster size above which the individual clusters have a self-similar shape. For this we propose to use a simple visual criterion. We have grown clusters in sizes of three different orders of magnitude, namely $6 \times 10^4$ to $6 \times 10^6$ particles, and plotted them with the same resolution. This is important in order not to fool the visual impression. The clusters are shown in fig. 2.

It is striking to note that the two last figures are virtually indistinguishable modulo statistical fluctuations. That means that over one order of magnitude in size difference self-similarity is convincingly present. This is not the case for smaller clusters.

With growing cluster size it gets more and more difficult to distinguish which of the clusters has more sites than the other. The shape of the small cluster is more influenced by fluctuations than that of the larger clusters. It can be seen that visual self-similarity is reached for clusters that contain at least several $10^5$ particles.

This suggests three conclusions. The first is that large off-lattice DLA clusters seem to be really self-similar for infinite sizes. The second is that a crossover behavior like in lattice DLA does not appear. Furthermore, one has to grow large clusters ($>10^5$ particles) to obtain results that are not strongly affected by finite-size effects. High-quality computing is needed to test DLA self-similarity.

## 4. Multiscaling

One feature of moderate-sized DLA clusters seems to be the existence of different scaling exponents for different quantities. By studying the width of

the active growth zone, Plischke and Rácz [8] found an exponent that differs from the overall exponent determined by the radius of gyration. Coniglio et al. [5] proposed the existence of a whole set of scaling exponents within the framework of multiscaling.

For that purpose we measure the radial density profile $g(r, R)$ which is defined as

$$g(r, R)\, \mathrm{d}^d r = \mathrm{d}N\,, \tag{2}$$

where $\mathrm{d}N$ is the number of particles in an infinitesimal volume element $\mathrm{d}^d r$ at distance $r$ from the origin of the cluster. The size $N$ of the cluster is implicitly given by the radius of gyration $R = R(N)$.

By analogy with critical phenomena one usually assumes a scaling behavior

$$g(r, R) = r^{-d+D} f\left(\frac{r}{R}\right), \tag{3}$$

with a scaling function $f(x)$ and the overall fractal dimension $D$. Coniglio and Zannetti [5] suggested to replace the overall fractal dimension by a more structured function $D = D(r/R)$ in order to determine the set of fractal dimensions within different shells. Thus they proposed a scaling form

$$g(r, R) = r^{-d+D(x)} f(x)\,, \qquad x = r/R\,. \tag{4}$$

One expects that well inside the frozen regions of the cluster $x \to 0$ the multiscaling exponent $D(0)$ is the same as the global fractal dimension measured before. On the other hand, it is not possible to predict a priori the behavior of $D(x)$ in the outer regions.

Recently this possibility was studied numerically using clusters of $10^5$ particles by Amitrano et al. [12]. Some evidence was given that the multiscaling dimension $D(x)$ is not a constant but depends continuously on $x$. As expected, for small $x$ the fractal dimensions $D$ and $D(x)$ agree very well. For increasing $x$ they obtained a small maximum at $x \simeq 1.4$ and a continuous drop between $x \simeq 1.7$ and $x \simeq 2.1$. In our study of the multiscaling behavior of large DLA clusters we grew 100 off-lattice DLA clusters of $10^5$ and of $10^6$ particles. The cluster growth was divided into 10 stages to give different values for the radius of gyration. From stage to stage the mass of the cluster was increased by a factor of 1.25. At each stage the cluster was divided into 30 shells in which we measured the mass $M(r_n, R)$, which is directly related to the density profile

$$M(r_n, R) = 2\pi r_n g(r_n, R)\, \Delta r\,. \tag{5}$$

A comparison of the radii of gyration of two subsequent growth stages leads to a scaling factor $l$ given by

$$l = R_{n-1}/R_n \,. \tag{6}$$

After rescaling the thickness and the radii of the shells by this factor one obtains an estimate of the fractal dimension within a given shell,

$$\begin{aligned} \Delta r_{n+1} &= l\,\Delta r_n \,, \\ r_{n+1} &= l r_n \,, \\ D\left(\frac{r_{n+1}}{R_{n+1}}\right) &= d + \frac{\ln[g(r_{n+1}, R_{n+1})/g(r_n, R_n)]}{\ln(l)} \,. \end{aligned} \tag{7}$$

Then we averaged over each growth stage of the cluster and over the different runs. The results obtained for both cluster sizes are shown in fig. 3.

At small $x$ we obtain for $D(x)$ a value that is, within the statistical error, very close to the overall fractal dimension: $D(0) = 1.69 \pm 0.02$ and $D = 1.712 \pm 0.003$. Here we obtained $D(0)$ by fitting a straight line to the values of $D(x)$ for small $x$ and extrapolating it to $x = 0$. For growing $x$ the multiscaling dimension remains fairly constant. For large values of $x$ one has to measure the outer region of the cluster where the measurement of the mass is very inaccurate since there are less particles. This results in large fluctuations and statistical error bars for $D(x)$.

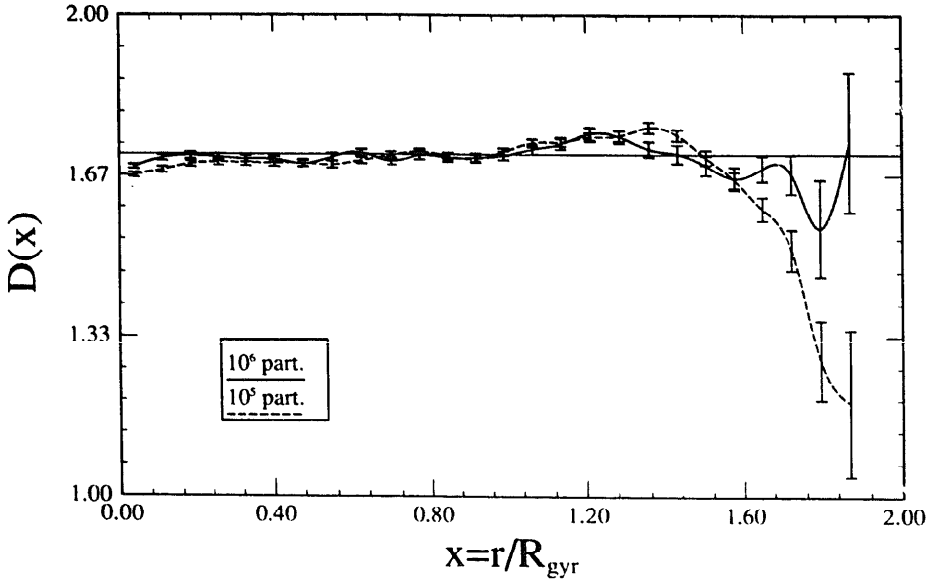


Fig. 3. Plot of the multiscaling dimensions $D(x)$ for 100 off-lattice DLA clusters with $10^6$ particles (solid curve) and for 100 off-lattice DLA clusters with $10^5$ particles (dashed curve). The thin solid line denotes $D = 1.712$.

For the small clusters of $10^5$ particles we reproduced the systematic drop of $D(x)$ at large $x$ described earlier. But for large clusters of $10^6$ particles this systematic deviation is much less pronounced and seems to disappear within the error bars. For large $x$ the estimates of the multiscaling dimensions seem to remain constant around the mean value of $D(0) = 1.69$, only fluctuating around this value. Our data therefore suggest that the multiscaling observed in ref. [12] is only a crossover behavior for clusters of the order of or smaller than $10^5$.

## 5. Conclusion

In the present paper we have presented a detailed description of an effective algorithm to grow large-sized off-lattice DLA clusters and produced the largest clusters so far. Using this algorithm we grew 100 clusters of size $10^5$ and $10^6$ particles and checked the multiscaling ansatz recently suggested [5]. For small clusters of size $10^5$ particles we found a systematic decrease in the multiscaling dimension $D(x)$ for large $x$. This systematic behavior disappeared for larger clusters. The multiscaling dimensions only showed statistical fluctuations around the value of $D = 1.712 \pm 0.003$. Thus we suggest that this effect might be a finite-size effect that disappears for large clusters.

Tolman and Meakin also showed that the exponent that describes the width of the active growth zone tends for large cluster sizes to be of the same value as the fractal dimension $D$. This is another hint indicating that some effects that were previously explained by the existence of several fractal dimensions may be simply crossover effects. Therefore one could speculate that also other effects like geometrical multifractality might be for off-lattice DLA only crossover effects for finite cluster sizes. More work in this direction is in progress.

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