Simulation of diffusion-limited aggregation: effects of launching boundary shape and non-fixed centre

Shyi-Long Lee 1 and Yeung-Long Luo

Institute of Chemistry, Academia Sinica, Taipei, Taiwan 11529, ROC
and Department of Chemistry, National Chung-Cheng University, Min-Hsiung, Chia-Yi, Taiwan 62117, ROC

Received 14 January 1992; in final form 6 May 1992

Simulations of the Witten–Sander model of diffusion-limited aggregation (DLA) were performed using modified versions in which a square launching boundary and a non-fixed centre were adopted. Square launching boundary leads to an isotropic fractal instead of the diamond-shape cluster found in the conventional simulation using circular releasing boundary. The nonfixed centre model displays a similar feature as that found in Levy-flight-trajectory simulations which bridge two limiting aggregation models, i.e., the Eden model and the Witten–Sander model.

1. Introduction

Fractal attributes in the Witten–Sander diffusion-limited aggregate (DLA) have been the focus of researcher's attentions [1–20] since its first appearance in 1981 [21]. During the last decade, factors influencing the DLA processes were studied thoroughly and several variations of the DLA model were proposed [22–25]. Most studies in this field were concentrated on revealing the geometric beauty of the fractal object itself. Recently, several groups started to investigate the physical properties [26] and chemical reactivities [27–30] of these fractal objects. In this Letter, we would like to report some preliminary results concluded from our recent effort in pursuing multifractal analysis of diffusion-limited reactions over surfaces of DLA clusters [31].

The Witten–Sander model is the simplest model which demonstrates how computer simulation can be used to study the fractal nature existing in many natural [32] and industrial [33] aggregates. For the case of two-dimensional DLA, a square lattice is used with a seed particle fixed at the center. The particle is then released, one at a time, from a large inner circular boundary. The particle then takes a random walk over the lattice until it either leaves the outer circular boundary or enters the neighborhood of the seed particle and becomes part of the growing DLA. In the former case, a new particle is released again and the process is restarted. With the help of computer, such a simple strategy can easily yield self-similar, fractal structures. Several variations of the original Witten–Sander model were suggested to test the efficiency of simulation algorithms [24], to generate different patterns [34–36] and to investigate the connection between the Witten–Sander model and other models [37]. For instance, Rosenberg et al. considered the effect of sticking probability on the fractal patterns [34,35]. Meakin [38] and Vicsek and Ketesz [39] investigated the effect of the noise reduction parameter on the fractal properties. Interesting generalization models were also proposed to combine all aggregate models into a unified type of simulation. For instance, by changing the step-length exponent in Levy-flight trajectories from 0 to ∞, one would obtain continuous results from the Vold–Sutherland ballistic aggregation [41,42] to Witten–Sander random-walk model [21]. Effects of fractal substrates on DLA were also discussed by Witten and Meakin [43]. In all the variations reported so far, a circular launching boundary and a fixed center were assumed. In this paper, we report the results from

Correspondence to: S.-L. Lee, Department of Chemistry, National Chung-Cheng University, Min-Hsiung, Chia-Yi, Taiwan 62117, ROC.

0009-2614/92 $ 05.00 © 1992 Elsevier Science Publishers B.V. All rights reserved.
simulations of non-fixed-seed version of DLA with square launching boundary.

2. Methods

Quantitative measure of the fractal attribute in a DLA is generally represented by a critical index, $D$, which is defined by the mass–length relation [44]

$$M(aL)^{1/D} = a^D M(L),$$

(1)

where $D$ is the fractal dimensionality and is always smaller than the Euclidean dimension, $d$. The fractal dimensionality is one of the important indices in the DLA simulation.

Recently, we constructed a modified version of the Witten–Sander model for DLA for the sake of saving computing time [45]. In this modified version, acceptable radii of the launching boundary, $R_{\text{in}}$, and the outer boundary, $R_{\text{out}}$, are adopted to optimize the cluster growth rate and minimize the CPU time consumption. When the cluster grows, the radii of the inner and outer boundaries expand accordingly. The relationship among the radii of the cluster, $R_{\text{max}}$, the launching boundary, and the outer boundary are kept to be $R_{\text{max}} = R_{\text{out}} = R_{\text{in}} = R_{\text{in}} + R_{\text{out}}$ during the simulation, where $R_{\text{max}}$ represents the maximum radius in the growing cluster. This model has been tested using several sets of ratios and scales of $R_{\text{in}}$ and $R_{\text{out}}$ [45]. Insignificant deviations in the fractal dimensionality are observed and the results are found to agree satisfactorily with other experimental works [46,47] and theoretical calculations [24,48,49]. This model was used in all our simulations. In our simulations, the initial radii of launching boundary $R_{\text{in}}$ and outer perimeter $R_{\text{out}}$ were taken to be 24 and 36 units of lattice constant.

In the conventional DLA model, a seed is used to be fixed at the centre of the square lattice. A particle is launched, one at a time, from a randomly selected point on a circle which is centered at the seed. The selected particle then undergoes a random walk on the lattice until it either reaches an unoccupied lattice site neighboring to the growing cluster or it detours a long distance on the lattice until it goes out of the outer perimeter. In these models, the simulations were frequently performed on a finite, discrete lattice. Thus, the particle-launching sites on the circular boundary are not equal-event sites, i.e. they are of different steps away from the seed. A set of launching sites with equal-step away from the seed would construct a diamond shape boundary as shown in fig. 1. In this paper, we report the effect of such a difference on the DLA.

The second effect we report is the effect caused by the non-fixed launching centre. In simulating this effect, we performed the modified DLA version as in the previous model where the center of the launching boundary is initially located at the seed site. However, during the growing process, a new center for the releasing boundary is set at random to be any site in the growing cluster whenever a new particle is going to be released from a launching boundary. Note that the radii of the inner and outer margins from the new seed are kept fixed. Here the particle is discarded only when its distance (the least steps) to each particle in the cluster are all greater than the radius of the outer boundary. A new center is then re-selected and a new particle is released to start the growing process over. When the cluster is growing and becomes more compact, some lattice sites may be occupied by the cluster particles and the launching particle could be one particle of the cluster. A new particle is re-selected until all the lattice sites of the launching boundary are completely populated by the cluster particles. Under such situation a new center and thus a new launching boundary is chosen to keep the aggregation process going. The apparent Hausdorff dimensions are then analyzed to demonstrate the variations of aggregation patterns. The resulting fractals are more compact compared to those obtained in fixed-centre DLA simulation. Analysis of the variation of apparent Hausdorff dimension at different cluster sizes of the growing cluster revealed

![Fig. 1. A comparison between square and circular launching boundaries. A square margin is equal-stepped from the centre in all directions but a circular one is a function of angles.](image-url)
that the apparent Hausdorff dimension changes continuously from $1.64 \pm 0.03$ to $1.94 \pm 0.02$. It might be expected that as the cluster size grows infinitively large, the cluster does not possess any fractal geometry. In one limiting case as extrapolated to zero cluster size, it corresponds to the Witten–Sander DLA model. In the other limit as the cluster size goes to infinity, we obtain, in fact, an Eden cluster.

3. Results and discussions

To demonstrate the effect of launching-boundary shape on DLA, we first performed the modified Witten–Sander model on a $700 \times 700$ square lattice with a circular launching boundary. A typical diamond-shape aggregate is displayed in fig. 2b. The reason of the anisotropic contour might be rationalized as we pointed out earlier that the releasing sites on the circular boundary are not equal-event sites. In fig. 2a, we show a typical DLA of our modified Witten–Sander model using a square launching boundary. As can be seen in fig. 2a, the square boundary gives a relatively less anisotropic cluster since all the particle-releasing sites on a square boundary are equal-event sites. A second difference between these two configurations with equal radii is that particles launched from a circular boundary have larger probabilities to stay inside and will squander much random walk time owing to its clumsy occupancy of lattice sites. Note that the radius for a square boundary is the steps away from its centre. Hence particles released from the square margin have prevailing chances to adhere to the cluster and thus better aggregation efficiency with respect to those released from a circular margin. Effect of boundary shape on DLA can also be found in simulations on any finite, discrete lattice. For instance, on a trigonal lattice, the equal-step sites form a hexagonal boundary. However, the effect on the shape of the resulting DLA is less pronounced on a trigonal lattice. This can be easily understood since a regular polygon would get closer and closer to a circle as the number of edges increases.

It is also interesting to observe that, although the form of the cluster is considerably changed, the fractal dimension is not. This fact can be rationalized as follows. Firstly, since DLA is basically a probabilis-

![Diagrams](image)
duction parameter or the mean field parameter is increased, the resulting DLA is exactly the same no matter what boundary is used [31].

For two-dimensional DLA with nonfixed seed, simulations were also performed on a 700×700 square lattice. The impetus behind this model is to generate a cluster with a continuously changing apparent Hausdorff dimension and to find the variation of cluster patterns. Analyzing the growing cluster at different cluster size, we found that the apparent Hausdorff dimension changed continuously [45]. This observation can be rationalized in the following way. Due to the randomness of the seed site, the screening effect in the fixed-center DLA simulation

![Graph (a)](image)

**Graph (a)**

![Graph (b)](image)

**Graph (b)**

Fig. 3. The apparent Hausdorff dimension analyzed as every 2000 particles were added to the growing cluster in 2D simulations of moving-centre model using (a) square and (b) circular launching boundaries.
is diminished, namely, the interior core of the growing cluster is filled up gradually during the growing process. The limiting cases in both directions might be viewed as a cluster with a compact interior when extrapolated to an infinite large cluster size and a cluster with no chance to attach to the interior core when extrapolated to very small cluster size. The former is analogous to an Eden cluster while the latter is a Witten–Sander DLA. The changes of fractal patterns with apparent Hausdorff dimension of our second model in two-dimensional simulations are illustrated in fig. 3 as we plotted the apparent Hausdorff dimension as a function of cluster size. This model has built a way from the Witten–Sander DLA aggregate to the Eden model. Our second model somehow displays the same features which were achieved by the simulations using Levy-flight trajectories [50]. The continuous change of the apparent Hausdorff dimension as the DLA cluster grows gives us a clue to generate a DLA having fractal dimensionality somewhere between 1.67 and 2 if we combine the fixed-center model and nonfixed-center model in an appropriate weighing ratio. We display in fig. 4 a series DLA generated in the way we just described. As can be seen from fig. 4, the apparent Hausdorff dimension in each cluster is found to vary continuously as the weighing ratios of the fixed to the non-fixed model change from 10:0, 9:1 to 0:10.

Finally, the fractal dimensions obtained from the simulations of our first model in two-dimensional simulations are found to be in good agreement with previous experimental works [46,47] and theoretical calculations [24,48,49]. A square launching boundary in two-dimensional simulations seems to be a more efficient way to generate larger clusters instead of the conventional circular one without changing the fractal characteristics. The non-fixed seed DLA model displays a continuously changing apparent Hausdorff dimension as the cluster grows and it provides a clue to develop a model to generate DLA cluster with apparent Hausdorff dimension between 1.67 and 2.

4. Conclusions

We performed DLA simulation on a two-dimen-
sional square lattice to study the effect of square launching boundary and non-fixed centre on DLA. A square boundary is found to be superior to a circular one for its vulnerability to initiate the first few aggregation events and less CPU consumption. The resulting clusters have comparatively isotropic contours other than the diamond-like ones obtained in the conventional DLA simulations using a circular particle-releasing boundary. The non-fixed-seed model gives us some clues from which we can bridge Witten–Sander DLA to Eden model. This has been done by combining fixed-seed and non-fixed seed models in an appropriate way in the simulations. By changing the weighing ratios of these two models, we obtain continuous change of the apparent Hausdorff dimension from the Witten–Sander limit to the Eden limit.

Acknowledgement

The authors thank the National Science Council, Taiwan, Republic of China, for financial support.

References

Letters 54 (1985) 1416.
[47] D.W. Schaefer, J.E. Martin, P. Wiltzius and D.S. Cannell,

[50] B.B. Mandelbrot, The fractal geometry of nature (Freeman,
San Francisco, 1982).