Bias-free simulation of diffusion-limited aggregation on a square lattice

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We identify sources of systematic error in traditional simulations of the Witten-Sander model of diffusion-limited aggregation (DLA) on a square lattice. We present an algorithm that reduces these biases to below $10^{-12}$. We grow clusters of 10$^8$ particles on 65536 × 65536 lattices. We verify that lattice DLA clusters inevitably grow into anisotropic shapes, dictated by the anisotropy of the aggregation process. We verify that the fractal dimension evolves from the continuum DLA value, $D = 1.71$, for small disk-shaped clusters, towards Kesten's bound of $D = 3/2$ for highly anisotropic clusters with long protruding arms.

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Diffusion-limited aggregation (DLA) is one of the most important models in nonequilibrium statistical physics, exhibiting self-organized criticality and complex pattern formation. In the DLA process, one begins with a cluster (“seed crystal”) immersed in a very dilute solution of particles (“molecules”). Each particle wanders around according to Brownian motion until it encounters the cluster, at which point it “freezes” and becomes part of the cluster. It is more likely that a diffusing particle will stick to a protrusion on the cluster than to a depression. Thus DLA has a natural instability resulting in pattern formation; protrusions grow quickly and spawn other protrusions, forming a treelike pattern somewhat like frost on a window pane. DLA and its variants have been used to model a whole host of nonequilibrium phenomena, including viscous fingering (pattern formation when one fluid is injected into a viscous fluid), electrodeposition, dielectric breakdown, and surface poisoning in ion-beam microscopy.

During the course of a DLA simulation, the radius of gyration of the cluster, $R$, and the cluster mass, $M$, are usually recorded. These data can usually be fit to a power law $R \sim M^\beta$, where $\beta$ is known as the radius-of-gyration exponent. Then one has $M \sim R^D$ where $D = 1/\beta$ is the fractal dimension of the DLA cluster $D$ (insofar as the fractal dimension can be defined for an inhomogeneous finite object). In two dimensions (2D), $\beta \leq 2/3$; this is one of the few rigorous results on DLA. Other results have been obtained using mean-field theories and iterated conformal maps, but these are uncontrolled approximations without small parameters.

The bulk of the literature involves numerical simulations. Early papers reported similar values ($\beta \approx 0.585$) for 2D continuum, square lattice, and triangular lattice DLA clusters. Later papers claimed that square lattice DLA clusters evolve from a roughly circular shape for small clusters towards diamond and cross shapes for larger clusters, and that $\beta$ approaches $2/3$ for very large clusters. Some numerical data suggested that DLA exhibits multiscaling, but later work suggested that multiscaling is a finite-size effect that is not intrinsic to DLA.

In Monte Carlo simulations of equilibrium systems, such as Ising models, it is essential to construct a Markov chain with the correct invariant distribution (e.g., by ensuring detailed balance). Any bias in the simulation in sampling the wrong probability distribution, giving wrong answers for thermodynamic quantities and critical exponents. Non-equilibrium situations such as DLA deserve the same amount of care. However, DLA studies to date have used approximations with errors potentially as large as 1%. The results were justified by noting that varying the severity of the approximation did not noticeably affect the results; nevertheless one may still be concerned that the approximations led to subtle effects that went unnoticed.

In this paper we present an algorithm for square lattice DLA where probability distributions are sampled with accuracies better than $10^{-12}$. We verify that DLA on a lattice produces anisotropic clusters, and that the anisotropy originates from the aggregation process rather than the diffusion process. We confirm that small circular clusters have a radius-of-gyration exponent $\beta = 0.585 = 1/1.71$, but as they mature into anisotropic shapes with arms extending outwards, the exponent tends towards $\beta = 0.667 = 2/3$.

I. BIASES IN TRADITIONAL DLA

The standard algorithm for square lattice DLA is as follows:

1. Let the initial cluster consist of a single seed particle at the origin of the lattice.

2. Launch a new particle on a launching circle of radius $R_L$ that contains the current cluster. In other words, generate an angle $\phi$ from the uniform distribution on $[0, 2\pi]$, and set $x = \text{round}(R_L \cos \phi)$ and $y = \text{round}(R_L \sin \phi)$.

3. Move the particle east, west, north, or south with equal probability.

4. If the particle is adjacent to the cluster, add it to the cluster, and go back to step 2.
5. If the particle has diffused outside the killing circle of radius $R_K$, discard it, and go back to step 2.

6. Go back to step 3.

The launching radius is typically taken to be $R_L = R_B + 5$ where $R_B$ is the radius of the bounding circle circumscribing the cluster. The killing radius may be as small as $R_K = 2R_B$ or as large as $R_K = 100R_B$.

Obviously, DLA is a stochastic process involving random numbers. Measurements of observables (such as $D$) are subject to random error, which cannot be eliminated, but can be reduced by averaging over many simulations, or by self-averaging as part of going to larger system sizes. However, one should be wary of systematic errors. These cannot be removed by any amount of statistical averaging. Moreover, emergent phenomena such as the self-organized critical behavior of DLA may be strongly affected by any bias inadvertently introduced by the algorithm. The original algorithm suffers from two potential sources of systematic error:

1. The launching circle only passes through a few lattice points. When launching a new particle, we must snap its coordinates to the grid, introducing roundoff error. For a particle accreting onto a cluster of linear size $10^2$ one may worry that the errors may be as large as $10^{-2}$.

2. For a 2D random walk, even if a particle has wandered outside the killing circle, there is a 100% probability that it will eventually re-enter the launching circle. The particle is more likely to enter at the near side of the circle than at the far side. By removing the particle from the killing circle and re-launching it from a uniform distribution on the launching circle, the algorithm introduces a bias that may affect results such as $D$. Even if the killing radius is $10^2$ times the cluster radius, the errors in the return probabilities may still be as large as $10^{-2}$.

II. ELIMINATING LAUNCHING BIAS

Snap-to-grid error due to launching circle: Let us first address the first source of systematic error. Suppose we launch a particle on a launching circle of radius $R_L$, and snap its coordinates to the grid as described earlier. The probability distribution of the point $(x, y)$ is

$$P_{x,y|0} = \int_{x_0 - \frac{1}{2}}^{x_0 + \frac{1}{2}} dx \int_{y_0 - \frac{1}{2}}^{y_0 + \frac{1}{2}} dy \delta(\sqrt{x^2 + y^2} - R_L).$$

(1)

Suppose we generate many particles from this distribution and let them diffuse via Brownian random walks. What is the steady-state concentration of particles within the launching circle? How far does it deviate from a uniform distribution?

This Brownian problem maps to an electrostatics problem. The source distribution maps to a charge distribution $Q_{x,y|0} = P_{x,y|0}$, and the steady-state distribution of particles maps to the electric potential

$$V_{xy} = \sum_{x',y'} G_{x-x',y-y'} Q_{x',y'}$$

(2)

where $G_{xy}$ is the Green function of the square lattice Poisson equation such that

$$4G_{xy} - G_{x+1,y} - G_{x-1,y} - G_{x,y+1} - G_{x,y-1} = \delta_x \delta_y.$$ 

(3)

Because of the long-range logarithmic divergence in 2D, $G_{xy}$ contains an infinite additive constant. Thus we define the regularized Green function $F_{xy} = G_{xy} - G_{xy}$.

The quantities $F_{xy}$ are related to the resistances between two points on a square lattice of resistors and as described in Appendix A it can be calculated to machine precision for any $x$ and $y$. Compare the potential with that at a reference point $(x', y')$, which might as well be the origin $(0, 0)$:

$$V_{xy} - V_{x',y'} = -\sum_{x',y'} (F_{x-x',y-y'} - F_{x''-x',y''-y'}) Q_{x',y'}.$$ 

(4)

We calculate the charges $Q_{x,y|0}$ numerically according to Eq. (1), and we perform a fast 2D convolution with $F_{xy}$ to obtain $V_{xy}$. Figures 1(a), 1(b), and 1(c) show the charges and potentials for a launching circle of radius 20. The ring of charge is distorted by snapping to the grid, leading to potential fluctuations on the scale of $10^{-4}$.

Eliminating bias using a fuzzy launching annulus: It is useful to take some insights from computer graphics. Early raster displays rendered oblique lines and circles with jagged edges. Modern displays eliminate this problem using antialiasing. In the context of DLA, one might hope that launching bias might be reduced by “antialiasing” the launching circle. The launching bias comes from the high-order Fourier components in $P(x, y) = \delta(\sqrt{x^2 + y^2} - R_L)$ that cannot be represented on the grid. Perhaps if we thicken the launching circle into an annulus and smear out its inner and outer boundaries, the resulting probability distribution will be smoother, and quantization error will be reduced. We will show that this is indeed true.

Suppose we pick a radius from the probability distribution

$$P_{rad}(r) = \frac{2}{R_{l2} - R_{l1}} P_{Kaiser}\left(\frac{2r - R_{l1} - R_{l2}}{R_{l2} - R_{l1}}\right)$$

(5)

where

$$P_{Kaiser}(x) = \frac{\Theta(1 - x^2)}{\int_{-1}^{1} \Theta(\beta \sqrt{1 - y^2}) dy} I_0(\beta \sqrt{1 - x^2})$$

(6)
where $J_0$ is the Bessel $I$ function. This distribution corresponds to to a normalized Kaiser-Bessel window function \cite{baker1996} on the interval $[R_{L1}, R_{L2}]$. We choose the Kaiser-Bessel window because it has very small spectral leakage beyond the central lobe, and because the distribution is easy to evaluate and sample compared to the optimal Dolph-Chebyshev window \cite{baker1996}. We also pick an angle $\phi$ from the uniform distribution on $[0, 2\pi]$, and set $x = \text{round}(R_L \cos \phi)$ and $y = \text{round}(R_L \sin \phi)$. The probability distribution of the point $(x, y)$ is then

$$P_{x_0y_0} = \int_{x_0-\frac{1}{2}}^{x_0+\frac{1}{2}} dx \int_{y_0-\frac{1}{2}}^{y_0+\frac{1}{2}} dy \frac{P_{\text{rad}}(\sqrt{x^2 + y^2})}{\sqrt{x^2 + y^2}}.$$  

(7)

We calculate $Q$ and $V$ as before. Figures 1(d), 1(e), and 1(f) show the charges and potentials for a launching annulus with blurred edges ($R_{L1} = 16, R_{L2} = 24, \beta = 15$). We see that the potential in the interior of the annulus ($r < R_{L1}$) is uniform to within $10^{-10}$. By increasing the inner radius and the thickness of the annulus, and by adjusting the parameter $\beta$, the potential can be made even more uniform. For an annulus with $R_{L1} = 40, R_{L2} = 80$, and $\beta = 24$, we find that $|V_{xy}| < 10^{-14}$ for all $r < R_{L1}$.

For practical purposes this means that the launching bias has been eliminated.

In our DLA simulations we use a launching annulus with $R_{L1} = 2R_B, R_{L2} = 4R_B$, and $\beta = 24$, where $R_B$ is the bounding radius of the cluster. Since the cluster is well within the interior of the annulus, launching bias is negligible.

We sample $x$ from $P_{Kaiser}(x)$ using rejection sampling \cite{baker1996} with a Gaussian envelope function. (In rejection sampling one must keep retrying until a move is accepted, unlike in the Metropolis algorithm. A better term would be “retrial sampling”.)

### III. ELIMINATING KILLING BIAS

The second source of systematic error is the killing-and-relaunching. We will eliminate this error by using an enormous killing circle of radius $R_K = 10^{14}$. 

![Diagram](image-url)
IV. ACCELERATING DIFFUSION OUTSIDE THE CLUSTER USING THE WALK-TO-LINE ALGORITHM

What is the catch in using large launching and killing circles? Recall that a particle executing Brownian motion has a r.m.s. displacement that grows very slowly with time, \( r_{\text{rms}} \propto \sqrt{t} \). If a particle is launched \( 10^9 \) sites away from the cluster, it will take at least \( 10^{18} \) timesteps before the particle has an appreciable probability of encountering the cluster! Thus, in order to make a DLA simulation feasible, we must find a way to accelerate the diffusion process – that is, we must “fast forward” through the random walk. We do this using “first passage theory.”

Electrostatic analogue of the first-passage problem: Suppose a particle starts at \((x_0, y_0)\) and executes a random walk until it encounters a “marked” site \((x_n, y_n)\) where \(n = 1, 2, 3, \ldots, N\). We wish to find the probability distribution \(p_{x_n,y_n}\) of the final position of the particle. This is known as the first-passage position, that is, the position at which an infinite random walk first passes through a marked site.

This Brownian problem maps to the following electrostatics problem. Suppose a charge is placed at \((x_0, y_0)\) and executes a random walk on a square lattice, and that the sites \((x_n, y_n)\) for \(n = 1, 2, 3, \ldots, N\) are held at zero potential. Solve the discrete Poisson equation:

\[
\begin{align*}
4V_{xy} - V_{x+1,y} - V_{x-1,y} - V_{x,y+1} - V_{x,y-1} &= Q_{xy}, \\
V_{x_n,y_n} &= 0, \quad n = 1, \ldots, N \\
Q_{x_0,y_0} &= 1, \\
Q_{x_n,y_n} &= Q_n \quad \text{(to be determined)}, \\
Q_{xy} &= 0 \quad \text{on all other sites}.
\end{align*}
\]

The charges \(Q_{x_n,y_n}\) give the desired first-passage probabilities. In other words, we are to find the charge distribution induced on a grounded conducting object by an external point charge. Rather than solving the discrete differential equation for the potential \(V_{xy}\) in all space, it is better to solve the discrete integral equation for the charges \(Q_j\) on the surface of the conductor. This takes the form of \(N\) simultaneous equations in \(N\) variables. Formally, we have

\[
V_i = \sum_j G_{x_i,x_j} - \delta_{x_i,y_j} Q_j + G_{x_i,x_j} - \delta_{x_i,y_j} - y_0
\]

where \(i, j = 1, 2, \ldots, N\) and \(G_{xy}\) is the Green function of the square lattice Poisson equation such that

\[
4G_{xy} - G_{x+1,y} - G_{x-1,y} - G_{x,y+1} - G_{x,y-1} = \delta_x \delta_y.
\]

The long-range logarithmic divergence in 2D poses two additional complications. First, \(G_{xy}\) contains an infinite constant. We regularize this by defining the resistance Green function \(F_{xy} = G_{00} - G_{xy}\). As described in Appendix A, \(F_{xy}\) can be calculated to machine precision for any \(x\) and \(y\). Take Eq. \(9\) and subtract the potential at a reference point \((x'', y'')\), which might as well be \((x_1, y_1)\). This gives

\[
V_i - V_{x''y''} = \sum_j (F_{x_i,x_j}, y_j - F_{x'', x_j}, y'', y_j) Q_j + F_{x_i,x_0}, y_0 - F_{x'', x_0}, y'', y_0.
\]

Second, in order for the potential to be well defined, the total charge in the entire system must be zero:

\[
\left( \sum_j Q_j \right) + 1 = 0.
\]

Although Eq. \(11\) and \(12\) contain \(N + 1\) equations, they form a linear system of rank \(N\), and so there is a unique solution for the \(N\) charges, \(Q_j\).

Walk-to-line algorithm: We now apply this formalism to the situation shown in Fig. 2(a). We will call this the walk-to-line (WtL) problem on a square lattice. It is analogous to the walk-to-plane algorithm \(39,40\) for 3D continuum Brownian diffusion \(39\).

Suppose a charge is located at \((0, h)\) and every site on the \(x\)-axis \((x, 0)\) is a conducting site held at zero potential. The potential everywhere in the upper half-plane is given by the method of images as \(V_{xy} = F_{x,y+h} - F_{x,y-h}\). The electric field along the bond \((x, 1) - (x, 0)\) is \(E_{x_1,x_0} = V_{x_1} - V_{x_0} = F_{x,h+1} - F_{x,h-1}\). Mapping this back to the Brownian problem, we see that if a particle is launched at \((0, h)\), the probability distribution of first passage to the \(x\)-axis is

\[
p_x = F_{x,h+1} - F_{x,h-1}.
\]

There are an infinite number of probabilities corresponding to all integer \(x\). We sample this distribution using rejection \(39,40\), sampling \(25\). In order to use rejection sampling,
we need an envelope function that resembles the target distribution (the probability distribution that we wish to sample from). To obtain a suitable envelope function, consider the continuum version of the walk-to-line algorithm. Suppose a particle starts at \((0, h)\) and executes continuum Brownian motion until it encounters the line \(y = 0\). The electrostatic analog is a unit charge at \((0, h)\) and a grounded conducting plane at \(y = 0\). Solve Poisson’s equation with Dirichlet boundary conditions using the method of images. The potential is

\[
V(x, y) = \frac{1}{2\pi} \ln \sqrt{x^2 + (y + h)^2} - \frac{1}{2\pi} \ln \sqrt{x^2 + (y - h)^2},
\]

and so the charge density on the line is \(\sigma(x) = -\frac{h}{\pi(x^2 + h^2)}\). Thus the first-passage probability distribution is \(P(x) = \frac{h}{\pi(x^2 + h^2)}\). The cumulative distribution function (CDF) is \(C(x) = \int_{-\infty}^{x} dx' P(x') = \frac{1}{2} \arctan \frac{x}{h} + \frac{1}{2}\). Therefore, we can generate a sample from \(P(x)\) using the inverse CDF method as \(x = h \tan \pi(u - \frac{1}{2})\), where \(u\) is a random number from the uniform distribution on \((0, 1)\). Now, since the target distribution is discrete, consider generating a sample using

\[
x = \text{round}(h \tan \pi(u - \frac{1}{2})).
\]  

This corresponds to the discrete envelope distribution

\[
q_x = \int_{x - \frac{1}{2}}^{x + \frac{1}{2}} dx' \frac{h}{\pi(x'^2 + h^2)} = \frac{1}{\pi} \left( \arctan \frac{x + \frac{1}{2}}{h} - \arctan \frac{x - \frac{1}{2}}{h} \right).
\]  

The rejection sampling algorithm is as follows:

1. Find a number \(c\) such that \(cp_x \leq q_x\) for all \(x\). For our purposes we can choose \(c = q_0/p_0\).

2. Draw a random integer \(x\) from the envelope distribution \(q_x\) (gray symbols in Fig. 3(a)).

3. Generate a uniform random number \(v \in [0, 1)\).

4. If \(v < cp_x/q_x\), return \(x\). Otherwise, go back to step 2.

The returned value of \(x\) is a sample from the target distribution \(p_x\).

**Application to square lattice DLA:** Suppose the diffusing particle is just outside the bounding rectangle of the cluster (see Fig. 2(b)). Apply the walk-to-line algorithm to return the particle to an infinite horizontal or vertical line parallel to the bounding rectangle. After a few iterations of this procedure usually suffice to return the particle to the bounding rectangle.

Now suppose the particle is a large distance \(r\) away from the cluster. Then, Eq. (14) implies that the walk-to-line algorithm is roughly equivalent to multiplying \(r\) by a random number \(\alpha\) drawn from a Lorentzian distribution:

\[
r_{\text{new}} = r \tan \pi(u - \frac{1}{2}) = r\alpha, \quad P_{\text{Lor}}(\alpha) = \frac{1}{\pi(1 + \alpha^2)}.
\]

Thus, the logarithm of the radius is incremented by a random number \(\gamma = \ln \alpha\) drawn from a sech distribution:

\[
\ln |r_{\text{new}}| = \ln |r| + \gamma, \quad P_{\text{sech}}(\gamma) = \frac{\text{sech} \gamma}{\pi}.
\]

The variance of the sech distribution is

\[
\int_{-\infty}^{\infty} d\gamma \gamma^2 \text{sech} \gamma = \frac{\pi^2}{4}.
\]

Therefore, \(\ln |r|\) executes a random walk with a step variance of \(\pi^2/4\). After \(M = 54\) iterations of the walk-to-line algorithm, the accumulated variance is \(M\pi^2/4\), and one might expect \(r\) to have increased or decreased by \(\exp(\sqrt{M\pi/2}) \approx 10^5\). If a walker somehow finds itself at a distance \(10^9\) from a cluster of linear size \(10^4\), after 54 iterations of walk-to-line, there is an appreciable probability that it will either have returned to the cluster (of radius \(10^4\)) or that it will have drifted outside the killing circle (of radius \(10^{14}\)).

In summary, if an errant particle finds itself a distance \(10^9\) away from the cluster, the original Witten-Sander algorithm would take about \(10^{18}\) steps to return it to the cluster, whereas the walk-to-line algorithm would take about 50 iterations. Although this is not perfect, it is certainly a great improvement.

**V. ACCELERATING DIFFUSION NEAR THE CLUSTER USING THE WALK-TO-SQUARE ALGORITHM**

Now let us consider another Brownian motion problem. Suppose a random walker begins at point \((x_0, y_0)\) within a square with corners \((0, 0)\) and \((l, l)\), as in Fig. 4. What is the probability that the walker makes first passage through the square at position \((x, y)\)?
The corresponding electrostatic situation is a point charge at the center of a grounded conducting square. We wish to solve the discrete Poisson equation with Dirichlet boundary conditions on a square:

\[ 4V_{xy} - V_{x+1,y} - V_{x-1,y} - V_{x,y+1} - V_{x,y-1} = Q_{xy}, \]
\[ V_{xy} = 0 \quad x_0 \in \{0, l\} \text{ or } y_0 \in \{0, l\}, \]
\[ Q_{xy} = \delta_{x-x_0}\delta_{y-y_0} \quad \{x, y\} \subseteq \{1, 2, \ldots, l - 1\}. \]  

This is a linear system involving a \((l-1)^2 \times (l-1)^2\) sparse matrix with integer coefficients. Brute force matrix algebra gives the solutions \(V_{xy}\) as rational numbers. For example, for \(l = 8\) the solutions are

\[
\{V_{xy}\} = \frac{1}{544} \begin{pmatrix} 2 \end{pmatrix}.
\]

A better approach is to separate variables in Cartesians and superpose eigenfunctions to obtain the Green function. Expand the charge distribution \(Q_{xy} = \delta_{x-x_0}\delta_{y-y_0}\) and the potential \(V_{xy}\) in Fourier sine series, and connect them via the discrete Poisson equation:

\[
\tilde{Q}_{pq} = 2 \sum_{x=1}^{l} \sum_{y=1}^{l-1} \frac{\sin \frac{\pi px}{l} \sin \frac{\pi qy}{l}}{l} Q_{xy} = 2 \sum_{x=1}^{l} \sum_{y=1}^{l-1} \frac{\sin \frac{\pi px}{l} \sin \frac{\pi qy}{l}}{l},
\]

\[
\tilde{V}_{pq} = \left(4 - 2 \cos \frac{\pi p}{l} - 2 \cos \frac{\pi q}{l}\right) \tilde{Q}_{pq},
\]

\[
V_{xy} = 2 \sum_{p=1}^{l-1} \sum_{q=1}^{l-1} \tilde{V}_{pq} \sin \frac{\pi px}{l} \sin \frac{\pi qy}{l}.
\]

We implement Eq. (23) using the fast 2D discrete sine transform (DST). This allows us to compute \(V_{xy}\) for all \(x\) and \(y\) in \(O(l^2 \ln l)\) time. This is faster than evaluating the double sums

\[
V_{xy} = \frac{4}{l^2} \sum_{p=1}^{l-1} \sum_{q=1}^{l-1} \frac{\sin \frac{\pi px}{l} \sin \frac{\pi qy}{l} \sin \frac{\pi px}{l} \sin \frac{\pi qy}{l}}{4 - 2 \cos \frac{\pi p}{l} - 2 \cos \frac{\pi q}{l}},
\]

which takes \(O(l^4)\) time. For \(l > 512\) the DST method takes a long time and accumulates roundoff errors of the order of \(10^{-12}\). Then it becomes preferable to calculate \(V_{xy}\) as a Madelung sum involving an infinite series of positive and negative image charges,

\[
V_{xy} = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} (-1)^{m+n} F_{x-(m+1)l, y-(n+1)l} t.
\]

For speed and accuracy, split \(F_{xy}\) into a \(\ln r\) part plus a correction due lattice anisotropy (Eq. (A12)). This gives \(V_{xy}\) as the solution to the continuum problem (in terms of the Jacobi \(cn\) function) plus a lattice correction, which is best evaluated by grouping the charges into quadrupoles and truncating the sum appropriately.

Having found \(V_{xy}\), we can find the electric field and hence the charge distribution on the boundary, \(Q_{x0} = E_{x1,x0} = V_{x1} - V_{x0}\). Thus the first-passage probabilities \(p_{xy}\) are given simply by the first row of the \(V_{xy}\) matrix, such as that in Eq. (20).

![Diagram](image_url)

**FIG. 4**: Geometry for walk-out-to-square algorithm. A particle starts at \((x_0, y_0)\) (black disk) and executes a random walk on the square lattice. We wish to find the probability distribution of the first intersection of this walk with a surrounding square of side \(l\) (gray disks).

We have tabulated the first-passage probabilities \(P_{l,x}^{eq} \) from the center of a square of side \(l\) to every point \((x,0)\) on the lower edge, for \(l \in \{2, 4, 8, 16, 32, 64, 128, 256, 512\}\). See Fig. 5. These distributions can easily be sampled using precalculated Walker alias tables.\[33\,34\]

**FIG. 5**: First-passage probabilities \(P_{l,x}^{eq} \) from the center of a square of side \(l\) to every point \((x,0)\) on the lower edge, for \(l = 8, 16, 32, 512\). Horizontal and vertical axes are scaled to show that \(l^2 P_{l,x}^{eq}\) approaches a universal function of \(x/l\) as \(l \to \infty\). The universal function is the charge distribution inside a grounded conducting square induced by a charge at its center.

**Application to square lattice DLA**: We store the
This means that we can move the particle by until we get to a level where all nine blocks are empty.

3. Launch a new walker on a fuzzy annulus of inner radius \( R_{L1} = 2R_B \) and outer radius \( R_{L1} = 4R_B \), where \( R_B \) is the bounding radius of the cluster (see Fig. 1(d)).

4. If the walker is now at a sticky site, freeze it (i.e., add it to the cluster and mark its neighbors as new sticky sites) and go to step 2. Otherwise, go to step 3.

In this algorithm all probability distributions are sampled with errors less than \( 10^{-12} \). Thus systematic error is practically eliminated, leaving statistical error and finite cluster size as the only sources of error.

We have implemented this algorithm in C++ (see Supplementary Material). We use 64-bit floating-point arithmetic, and we represent \((x, y)\) coordinates by 64-bit integers to allow the killing circle radius to be \( R_K = 10^{14} \). We assume nearest-neighbor diffusion, such that the diffusing particle only moves horizontally or vertically (Fig. 6(a)). We try various aggregation rules (Figs. 6(b), 6(c), 6(d), and 6(e)); square lattice DLA studies in the literature typically use the 4-neighbor rule, where sticky sites are horizontally or vertically adjacent to a cluster site. At each level of the hierarchy we store the pattern of frozen/sticky sites using a bit array. For simplicity we do not distinguish frozen sites from sticky sites.

FIG. 6: (a) The diffusing particle moves to one of 4 neighboring sites with equal probability. (b,c,d,e): When the particle freezes at a sticky site (black), 2, 3, 4, or 8 neighboring sites (gray) are marked as sticky sites according to the aggregation rule.

In this work we have used a built-in system random number generator, which is a non-linear additive feedback generator with a period of approximately \( 16(2^{31} - 1) \). We have not tested the effect of different random number generators.

### VII. RESULTS

**Cluster shape:** Figures 7(a), 7(b), 7(c) and 7(d) show square lattice DLA clusters grown using different...
aggregation rules. The 2-neighbor and 3-neighbor aggregation rules clearly manifest themselves by producing L-shaped and T-shaped clusters. The 4-neighbor aggregation rule produces faster growth along horizontal and vertical directions, whereas the 8-neighbor aggregation rule produces faster growth along diagonal directions; both these rules lead to a cos 4\(\phi\) asymmetry in the angular mass distribution.

We have tried starting with seed clusters of various shapes (\(\diamond, +, \times, -, /\)). Regardless of the shape of the seed cluster, the growing cluster evolves toward a shape determined by the aggregation rule. Thus the asymptotic shape of the cluster is governed by the aggregation rule (the way in which particles stick together) and not by the diffusion rule, nor by the seed cluster shape.

Various authors have reported that a “square deposition habit” leads to a+ and cluster shapes, whereas a “diagonal deposition habit” leads to \(\times\) shapes. For off-lattice DLA, it was found that the ratio of the principal radii of gyration tends to unity for large clusters – i.e., if a cluster happens to start off with an elliptical shape, it evolves toward a circular shape. Our results agree with these statements.

**Fractal dimension**: Figure 8(a) shows the radius of gyration \(R\) as a function of the cluster mass \(M\), during the growth of a single cluster, for various aggregation rules. The data are roughly consistent with a power law \(R \propto M^\beta\) somewhere between \(\beta = 0.585 = 1/1.71\), which is the exponent for 2D continuum DLA, and \(\beta = 0.667 = 2/3\), which is Kesten’s upper bound for 2D DLA. Figure 8(b) shows \(\beta(M) = d(\ln R)/d(\ln M)\) estimated from ratios between successive \((R, M)\) data points. For 2- and 3-neighbor aggregation rules, \(\beta(M)\) is close to 2/3 for large \(M\). For 4- and 8-neighbor aggregation rules \(\beta(M)\) appears to be close to 0.585 for moderate \(M\), but for very large \(M\) it appears possible that \(\beta(M)\) is increasing towards 2/3.

Meakin et al. reported that \(\beta\) evolves from 0.585 towards 0.667 = 2/3 during the growth of the cluster for square lattice DLA. Menshutin et al. also reported that \(\beta \to 2/3\) for a variant of DLA in which particles diffuse via continuum 2D Brownian motion but aggregate onto lattice sites using an “antenna” rule. Our results are consistent with these statements.
VIII. CONCLUSIONS

We present an improved algorithm for 2D lattice DLA that reduces systematic errors in probabilistic sampling below \(10^{-12}\). We build clusters of \(10^8\) particles on lattices of size \(65536 \times 65536\). We verify that the anisotropy of the aggregation process leads to anisotropy of the cluster shape, so that the radius-of-gyration exponent evolves from \(\beta = 0.585 = 1/1.71\) towards \(\beta = 0.667 = 2/3\).

Our unbiased DLA algorithm can be generalized to triangular lattices, cubic lattices, and other lattices. There are analytic expressions for triangular lattice Green functions and Green functions on 3D lattices can be calculated numerically.\[22,23\]

We are grateful to William Schwalm for helpful discussions.

Appendix A: Square lattice resistance Green function

In this appendix we consider the Green function

\[
G_{xy} = \int_0^{2\pi} \frac{dp}{2\pi} \int_0^{2\pi} \frac{dq}{2\pi} \frac{e^{ipx+ipy}}{4 - e^{ipx} - e^{ipy} - e^{-ipx} - e^{-ipy}}.
\]

(A1)

and the regularized Green function

\[
F_{xy} = \int_0^{2\pi} \frac{dp}{2\pi} \int_0^{2\pi} \frac{dq}{2\pi} \frac{1 - e^{ipx+ipy}}{4 - e^{ipx} - e^{ipy} - e^{-ipx} - e^{-ipy}}.
\]

(A2)

Recursion relations: By symmetry it can be shown that \(F_{00} = 0\) and \(F_{10} = \frac{1}{4}\). Using complex variable techniques it can be shown that\[22\]

\[
F_{xx} = \frac{1}{\pi} \sum_{n=1}^{x} \frac{1}{2n-1} = \frac{2H_{2n} - H_x}{2\pi}
\]

(A3)

where \(H_x = 1 + \frac{1}{2} + \frac{1}{3} + \ldots + \frac{1}{x}\) are the harmonic numbers. \(F_{xy}\) also satisfies the discrete Poisson equation

\[
4F_{xy} - F_{x+1,y} - F_{x-1,y} - F_{x,y+1} - F_{x,y-1} = -\delta_x\delta_y.
\]

(A4)

In principle, Eqs. (A3) and (A4) allow one to compute \(F_{xy}\) for all \(x\) and \(y\). However, this procedure is unstable to roundoff error if implemented numerically. Thus, we implement the recursion relations using symbolic algebra, and use extra-precision arithmetic to convert the results to floating-point numbers. The first few \(F_{xy}\) are shown in Table \[A2,23\].

Series approximation at large distances: For large values of \(x\) and \(y\), the behavior of Eq. (A1) is dominated by small \(p\) and \(q\). Expand the denominator in powers of \(p\) and \(q\).

\[
G_{xy} = \frac{1}{(2\pi)^2} \int_0^{2\pi} dk \int_0^{2\pi} d\phi e^{ik\cos(\phi-\theta)}
\]

\[
\left[ \frac{1}{k^2} + \left( \frac{1}{16} + \cos^4\phi \right) + \frac{k^2}{4608} \cos 4\phi + \frac{4\cos 8\phi}{4608} \right] + \ldots
\]

(A7)

Take Eq. (A1) and extend the domain of integration to the entire \((p, q)\) plane. Let \(x = r\cos\varphi\) and \(y = r\sin\varphi\). Then

\[
F_{xy} = \frac{1}{(2\pi)^2} \int_0^{2\pi} dk \int_0^{2\pi} d\phi e^{ik\cos(\phi-\theta)} \left[ \frac{1}{k^2} + \left( \frac{1}{16} + \cos^4\phi \right) + \frac{k^2}{4608} \cos 4\phi + \frac{4\cos 8\phi}{4608} \right] + \ldots
\]

(A8)

Now let us derive an identity for the Fourier transform of a 2D power law function,

\[
\frac{1}{(2\pi)^2} \int_0^{2\pi} dk \int_0^{2\pi} d\phi e^{ikr \cos(\phi-\theta)} \left[ \frac{1}{k^2} + \left( \frac{1}{16} + \cos^4\phi \right) + \frac{k^2}{4608} \cos 4\phi + \frac{4\cos 8\phi}{4608} \right] + \ldots
\]

(A9)

This gives

\[
2\pi G_{xy} = c_1 + \ln \frac{1}{r} + \frac{\cos 4\phi}{12r^2} + \frac{3\cos 4\phi}{40r^4} + \frac{5\cos 8\phi}{48r^4} + \ldots
\]

(A10)

The constant \(c_1\) is infinite, but the other terms are finite. Thus the regularized Green function has the form

\[
2\pi F_{xy} = c_2 + \ln r - \frac{\cos 4\phi}{12r^2} - \frac{3\cos 4\phi}{40r^4} - \frac{5\cos 8\phi}{48r^4} - \ldots
\]

(A11)
where $c_2$ is a finite constant. By matching this to the inverse power series for the harmonic numbers, Eq. (A3), it can be shown that

$$2\pi F_{xy} = \gamma + \ln \sqrt{2} + \ln r - \frac{\cos 4\phi}{12r^4} - \frac{1}{r^2} \left( \frac{3\cos 4\phi}{40} + \frac{5\cos 8\phi}{48} \right)$$

$$- \frac{1}{r^4} \left( \frac{51\cos 8\phi}{112} + \frac{35\cos 12\phi}{72} \right)$$

$$- \frac{1}{r^6} \left( \frac{217\cos 8\phi}{520} + \frac{45\cos 12\phi}{8} + \frac{1925\cos 16\phi}{384} \right)$$

$$- \frac{1}{r^8} \left( \frac{38859\cos 12\phi}{1108} + \frac{3795\cos 16\phi}{32} + \frac{350035\cos 20\phi}{384} \right) - \ldots$$

(A12)

where $\gamma \approx 0.577216$ is the Euler-Mascheroni constant.

For $r = 60$, the $1/r^{10}$ terms in Eq. A12 have absolute value smaller than $10^{-16}$. Therefore, truncating the series at the $1/r^8$ term allows us to evaluate $F_{xy}$ to machine precision for all $r > 60$. In our DLA simulations we obtain $F_{xy}$ by table lookup for $x < 60$ and $y < 60$ and using the series otherwise.

**Appendix B: Alternative methods**

In this appendix we discuss other approaches to bias-free lattice DLA, which are less efficient than the algorithm we have presented.

**Solution of Laplace’s equation for an arbitrary cluster:** For a particle launched at infinity, the first-passage probabilities to the sticky sites (sites adjacent to cluster sites) can be computed exactly by solving Laplace’s equation. One can then add a particle at a position picked directly according to these probabilities. However, for a cluster of $N$ sites, solving Laplace’s equation is a dense linear algebra problem taking $O(N^3)$ time. Even if the Sherman-Morrison formula is used to update the inverse matrix incrementally, the problem still takes $O(N^2)$ time for every particle that is added to the cluster. This is prohibitively slow.

**Walk-in-to-circle methods:** For 2D or 3D continuum DLA, it is easy to return a particle to the bounding circle or sphere of the cluster. The electrostatic problem is easily solved by the method of images, and the return probability distribution can be evaluated and sampled analytically. This is exploited in a killing-free algorithm for continuum DLA where particles that escape from the launching circle are immediately returned to the launching circle. For lattice DLA, however, circular or spherical boundaries do not fit naturally on the lattice. Snapping to the grid leads to large errors, as we have shown. It may be possible to reduce these errors by returning the particle to a fuzzy annulus; we have not investigated this completely.

**Walk-in-to-square methods:** What if we wish to return a particle to a bounding rectangle, square, or cube? This requires finding the charge distribution on a conductor induced by an *exterior* point charge. Whereas interior electrostatics problems are amenable to a variety of methods (images, separation of variables, and conformal mapping), exterior electrostatics problems are notoriously difficult even in the continuum. The most accurate results for the capacitance of a cube have been obtained by mapping the electrostatic problem back to a random walk problem and using Monte Carlo techniques. It is probably futile to search for a simple analytic formula for the lattice problem (see Fig. 9).

The walk-in-to-square problem can be solved numerically, but this takes $O(l^3)$ time, where $l$ is the perimeter of the boundary. In comparison, the iterated walk-to-line method may take several hundred iterations to return the walker to the bounding box of the cluster, but this number of iterations is independent of cluster size. Thus we prefer the walk-to-line method.

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