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Probing surface characteristics of diffusion-limited-aggregation clusters with particles of variable size

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We develop a technique for probing the harmonic measure of a diffusion-limited-aggregation (DLA) cluster surface with variable-size particles and generate 1000 clusters with 50×10^6 particles using an original off-lattice killing-free algorithm. Taking, in sequence, the limit of the vanishing size of the probing particles and then sending the growing cluster size to infinity, we achieve unprecedented accuracy in determining the fractal dimension $D=1.7100(2)$ crucial to the characterization of the geometric properties of DLA clusters.

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Kinetic interfaces that evolve into two-dimensional fractals via diverse stochastic growth processes are ubiquitous to nature. The systems and physical processes that exhibit kinetic roughening and fractal structure range from firefronts and bacterial colonies to dendrites of various nature, to domain walls in magnets and ferroelectrics, to liquids penetrating porous media, and many others. The study of two-dimensional fractals associated with kinetic roughening is an exciting and mature branch of statistical physics—see the excellent works [1,2] for exhaustive reviews. The generic process governing a good part of these phenomena is the so-called two-dimensional aggregate growth, which is commonly modeled as diffusion-limited aggregation (DLA) [3] and its generalization dielectric breakdown model (DBM) [4], capturing well most of the properties of the random aggregates [2]. Past analytical and numerical studies have impressively advanced our understanding of DLA (see again [1,2]), yet there are still several critical issues that remain unresolved, like the controversies related to the multiscale and fractal nature of DLA, to name a few. One of the central questions is the precise value of the DLA fractal dimension D, knowledge of which is crucial for a full description of the geometric properties and characterization of DLA clusters. In particular, an exact value of D is necessary for evaluating DLA lacunarity at large growth times.

In the planar, $d=2$, geometry analytical results (see, for example, [5]) suggest that the DLA fractal dimension lies in the range $D=1.67-1.72$; certain rational values like $D=5/3$, in [6], or $D=17/10$, in [7], were also predicted. On the other hand, Mandelbrot [8] argued that DLA clusters fill the whole space—i.e., that $D=2$. Direct simulations usually produce $D=1.715(4)$ for the DLA fractal dimension [9,10]; simulations [11] based on conformal mapping [12,13] yield $D=1.713(5)$.

Conventionally the fractal dimension D is determined from a fit of the growing aggregate (cluster) size R to the functional dependence:

$$R \propto N^{1/D}, \tag{1}$$

where N is the number of particles in the cluster. The cluster size R can be defined as the radius of the deposition, $R_{dep}=\langle r_i\rangle$, where r_i is the position of the ith particle and brackets stand for averaging over the ensemble of clusters. The accuracy achieved in the determination of D in past publications is characterized by the fluctuations [14,15] $\mathcal{F}_D=(\langle D^2\rangle-\langle D\rangle^2)/\langle D\rangle^2$. The latter decays as $\mathcal{F}_D\propto N^{-0.33}\simeq N^{-1/3}$ (rather than the naively expected $\propto 1/N\ln N$). As a matter of practice, this implies that in order to achieve the next level of accuracy [one more (fourth) digit] one is required to consider clusters with the number of particles exceeding by a factor of 1000 those used in the simulations of Refs. [9–11]. Clusters of such a size, about $N=10^9$, are not accessible via standard approaches due to computational speed and computer memory limitations.

In this Rapid Communication we develop and report on an alternative approach allowing us to reach a higher accuracy of the fractal dimension measurement. We exploit the fact that in simulations the diffusing particles always have some finite physical size δ and that, while the true fractal dimension D should not depend on δ, the results of simulations appear to depend on the size of the particles probing the harmonic measure. Our idea is to use this dependence in order to parametrize the fractal dimensionality as a function of δ and, upon finding $D(\delta)$ in a series of numerical experiments, define the fractal dimension[1] as $D=\lim_{\delta\to0}D(\delta)$. We will show that our approach allows for a dramatic improvement in the precision in determining D.

The accessibility of a particular set of the points at the cluster interface is characterized by the probabilities p_k for a particle diffusing from infinity to hit the cluster at this given subset Γ_k of the surface. For an interface of the form of an ideal circle (and the symmetric diffusion), the probabilities are distributed uniformly and the probability density is just $1/2\pi$ (the harmonic measure). In an irregular cluster most of the probability density is concentrated around the cluster's tips, whereas the fjords are screened (this effect is often referred to as the "tip effect" and/or "Faraday screening" [4,16–18]). The conventional approach to probing the harmonic measure is as follows: (i) A DLA cluster containing N

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[1]Our definition of the fractal dimension does not depend upon the size of the particles the cluster itself is composed of. Therefore, we let the size of the particles in the cluster be unity and measure the size of the probing particles in units of the cluster particles.

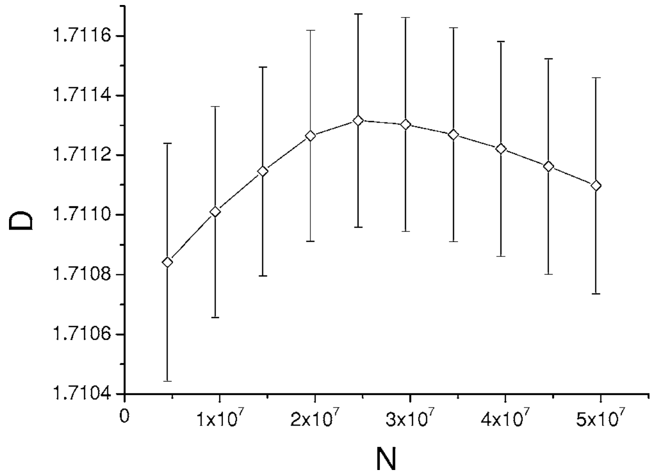

FIG. 1. Fractal dimension with error bars as a function of the cluster size, computed with R_{dep}. The solid line connecting circles is a guide for the eye.

particles is generated. (ii) The positions r_i where the next M particles hit the border of the cluster for the first time are stored but the particles do not remain attached to the cluster. (iii) The deposition radius is calculated as

$$R_{dep}(N) \approx \frac{1}{M}\sum_{i=1}^{M} r_i, \tag{2}$$

and the sum converges to the integral over the harmonic measure $R_{dep}(N)=\int dqr$ for sufficiently large M.

Figure 1 shows a typical variation of D calculated using relation (1) with R_{dep} and representing the half period of the oscillations of fractal dimension D with the size of the cluster. The oscillations are related to the spatially nonuniform growth of the cluster: different branches grow with different speed, and the newborn subbranches often outgrow the parent branches. The amplitude of the oscillations decreases slowly with cluster size, thus complicating a precise determination of the value of D.

Figure 2 shows part of the cluster branch. The spots where the probe particles hit the surface are marked with intensity proportional to the logarithm of the particular probability p_k for the particle to hit the segment Γ_k. For the sake of better visualization we choose the length of segments to be equal to one pixel of the figure. Uncoupled segments Γ_k (see Fig. 2) constitute only the part of the surface accessible to the diffusing particles. The total length of the accessible cluster interface depends on the size of the probe particles. We choose the probe particle size δ as a parameter of the particular measurement. The value of δ controls two processes: (i) the "geometrical" process which is the penetration of the particles inside the fjords where the geometrical bottleneck of the fjords may prevent [17,18] sizable particles from going through and (ii) the probabilistic process of screening; the latter becomes more effective with the growth of the particle size δ.

It is important to stress the difference between the measurement of the length of the fractal surface [19] and the measurement of the harmonic measure on the surface within

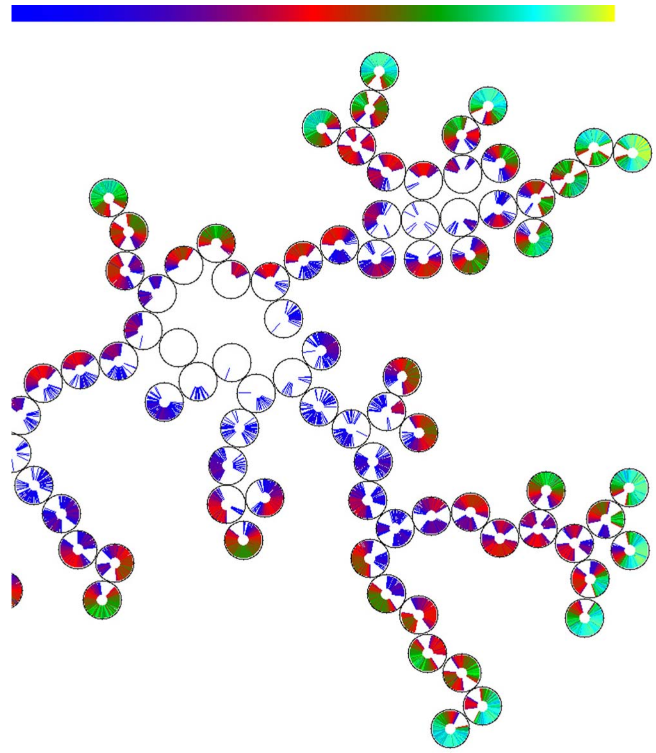

FIG. 2. (Color online) Fragment of the cluster with $N=10^4$ particles and positions of hits by probe particles with radius $\delta=1$. The intensity is proportional to the logarithm of the hit probabilities, denoted accordingly by the intensity bar at the top. Probabilities are larger near the tips and smaller inside the fjords.

our approach. In the former case, the total length of the surface grows with decreasing scale division value [19] (i.e., the length of the subsets Γ_k is equal to the ruler size). In the latter case, the probability p_k for the particle to hit the subset Γ_k saturates as $\delta \rightarrow 0$.

Figure 3 shows the number of the surface particles having been touched by the probe particles as a function of the probing particle size. The solid line is given by the expression $N_{reach}=N_{surf}/(1+\delta/\delta_0)^{\alpha}$, with $\alpha=0.69(2)$ and $\delta_0=2.2(1)$.

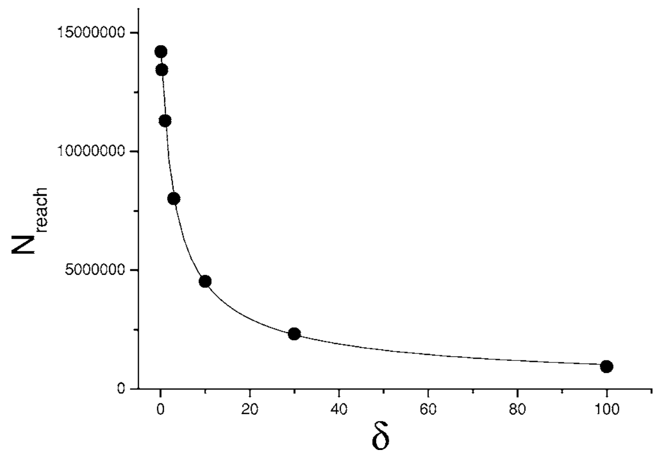

FIG. 3. Number of reachable sites of the cluster as a function of the probe particle radius (circles) with the fit described in the text (solid line).

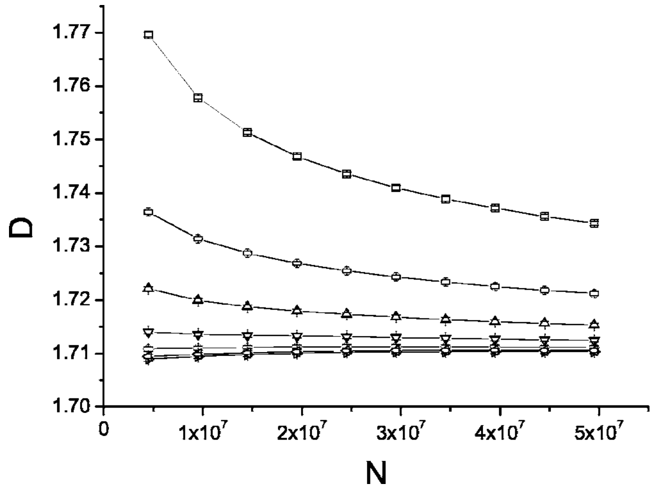

FIG. 4. Fractal dimension (symbols) as a function of N for δ=0.1, 0.3, 1, 3, 10, 30, 100 from bottom to top. Solid lines connecting circles are a guide for the eye.

The limit of vanishing size $\delta \to 0$ gives the limiting number of the reached particles as the total number of surface particles, $N_{surf} \approx 14\,662\,525$ (out of total 20×10^6 in the cluster).

The dependence of D upon N for different δ is shown in Fig. 4. As we have already mentioned, the dependence on N within the given interval of N and for fixed δ is not monotonic for $\delta < 3$. Thus, we fit results by the formula

$$D(\delta;N) = D(N) + A\delta^{\beta} \quad (3)$$

and take the limit of $\delta \to 0$ for the fixed values of the cluster size N. The resulting values of $D(N)$ are shown in Fig. 5. Note that now the dependence $D(N)$ has become monotonic. This can be understood as the result of the effective averaging of the competition between the growing branches. We have examined an ensemble of 1000 clusters with 50×10^6 particles for each value of δ. The number of particles, M, in each event of the measurement necessary to achieve the desired accuracy in R_{dep} of about 0.1% was typically several tens of thousands. We have found no difference in results when using a larger number of probe particles. The error bars represent combined errors from both the ensemble average and the fit. Thus from Fig. 5 one finds at the end of the day the ultimate value of the fractal dimension is $D = 1.7100(2)$. This is an unprecedented accuracy in the measurements of D, exceeding, by an order of magnitude, the results known from the literature.

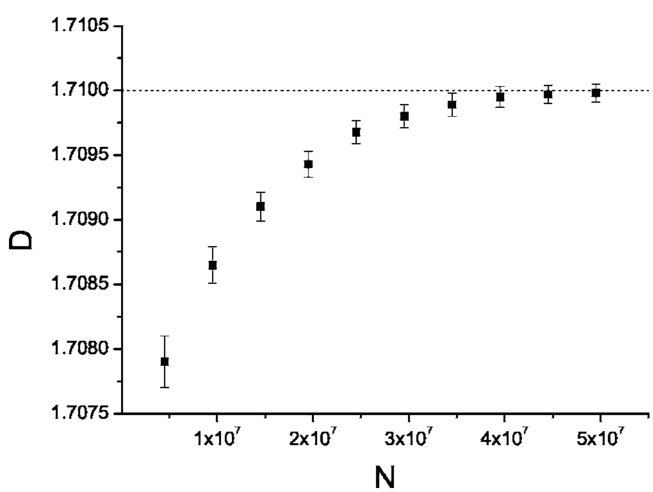

FIG. 5. Fractal dimension as a function of N for the limiting value of δ=0. It reaches the value $D = 1.7100(2)$ (plotted with the dotted line) in the limit of large cluster size N.

TABLE I. Fractal dimension estimated by the standard method using the reference frames centered at the seed particle (left column) and at the center of gravity (right column), respectively.

	r to seed	r to center of mass
R_{dep}	1.7098(12)	1.7111(6)
R_2	1.71155(56)	1.71149(54)
R_g	1.71149(30)	1.71133(30)

It is instructive to use the same ensemble of clusters in order to evaluate the fractal dimension via the traditional approach introducing the deposition radius as $R_{dep} = \langle r \rangle$, the mean-square displacement $R_2 = \sqrt{\langle r^2 \rangle}$, and the radius of gyration $R_g = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\langle r^2 \rangle}$. The results of the fit to the form (1), where R stands for one of the above radii, are presented in Table I. Note that all the obtained values of D are larger than that of $D = 1.7100(2)$ derived by the method of the present work.

Since DLA clusters grow randomly, a center of the cluster mass $R_M = \sqrt{\frac{1}{N}\left|\sum_{i=1}^{N} r_i\right|}$ performs random walks in the plane. Accordingly, the distance from the original position of a seed particle to the center of mass grows as $\sqrt{N}$ and the number of particles is proportional to the time of the random walk.[2] The average value of R_M for $N = 5 \times 10^7$ is $\langle R_M \rangle \approx 1000$ which should be compared to $\langle R_g \rangle \approx 30\,000$ and the penetration depth $\xi \approx 7000$. The average angular position of the center of mass (averaged over an ensemble) is also a stochastic function of time, although at each realization of the cluster angular correlations are observed (some of the branches grow faster within a given time interval [20]).

The important question now is whether the choice of the coordinate frame influences the final result and the value of the fractal dimensionality. Indeed, when determining D one can choose the origin at either (i) the position of the seed particle, (ii) at the (evolving with time) position of the center of gravity, or else (iii) at the "center of the charge gravity" (the latter is most appropriate for the DBM case). We have performed averaging according to Eq. (2), finding D from the

[2] There are some attempts in the literature of extracting the fractal dimension of the cluster using the fit $R_M \propto N^{1/D}$. However, no justification for such a fit is available to the best of our knowledge. One rather expects the center of the cluster mass to perform a conventional random walk.

fit to $\widetilde{R}_{dep}$, $\widetilde{R}_2$, and $\widetilde{R}_g$, placing the origin of the reference frame to the seed particle (left column of Table I) and to the center of gravity (right column). One sees that for all quantities the choice of reference frame is irrelevant (within the accuracy of computation), although the ensemble of clusters should be large enough to ensure this convergence.

In conclusion, we have developed a technique for the high-precision analysis of the geometrical properties of DLA clusters, in particular the evaluation of its lacunarity in the long-time limit. Our approach offers a perfect tool for further advancing our understanding of the fjord screening behavior. In particular, the long-standing problem of behavior of p_{min}, which is the minimal growth probability (in DBM language) or probability to hit a given segment of the cluster surface (in DLA language), can be efficiently addressed via the developed approach. The behavior of the latter probability is related to the phase transition in the multifractal spectrum [21]. To the best of our knowledge, this probability was estimated only within the "tunnel configuration" [16] technique and had never been measured in simulations of the "typical configuration" [22].

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