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Deviations from Self-Similarity in Plane DLA and the «Infinite Drift» Scenario.

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Abstract. – The behavior of very large clusters of diffusion-limited aggregation (DLA) was investigated to help discriminate between the two geometric scenarios recently described by Mandelbrot: finite transient and infinite drift. Using 50 DLA clusters of 1 million particles, we follow the increase during growth of the maximum radius of the clusters and of various relative moments. One can distinguish two regions: an inactive completely grown core and an active growing region. In the growing region, scale factors were defined the moments of the atoms distances from the original «seed». They do not cross-over to the behavior characteristic of self-similarity for finite sizes and support the novel «drift» scenario that postulate an infinite continuing «transient». The moment's «misbehavior» may help understand the disagreement between previous estimates of the clusters' fractal dimension.

In the last ten years a considerable effort has been devoted to the analysis of fractal-growth phenomena [1]. The reason of this interest is that a large number of non-equilibrium aggregation phenomena like dendritic solidification, polymerization, electric breakdown and many others may be described by means of simple models showing a variety of fascinating characteristics. The first model of fractal growth based on a well-defined process is diffusion-limited aggregation (DLA) [2]. For the sake of completeness, let us recall that in DLA growth an «atom» executes Brownian motion until it hits, and becomes attached to, the curve that bounds a given «target» or «seed». Another atom is then launched towards

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the enlarged seed, and the whole process repeats. Witten and Sander [2] believed that DLA clusters are self-similar [3], *i.e.* that their complication is about the same at all scales of observation sufficiently larger than the scale of the atoms. However, departures from self-similarity were soon observed (see [1, 4]). Eventually, a widespread belief arose that the early DLA clusters should be viewed as «prefractal» approximations; this implies that there exists a finite cross-over to a self-similar range. The cross-over to this range was beyond the sample sizes obtained until very recently, but now it can be investigated. However, asymptotic self-similarity of every characteristic of DLA is not the only possible scenario. As an alternative ref. [5] has argued that it is conceivable, at least theoretically, that as samples grow some properties of DLA drift continually. This scenario implies that departures from simple self-similarity will be observed for any finite size of DLA clusters, even if very large. Moreover, it is still unclear if more than one exponent is needed to characterize the scaling properties of the resulting asymptotic structure.

To gain a deeper understanding of these problems, the Yale group has undertaken a systematic study [6, 7] on the properties of very large clusters of off-lattice diffusion-limited aggregation (DLA). This article investigates distributions that we call «radial density profiles»; its tools are traditional, namely moments analysis, instead of the new approach based on ϵ -neighborhoods [5]. The study is based on 50 clusters of 1 M particles grown under meticulous control to avoid biases due to approximations in the algorithm [8]. The present conclusion is that our mental picture must allow different numerical characteristics of DLA to have different cross-over to self-similarity. Thus, one should not be surprised if for given cluster size different viewpoints disagree, some suggesting self-similarity while others do not. In particular, DLA clusters show two very different regions: a fully grown cluster core that can be considered «frozen» and an outer «active» region where the dynamical features of the model play a major role [9]. We view these dynamical aspects as responsible for the infinite «drift» deviating from the simple self-similarity observed for some of the properties we can study. The overall conclusion is that the results reported in earlier studies are often affected or even dominated by transients.

Given a cluster of N particles, let $F(R, N)$ be the number of particles at a distance $\leq R$ from the seed, plotted as a function of R . A *cluster shell* is the collection of particles that have become part of the cluster when cluster size ranged between $N - \Delta N$ and N . The *radial cluster shell profile* is

$$\Delta F(R, N, \Delta N) = F(R, N) - F(R, N - \Delta N). \quad (1)$$

For $\Delta N = N$, the cluster shell fills the cluster. For small ΔN , the cluster shell profile is a form of the finite difference of $F(R, N)$. The function $F(R, N)$ is a *cumulative* distribution relative to distances $\leq R$. Often, it is better to deal with a density-like function. For that, one divides $\log R$ into uniform bins and plots the number of atoms (in each bin).

Letting R_k be the distance from the seed to the k -th particle (in order of absorption into the cluster), the moment-based scale factors of the cluster shell will be defined as

$$\sigma_q(N, \Delta N) = \left[\frac{1}{\Delta N} \sum_{k=N-\Delta N+1}^N \left| R_k - \frac{1}{\Delta N} \sum_{n=N-\Delta N+1}^N R_n \right|^q \right]^{1/q}. \quad (2)$$

In all cases, the $q \leq 0$ values of σ_q are without interest. In fact, it is obvious that $\sigma_0 = 1$, and it is easy to show that $q < 0$ yields $\sigma_q \sim N^{1/q}$ because σ_q is dominated by the inner cut-off due to the atoms' positive size. On the contrary, when $q > 0$ and $N \gg 1$, the atom's size no longer matters. For $q = 0$, σ_q can be used to measure the thickness of the cluster's growing region, a notion pioneered in [9]. As $q \rightarrow \infty$, $\sigma_q(N)$ converges to $R_{\max}(N)$, the largest distance from the seed to a particle in a cluster. It is important to notice that shell analysis is focussed

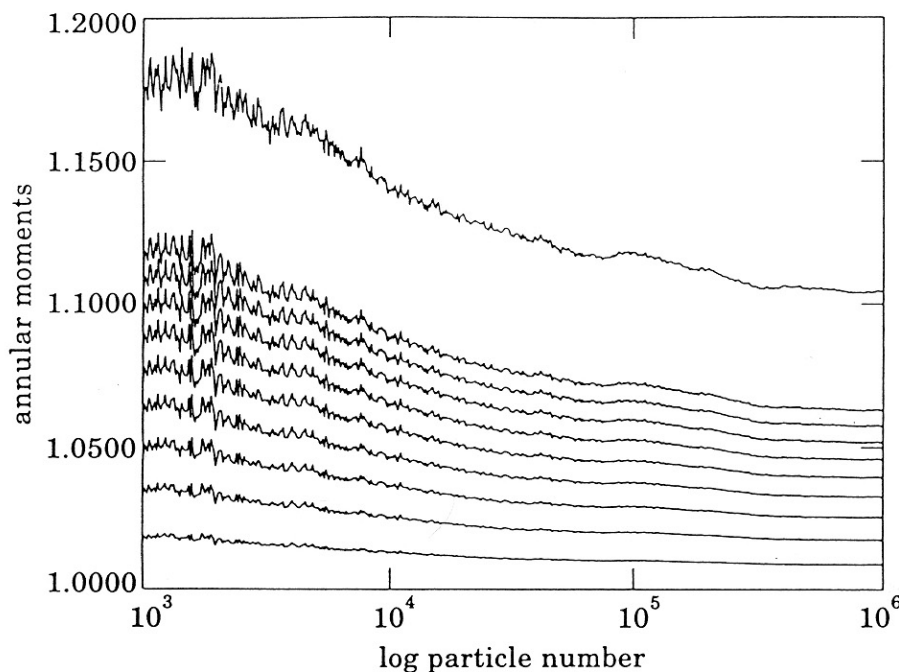


Fig. 1. – Analysis of DLA clusters based on the annular-moment behavior. The various moments are normalized with respect to the first one and averaged over 50 one-million-particle clusters.

particularly on the active region of the DLA cluster, *i.e.* where new particles become part of the aggregate.

If the cluster had been statistically self-similar, it would have been characterized by a single well-defined D , and quantities $\sigma_q(N, \Delta N)$ would have been proportional (for large N) to $N^{1/D}$ and to each other. The first inference from our data is a very familiar one. We find, as previous authors observed again and again, for $\sigma_1(N) = (1/N) \sum_{k=1}^N R_k$, that $\sigma_1(N) \sim N^{1/D}$, where $D = 1.71$. Nevertheless, $\sigma_q(N)$ shows a substantial amount of sample fluctuation, even after averaging data for 50 clusters of 1 Mp each. In order to study the behavior of the higher moments, we write them in terms of $\sigma_1(N)$ by using a proportional factor $\lambda_q(N)$

$$\sigma_q(N) = \sigma_1(N) \lambda_q(N), \quad \text{and} \quad R_{\max} = \lim_{q \rightarrow \infty} \sigma_1(N) \lambda_q(N), \quad (3)$$

Where, for given N , the factors λ_q necessarily increase with q . By studying $\lambda_q(N)$, it is, therefore, possible to analyze the moments' behavior. A necessary but not sufficient condition for the clusters being self-similar is that each $\lambda_q(N)$ tends to a limit as $N \rightarrow \infty$.

To test whether or not $\lambda_q(N) \rightarrow \text{limit}$, we evaluated these quantities for logarithmically spaced values of N and plotted them in logarithmic doubly coordinates (see fig. 1).

The expression $\sigma_2(N)$ is closely akin to the width ξ of the active zone where new particles stick. Plischke and Ra  cz [9] introduced the division of DLA clusters in «frozen» and active region and found that ξ scales with N as $\xi \sim N^\nu$, with $\nu \approx 0.484 \neq (1.71)^{-1}$. Subsequent larger-scale simulations [10] indicated that ν increases for larger clusters and seems to approach $1/D$ asymptotically. Recently Ossadnik [11] investigated clusters up to 200 000 particles and claimed consistency with a scaling form with logarithmic corrections. However the true asymptotic scaling behavior of the width of the active region is still unclear. We also find that

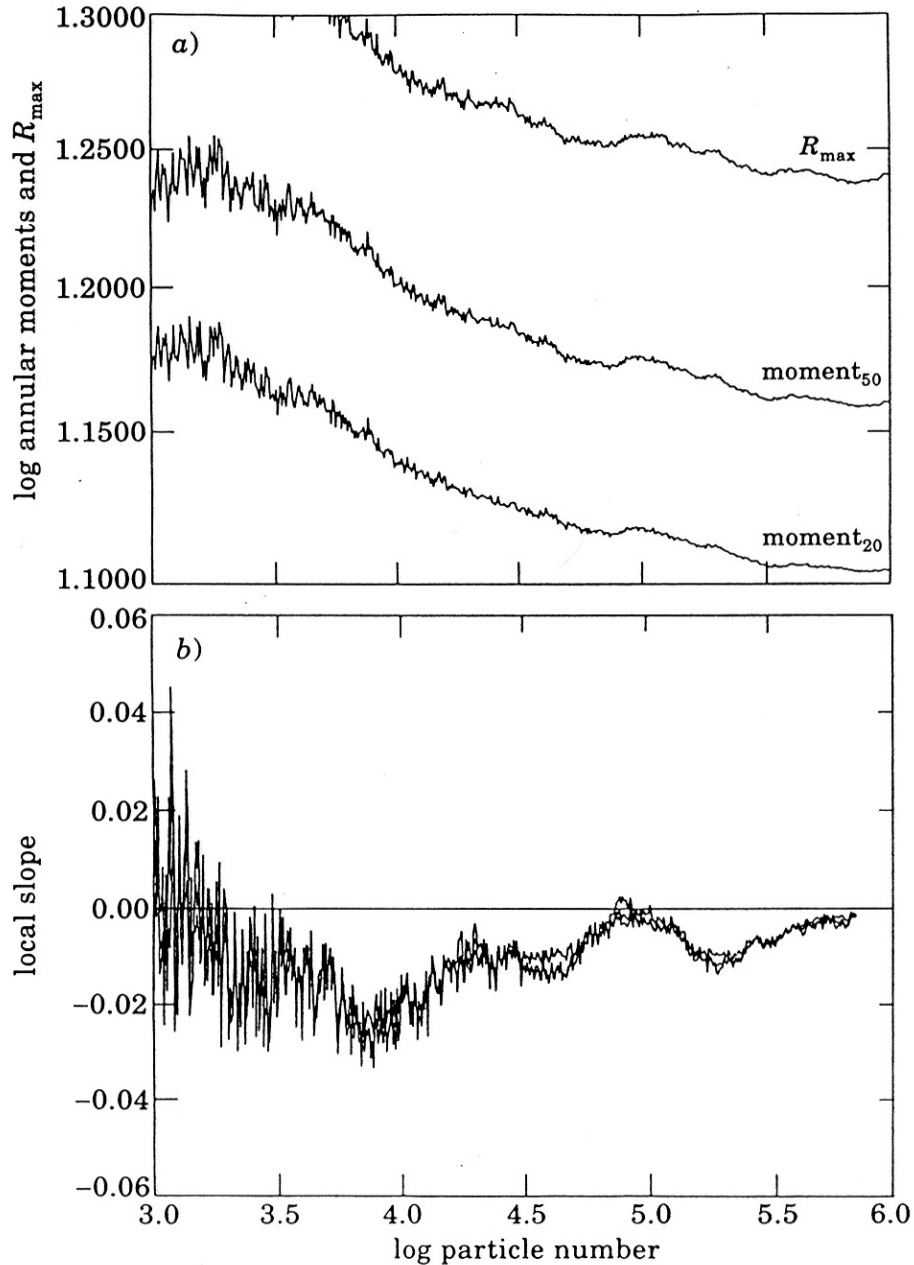


Fig. 2. - *a*) Magnified plots of the moments behavior for $q = 20$, $q = 50$ and $q \rightarrow \infty$. *b*) Local-slope analysis of the moments behavior. Apart from an initial region (small-size effect), the local slope is appreciably and definitively lower than zero.

$\lambda_2(N)$ begins by a near linearly decrease on logarithmic coordinates. Hence, one can fit $\lambda_2(N)$ by $N^{\Delta\nu}$, therefore fit $\sigma_2(N)$ by N^{ν_2} , with $\nu_2 = \nu_1 - \Delta\nu < 1/D$. Extended to infinity, this implies $\lambda_2(N) < 1$ for large enough N , which is impossible. In fact, our data show that $\Delta\nu$ depends on N , and the «local» $\nu_2(N)$ decreases as N grows. Our data on $\lambda_2(N)$ do not exclude that $\lambda_2(N) \rightarrow \text{limit} > 1$ after a long but finite transient, but they do not exclude, either, that $\lambda_2(N)$ continues to decrease very slowly in a non-trivial way. In the last case, the growing region is progressively smaller and its approach to the asymptotic limit is not governed by a finite cross-over.

Our most striking conclusion is that $\lambda_q(N)$ continually decrease for every value of $q > 2$, including $q \rightarrow \infty$. In fig. 2, it is easy to note the curvature of the $\lambda_q(N)$ behavior up to the limit

size of our samples. In order to visualize this effect, we perform a local-slope analysis of $\lambda_q(N)$ (fig. 2b)). The local slope is definitively different from zero even for $N \approx 10^6$, and does only approach this value for very large size clusters. The crossover from fast to slow decrease depends on q . For large q , $\lambda_q(N)$ continues to decrease rapidly, even in the range where it might have been argued that $\lambda_2(N)$ has settled down. Thus, λ_q continues to decrease non-trivially up to the size of our simulations. Moreover, we have tested the possibility of a logarithmic behavior of the $\lambda_q(N)$ curves. An accurate analysis shows that this behavior seems consistent up to $N \approx 10^4$, but not for larger clusters. Therefore, these results support the idea of an «infinite drift» scenario which shows persistent deviations from self-similarity for arbitrary large finite-size samples. This scenario could account for several corrections to scaling which are non-trivially related and reflect the dynamical aspects of the problem.

Additional information is yielded by the radial cluster shell profiles. For instance, an important feature of DLA clusters is confirmed by the analysis of the function $F(R, N) R^{-1/D}$ for several values of N . It is observed that each of the contributing graphs begins by a piece that is indistinguishable from the preceding contributing graph. In other words, among the atoms that joined the cluster between the $(N - \Delta N)$ -th and the N -th, very few reach the central portion. This confirms the fact that the central portion can be viewed, in effect, as having stopped growing. In addition, by inspecting the distribution $\Delta F(R, N, \Delta N)$ it is also possible to discuss several geometric features of very large clusters. These results will be discussed elsewhere.

From the previous analysis of very large DLA clusters we can draw the following picture. DLA is mainly a non-equilibrium phenomenon in which the dynamical aspects play a major role. These dynamical aspects are present from the early stages of the growth process up to the very large sizes considered in our simulations, and are responsible for the infinite-«drift» scenario suggested by the analysis in ref. [5] and in this paper. In fact, DLA shows two different cluster regions. The first is a fully grown core that will not be further modified by growth. The second region is the active zone of the cluster where the growth processes are still occurring. This region is clearly far from asymptotic and contains the dynamical properties of the DLA model. Our moment analysis is focussed on this second region and supports the novel «scenario» [5] in which the dynamical transient continues forever, showing infinite persistent deviations from the simple self-similarity. In fact, we found that the moment-based scale factors of the cluster shell show corrections to a simple self-similar scaling up to $N \sim 10^6$. These corrections decrease very slowly in a non-trivial way (no observed finite cross-over), and allow a scenario in which, for every finite-size samples, it is possible to observe departures from the simple self-similarity.

The situation we have described is completely different with respect to the usual equilibrium problems, such as percolation or Ising clusters, where there is no distinction between cluster's regions. The inner region of the DLA clusters is completely «frozen», and it may be expected to be «self-similar». However, this «old» part of the cluster had been young, and preserves a memory of the dynamical process by which it has been generated. As pointed out in ref. [5] this can be reflected in a power law behavior in the prefactor that measures the mass lacunarity and that supports the scenario of limitless drift. In this case the fractal dimension estimated from the mass-radius relation is biased by a correction term that could explain the disagreement, both from numerical simulations [1] and theoretical approach [12], between the various estimates of the fractal dimension D .

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