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LETTER TO THE EDITOR

Two-dimensional diffusion limited aggregation: a finite-size scaling approach

Loïc Turban and Jean-Marc Debierre

Laboratoire de Physique du Solide†, ENSMIM Parc de Saurupt, F-54042 Nancy Cedex, France and Université de Nancy I, BP 239, F-54506 Vandoeuvre les Nancy, France

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Abstract. Finite-size scaling in the diffusion-limited aggregation model of Witten and Sander is studied in two dimensions via Monte-Carlo simulations on semi-infinite strips of width $n = 2$–20. Due to a crossover between self-avoiding walk-like growth for small n and dendritic growth for large n, wide strips ($n = 8$–20) are needed to deduce the Witten–Sander fractal dimension $D \sim \frac{5}{3}$ from the finite-size scaling analysis.

The irreversible aggregation of small particles to build randomly ramified clusters is of interest in a wide variety of problems ranging from the coagulation of smoke particles (Forrest and Witten 1979) to the growth of crystals from an undercooled melt or a supersaturated solution (Langer 1980). Since the diffusion of the particles towards the cluster surface is often the rate-limiting process, Witten and Sander (1981, 1983) considered a simple lattice model in which a seed particle is placed at the centre of a large hypersphere at $t = 0$, then a new particle is released at random on the sphere and performs a random walk on the lattice until it reaches a site adjacent to the seed where it stops, building a two-particle cluster. A new particle is then launched on the sphere and the process is continued until the required cluster size is reached.

Perimeter sites deep inside the cluster are screened by peripheral ramifications so that compact clusters are unstable and a dendritic structure results. At scales much larger than the particle size (or lattice parameter) there is no natural length scale in the problem and a self-similar structure results. A large N-particle cluster has a radius $R(N)$ given by:

$$N \sim R(N)^D \tag{1}$$

where D is the fractal dimension of the cluster (Mandelbrot 1982). This property largely explains the popularity of the diffusion-limited aggregation (DLA) model; it was recognised by the initiators who obtained $D \sim \frac{5}{3}$ through two-dimensional (2D) Monte Carlo simulations. Monte Carlo simulations in higher euclidean dimensions d (Meakin 1983a) are consistent with

$$D \sim \tfrac{5}{6}d \qquad (d = 2\text{–}6) \tag{2}$$

whereas a mean-field approximation (Ball *et al* 1983) gives

$$D = d - 1 \qquad (d > 2). \tag{3}$$

† Laboratoire associé au CNRS no 155.

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Some arguments have been given (Witten and Sander 1983) suggesting that DLA has no upper critical dimension. A real-space renormalisation group approach has been proposed recently (Gould *et al* 1983) showing that DLA and lattice animals are in different universality classes; difficulties occur with this method in three and higher dimensions (Sahimi and Jerauld 1983).

The present work is devoted to a study of finite-size scaling on 2D lattice strips, DLA clusters being generated via Monte Carlo simulations. Our aim is to test the finite-size scaling assumptions on the kinetically defined DLA clusters and to see whether finite-size scaling, combined with Monte Carlo simulations†, could provide a reliable value of the factal dimension with low computational efforts.

DLA clusters are generated on semi-infinite strips with width n ($n = 2$–20) with either periodic or free boundary conditions (figures 1 and 2). A cluster is grown on the right of the first column which is initially occupied by n adjacent seed particles. A single main branch grows when n is small and, although secondary branches may occur on the largest strips, they quickly die off due to the screening effect and the long term results remain unaffected by this particular choice of initial conditions. Since a particle diffusing from a point at a large distance on the right of the cluster intersects the columns near to the cluster for the first time at random positions, the $(N+1)$th particle is released at random at $R_n(N)+1$ where $R_n(N)$ is the cluster 'radius' i.e. the position of the extreme particle in the cluster. When particles diffuse away at distances greater than $2n$ they are eliminated and a new particle is launched at $R_n(N)+1$. This value was increased without noticeable change in the cluster structure.

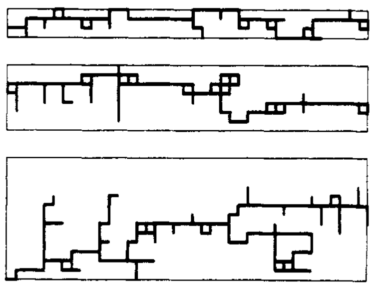

Figure 1. Parts of DLA clusters generated by Monte Carlo simulations on strips with width $n = 4, 8, 14$ and free boundary conditions.

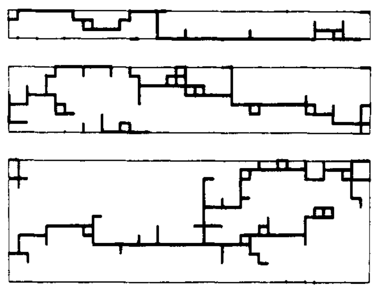

Figure 2. As figure 1 with periodic boundary conditions.

Since the system is actually 1D, a linear growth of the cluster 'radius' $R_n(N)$ with N is obtained (figure 3):

$$R_n(N) = pN + \alpha \qquad (N \text{ large}) \tag{4}$$

where the small shift α is due to end effects. The variation of the slope p with n is shown in figures 4 and 5. p is obtained by a least square fit of the data for each sample ($N = 2500$–4000) and by averaging over 8 to 10 samples for each point. The error bars give the standard deviations.

† Finite-size scaling with N has been recently used (Botet *et al* 1983) to study DLA as well as cluster–cluster aggregation (Meakin 1983b, Kolb *et al* 1983).

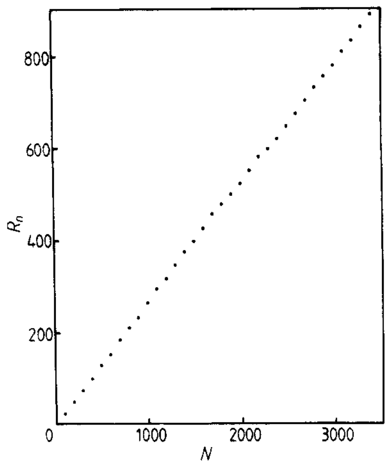

Figure 3. Linear growth of the cluster radius $R_n(N)$ with N on a strip of width $n = 20$ (data taken from a single Monte Carlo sample).

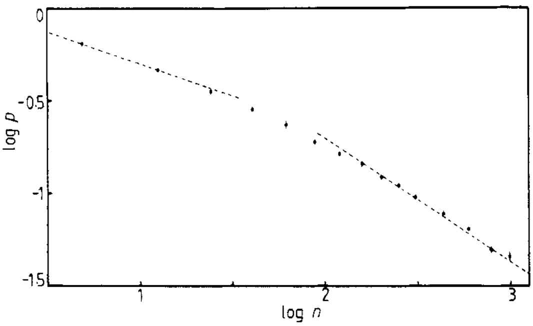

Figure 4. Variations of the logarithm of the growth rate $p = R_n(N)/N$ with ln (n) on a strip of width n and free boundary conditions. The broken lines give the slopes expected for SAW (small n values) and DLA (large n values).

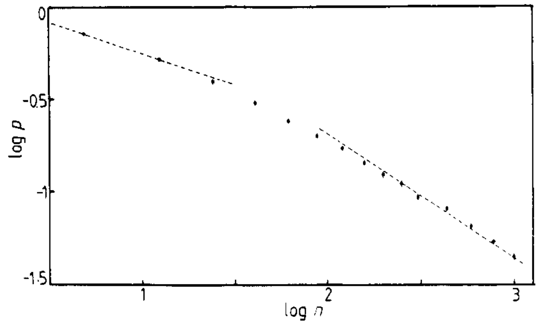

Figure 5. As figure 4 with periodic boundary conditions.

According to equation (1), an unconfined cluster grows with N like

$$R_\infty(N) \sim N^{1/D}. \tag{5}$$

The finite-size scaling assumption reads

$$R_n(N)/R_\infty(N) = f(n/R_\infty(N)) \qquad (N \text{ large}) \tag{6}$$

where

$$\lim\,(x \to \infty)\, f(x) = 1 \qquad \text{(unconfined growth)} \tag{7}$$

$$f(x) \sim x^u \qquad (x \ll 1). \tag{8}$$

Linear growth on a strip requires $u = 1 - D$ so that

$$p = R_n(N)/N \sim n^{1-D}. \tag{9}$$

This result is easily rederived using the 'blob' picture (de Gennes 1981) in which the confined cluster is supposed to be built up by a succession of circular blobs of radius n with bulk internal correlations so that inside a blob there are $g \sim n^D$ particles and the cluster radius is

$$R_n(N) \sim nN/g \sim Nn^{1-D} \tag{10}$$

as above.

According to this picture ln (p) should be linear in ln (n) with a slope $1 - D_{\rm DLA} \simeq -\frac{2}{3}$. This is what is observed with both types of boundary conditions for sufficiently large n values (figures 4 and 5) whereas for narrow strips the initial slope is near to $-\frac{1}{3}$ with a crossover region for intermediate values ($n \sim 4$–8). The finite-size scaling law

$$f(x) \simeq Ax^{1-D_{\rm DLA}} \tag{11}$$

with $R_\infty(N) = N^{3/5}$ is verified with both types of boundary conditions for sufficiently large n values ($n = 6$–20) (figures 6 and 7). The data, which were obtained by averaging $R_n(N)$ over 8 to 10 samples with N ranging from 200 to 4000, lead to

$$A = 1.85 \pm 0.05 \tag{12}$$

A progressive smearing of the points is observed when one enters the crossover region.

This crossover may be traced to an enhancement of the screening effect on narrow strips leading to an essentially linear structure with few side ramifications (figures 1 and 2). The dendritic structure, which is characteristic of the DLA is lost and local correlations are more like in confined self-avoiding walks (SAWs). The initial slopes in figures 4 and 5 give a fractal dimension $D = 1.33$–1.34 near to the SAW value†.

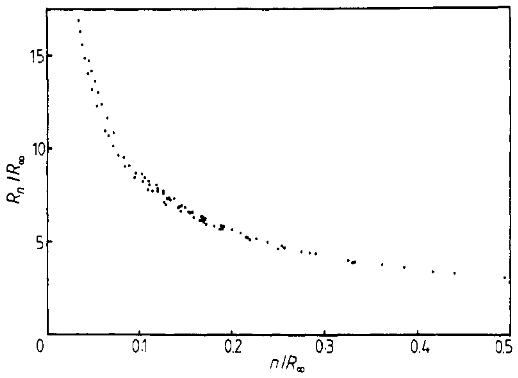

Figure 6. Finite-size scaling of the cluster radius on wide strips ($n = 6$–20) with free boundary conditions.

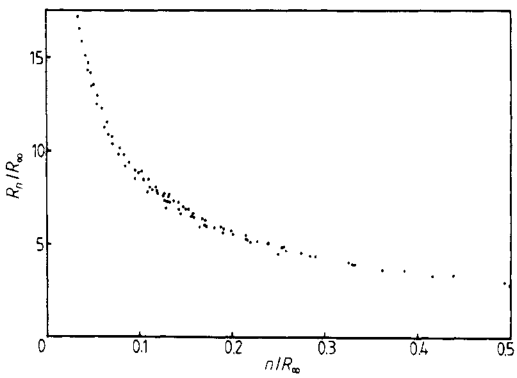

Figure 7. As figure 6 with periodic boundary conditions.

References

Ball R, Nauenberg M and Witten T A 1983 *Preprint Santa Barbara NSF-ITP 83-87*
Botet R, Jullien R and Kolb M 1983 *Preprint, Orsay*
Forrest S R and Witten T A 1979 *J. Phys. A: Math. Gen.* **12** L109–17
de Gennes P G 1981 *Scaling Concepts in Polymer Physics* (Ithaca: Cornell University Press)

† Confined SAWs are known to obey finite-size scaling for quite small values of n (Wall *et al* 1978).

Gould H, Family F and Stanley H E 1983 *Phys. Rev. Lett.* **50** 686–9
Kolb M, Botet R and Jullien R 1983 *Phys. Rev. Lett.* **51** 1123–6
Langer J S 1980 *Rev. Mod. Phys.* **52** 1–28
Mandelbrot B B 1982 *The Fractal Geometry of Nature* (San Francisco: Freeman)
Meakin P 1983a *Phys. Rev.* A **27** 1495–507
—— 1983b *Phys. Rev. Lett.* **51** 1119–22
Sahimi M and Jerauld G J 1983 *J. Phys. A: Math. Gen.* **16** L419–25
Wall F T, Seitz W A, Chin J C and de Gennes P G 1978 *Proc. Natl. Acad. Sci.* **75** 2069–70
Witten T A and Sander L M 1981 *Phys. Rev. Lett.* **47** 1400–3
—— 1983 *Phys. Rev.* B **27** 5686–97