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How to grow isotropic on-lattice diffusion-limited aggregates

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Abstract

We consider the problem of on-lattice cluster anisotropy in the diffusion-limited aggregation (DLA) model. On the basis of a recent paper (Bogoyavlenskiy V A 2001 *Phys. Rev.* E **64** 066303), we derive an *isotropic quadratic ratio* for a set of aggregation probabilities, in order to grow on-lattice DLA clusters without anisotropy.

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The basic model adopted for stochastic simulations of nonequilibrium growth processes in various natural Laplacian systems, diffusion-limited aggregation (DLA) [1, 2], is known to produce anisotropic on-lattice clusters—the anisotropy seems to be unavoidable when DLA algorithms are applied on a grid, so resulting patterns range from weakly directional (for a classic DLA by Witten and Sander [3–6]) to strongly anisotropic (for a multiple-hit averaging DLA by Tang [7–12]). While the lattice issue would be considered physical for modelling nonequilibrium growth in solids (e.g., snowflake-type dendritic crystallization [13–16]), it raises a fundamental problem when one has to simulate properties of natural systems which behave as isotropic liquids or quasi-liquids—this is especially important for modelling such phenomena as dielectric 'breakdown' [17], formation of bacteria colonies [18] and viscous 'fingering' in Hele–Shaw cells [19] and in porous media [20].

The simplest solution avoiding lattice anisotropy for DLA clusters is to proceed from on- to off-lattice growth algorithms [21] which are intrinsically isotropic [22, 23]. The related substitution, however, is fraught with serious drawbacks: (i) first, off-lattice DLA simulations imply a substantial increase of computational time, which limits both their efficiency and their applicability; (ii) second, the off-lattice approach considerably hampers a multiple-hit (ensemble) averaging procedure [24], being essential for the reduction of stochastic

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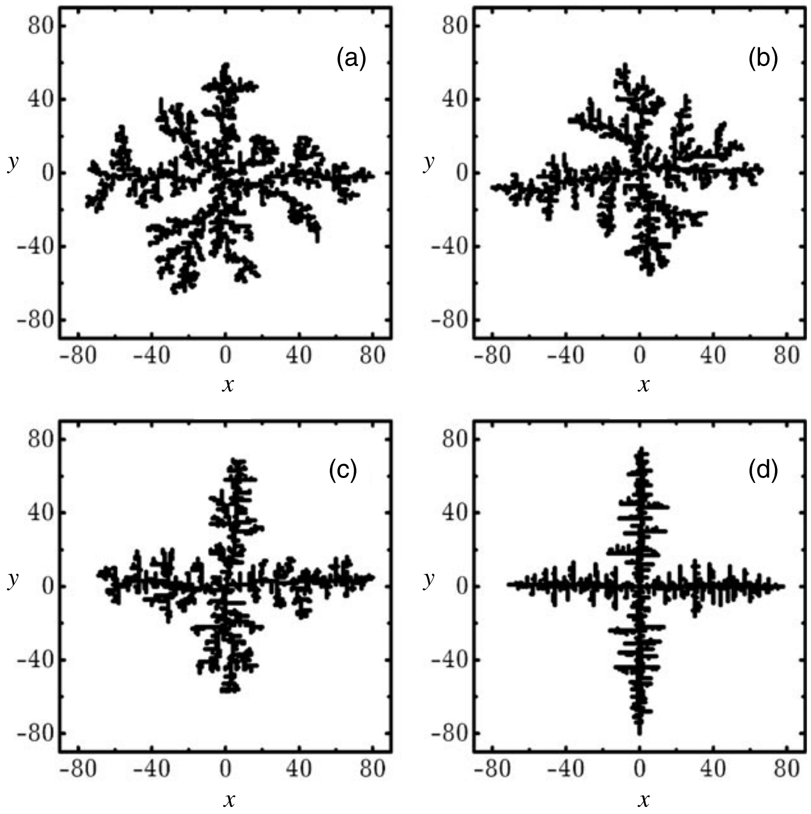

Figure 1. Typical DLA clusters grown on a square grid (x, y) of spacing $a = 1$ up to gyration radii $r_g = 80a$ (number of particles attached N varies from 1000 to 2000); aggregation probabilities $\{P_i\}$ for lattice sites with different numbers $i = 1, \ldots, 3$ of nearest occupied neighbours are given by the regular set, $P_1 = P_2 = P_3 = 1$. We show results for the classic Witten–Sander algorithm in plot (a) and for the Tang multiple-hit averaging with parameter $M = 2^1$, 2^2 and 2^4 in plots (b), (c) and (d), respectively.

noise [7–12]; (iii) finally, and most crucially, there is no opportunity to vary a characteristic length scale for off-lattice patterns, in contrast to on-lattice ones, for which a variable capillary length can be successfully introduced [13–16]. So all the above forces us to seek to elaborate a method for growing isotropic DLA clusters still in lattice terms—our goal for the present work.

For that purpose, we are going to use a mean-field generalization of the original DLA model recently introduced and explored [25]. This generalization advances a discrete theory of DLA by a quasicontinuum framework; as a remarkable outcome, resulting on-lattice patterns are demonstrated to be fully independent of the underlying grid, i.e. isotropic for any lattice. Thus to derive an isotropic version of the discrete DLA, we just have to transform relevant growth rules and conditions accordingly.

A quasicontinuum lattice-independent extension of the DLA model is governed by the following principal rule: 'the probability of a walker aggregation P is directly proportional to the squared mean cluster density (being a continuous function) in a lattice neighbourhood of that walker' [25]. For the discrete DLA, i.e. for a stairlike spatial distribution of a cluster density

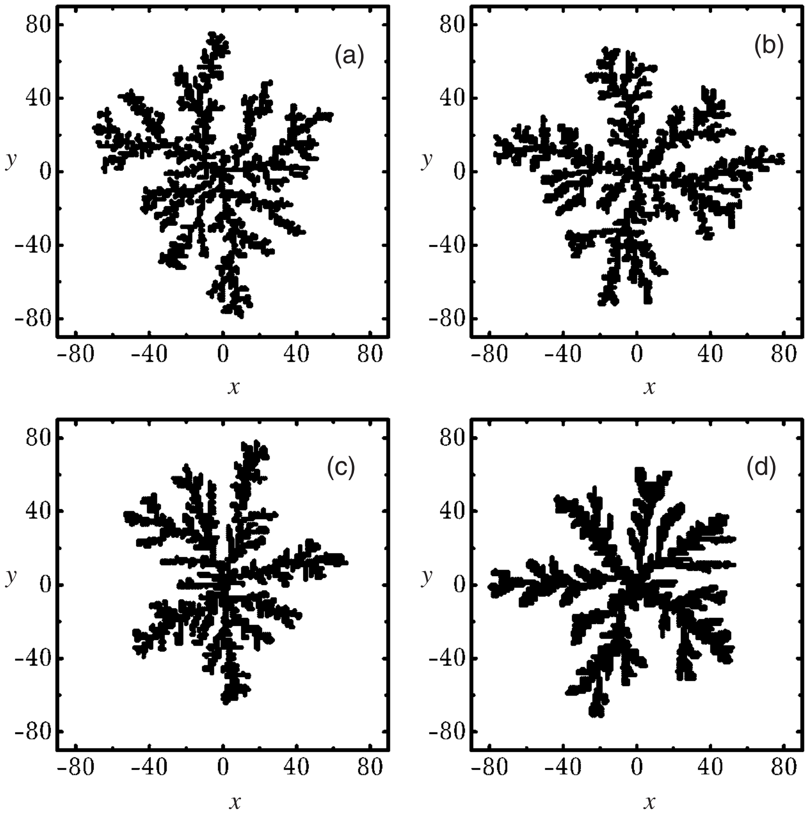

Figure 2. Typical DLA clusters grown on a square grid (x, y) of spacing $a = 1$ up to gyration radii $r_g = 80a$ (number of particles attached N varies from 2000 to 3000); aggregation probabilities $\{P_i\}$ for lattice sites with different numbers $i = 1, \ldots, 3$ of nearest occupied neighbours obey the *isotropic quadratic ratio* requirement of equation (1): $P_1{:}P_2{:}P_3 = 1{:}4{:}9$. We show results for the classic DLA algorithm (plot (*a*)) and for the Tang multiple-hit averaging: parameter $M = 2^1$, 2^2 and 2^4 for plots (*b*), (*c*) and (*d*), respectively.

field (either 1 or 0 at occupied or unoccupied lattice sites), this rule is therefore transformed to the next one: 'the aggregation probability P is directly proportional to the squared number of occupied sites neighbouring that walker'; in other words, the set of aggregation probabilities $\{P_i\}$ for lattice sites (e.g., of having one occupied neighbour, P_1, two occupied neighbours, P_2, three occupied neighbours, P_3, etc) should obey the relation

$$P_1{:}P_2{:}P_3{:}\cdots{:}P_i = 1^2{:}2^2{:}3^2{:}\cdots \qquad i^2 = 1{:}4{:}9{:}\cdots, \tag{1}$$

to provide isotropic growth of on-lattice DLA clusters.

To demonstrate the validity of the relation derived, let us consider the DLA taking place on a square grid (x, y) and assume there only nearest-neighbourhood interactions (i.e. each lattice site has four equivalent neighbours) [1]; corresponding patterns are presented in figures 1 and 2. DLA clusters simulated with a regular set of aggregation probabilities, $P_1 = P_2 = P_3 = 1$, are shown in figure 1—we plot typical patterns grown by the classic Witten–Sander algorithm (figure 1(*a*)) and according to the multiple-hit averaging of Tang (figures 1(*b*)–(*d*)); all the patterns obtained are characterized by an anisotropic behaviour which increases monotonically with the parameter $M = 2^1, \ldots, 2^4$, a counter of the multiple-hit averaging [7]. One can resolve

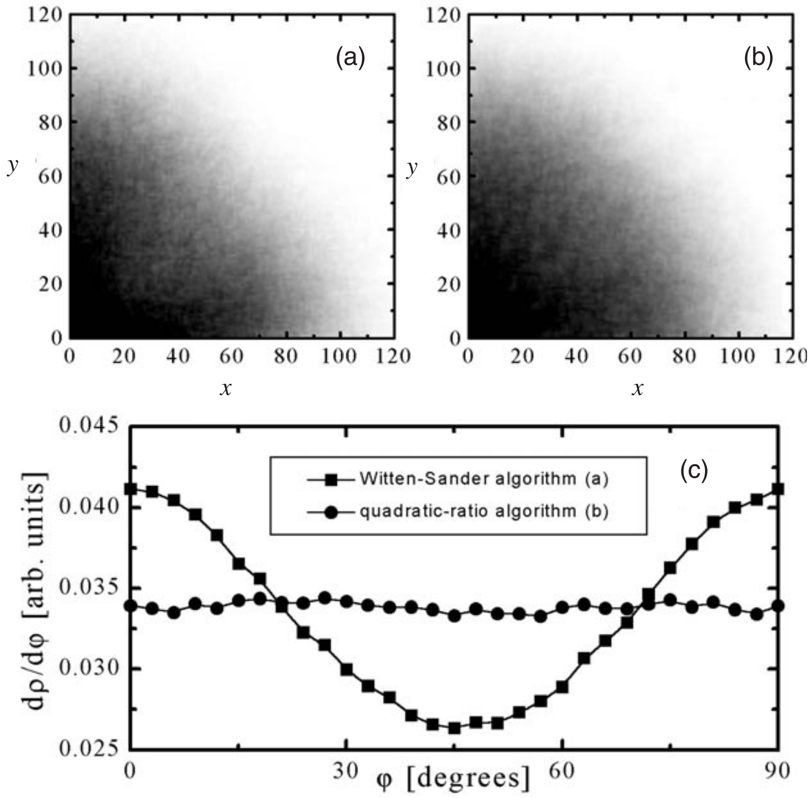

Figure 3. Statistical analysis of DLA clusters grown on a square grid (x, y) of spacing $a = 1$ up to gyration radii $r_g = 120a$ (number of particles attached N varies from 4000 to 5000). (a), (b) Spatial distribution of an average cluster density $\rho(x, y)$ over an ensemble of 1000 similar clusters, shown for the first quadrant of the square grid, $x > 0$ and $y > 0$ (the density increases with palette darkness); aggregation probabilities $\{P_i\}$ obey either the regular Witten–Sander law, $P_1 = P_2 = P_3 = 1$ (plot (a)), or exhibit the *isotropic quadratic ratio* given by equation (1), $P_1{:}P_2{:}P_3 = 1{:}4{:}9$ (plot (b)). (c) Angular distribution of the average cluster density, $d\rho/d\varphi$, computed for clusters grown according to the regular Witten–Sander algorithm (see plot (a)) and the quadratic ratio one (see plot (b)).

a preferred growth in the main lattice directions, $\langle 10\rangle$, $\langle 01\rangle$, $\langle \bar{1}0\rangle$ and $\langle 0\bar{1}\rangle$, i.e. regular DLA algorithms with noise reduction simulate anisotropic (dendritic) patterns [8–12]. In contrast, DLA clusters in figure 2 simulated with the set of aggregation probabilities $\{P_i\}$ according to equation (1), $P_1{:}P_2{:}P_3 = 1{:}4{:}9$, are reported to be isotropic in case of the multiple-hit averaging (figures 2(b)–(d)) as well as in case of the classic DLA (figure 2(a)); only the capillary length of these patterns is varied, increasing with M, whereas no preferred growth directions are observed.

In order to give a quantitative proof for our *isotropic quadratic ratio* given by equation (1), let us focus on an ensemble statistics of DLA clusters; corresponding results are summarized in figure 3. As seen, the ensemble-averaged cluster density $\rho(x, y)$ for regular Witten–Sander patterns demonstrates preferred growth along the x- and y-axes (figures 3(a) and (c))—angular distribution of the cluster density $d\rho/d\varphi$ is maximal in the main lattice directions ($\varphi = 0^\circ$ and 90°) and is at its minimum along the $x = y$ diagonals ($\varphi = 45^\circ$) [6]. In contrast, for quadratic ratio DLA patterns, one can observe purely isotropic spatial behaviour (figures 3(b) and (c))—

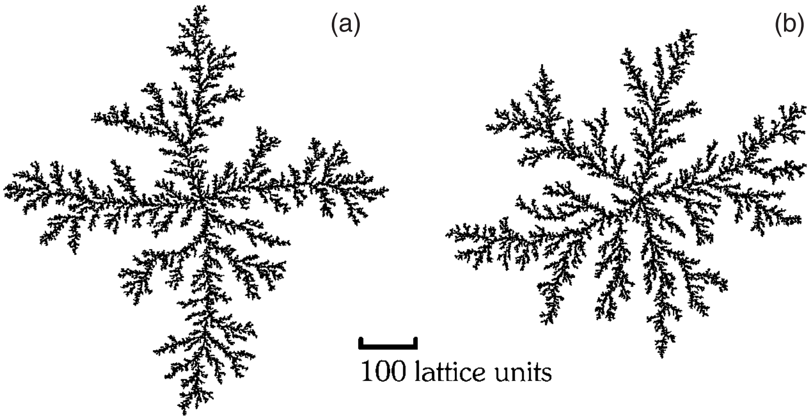

Figure 4. Typical large-scale DLA clusters containing $N = 100\,000$ particles grown on a square grid (x, y) of spacing $a = 1$ (gyration radii $r_g \approx 1000a$); aggregation probabilities $\{P_i\}$ obey either the regular Witten–Sander law, $P_1 = P_2 = P_3 = 1$ (plot (*a*)), or exhibit the *isotropic quadratic ratio* given by equation (1), $P_1{:}P_2{:}P_3 = 1{:}4{:}9$ (plot (*b*)).

the angular density distribution $\mathrm{d}\rho/\mathrm{d}\varphi$ behaves as an approximately constant function slightly perturbed by stochastic noise.

As an additional confirmation of the conclusions derived above from the analysis of medium-scale DLA clusters presented in figures 1–3 (gyration radii $r_g \approx 100$ lattice units), we have also extended our simulations to large-scale DLA clusters ($r_g \approx 1000$ lattice units) containing up to $N = 100\,000$ particles; corresponding patterns are shown in figure 4. On such length scales, one can clearly resolve for a regular Witten–Sander cluster (figure 4(*a*)) preferred growth along the main lattice directions, $\langle 10\rangle$, $\langle 01\rangle$, $\langle \bar{1}0\rangle$ and $\langle 0\bar{1}\rangle$, which is always reported for the square grid [3–6]. In contrast, for a quadratic-ratio DLA cluster (figure 4(*b*)) there is absolutely no anisotropy and the pattern obtained looks very similar to the off-lattice ones [21] (it is possible even to resolve a kind of fivefold symmetry known for off-lattice DLA clusters in two dimensions [26, 27]).

Thus we conclude that the *isotropic quadratic ratio* derived for the DLA model (equation (1)) is satisfactorily verified by three independent techniques: (i) multiple-hit averaging by Tang's algorithm; (ii) statistical analysis of a cluster ensemble; and (iii) large-scale simulations. We believe that the application of our on-lattice isotropic scheme will be extremely useful for modelling very large DLA fractals [28].

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