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Branch distribution in diffusion-limited aggregation: a maximum entropy approach

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Abstract

A new approach to the branching structure of diffusion-limited aggregation (DLA) clusters is proposed, in which the stress is laid not on the (traditionally used) order of the branches, but on their mass. The branch distribution $n(s, M)$ (to be defined) of DLA is computed and its properties are compared with those found in self-similar deterministic fractal sets. A power-law behavior is found in both cases. DLA also shows a striking crossover, which is independent of the cluster size. The Maximum Entropy formalism, a well-known method in statistical physics, is applied in order to derive the functional form of $n(s, M)$. The fit is achieved by means of a constraint concerning the information in the ensemble of all DLA clusters. We believe this constraint is a preliminar hint towards a new conceptual framework for the study of fractal growth phenomena.

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1. Introduction

A great deal of attention has been paid in the last decade to the processes of aggregation of initially dispersed particles to form fractal [1,2] aggregates (i.e. fractal growth phenomena [3]). This has been especially so since the development of computer models, the most remarkable and important being the diffusion-limited aggregation (DLA) model of Witten and Sander [4–6].

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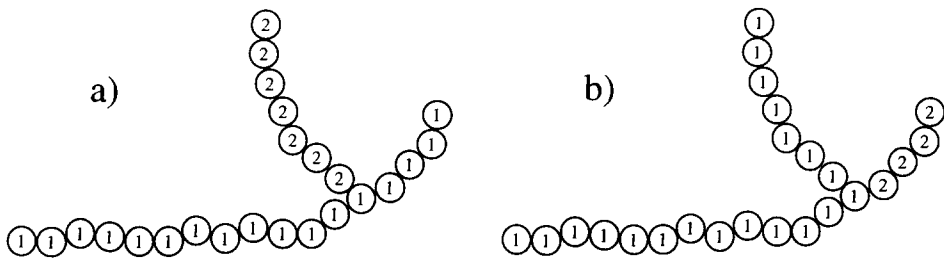


Fig. 1. Simple DLA branch structure with two alternative configurations: (a) stem of mass $m_1 = 17$, side branch of mass $m_2 = 7$; (b) stem of mass $m'_1 = 20$ and side branch of mass $m'_2 = 4$. In our classification, configuration (b) will be preferred, since it picks up the largest possible branch.

In spite of its apparent simplicity, DLA is still not fully understood. Among the different theoretical approaches to its study, we can mention the fixed-scale transformation [7], real-space renormalization techniques [8,9], mean-field theories [10], growth histories and overlapping distributions [11], the dynamics of screening of competing branches [12,13], etc. Especially noteworthy is the new method introduced by Hinrichsen et al. [14] and Vannimenus and Viennot [15], and subsequently developed by Ossadnik [16]. Within this approach, which is based on the surprisingly tree-like aspect of DLA, clusters are divided into branches and characterized in terms of a hierarchy of *branch orders*. This concept is intimately related to the Horton-Strahler ordering of the branches of a tree [17,18], and it was previously applied to the study of river networks. Following Ref. [16], a branch is defined by the unique continuous line which starts at the tip of the branch and ends on another branch of a higher order. In order to classify them, branches with no side branches have been assigned order 0, branches that have only side branches of order 0 have been assigned order 1, and so on. As it is shown in Fig. 1, this definition is at some extent arbitrary. Fig. 1a depicts some DLA branch of mass m_1 (that is, composed by m_1 monomers), which has a smaller side branch of mass m_2 attached. It is clear that this is not the only possible branch configuration, since as Fig. 1b shows, we can also consider a larger main branch (the stem) of mass $m'_1 > m_1$, with an attached side branch of mass $m'_2 < m_2$. Indeterminacies arise when more than one branch meets at a given point (a *branching site*). In these points, different rules can be prescribed for determining the order of the branches. In Ref. [16], when any N branches with orders $\{n_1, \dots, n_N\}$ meet, the longest branch, say number 1, is considered to be the stem and assigned the highest order $n'_1 = \max(n_1, n_2 + 1, \dots, n_N + 1)$, while the other branches maintain their respective orders. On the other hand, in Ref. [14] the branch with the highest order is always considered to be the stem, and only when branches with the same order n meet, is the longest one assigned the higher order $n + 1$. For a description of algorithms implementing these prescriptions see [16].

By means of this scheme, information can be extracted about the self-similar nature of DLA. This information is expressed in terms of the bifurcation and length ratios and the ramification matrix [15]. In the aforementioned works it is found that the bifurcation ratio r_N , which is defined as the quotient between the number of branches

of two successive orders, is constant [16,19]. In turn, the length ratio r_L between successive orders is also a constant. In Ref. [14] these results are interpreted in terms of a *similarity dimension* $D = \log(r_N)/\log(1/r_L)$, which is found to be close to the numerically computed fractal dimension of DLA. In Ref. [16] the stress is laid on the *metric* properties of the branching structure of DLA clusters, and it is found that not only the number and length of the branches follow a power law, but also the width and mass ratios. Similarly, by analyzing the ramification matrix, a self-similar relation is found between branches and stems. On the other hand, Ref. [19] emphasizes the *topological* properties of the branching structure. The calculations are carried out with very large clusters (up to 10^8 particles) and it is also found that the bifurcation ratios relax to constant values for cluster sizes around 200,000 particles. DLA is thus found to converge to a topologically self-similar structure at the limit of very large cluster sizes.

In the aforementioned works the branching analysis is carried out by classifying the branches according to their *order*. Even though they throw some light on the self-similar nature of the DLA, these classifications present some drawbacks, however:

- (i) The extent of the classification is extremely short. It covers only 9 or 10 orders even for 10^6 -particle clusters [16].
- (ii) The order of the biggest branches widely fluctuates and is strongly dependent on the configuration of the cluster in the vicinity of the seed.
- (iii) The branching properties stabilize only for large clusters and for very low order (small mass) branches, because only for those orders branches belonging to the same class share approximately the same structural properties, such as mass or length [16]. For high order (large mass) branches these classifications become less and less accurate.
- (iv) The mass (number of particles) of the branches of a given order is not a well defined magnitude, but a mere average over the ensemble of branches of that order.
- (v) The results obtained are strongly dependent upon the branch prescription chosen, with the variations in the numerical differences in the computed values of r_N and r_L between 10% and 20% in value.

Our purpose in the present paper is twofold. First, we introduce a new classification scheme for the branch structure of DLA clusters (and, in general, for tree-like sets), which endeavours to overcome the difficulties shown by previous approximations. We focus our attention on the *mass* of the branches, rather than on their *order*. Branches are thus defined and classified according to their mass, in order to obtain what we call the *branch distribution* of the set. This magnitude leads to stable results for a wide range of branch masses and for not too large cluster sizes (up to 10^5 particles in our simulations). Apart from its better convergence, the branch distribution is a magnitude that seems to be related not only to the topological or metric properties of the cluster, but also to other dynamical qualities, like the distribution of mass in the cluster. Using this distribution as a starting point, we propose to apply to DLA a well-known and powerful theoretical method in statistical physics, the so-called *Maximum Entropy* [20] principle. As we prove in this paper, this idea provides a theoretical derivation of the functional form of the branch distributions. In other words, we believe that fractal growth phenomena can

be understood in this light of rather fundamental principles in physics.

Our paper is arranged as follows. In Section 2 the concept of branch distribution is defined and exemplified with deterministic fractal sets. Section 3 analyzes the branching properties of DLA under this new prism, comparing the results obtained with those found in previous deterministic cases. Section 4 introduces the Maximum Entropy principle and applies it to a theoretical study of the branch distribution of growing fractals. Finally, Section 5 presents a summary along with our conclusions.

2. Branch distribution in tree-like sets

Consider any tree-like set which has assigned to it a certain total mass M ; in a growing cluster constructed by adding particles to a given seed, according to a certain set of rules, this mass is established by the number of monomers of which the cluster is composed. As usual, a branch is defined by the **unique path starting at the tip of the branch and ending on another branch** (or on the seed, in the case of a growing fractal). When N branches of masses s_1, \dots, s_N meet at the same point, then **the largest is considered to be the stem, while the others are considered to be side branches** of that particular stem. By doing so we ensure that the largest branch that can be constructed in a given set is always present in the branch classification. When all branches have been finally processed, they are grouped and classified according to their mass s , in order to obtain the *branch distribution* $n(s, M)$, namely **the number of branches of mass s included in a cluster of total mass M** . For a random fractal like DLA the branch distribution is defined as an average over the ensemble of all clusters of mass M .

In the following subsections we will proceed to compute the branch distribution for two well-known deterministic fractal sets showing a branching structure.

2.1. Deterministic iterative tree-like fractal

Consider first the self-similar fractal tree of Mandelbrot and Vicsek [21], which is constructed by the following algorithm: starting from a line segment of length 1 (stage $k = 0$), the construction proceeds by recursively replacing each line segment by three new lines reduced by a factor $1/2$ (or, in other words, by rooting in the middle of each line segment a new segment of halved length). This procedure leads to a self-similar tree-like set of fractal dimension $D = \log 3 / \log 2 \simeq 1.58$. Fig. 2 shows the first steps in the construction of this set.

Consider now the stage k of the iterations (what is commonly called a *k-prefractal* [2]). Because of its recursive construction, it is found that all branches within the same order i possess the same mass. Therefore, both classifications (either according to the order or to the mass) will lead to analogous results. It is easy to check that the k -prefractal has $k + 1$ different orders, labelled $i = 0, \dots, k$, respectively. Let $n_k(i)$ be the number of branches of order i , and $s_k(i)$ their corresponding mass (we actually measure the length, but keep the name “mass” for the sake of clarity). We assign order

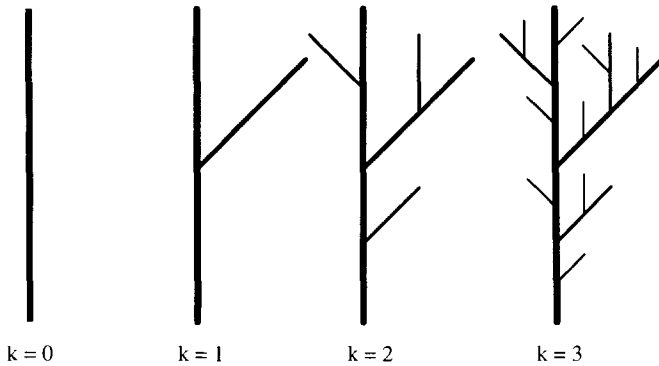


Fig. 2. First four iterations of a deterministic tree-like fractal. At each stage the construction proceeds by replacing each line segment by three new lines reduced by a factor $1/2$. Branches of different mass have been drawn with lines of different thickness.

0 to the largest branch (the stem), order 1 to the second largest ones and so on. We can see from Fig. 2 that the passage from the stage $k - 1$ to k is performed by merely adding 3^{k-1} new line segments of length 2^{-k} . In the k -prefractal, these new segments correspond to the branches of order k , the rest of the branches keeping their former orders and masses. Then we have

$$n_k(i) = 3^{i-1}, \quad i = 1, 2, \dots, k, \quad (2.1)$$

$$s_k(i) = 2^{-i}, \quad i = 1, 2, \dots, k. \quad (2.2)$$

For the stem (order 0 branch) we obviously have $n_k(0) = s_k(0) = 1$ for any k . From this distribution we can compute the total mass (length) M_k of the k th iteration

$$M_k = \sum_{i=0}^k n_k(i) s_k(i) = 1 + \sum_{i=1}^k 3^{i-1} 2^{-i} = (3/2)^k. \quad (2.3)$$

We have $M_k \rightarrow \infty$ when $k \rightarrow \infty$. Similarly, we can compute the number of branches Q_k present in the k -prefractal

$$Q_k = \sum_{i=0}^k n_k(i) = 1 + \sum_{i=1}^k 3^{i-1} = \frac{1}{2}(3^k + 1). \quad (2.4)$$

We can express this last result as a function of the mass M_k by noticing that

$$3^k = [(3/2)^k]^{\log 3 / \log(3/2)} = M_k^{D/(D-1)}, \quad (2.5)$$

where $D = \log 3 / \log 2$ is the fractal dimension of the set. Thus we have

$$Q_k = \frac{1}{2} [M_k^{D/(D-1)} + 1]. \quad (2.6)$$

The average mass per branch $\langle s_k \rangle$ is defined by the quotient

$$\langle s_k \rangle = \frac{M_k}{Q_k} = \frac{2M_k}{M_k^{D/(D-1)} + 1}. \quad (2.7)$$

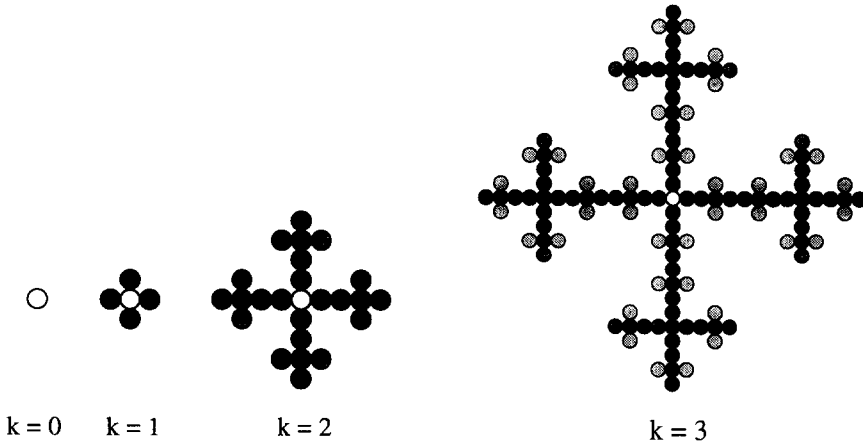


Fig. 3. First four iterations of a deterministic cluster-like fractal. The k stage proceeds by joining and rearranging five copies of the structure at the $k - 1$ stage. Branches of different masses have been colored in different dark tones.

For large mass M_k (large k) we have

$$\langle s_k \rangle \sim 2M_k^{-1/(D-1)}. \quad (2.8)$$

So

$$\langle s \rangle = \lim_{M_k \rightarrow \infty} \langle s_k \rangle = 0, \quad (2.9)$$

as $D > 1$. That is, even though the limit fractal has an infinite mass, its asymptotic average mass per branch is indeed vanishing.

Provided that mass and order are unambiguously related to each other, we can remove the i dependence in Eqs. (2.1) and (2.2):

$$n_k(i) = \frac{1}{3} 3^i = \frac{1}{3} (2^i)^D = \frac{1}{3} [s_k(i)^{-1}]^D. \quad (2.10)$$

If we rename $s_k(i) \equiv s$, then the branch distribution in a fractal of mass M is given by

$$n(s, M) = \frac{1}{3} s^{-D}. \quad (2.11)$$

We observe a universal behavior of the branch distribution, which is a scaling (power-law) function independent of the total cluster mass.

2.2. Deterministic growing cluster-like fractal

In this section we analyze the Vicsek fractal [22], the first steps of the construction of which are depicted in Fig. 3. The construction of this growing fractal starts from a seed configuration ($k = 0$) and proceeds in the stage k by joining and rearranging 5 equal copies of the structure on the stage $k - 1$. The set constructed by iterating this procedure resembles a real growing DLA cluster because of its open branching structure.

Therefore, the results we will obtain from it will more likely reproduce those observed in real DLA clusters than those from the deterministic tree previously studied.

If we denote by L_k the linear length of the k -prefractal, and by M_k its total mass (the total number of monomers of which it is composed), we have $L_k = 3^k$ and $M_k = 5^k$. From these values we may define a fractal dimension D through the relation $M_k = L_k^D$ [3], where $D = \log 5 / \log 3 \simeq 1.46$. In order to identify the branching structure of the cluster, and because of its rotational symmetry, we first remove the seed particle at its centre. The k -prefractal has now k different orders, which we label $i = 0, \dots, k - 1$. It is easy to check that

$$n_k(0) = 4, \quad n_k(1) = 8, \quad (2.12)$$

$$s_k(0) = (3^k - 1)/2, \quad (2.13)$$

for any value of k . Any branch of order $i > 0$ in the k -prefractal was already present in the previous $k - 1$ iteration with an order one unit smaller. So

$$s_k(i) = s_{k-1}(i - 1), \quad i = 1, 2, \dots, k - 1. \quad (2.14)$$

Furthermore, when proceeding from the $k - 1$ iteration to the k , the $(i - 1)$ th branches are repeated 5 times and promoted to i th order. So

$$n_k(i) = 5n_{k-1}(i - 1), \quad i = 2, 3, \dots, k - 1. \quad (2.15)$$

From the recursion relations (2.14) and (2.15), together with the initial conditions (2.12) and (2.13), we get

$$n_k(i) = 8 \times 5^{i-1}, \quad i = 1, 2, \dots, k - 1, \quad (2.16)$$

$$s_k(i) = (3^{k-i} - 1)/2, \quad i = 0, 1, \dots, k - 1. \quad (2.17)$$

To verify this distribution, let us compute the total number of particles in the set of branches

$$\sum_{i=0}^{k-1} n_k(i) s_k(i) = 4 \frac{3^k - 1}{2} + 8 \sum_{i=1}^{k-1} 5^{i-1} \left(\frac{3^{k-i} - 1}{2} \right) = 5^k - 1 = M_k - 1. \quad (2.18)$$

This result is indeed correct, since the seed particle was not taken into account in computing the branch distribution. The number of branches Q_k is given by

$$Q_k = \sum_{i=0}^{k-1} n_k(i) = 4 + 8 \sum_{i=1}^{k-1} 5^{i-1} = 2 \left(\frac{5^k}{5} + 1 \right) = 2 \left(\frac{M_k}{5} + 1 \right). \quad (2.19)$$

That is, the total number of branches grows as a linear function of the cluster total mass. The average mass per branch is

$$\langle s_k \rangle = \frac{M_k}{Q_k} = \frac{5M_k}{2(M_k + 5)}. \quad (2.20)$$

In the limit of large mass

$$\langle s \rangle = \lim_{M_k \rightarrow \infty} \langle s_k \rangle = 5/2. \quad (2.21)$$

In the case of a growing fractal, we obtain an asymptotic average mass per branch that is constant and independent of M_k . Its low value is accounted for by the overwhelmingly large number of very small branches of a high order.

By taking logarithms and dividing both expressions, we can express $n_k(i)$ as function of $s_k(i)$ in Eqs. (2.16) and (2.17)

$$\log\left[\frac{5}{8}n_k(i)\right] = \log\{3^{-k}[2s_k(i) + 1]\} \left(-\frac{\log 5}{\log 3}\right) \quad (2.22)$$

$$= \log\{M_k[2s_k(i) + 1]^{-D}\}, \quad (2.23)$$

where D is the fractal dimension of the set. Then we obtain a branch distribution

$$n(s, M) = (8/5)M(2s + 1)^{-D}, \quad (2.24)$$

where we have explicitly denoted the dependence on the total mass M . We note that the branch distribution scales linearly with M ; this fact is due to the growing construction of the fractal. The ratio $n(s, M)/M$ presents a universal behavior, which is independent of M . This universal relationship can be restated in terms of the mass of the largest branch s_M

$$s_M \equiv s_k(0) = \frac{1}{2}(3^k - 1) = \frac{1}{2}[(5^k)^{\log 3 / \log 5} - 1] = \frac{1}{2}(M_k^{1/D} - 1). \quad (2.25)$$

For large masses we obtain $s_M \sim M^{1/D}$. This can be explained by the relation between the mass (length) of the largest branch and the radius of gyration R_g of the cluster. If we assume a proportional relation, then $s_M \sim R_g \sim M^{1/D}$, thus recovering the previous result. Introducing the expression of s_M in Eq. (2.24), we get

$$n(s, M) = \frac{8}{5} \left(\frac{s + \frac{1}{2}}{s_M + \frac{1}{2}} \right)^{-D}. \quad (2.26)$$

This rescaled function represents the finite size effects on the clusters analyzed: for large clusters we have $n(s, M) \sim (s/s_M)^{-D}$ for $1 \ll s < s_M$, and $n(s, M) = 0$ for $s > s_M$.

To sum up, for the deterministic fractals analyzed we find in both a branch distribution exhibiting a power-law behavior of the form $n \sim s^{-\alpha}$, for large values of s . The exponent α coincides with the fractal dimension D of the set. For the cluster-like fractal of Vicsek, which is a better approximation to a real DLA cluster, we also find that $n(s, M)$ actually scales linearly with the mass M , $n(s, M) \sim Ms^{-\alpha}$; this fact is obviously due to the growing nature of the set. Moreover, we find a correction to the scaling for small s , $n(s, M) \sim M(s + b)^{-\alpha}$, the source of which is the removal of the seed particle (and, at the last instance, the rotational symmetry of the set). In analyzing DLA clusters in the following sections, this correction to the scaling is expected to happen.

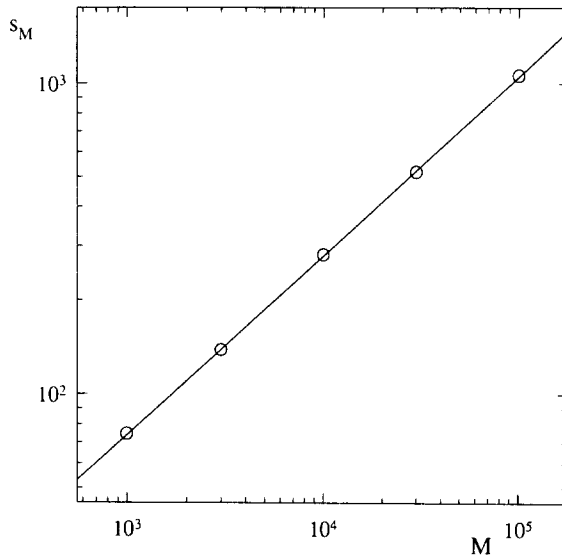


Fig. 4. Mass of the largest branch s_M as function of the total mass of the cluster M . The solid line corresponds to a least-squares fitting of the form $s_M \sim M^{\nu_m}$, where $\nu_m^{-1} = 1.74 \pm 0.03$ is very close to the fractal dimension of DLA (see text).

3. Branch distribution in DLA clusters

Bearing these results in mind, we undertake the study of the branch distribution in DLA. For this purpose, we have simulated 700 off-lattice two-dimensional DLA clusters of 10^5 particles, constructed by means of standard algorithms described elsewhere [6]. Given the actual “state of the art” of computer science, it is possible to generate DLA cluster up to 100 million particles within a reasonable computational effort [19]. However, instead of generating a small number of huge clusters, in this case we prefer to grow a large number of medium-sized aggregates. We indeed require large statistics of branches in order to estimate the branch distribution as accurately as possible, since the number of large branches in a given cluster is very scarce. As a consistency check, we advance here that the branch distribution converges to a stable result for the cluster sizes analyzed.

We find that the properties related to the branch distribution stabilize for large branch masses and relatively small cluster sizes. As noted in Ref. [16], this is because branches are actually classified according to a physically meaningful magnitude: their mass. In the first place, we analyzed the behavior of the mass of the largest branch s_M . In Fig. 4 we plot s_M as a function of M . We conclude a power-law dependence of the form $s_M \sim M^{\nu_m}$, with $\nu_m = 0.576 \pm 0.001$. Given the relation $s_M \sim M^{1/D}$ pointed out in Section 2.2, we have $\nu_m^{-1} = D$. From our simulations, we compute $\nu_m^{-1} = 1.74 \pm 0.03$, which is in fact quite close to the well-known value of the radius-of-gyration dimension $D_g = 1.71$ [6].

Fig. 5 depicts the total number of branches $Q(M)$ in a cluster as a function of M ,

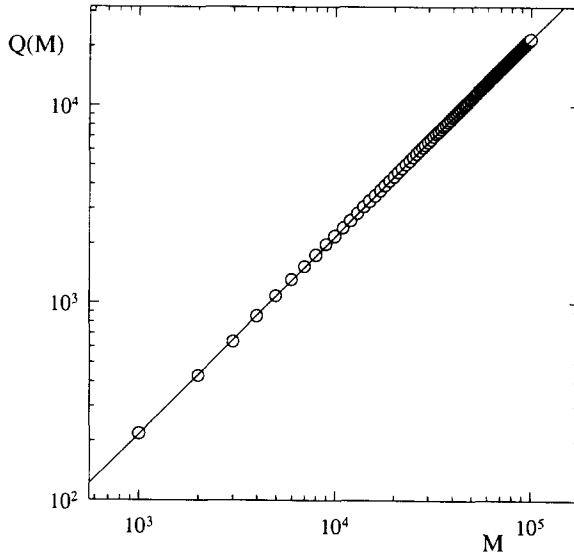


Fig. 5. Average total number of branches $Q(M)$ in a cluster, as function of its mass M . The solid line corresponds to a least-squares fit of the form $Q(M) \sim M/\langle s \rangle$, with an average mass per branch $\langle s \rangle = 4.605 \pm 0.002$.

which is defined as

$$Q(M) = \sum_s n(s, M). \quad (3.1)$$

This plot shows a quite remarkable linear dependence between $Q(M)$ and M . A least-squares fitting of the form $Q(M) \sim M^\gamma$ provides a value $\gamma = 1.000 \pm 0.001$; a linear fit of the form $Q(M) \sim (1/\langle s \rangle)M$ yields a value for the average mass per branch $\langle s \rangle = 4.605 \pm 0.002$, which is indeed independent of M and not so far from the limit value found for the deterministic cluster-like fractal we analyzed in Section 2.2.

In view of the discussion in Section 2, we should expect a power-law dependence of $n(s, M)$ on s . In order to further explore this issue, we plotted the reduced branch distribution $n(s, M)/M$ as function of s , for different values of M (Fig. 6). We observe that the plots collapse into the same function, given by the limit case $M \rightarrow \infty$.

In order to further explore the behavior of this limiting curve, we fitted our data to several different functions. Given the similarity of DLA to the cluster-like fractal in the previous section, we first tested the functional form

$$\frac{n(s, M)}{M} \sim (s + b_0)^{-\alpha_0}. \quad (3.2)$$

The better fit is achieved for $s < 20$, the parameters being $b_0 = 0.74 \pm 0.01$, $\alpha_0 = 2.15 \pm 0.01$. The best-fit curve is depicted in Fig. 7 (dotted line). On the other hand, for values $s > 20$ the best fit is provided by the function

$$\frac{n(s, M)}{M} \sim s^{-\alpha_1}, \quad (3.3)$$

$n(s, M)/M$

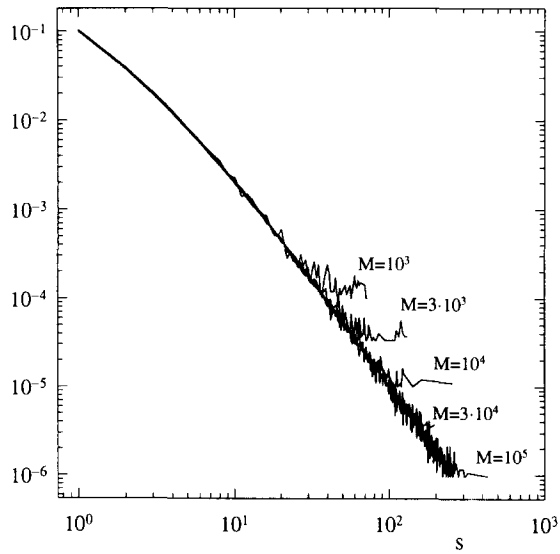


Fig. 6. Reduced branch distribution $n(s, M)/M$ as function of the mass s , for different values of the cluster mass $M = 10^3$, 3×10^3 , 10^4 , 3×10^4 , and 10^5 . The plot for $M = 3 \times 10^4$ is partly hidden by that corresponding to $M = 10^5$.

$n(s, M)/M$

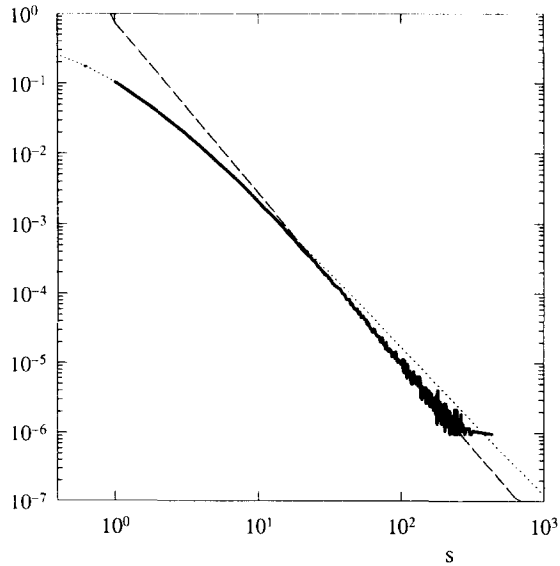


Fig. 7. Reduced branch distribution $n(s, M)/M$ for the largest cluster size simulated $M = 10^5$ (thick line). The dotted line corresponds to a best fit of the form $(s + b_0)^{-\alpha_0}$ for small branches. The dashed line is a best fit of the form $s^{-\alpha_1}$ (power-law) for large branches (see text).

with $\alpha_1 = 2.43 \pm 0.02$ (Fig. 7, dashed line). This seems to be a ceiling stable behavior up to the cluster sizes simulated ($M = 10^5$).

In view of these results, the behavior of the branch distribution can then be summarized as follows:

(i) For s small

$$\frac{n(s, M)}{M} \sim (s + b_0)^{-\alpha_0}, \quad (3.4)$$

where $b_0 \sim 1$ and $\alpha_0 = 2.15 \pm 0.01$. For the smallest branches we recover the behavior already found in the cluster-like deterministic fractal. The qualitative behavior is accounted for by the rotational symmetry of DLA. The exponent, however, does not coincide with the fractal dimension; it is even greater than 2 (the dimension of the embedding space).

(ii) For s large

$$\frac{n(s, M)}{M} \sim s^{-\alpha}. \quad (3.5)$$

The branch distribution shows a power-law behavior.

We notice at this point the striking crossover, independent of the cluster size, shown in the branch distribution at a mass $s \sim 20$, where α changes from $\alpha_0 = 2.15$ to $\alpha_1 = 2.43$, values which are clearly different, out of the error bars. These two results, the large value of the scaling exponent and the apparent crossover, could be accounted for by the fact that DLA is not a strictly self-similar set, and therefore order and mass classification schemes do not exactly match, as it was the case in the deterministic model. Another explanation for the crossover could be: there are many fewer large branches than small branches, so the statistics for the latter are worse than for the former. We cannot utterly reject the possibility that an increased accuracy in the determination of $n(s, M)$, achieved by analyzing a far larger ensemble of clusters, might prove that the observed crossover is indeed fictitious, yielding that α_0 is actually equal to α_1 .

Our results can be compared with the branch analysis of DLA by Alstrøm et al. [23]. In that paper, the boundary of a cluster is partitioned into an extinct phase where no further growth occurs, and a surviving phase, where growth can occur at some later time. The surviving paths of the cluster are constructed by tracing the surviving sites back to the seed. When removing these surviving paths, the cluster splits into subclusters, called *extinct branches*. The size distribution of these extinct branches is found to follow the power-law $D(s) \sim s^{1-\tau}$, with an exponent $1 - \tau \sim -1.5$. This result differs from ours due to the different classification scheme in both approaches. Our approach is even more general, since we take into account *all* the branches in a cluster, either coming from an extinct or a surviving branch.

4. The maximum entropy principle and branch distribution in DLA

The Theory of Information [24], entropic magnitudes and the Maximum Entropy (MaxEnt) Principle [20] are time-honored tools for the study of complex systems, especially in those situations where there is a considerable lack of information. They have been successfully applied in the prediction of average magnitudes in statistical mechanics [20], the reconstruction and analysis of signals [25], the prediction of stationary states in ecological systems [26] and models of growth and differentiation [27], etc.

From the point of view of the Theory of Information, many complex natural systems can be represented by a set of n generic *nodes* i , each one characterized by a certain magnitude x_i , and which have assigned some *structural probabilities* $p(x_i)$, $i = 1, \dots, n$. For example, in statistical mechanics we have a set of states described by an energy E_i , and which occur with a probability $p(E_i)$; in an ecological energy-flow network [26] the nodes i represent compartments in a biologically meaningful partition of the ecosystem (individuals, species, groups, etc.), which are characterized by its energy x_i and by the probability (ratio) of exchange of energy $p(x_i)$. From this view, the whole system X is characterized by its total *entropy* [24]

$$H(X) = - \sum_{i=1}^n p(x_i) \log_2 p(x_i), \quad (4.1)$$

which can be interpreted as a measure of the uncertainty in our description of the system.

On these foundations, the Maximum Entropy Principle as stated by Jaynes says that [20]: “The least biased and more likely probability assignment (the structural probability distribution $p(x_i)$ in our case) is that which maximizes the total entropy (4.1) subject to the constraints imposed on the system”.

Besides the trivial normalization condition $\sum_{i=1}^n p(x_i) = 1$, the additional constraints imposed on the system have to be understood as the global effect of the physical laws intervening in the process. For instance, in statistical mechanics the constraint of constant average energy ($\sum_i E_i p(E_i) = \text{const.}$) provides the well-known canonical distribution $p(E_i) \sim \exp(-\beta E_i)$.

We now apply the MaxEnt formalism to DLA. Consider an aggregate composed of M particles, the branch structure of which has been resolved, so that the cluster turns out to be composed of Q^* branches, having $n^*(s)$ branches of mass s . Now consider the set of all possible DLA clusters of M particles. This ensemble will have an average number of branches $Q(M)$, and they will be distributed with a branching distribution (average number of branches of mass s) given by $n(s, M)$; we have explicitly introduced the dependence on the total mass M .

The probability of a cluster having a branch of mass s or, in other words, the probability of a branch in a given cluster having mass s , will be given by

$$p(s, M) = \frac{n(s, M)}{Q(M)}. \quad (4.2)$$

Given that Q does not depend on s , we have $p(s, M) \sim n(s, M)$, as functions of s . This is a well defined probability distribution, fulfilling the normalization condition

$$\sum_{s=1}^{s_M} p(s, M) = 1, \quad (4.3)$$

where s_M stands for the mass of the largest branch in a cluster of M particles.

We choose as our structural probabilities characterizing DLA aggregates the probability distribution (4.2); when determining these probabilities, we will obtain a complete description of the distribution of the branches over the cluster. The *branch entropy* associated with a cluster will then be

$$H(M) = - \sum_{s=1}^{s_M} p(s, M) \log_2 p(s, M), \quad (4.4)$$

a magnitude which depends in principle on the cluster mass M . The maximization of the branch entropy (4.4), subject to the constraints operating on the system, will provide the most likely theoretical branch distribution compatible with those very constraints.

In order to apply the MaxEnt formalism, we first explore the constraints to be imposed on the system. We first take into account the trivial normalization condition (4.3). Further constraints will emerge by considering the nature of the very growth process. DLA clusters are, in a certain statistical sense, *self-similar objects*. That is to say, the structure of the whole cluster is *statistically* similar to the structure of a small part of it. In other words, the amount of *information* of the whole cluster is, because of its self-similar essence, small and nearly equal to the information contained in any small portion of the aggregate. This information could be understood in terms of the *algorithmic complexity* [28] required to fully specify the structure of the cluster. The situation is quite similar to the process of construction of deterministic fractal sets by means of iterative algorithms, the so-called *Iterated Function Systems* [29]. All the information needed to construct a complex fractal set can be compressed into a small set of contraction functions and, in the simplest case, into a small set of real numbers; therefore these deterministic fractals do indeed contain a small amount of information.

We can then assume that the information contained in a DLA cluster does not increase substantially when the total mass of the aggregate grows. This information I is a candidate for being a constant, not only as the cluster grows by increasing its mass, but also *within the ensemble of clusters* compatible with a given value of M .

Let us express the information content I of a cluster in terms of our structural probabilities $p(s, M)$, i.e. in terms of its branch structure. Consider a given branch of mass s . It is composed of s particles, ordered in a certain way. If the particles are considered to be indistinguishable, the amount of information needed to specify their order is then given by [24]

$$I_s = \log_2 s. \quad (4.5)$$

The average over the whole cluster will then be the average of the previous expression over the distribution (4.2)

$$I = \sum_{s=1}^{s_M} I_s p(s, M) = \sum_{s=1}^{s_M} p(s, M) \log_2 s. \quad (4.6)$$

This function will depend in principle on the mass M through s_M and $p(s, M)$. Our fundamental assumption concerning the essence of DLA process is that

$$I = I^* \equiv \text{const.} \quad (4.7)$$

is a constraint acting on the system. We will further assume that no other relevant constraint plays an essential role.

The MaxEnt Principle will finally read as follows: the most likely probability assignment is given by the maximization of the branch entropy (4.4), subject to the constraints

$$\sum_{s=1}^{s_M} p(s, M) = 1, \quad (4.8)$$

$$\sum_{s=1}^{s_M} p(s, M) \log_2 s = I^*. \quad (4.9)$$

The maximization is worked out by means of the Lagrange multipliers method, computing the extremes of the auxiliary function

$$\begin{aligned} \Phi = & - \sum_{s=1}^{s_M} p(s, M) \log_2 p(s, M) \\ & + \lambda \left(I^* - \sum_{s=1}^{s_M} p(s, M) \log_2 s \right) + \lambda' \left(1 - \sum_{s=1}^{s_M} p(s, M) \right), \end{aligned} \quad (4.10)$$

where λ and λ' are Lagrange multipliers. The extreme is given by the condition

$$\frac{\partial \Phi}{\partial p(s, M)} = 0, \quad (4.11)$$

which yields the equation

$$-\log_2 p(s, M) - \log_2 e - \lambda \log_2 s - \lambda' = 0, \quad (4.12)$$

from which

$$p(s, M) = e^{-1} 2^{-\lambda'} s^{-\lambda} \sim s^{-\lambda}. \quad (4.13)$$

which indeed fits the power law behavior observed empirically.

Given the constraint (4.7), we can deduce theoretically, through the MaxEnt formalism, the asymptotic functional form of the branching distribution, $n(s, M) \sim p(s, M) \sim s^{-\alpha}$, with an exponent α which is given by the Lagrange multiplier λ defined above.

5. Conclusions

In this paper we have investigated both numerically and theoretically the properties of a new way of analyzing the branching structure of DLA clusters. The branch distribution $n(s, M)$, which is defined as the average number of branches of mass s in a cluster of M particles, is computed for off-lattice two-dimensional DLA aggregates. The branch distribution of DLA matches the behavior found in a deterministic self-similar model. For large branch mass s , we find a power-law behavior $n/M \sim s^{-\alpha}$, with a scaling exponent greater than the dimension of the embedding space. For small s , a correction to the scaling shows up, $n/M \sim (s + b)^{-\alpha}$, which is due to the particular method of counting branches. Surprisingly a crossover, occurring at a mass $s \sim 20$ and independent of the cluster size, is found. This crossover could be due to a departure of DLA from the strict self-similarity or, perhaps, to a lack of accuracy to be remedied by improving the statistics, which is necessarily poor for the large branches. This is a question that merits further study in greater detail and depth. Our results differ from those in Ref. [23] due to the different definition of branch adopted in that paper.

We have also applied the MaxEnt formalism to the study of the branch distribution of a generic branching fractal. The maximization on the branch entropy, subject to the constraint of a constant amount of information in the ensemble of clusters of size M , Eq. (4.7), yields a power-law behavior for $n(s, M)$, which is indeed found in our simulations, at the limit of large branches. The MaxEnt formalism is applied here as a tool to derive the functional form of our structural probabilities, starting from first principles (the constraints). But it can also be considered in the opposite way: applying the MaxEnt formalism, we can deduce the dependence of $n(s, M)$ by imposing the constraint of constant information Eq. (4.7). This is a hint towards a characterization of fractal growing structures as *systems with a very small and constant amount of structural information*. In particular, the frequently observed power laws in this type of complex system, i.e. fractal growth phenomena, Zipf law, etc., are here related to a variational principle characterized by a very specific constraint, namely the average information of the elements belonging to the parts of the system. This also explains the general stability of distributions of this kind.

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