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# Nonuniversal diffusion-limited aggregation and exact fractal dimensions

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In analogy to recent results on nonuniversal roughening in surface growth [Lam and Sander, Phys. Rev. Lett. **69**, 3338 (1992)], we propose a variant of diffusion-limited aggregation (DLA) in which the radii of the particles are chosen from a power-law distribution. For very broad distributions, the huge particles dominate and the fractal dimension is calculated exactly using a scaling theory. For narrower distributions, it crosses back to DLA. We simulated 1200 clusters containing up to 200 000 particles. The fractal dimensions obtained are in reasonable agreement with our theory. This variant of DLA might have relevance to the cluster-cluster aggregation model.

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Diffusion-limited aggregation (DLA) [1] is an important prototype of fractal growth [2]. In two dimensions, its fractal dimension is determined to be $1.712 \pm 0.003$ from large scale off-lattice simulations [3,4]. There exists no exact formula for the fractal dimension. In spite of intensive studies, the task of obtaining accurate estimates of the fractal dimension by analytical means remains very challenging [2,5].

In this work, we investigate a class of variants with *exactly* solvable fractal dimensions for a certain range of a model parameter. In another range, the model crosses back to DLA. The transition is associated with an interesting morphology change. The model might have relevance to cluster-cluster aggregation (CCA) models which simulate colloidal aggregation [2]. More importantly, DLA and most previous nontrivial variants are not expected to have exactly solvable fractal dimensions. Our variant might have a particular role in testing theoretical approaches of branched growth [2,5]. However, even though the variant has an exact dimension for a certain regime which extrapolates continuously to DLA, our approach is not capable of calculating the fractal dimension, $D_{\mathrm{DLA}}$, of DLA. The reason is that the transition point is not known *a priori* and has to be expressed in terms of $D_{\mathrm{DLA}}$. We concentrate on the two dimensional case, while the results can be generalized easily to higher dimensions.

Our variant of DLA is motivated by recent results on Zhang's model of surface growth with power-law noise [6,7]. The algorithm is very similar to standard DLA. Particles are launched one by one and carry out Brownian motion. Starting from an immobile seed, the aggregate grows when a walker hits it and becomes part of it. Usually, all the particles launched have the same radii. The asymptotic scaling properties and the morphology are not expected to change if the particle radii are random but bounded. However, the universality can be broken if the probability distribution of the radii is very broad. This leads us to characterize our variant by the following power-law distribution, $P(r)$, of particle radii, $r$:

$$P(r) = \begin{cases} \mu/r^{\mu+1} & \text{for } r \geq 1 \\ 0 & \text{for } r < 1. \end{cases} \tag{1}$$

It recovers the standard DLA algorithm as $\mu \to \infty$. In general, the walkers can be fractals themselves with dimension $D_p$. An interesting example is the CCA model in which, for some regimes, the radii of the ensemble of clusters can have a power-law distribution [2]. The walkers in our variant then correspond to the wandering clusters in the CCA model. In this case, the fractal dimension of the walkers and the final aggregate should be the same. This property follows naturally from our scaling theory in the appropriate regime.

We focus on the case that the aggregate and the individual particles are dense enough so that they are not transparent to each other. This is generally true in low dimensions. For programming convenience, we further assume in our simulations that the wandering particles have a circular outer boundary. This simplification should not alter the scaling properties.

The simulation of off-lattice DLA with the power-law distribution of the particle radii in Eq. (1) is complicated due to the absence of an upper cutoff for the particle radii. To determine accurately whether a walker has touched the cluster, it is no longer sufficient to search in a finite neighborhood for centers of other particles. In order to obtain an efficient algorithm, the focus must be shifted from the centers of the particles to their perime-

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ters, which are instead stored in a hierarchical map structure [3,4]. We can thus check efficiently whether a walker with a given radius overlaps with a perimeter site of some particle on the cluster. However, this procedure significantly increases both the storage requirements and the run time of the simulation, especially for a small power-law exponent $\mu \to 1$. Therefore we had to restrict our simulations to clusters with masses between 100 000 and 200 000 particles.

Figure 1 shows three typical clusters grown for exponents $\mu = 2.5$, $\mu = 1.713$, and $\mu = 1.3$. Each of them contains 100 000 particles. The choice of the values of $\mu$ is to illustrate a morphology transition which will be explained later using a scaling theory. For $\mu = 2.5$ [Fig. 1(a)], the presence of the large particles results in a cluster significantly more noisy than DLA. However, the small particles are abundant enough to dominate the geometry and the overall branching structure is very similar to DLA. There exists a number of well defined main branches emanating radially from the center of the cluster. We observe that the ratio between the size of the largest particles and that of the cluster decreases as the number of particles, $N$, increases. In fact, we will explain that the cluster becomes indistinguishable to DLA for very large $N$. In contrast, for the very broad distribution at $\mu = 1.3$ [Fig. 1(c)], the morphology is completely altered by the very big particles. A well defined geometrical center of the cluster no longer exists. The size of the largest particles is comparable to that of the cluster and dominates the structure completely. The morphology is more similar to that of CCA than DLA. We will show that the transition between the two different morphologies occurs at $\mu = D_{\rm DLA} \simeq 1.713$ [Fig. 1(b)]. Here, the DLA type morphology holds marginally and the size of the largest particles compared to the cluster size decreases very slowly as $N$ increases.

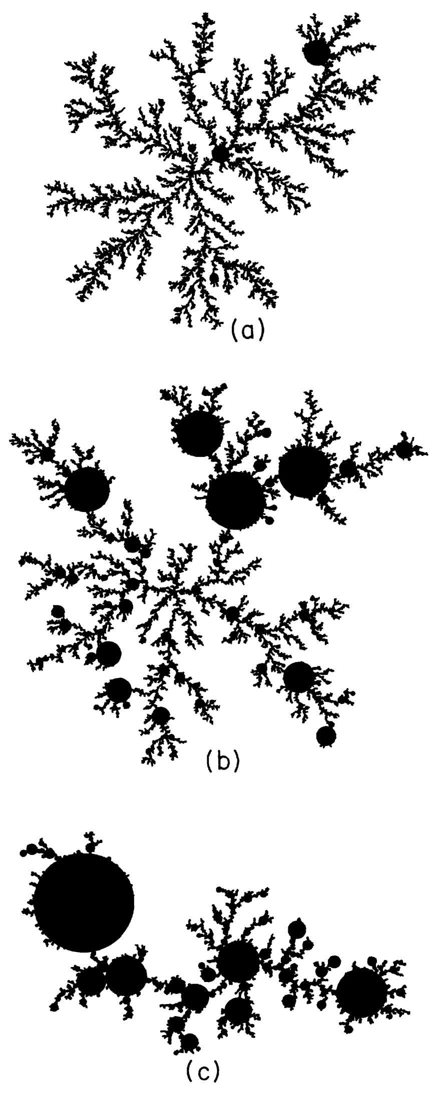


FIG. 1. Typical clusters at (a) the small particles dominating regime ($\mu = 2.5$), (b) the transition point ($\mu = 1.713$), and (c) the large particles dominating regime ($\mu = 1.3$).

We now present a scaling theory for the variant, which predicts a transition from a regime dominated by small particles to one with dominating large ones as $\mu$ decreases. Consider the scaling form

$$R_G \sim N^{1/\gamma}, \tag{2}$$

where $R_G$ is the radius of gyration of the cluster and $N$ is the number of particles. For cases such as $D_p = 0$ or $\mu \to \infty$, the exponent $\gamma$ reduces to the fractal dimension. The general relationship will be worked out later.

We first examine a broad distribution with $\mu < D_{\rm DLA}$. We are going to show that $\gamma$ is *exactly* given by $\gamma = \mu < D_{\rm DLA}$. The idea of the proof to be presented below can be sketched out briefly as follows: If it were true that $\gamma > \mu$, the cluster radius $R_G$ would be even smaller than the typical size of the largest particle inside the cluster. If $\gamma < \mu$, $R_G$ would be too large to be accounted for by the large particles. This leads to a domination of small particles, which again can be proved to be wrong. Our derivation is closely related to the analogous one for surface growth with power-law noise, in which case Lam and Sander [7] proved the exactness of a formula for the scaling exponent suggested independently by Zhang [8] and Krug [9].

We now give our arguments in more detail. It is easy to show that $\gamma \neq D_{\rm DLA}$, which necessarily implies a nonuniversal behavior $\mu < D_{\rm DLA}$. For a cluster of $N$ particles, the expected radius of the largest particle, $r_{\rm max}$, sampled from the power-law distribution in Eq. (1), follows $r_{\rm max} \sim N^{1/\mu}$. The proposition $\gamma = D_{\rm DLA}$ implies $R_G \sim N^{1/D_{\rm DLA}}$. This is impossible for $\mu < D_{\rm DLA}$ because at sufficiently large $N$, the largest particle would even be bigger than the cluster itself ($r_{\rm max} > R_G$). The same argument shows more generally that $\gamma > \mu$ is false when $\mu < D_{\rm DLA}$.

In fact, the huge particles are not only relevant to the scaling, as proved above, but also dominate the geometry completely. It is plausible that the largest particle sets the scale of the cluster: $R_G \sim r_{\rm max}$. This assumption immediately leads to $\gamma = \mu$, since $r_{\rm max} \sim N^{1/\mu}$. We will show that this simple picture is indeed correct asymptotically.

The conventional way to compare the visual appearance of DLA of different sizes is to rescale them to a standardized radius of gyration. Instead, we now rescale the clusters by a factor $N^{-1/\mu}$ and examine the dependence of the radii of the clusters on $N$. In this rescaling scheme, the size of the biggest particle is independent of $N$. Furthermore, the radii, $r'$, of the rescaled constituent particles follow a new probability distribution $P'(r')$. In a cluster of $N$ particles, the number density of particles per unit $r'$ is $n(r') = NP'(r')$ given by

$$n(r') = \begin{cases} \mu/r'^{\mu+1} & \text{for } r' \geq r_m \\ 0 & \text{for } r' < r_m, \end{cases} \tag{3}$$

where the lower cutoff radius, $r_m$, is a function of $N$ given by $r_m(N) = N^{-1/\mu}$. This implies that not only $r_{\max}$ but also the whole distribution $n(r')$, except for the lower cutoff $r_m$, is independent of $N$. The simple picture of the domination of the large particles corresponds to the assumption that the variations of the cutoff can be neglected asymptotically. If this is true, $n(r')$ is completely independent of $N$ as $N \to \infty$ and both, the self-similarity and $\gamma = \mu$, become obvious.

For narrower distributions with $\mu > D_{\rm DLA}$, the small particles dominate. We have $\gamma = D_{\rm DLA}$ and the morphology is the same as DLA. The huge particles are irrelevant to the geometry. The radius of the largest particle vanishes compared with the cluster size as $N$ increases. In summary, we have

$$\gamma = \min\{\mu, D_{\rm DLA}\}. \tag{4}$$

Although the complication about the lower cutoff does not alter the exponent, it leads to strong crossover effects. Using the above rescaling scheme with the factor $N^{-1/\mu}$, as $N \to \infty$ the rescaled cluster radius, $R'$, converges for $\mu < D_{\rm DLA}$ but diverges for $\mu > D_{\rm DLA}$. The $\mu = D_{\rm DLA}$ case is marginal and $R'$ is expected to diverge logarithmically, and by analogy with the results for surface growth [7] we postulate a logarithmic correction to scaling at $\mu = D_{\rm DLA}$:

$$R_G \sim N^{1/D_{\rm DLA}}[\ln(N)]^{1/2}. \tag{5}$$

Now, we compute the fractal dimension $D$ of the cluster from the relation $M \sim R_G^D$, where $M$ is the mass of the aggregate. Using the distribution of the particle radii in Eq. (1) and the assumption that the constituent particles are fractals of dimension $D_p$, we get

$$M \sim \begin{cases} N, & D_p < \mu \\ N^{D_p/\mu}, & \mu < D_p \end{cases} \tag{6}$$

where the averaged particle mass diverges for small $\mu$. At $\mu = D_p$, the divergence is marginal:

$$M \sim N \ln N. \tag{7}$$

Combining Eqs. (2), (4), and (6), the fractal dimensions are obtained for four different cases:

$$D = \begin{cases} D_{\rm DLA}, & D_p, D_{\rm DLA} < \mu \\ D_p D_{\rm DLA}/\mu, & D_{\rm DLA} < \mu < D_p \\ \mu, & D_p < \mu < D_{\rm DLA} \\ D_p, & \mu < D_p, D_{\rm DLA}. \end{cases} \tag{8}$$

The variant crosses back to DLA for narrower distributions of $D_p, D_{\rm DLA} < \mu$. For $D_{\rm DLA} < \mu < D_p$, even though the morphology is the same as DLA, the fractal dimension is different since the averaged particle mass diverges. For the other two cases of broad distributions, the morphology is nonuniversal. It is particularly interesting that for $\mu < D_p, D_{\rm DLA}$, $D = D_p$ follows. It is precisely how it should be when the walker represents the clusters in the CCA model. This sets an upper bound for $\mu$ if the variant describes some regime of CCA. Simulations of CCA in general give $\mu$ or its effective value well within this bound [2].

We test our scaling theory numerically for the case $D_p = 2$. Equation (8) then reduces to

$$D \sim \begin{cases} D_{\rm DLA}, & 2 < \mu \\ 2D_{\rm DLA}/\mu, & D_{\rm DLA} < \mu < 2 \\ 2, & \mu < D_{\rm DLA}. \end{cases} \tag{9}$$

The verification of Eq. (9) also establishes the validity of Eq. (4) and the general result in Eq. (8), since they are all related by the trivial Eq. (6). The logarithmic corrections in Eqs. (5) and (7) at the transition points give respectively:

$$M \sim \begin{cases} R_G^{D_{\rm DLA}}/\ln(N), & \mu = D_{\rm DLA} \\ R_G^2 \ln(N), & \mu = 2. \end{cases} \tag{10}$$

In our naive computation of $D$ from the slope of the best fitted straight line in the log-log plot of $M$ against $R_G$, these corrections cause an underestimation at $\mu = D_{\rm DLA}$ and an overestimation at $\mu = 2$.

Let $r_i$ and $\vec{x}_i$ be respectively the radius and the position of the $i$th particle in a cluster with $N$ particles. Assuming that every particle has uniform unit density, the mass of the individual particle is $m_i = \pi r_i^2$. Since the particles are disks instead of points, the mass and radius of gyration of the cluster is given by

$$M = \sum_{i=1}^{N} m_i, \tag{11}$$

$$MR_G^2 = \sum_{i=1}^{N} m_i[(\vec{x}_i - \vec{x}_{\rm c.m.})^2 + \tfrac{1}{2}r_i^2], \tag{12}$$

where $\vec{x}_{\rm c.m.}$ is the center of mass of the cluster.

We have grown a total of 1200 clusters for exponents $\mu$ in the range $1.0 \leq \mu \leq 5.0$. For various cluster sizes $N$, we compute the ensemble averaged cluster mass and radius of gyration. Each data point in the $R_G$ vs $M$ plot is obtained from ensemble average over clusters of fixed $N$. However, the averaging has to be done with caution to avoid divergence. For example, Eq. (1) implies that the probability distribution, $P(m)$, of the mass, $m$, of the walkers follows the power law: $P(m) \sim 1/m^{\mu/2+1}$. For $\mu < 2$, the arithmetic mean of $m$ diverges. However, the geometrical ensemble average, $\exp\langle \ln M \rangle$, is well defined, where the bracket denotes the arithmetic mean. Similarly, we also take the geometrical average $\exp\langle \ln R_G \rangle$ for the radius of gyration $R_G$. Figure 2 shows the geometrical ensemble averages $M$ against $R_G$ in a log-log

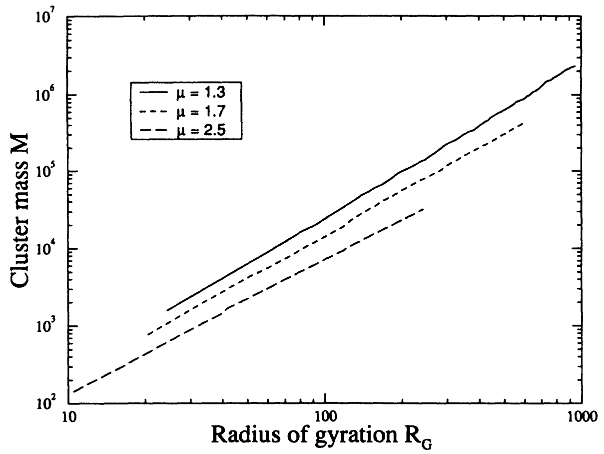


FIG. 2. Dependence of the cluster mass $M$ on the radius of gyration $R_G$ for three selected values of $\mu$. The geometrical mean is adopted for the ensemble averaging.

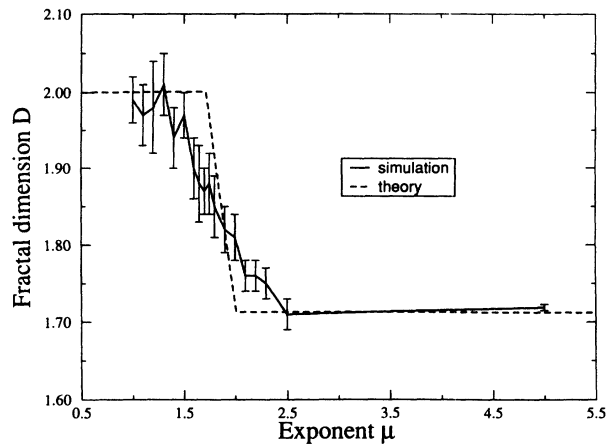


FIG. 3. Dependence of the fractal dimension $D$ on the exponent $\mu$. The solid line denotes our numerical results, whereas the dashed line marks the prediction of the scaling theory. The systematic discrepancies at the transition points $\mu \simeq 1.713$ and $\mu = 2$ are due to finite size effects in the form of logarithmic corrections.

plot for the selected values $\mu = 1.3$, $\mu = 1.7$, and $\mu = 2.5$. The numbers of clusters used are 50, 104, and 25, respectively. For all values of $\mu$ we investigated, we obtain a reasonable scaling behavior.

Figure 3 shows the measured fractal dimensions $D$ as a function of $\mu$. We computed $D$ by averaging over the dimensions for each individual cluster, obtained from the corresponding scaling plot of $R_G$ against $M$. The error bars were obtained from the statistical fluctuations. Quantitatively the same result is obtained when we compute $D$ from the slopes of the geometrically averaged $R_G$ vs $M$ plots (Fig. 2). Also shown in Fig. 3 is the prediction of the scaling argument in Eq. (9). Good agreement with our theory is observed far away from the transition points for $\mu \simeq 1$ and $\mu \gtrsim 2.5$. At the transition points $\mu = D_{\rm DLA}$ and 2, the expected discrepancies due to the logarithmic corrections in Eq. (10) are observed.

In summary, we propose a variant of DLA in which the random walkers have random radii of very broad power-law distribution. A scaling theory predicts that, as the distribution becomes narrower, there exists a transition between regimes dominated by large and small particles. The fractal dimension can be calculated exactly for the former regime. At the transition point we find a logarithmic correction to scaling. An analogous scaling theory leading to a similar transition has been verified numerically for the case of surface growth with power-law noise. We generated 1200 clusters of our DLA variant. When huge particles dominate, the morphology of the cluster is different from that of DLA and might be related to that of the cluster-cluster aggregation model. The measured fractal dimension is in reasonable agreement with the scaling theory. The numerical precision is limited by strong statistical fluctuations and finite size effects, which manifest themselves as logarithmic corrections at the transition points.

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