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Self-similarity of the branching structure in very large DLA clusters and other branching fractals

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Abstract. We study the branching structure of very large DLA clusters, of up to 100 million particles. The Horton–Strahler ordering of the branches in these clusters shows a relaxation towards a state with the stream numbers forming a geometric series. This behaviour is compared with those of several self-similar trees. It indicates that DLA clusters converge to topologically self-similar objects.

1. Introduction

This is one of several reports from the Yale group on the properties of very large clusters of off-lattice diffusion-limited aggregation (DLA). For the sake of completeness, let us recall the underlying process. In DLA growth, an ‘atom’ executes Brownian motion until it hits, and is attached to, the curve that bounds a given ‘target’ or ‘seed’. Another atom is then launched, and the whole process repeats. Initially, the growth rule and the pattern are very simple, but both become extremely complex in time.

Witten and Sander [1] believed that DLA clusters are self-similar, i.e. that their complication is about the same at all scales of observation that are sufficiently above the scale of the atom. More precisely, consensus arose that the clusters are ‘prefractal’ approximations that eventually cross over to a self-similar structure. A prototype of such behaviour is given by the samples of a random walk, which are prefractal approximations that cross over to Brownian motion. In mathematics, this process of approximation is called weak, or vague, convergence; it is discussed in detail in [2, chapter 36].

However, departures from self-similarity were soon observed (see [3,4]). A natural and tempting scenario assumes that the crossover to a self-similar range lies beyond the sample sizes investigated until very recently. We would like to elaborate on this scenario, by suggesting that the crossover to self-similarity may occur at different cluster sizes for different properties of DLA. Some characteristics may cross over quickly, for relatively small clusters, while others cross over slowly, for very large samples.

This last scenario is not the only one possible. In [4], one of us has put forward an alternative to asymptotic self-similarity. This alternative assumes that as a DLA cluster grows, some properties of the cluster may attain a limit, but others may ‘drift’ without limit. It is indeed conceivable, at least in theory, that as sample size grows, some properties of DLA clusters do not attain a limit.

With the above ideas in the background, the Yale group has undertaken a systematic study of very large off-lattice DLA clusters. One of the aims set is to determine which

properties develop the signatures of self-similarity, and which fail to do so. Part of the study is based on 50 clusters of 1 million particles, while another part is based on smaller numbers of 100 million particle clusters.

In theoretical off-lattice DLA, i.e. when the incoming particles perform Brownian motion in the continuous plane, an incoming particle adheres to one and only one particle in the cluster. This gives rise to a tree structure, with the initial nucleus particle as the root and each particle being the descendant in the tree of the particle on which it stuck to in its aggregation to the cluster. In practice, due to limited computer precision, there is a finite probability that a new particle will come in contact with more than one particle in the cluster. In our simulations, the resulting closed loops are of negligible number. In the case of on-lattice DLA, many loops are present, although even those may be disposed of by arbitrarily choosing a unique parent for a new particle sticking to the cluster.

This article centres on off-lattice DLA clusters. For the sake of background and comparison and because of their intrinsic interest, the paper also discusses several self-similar tree constructions for which exact results exist.

We begin with a statistical study of branching rates in DLA clusters, i.e., the number of child particles associated with each parent particle. These rates seem to be constant during its growth. The branching rates are also homogenous spatially, at different distances from the origin. These results are consistent with self-similarity.

Next we define and study the branches of the DLA clusters from the viewpoint of Horton–Strahler ordering [5, 6]. Several authors have tackled this task [7–9]. However, our analysis of very large DLA clusters shows that the earlier results concerned transients in the growth process. Our simulations show that numerical values related to the Horton–Strahler ordering do not relax to constant values until the clusters attain sizes of about 200 000 particles. Compared with what is known for other self-similar branching structures, our findings show that certain structural aspects of very large DLA clusters do converge to signatures of self-similarity. Recently Ossadnik [10] studied properties of the branching structure of large DLA clusters. His work was mainly focused on metric properties of the clusters, while the issues addressed here are almost purely topological.

In an appendix we sketch the methods we use to simulate extremely large DLA clusters, in particular those of 100 million particles.

2. Horton–Strahler ordering of the branches of a tree

To study river networks, Horton [5] devised a scheme for indexing the hierarchical structure of the streams. Streams starting from the sources of a river network are assigned the order 1 and, moving downstream, a confluence of streams raises the order of the resulting stream. Strahler [6] slightly modified this ordering scheme, to make it independent of metric or directional properties of the streams. Either scheme applies to all tree-like structures, where the terms *leaf*, *branch* and *root* replace the corresponding terms in river networks: *source*, *stream* and *outlet*. This work uses the Strahler ordering scheme.

Given a rooted tree structure, Strahler orders the branches recursively

- (1) Each leaf is assigned the order $i = 1$.
- (2) The order i of a subsequent branch is determined by the orders i_1, i_2 of its two sub-branches: if $i_1 \neq i_2$ then $i = \max\{i_1, i_2\}$; otherwise $i = i_1 + 1$.

When the order of a branch is equal to that of one of its sub-branches, it is considered to be a continuation of this branch, otherwise it is considered to be a new branch. The

order of a whole tree is defined to be the order of the root, its lowest-lying branch. When a branch has more than two sub-branches, only the two of highest order are considered.

Consider the number of branches N_i of given Strahler order i in a tree (*stream numbers*). N_1 is equal to the number of leaves. If I is the order of the whole tree (i.e. of its root) then $N_I = 1$. The bifurcation ratio B_i of branches of order i and $i + 1$ is defined by

$$B_i = N_i/N_{i+1} . \tag{1}$$

The geometric mean of the B_i 's is

$$B = \left[\prod_{i=1}^{I-1} B_i \right]^{1/(I-1)} = N_1^{1/(I-1)} . \tag{2}$$

Evidently, the Strahler analysis disregards metric properties of river networks and focuses on the topological properties pertaining to their tree-like structure. Yet this partial information might point out any universal behaviour of such branching structures.

Studies show that for many river networks, the stream numbers $\{N_i\}$ are very well approximated by a geometric series

$$N_i \approx B^{I-i} \tag{3}$$

otherwise stated as

$$B_i \approx B \tag{4}$$

for all i . The observed values of B for different river networks vary between 3 and 5.

Using variants of self-avoiding random walks in two dimensions to generate tree-like models of river networks, several authors [11–14] found bifurcation ratios varying between 3.63 and 4.11, depending on the variant. The numbers of lowest order streams—far from the roots—did form geometric series.

3. Strahler ordering of self-similar trees

The stream numbers are very easily computed for strictly self-similar trees constructed by recursive processes.

The simplest example is a complete binary tree, where each node branches in two. For a tree of height I the stream numbers are

$$N_i = 2^{I-i} \tag{5}$$

forming a geometric series.

Similarly, a Koch tree [15], where each tip branches into 3 branches, yields $B_i = 3$ for all i .

The self-similar tree introduced by Mandelbrot and Vicsek [16] is more complex, and instructive. In the underlying recursive procedure, each line segment of length λ is replaced by a line segment with a branch of length $\lambda/2$ rooted in its middle. This iterative procedure leads to a self-similar fractal tree of self-similarity dimension $D = \log 3/\log 2$. Figure 1

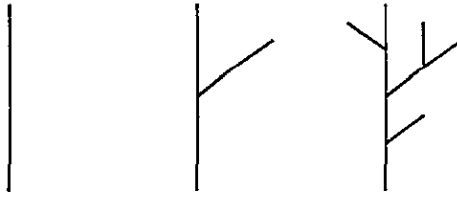


Figure 1. The first three stages of iteration of the self-similar fractal tree of Mandelbrot and Vicsek [16].

shows the first three steps in the construction. After the t th iteration of this substitution rule, the stream numbers are given by the recursion relation

$$N_i^t = 3N_i^{t-1} - 1 \quad (6)$$

for $i \leq t$, with the initial conditions

$$N_i^t = \begin{cases} 1 & i = t + 1 \\ 0 & i > t + 1. \end{cases} \quad (7)$$

The solution of this recursion relation is

$$N_i^t = \begin{cases} \frac{1}{2}[3^{t-i+1} + 1] & i \leq t + 1 \\ 0 & i > t + 1. \end{cases} \quad (8)$$

Therefore, at any step t of the iteration, and for any value of $i \leq t$, the bifurcation ratios are

$$B_i^t = [3^{t-i+1} + 1] / [3^{t-i} + 1] = 3 + O(3^{-(t-i)}). \quad (9)$$

As long as $t \gg i$, the bifurcation ratios tend asymptotically to 3. Note that the order of the whole tree at any stage of the iteration is $I = t + 1$. Denote by n the number of first order branches at time t , $n = N_1^t$. The order I of the whole tree depends logarithmically on n ,

$$I = 1 + \log_3(2n - 1). \quad (10)$$

When describing a structure as being statistically self-similar, one may start with the whole structure, and assume that any part of the system is similar, up to some scaling factor, to the whole.

One may also start at the shortest length scale, eliminate this length scale by performing some kind of average, and then scale down the system. The resultant *coarse-grained* system is then supposed to be similar to the original one. This is the method used when performing coarse-graining or renormalization on spin systems: several spins are clumped together to form a pseudo-spin, and the system is scaled down.

It is natural to use coarse-graining in the study of Strahler ordering. In the beginning, all branches of order 1 are at the tips of the tree. These are counted and then pruned off. The resulting tree has branches of order 2 at its tips. Pruning the tree recursively in this manner counts its stream numbers. If the tree is statistically self-similar, one should find that, at any stage, the pruned tree has the same statistical properties, up to some scale factor—the bifurcation ratio.

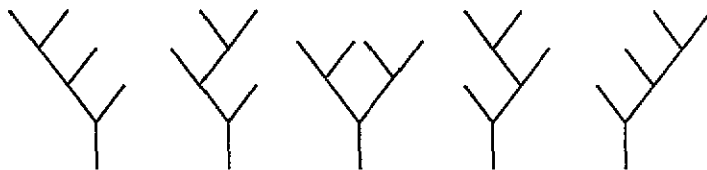


Figure 2. All five distinct binary trees of magnitude 4.

The assumption that such a tree is self-similar has as a corollary that the bifurcation ratios are equal (and constant), at least asymptotically, and far from the root of the tree. However, the converse is not true. The bifurcation ratios may be asymptotically equal even if the tree fails to be self-similar, this being a necessary condition but not a sufficient one. This possibility will be very important when we come to DLA.

An example of a statistically self-similar structure is a random binary tree. Consider the ensemble of all distinct rooted binary trees of a given magnitude (number of sources, or leaves). Assigning to each of these trees the same statistical weight defines the random binary tree model. Figure 2 shows all five distinct binary trees with four sources.

Shreve [17] was first to use random binary trees as a model for river networks. He found empirically that the bifurcation ratios tend asymptotically to 4. He also noted that the typical order of a tree of magnitude n was very close to

$$I_{\text{typ}} = \lfloor \log_4 n \rfloor . \quad (11)$$

These findings were later substantiated by analytical studies of random binary trees by Kemp [18], Flajolet *et al* [19] and Meir *et al* [20]. Moon [21] had shown that the ratio of the expectation values of successive stream numbers tended to 4. Wang and Waymire [22] have recently given proof that the first bifurcation ratio B_1 tends to 4 in a stronger sense. Two of the authors of the present paper have shown [23] that this is also the case for B_2 . This proof can be extended to higher, finite orders, but involves very cumbersome algebraic computations. It seems reasonable to expect the same property for any order $i \ll I_{\text{typ}}$. For branches lying close to the root of a tree, i.e. of order close to I_{typ} , the bifurcation ratio is different from 4. The expectation value of the lowest-lying bifurcation ratio $B_{I-1} (= N_{I-1})$ is less than 4, becoming asymptotically a periodic function of $\log_4 n$, with mean 3.34 and amplitude 0.19 .

4. Strahler ordering of the branches in DLA clusters

The results we discuss now were gathered from DLA clusters of either 1 million or 100 million particles. The 1 million particle clusters were generated as off-lattice DLA using a floating-point representation of particle positions. We use data averaged over 50 such clusters.

Generating 100 million particle clusters requires extremely long computing times and an enormous amount of memory. In order to minimize storage requirements, while conserving accuracy, particle positions were represented by a hierarchical tree of lattices of increasingly fine resolution. These DLA clusters are on-lattice, but the lattice spacing at the lowest level of the hierarchy is $\frac{1}{32}$ of a particle diameter. One can most probably neglect anisotropy effects, as an incoming particle may stick to another particle from approximately 100 directions.

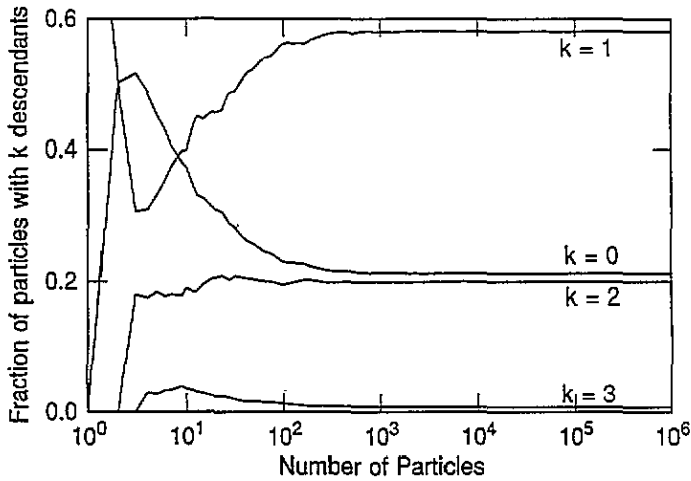


Figure 3. Fractions of the particles with different numbers of descendants as a function of the number of particles in the DLA cluster. The distributions are averaged over 50 clusters of 1 million particles each.

To deal with the long computation times, we replaced usual DLA by a variant we call parallel DLA. The clusters were generated on an IBM PVS computer which uses 32 RS/6000 RISC processors in parallel, with 512 megabytes of shared random access memory. Each processor handled the random walk of a single particle. Particles attempting to stick to the cluster while in overlap with a newly attached particle of the cluster were rejected. It takes 16 hours to generate a 100 million particle 'parallel DLA' cluster. Due to memory and time limitations, we did not sample these large clusters at many instants during their growth.

Measurements of the mass-radius relation of these parallel DLA clusters conform with the known result of the fractal dimension of DLA

$$D \approx 1.71. \quad (12)$$

Nevertheless, the overlap between the particles random-walking in parallel might induce some bias, relative to the original 'sequential' version of DLA—with particles sent one by one. A more detailed account of our methods of simulation, as well as comparison between 'sequential' and 'parallel' DLA growth, will be presented elsewhere [24].

First we checked for the number of descendants of each particle. The number of descendants is bounded by 0 (for a particle at the edge of the cluster) and 5 (including the parent particle, 6 is the maximal number of equally sized disks which can surround a disk of the same size). Figure 3, which refers to averages over 50 DLA cluster of 1 million particles, plots the fraction of particles with k descendants, for $0 \leq k \leq 3$, as a function of the number of particles in the clusters, as they are growing. The different curves begin with a transient which settles off when there are about 1000 particles in the cluster. The curves then remain constant throughout the growth of the clusters. The curve of the fraction of particles with 4 descendants is indistinguishable from the x -axis, as their number in a whole cluster of 1 million particles is less than 10.

Retaining only the particles with 2 or more descendants, we found that the branching rates are constant throughout the cluster, apart from the initial transient. From this data one can calculate the average link length (i.e. the number of particles along a chain

between successive nodes of the tree). We find that this is approximately equal to 2.35 particles. Particles with 2 descendants account for 96.5% of the branching in the cluster, the remaining being essentially due to branching into 3 branches. We conclude that, to a good approximation, DLA clusters are binary trees. It seems that under 100 000 particles, clusters are not yet stabilized, in as much as the branching rates are concerned. For larger clusters, the branching rates are uniform outside this (relatively) small inner core.

Next we calculated the Strahler orders of the branches in DLA clusters. In analysing these results, one should take into account two factors. The first is that the statistical fluctuations are larger for the higher Strahler orders. The reason is that the stream numbers decrease exponentially with the order, and that we deal with an object generated by a random process. The second factor is that an asymptotic value of a bifurcation ratio cannot be achieved until the Strahler order in question is much smaller than the order of the root. This was seen for the Mandelbrot and Vicsek fractal tree, as well as for random binary trees.

Figure 4 plots the bifurcation ratios $B_i = N_i/N_{i+1}$ for $i = 1, 2, 3, 4$ as a function of the number of particles in the cluster, using averaged data of 50 one million particle clusters. B_1 has settled to a constant value of 5.34. The ratios B_2 and B_3 seem to be attaining a different value, 5.2, while the ratio B_4 is still in a transient, with relatively large fluctuations. Figure 5 shows a similar curve for a single 100 million particle cluster. From it we see that B_1 takes an asymptotic value of 5.33, compatible with the result obtained from the smaller cluster, but clearly distinct from the value 5.2 to which B_i for $i = 2, 3, 4$ seem to converge. The order of the root particle grows approximately as $\log_5 N$.

Note that the bifurcation ratios are larger in DLA than in any previously studied structure (of course one may artificially construct trees with larger bifurcation ratios).

The first conclusion is that the topological branching structure of DLA clusters does have an asymptotic behaviour, as far as can be concluded from our simulation results. The ratios of stream numbers converge. For all practical purposes, each asymptotic value is reached for a finite cluster size, that increases with the Strahler order being considered. Except for the fact that the value of the first ratio differs from the value attained by the following ones, we could have asserted from figures 4 and 5 that the limit structure is topologically self-similar.

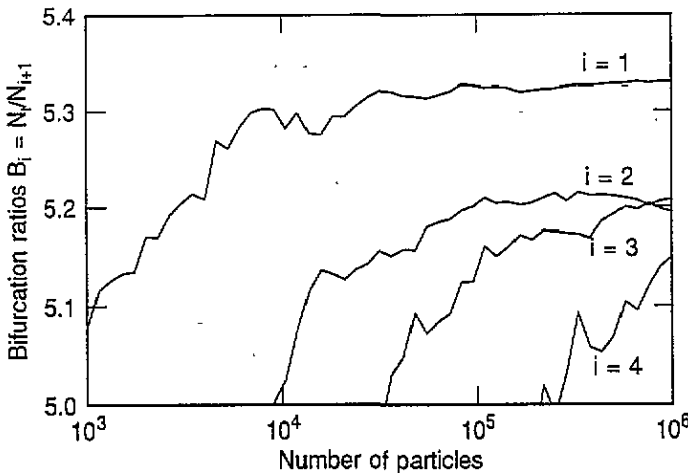


Figure 4. Bifurcation ratios in a DLA cluster as it grows. Data are averaged over 50 clusters of 1 million particles each.

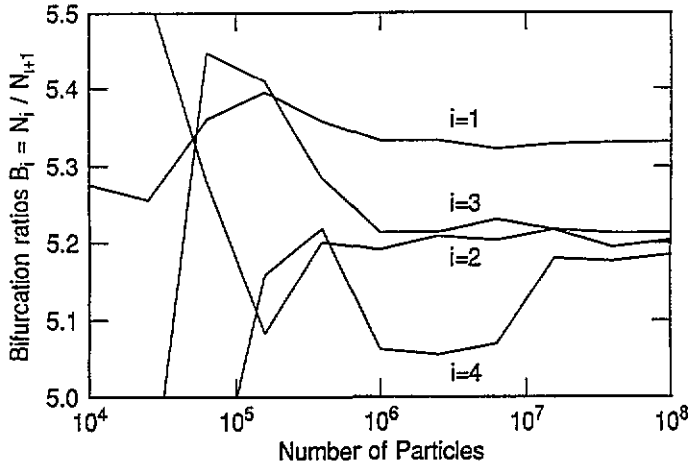


Figure 5. Bifurcation ratios in a DLA cluster of 100 million particles, as it grows.

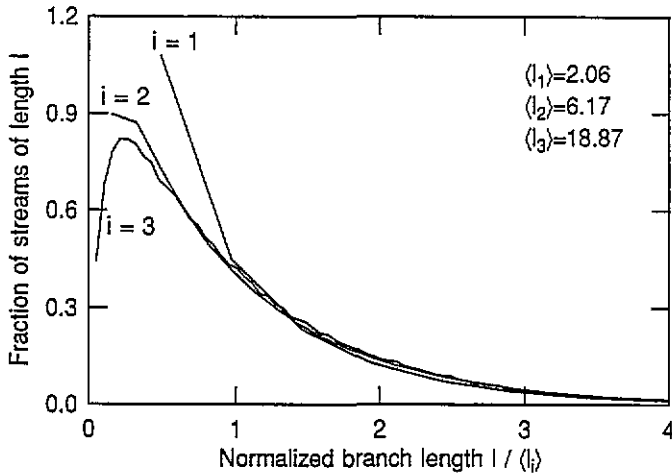


Figure 6. Distributions of lengths of branches of different orders in a DLA cluster of 1 million particles, averaged over 50 such clusters. Each distribution is scaled by the corresponding average branch length.

Why is the value of the first bifurcation ratio higher than those of the other ratios? That is to say, why are there more first order branches than expected for a self-similar tree, as seems to be indicated by the other ratios?

We calculated the distributions of branch lengths (measured by the number of particles in a branch) for branches of different orders. These were averaged over 50 DLA clusters of 1 million particles each. Figure 6 shows these distributions for orders $i = 1, 2, 3$. Each distribution was scaled by the average length of branches $\langle l_i \rangle$ of the respective order. The average lengths of branches of orders $i = 1, 2, 3, 4$ were, respectively, 2.05, 6.15, 19.65 and 55.51, leading to an approximate law

$$\langle l_i \rangle \sim 2 \times 3^i . \tag{13}$$

The tails of the three distributions in figure 6 are quite well approximated by an exponential

decay. The forms of the distributions differ for the low values. The first data point in the length distribution of first-order branches stands out, being significantly higher than for the other distributions. This data point represents branches of order 1 consisting of single particles. These are seen to be relatively abundant in the DLA clusters, and can account for the discrepancy between the value of the first bifurcation ratio B_1 and the values of successive bifurcation ratios. Although we have not checked this explicitly, many of these short branches may be situated at threefold branchings in the tree. Screening by the other two branches may have prevented them from growing any longer. Discounting this excess of first-order branches of one particle length, the stream numbers of the remaining structure form a geometric series, indicating self-similar behaviour.

5. Conclusion

This paper investigated the complexity of branching structures using the Horton–Strahler ordering scheme. For topologically self-similar trees, the stream numbers should form a geometric series asymptotically. We have shown this explicitly for several self-similar fractal tree constructions. Our study of very large off-lattice DLA clusters shows that statistics of the Horton–Strahler ordering of their tree structure does indeed relax to a geometric series. This indicates that, from the point of view of their topological branching structure, very large DLA clusters behave as self-similar objects. By this it does *not* follow that these clusters are metrically self-similar. The analysis of other characteristics of these clusters [25] shows no convergence to the asymptotic behaviour expected from self-similarity.

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Appendix

This appendix describes shortly the methods used by the Yale group to simulate very large DLA clusters. Some of these methods have already been used previously by different authors, while others are, to our knowledge, novel.

(i) Particles are set off on random walks from a circle of radius R_{birth} centred on the origin. Setting R_{birth} greater than R_{max} , the radial extent of the cluster, is equivalent to sending the particles off from infinity, as the probability of first passage of this circle is uniform in the angular direction.

(ii) The step size of a particle is taken to be slightly smaller than the distance of the particle to the cluster, in a direction chosen at random. If the particle is at a distance from the cluster of less than 1/20th of a particle diameter, it is stuck to the nearest particle in the cluster.

(iii) A random walking particle that moves outside a circle of radius R_{reb} ($> R_{\text{max}}$) is projected back onto this circle using the Poisson kernel

$$K(R, d, \theta) = \frac{(R + d)^2 - R^2}{(R + d)^2 + R^2 - 2R(R + d) \cos \theta}. \quad (\text{A1})$$

This kernel gives the probability that a random walker at a distance d from a circle of radius R cross this circle for the first time at an angle θ relative to its original angular position. It allows particles to take large steps while guarding the same boundary conditions at infinity.

(iv) Particle positions were represented by a lattice made of a hierarchical tree of square tiles. Each tile is subdivided into 4 tiles of relative side $\frac{1}{2}$. The subdivision of a tile is initiated only if a particle from the cluster is present inside the tile. The smallest tile is eight particle diameters wide. The position of particles within this tile is specified to an accuracy of 1/32nd of the particle diameter.

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