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Diffusion Limited Aggregation: Algorithm optimization revisited

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ABSTRACT

The Diffusion Limited Aggregation (DLA) model developed by Witten and Sander in 1978 is useful in modeling a large class of growth phenomena with local dependence. Besides its simplicity this aggregation model has a complex behavior that can be observed at the patterns generated. We propose on this work a brief review of some important proprieties of this model and present an algorithm to simulate a DLA aggregates that simpler and efficient compared to others found in the literature.

1. Introduction

The Diffusion Limited Aggregation (DLA) was proposed by Witten and Sander [1,2], while working with aggregation processes. The DLA model is a good representation of processes where particles get attached by simple contact. For example, studies of polymer behavior [3] on a viscous media, electrodepositon phenomena [4,5], neuron growth [6,7], bubbles of Helium moving into a liquid media [8], and chemical reactions [9] all explained by some simulations based on a modified DLA model.

As would be show in the next paragraphs we are going to describe two simple algorithms to develop simulations of DLA aggregates, in 2 and 3 dimensions. The efficiency of the proposed algorithm is compared to the method used is Ref. [14] to generate 2-dimensional aggregates. As results we present and characterize an aggregate for the 2-dimensional case.

2. DLA – model and algorithms

The Diffusion Limited Aggregation is a simple model used to describe dendritic growths. As other growth models it has a power-law correlation function associated with the aggregated particles. The morphology of the formed objects has low density and a huge number of singularities [1]. This characteristics of the DLA model is responsible for its invariance under scale transformation [10]. A self-similar behavior showing an intrinsic fractal dimension of order $D_f \approx 1.71$ [11] is observed in this model. Some DLA based model can present multifractal scaling behavior [12] but still the optimization here presented can be also used.

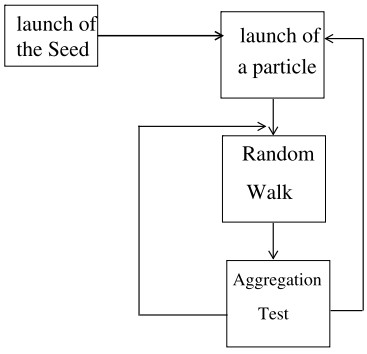

Fig. 1. Flowchart of the main algorithm to generate a DLA aggregate.

The main characteristics of this model are: (a) free particles execute random walks and (b) the aggregation of particles occurs by simple contact.

To generate a DLA aggregate there is a main algorithm as described in the flowchart, represented in Fig. 1.

On this model all the particles have radius r_p and execute a random walk until they get in contact with the aggregate. In this work all steps have constant size a, but it could be variable [13]. When this event occurs the particle is aggregated and cannot be removed from its position.

After allocating the seed at the origin of the coordinated system, next step is launch a particle on a circle of radius $R_l = R_a + \delta r$. Here, R_a is the radius of the aggregate and $\delta r > 0$, as shown in Fig. 2.

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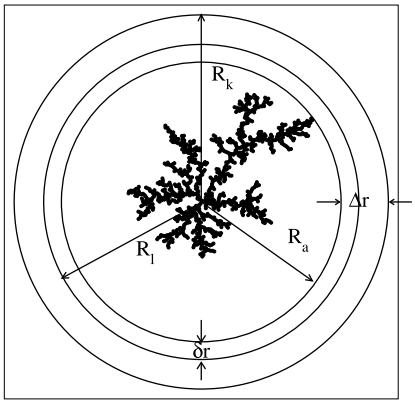


Fig. 2. A 2-dimensional scheme of the active regions on a DLA simulation.

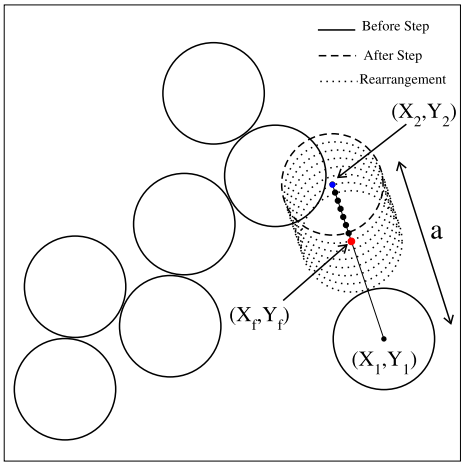


Fig. 3. Scheme of the algorithm described by Alves et al.

After each step of walk we must make the aggregation test. The time spending on simulations is due to the logical procedures involved at this part. In general, optimizations on the DLA algorithm are done trying to make this test more efficient [14].

If a discrete lattice is used to simulate the DLA model, the aggregation test consists on the simple inspection of the nearest neighbors of the site occupied by the particle. If some of them are occupied the particle is aggregated, otherwise, it continues the random walk. On the other hand, if you are using an off-lattice simulation the aggregation test is done by checking the distance between the center of walking particle and the center of all aggregated particles. If one of these distances is less or equal to $2r_p$ the particle is aggregated. If not the particle continues the random walk. The singular situation occurs when this distance is less than $2r_p$. To avoid superposition, the position of walking particles has to be rearranged.

There is a third event on the DLA model, the extinction of a walking particle. This occurs when a particle attached a distance r from the seed so that $r > R_k = R_a + \Delta r$, here $\Delta r \gg \delta r$. This simple modification, proposed by Lee et al. [15], in original model can save computational time.

At the work developed by Alves et al. [14], the rearrangement of the particle position is done by several backward steps along the direction of the last jump of the particle. Suppose a 2-dimensional DLA, and a particle is at the position (X_1, Y_1) very near the aggregate, executes a step of size a, and reaches the position (X_2, Y_2), as showed in Fig. 3. The correct position for the aggregation is the point (X_f, Y_f). The direction of the last step is stored in the format of an angle. To reach the correct position the particle executes the small steps of size γa (here $\gamma < 1$), until the distance between the particles is greater than $2a$, as observed in Fig. 3.

This method demands a great computational processing because of consecutive tests. We propose in this work a simple rearrangement of the particles by using a vectorial summation and an algebraic trick.

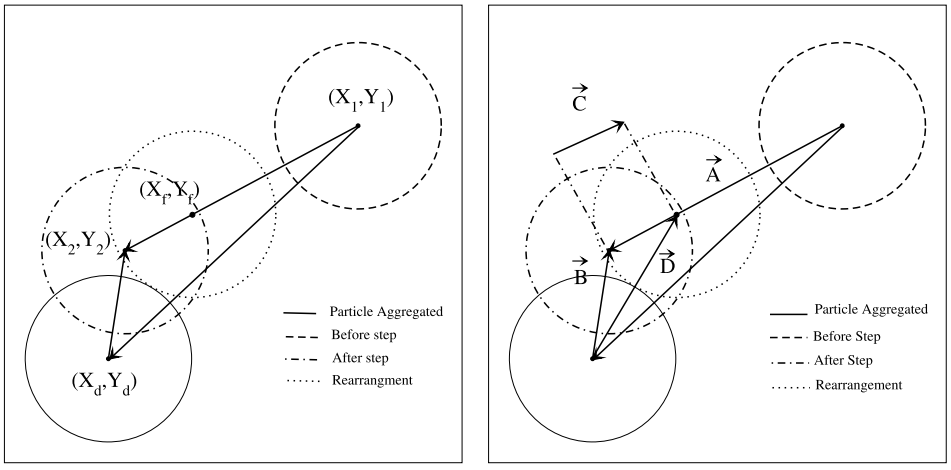
First consider two particles, A and B at the positions (X_d, Y_d) and (X_1, Y_1). They have this configuration before the step of size a of particle B. After the step particle B is located at position (X_2, Y_2). We can determine a useful set of vectors, as represented in Fig. 4(a). Notice that $|\vec{C}| < 2r_p$, and $|\vec{D}|$ must be equal to $2r_p$.

Considering the vectorial operations:

$$\vec{C} = \alpha \vec{A}$$
$$\vec{D} = \vec{B} + \vec{C} \tag{1}$$

if α is determined, the final position (X_f, Y_f) after the rearrangement is correctly determined. Imposing that $|\vec{D}| = 2r_p$, we find the following polynomial equation

$$4r_p^2 = B^2 + \alpha^2 A^2 + 2\alpha \vec{A} \cdot \vec{B} \tag{2}$$



(a) (b)

Fig. 4. (a) Schematic aggregation test. (b) Vectorial diagram for the rearrangement of the particle aggregated.

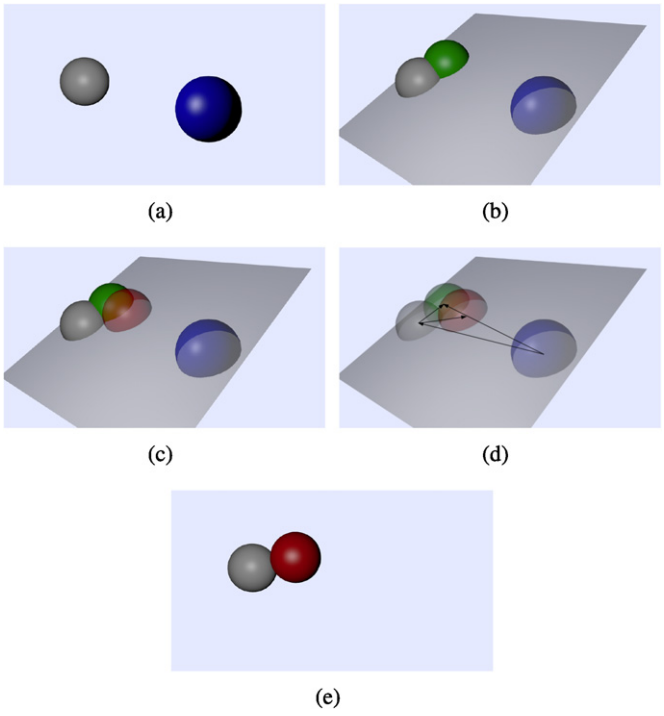


Fig. 5. The filled sphere represents the real position of a particle and the empty sphere represents future or past position of a particle. (a) One step after the blue particle sticks in the aggregate, (b) superposition of the green and gray particle, the blue sphere is the past position of the green particle, (c) the red sphere represents the desired position of the green particle to avoid superposition, (d) the empty spheres show that there are no superposition between the gray sphere and the red sphere and (e) shows the final position of the new particle aggregated. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

making $\theta = 2\vec{B}\cdot\vec{A}$, $\psi = B^2 - 4r_p^2$ and $\chi = A^2$, there are two roots,

$$\alpha_{1,2} = \frac{-\theta \pm \sqrt{\theta^2 - 4\psi\chi}}{2\chi} \tag{3}$$

The nearest position from the point (X_1, Y_1) is the correct rearranged position. The root of Eq. (2) that has absolute value smaller than the unit satisfies the previous condition. With this result the coordinates (X_f, Y_f) are,

$$\begin{aligned} X_f &= X_d + B_x + \alpha A_x \\ Y_f &= Y_d + B_y + \alpha A_y \end{aligned} \tag{4}$$

here, A_i and B_i are the components of the vectors.

As can be observed, Eqs. (1), (2) and (3) are independent of the space dimension. Then, for the 3-dimensional case, if the initial position was (X_d, Y_d, Z_d), the new coordinates are,

$$\begin{aligned} X_f &= X_d + B_x + \alpha A_x \\ Y_f &= Y_d + B_y + \alpha A_y \\ Z_f &= Z_d + B_z + \alpha A_z \end{aligned} \tag{5}$$

The entire process described in the proposed algorithm for the 3-dimensional case is shown in Fig. 5. In Fig. 5, the gray sphere represents an aggregated particle. The position of the particles before the aggregation event is shown in Fig. 5(a), after a step of size a, the blue particle reaches the position of the green particle as presented in Fig. 5(b). As can be seen, even in 3 dimensions the problem can be simplified in a 2-dimensional case because the three set of coordinates can be used to determine a plane crossing the spheres. The desired position of the green particle is the position of the empty red sphere in Fig. 5(c). As observed in Fig. 5(d), the empty red sphere and gray sphere just intercept each other at one point, not presenting superposition. Finally, the position of the new aggregated particle is shown in Fig. 5(e).

Table 1
Table of the simulations using a PC with an AMD Athlon 3400+ processor and 1.0 Gb of RAM memory. The last line is a power-law for the simulation time compared to the number of particles aggregated.

N^o of particles	Alves et al.	Algorithm proposed
1×10^3	3.9	3.7
2×10^3	12.8	18.4
5×10^3	84.9	92.2
1×10^4	330	175.4
2×10^4	2480	832.1
5×10^4	14 000	3600
	$T \sim N^{2.1}$	$T \sim N^{1.3}$

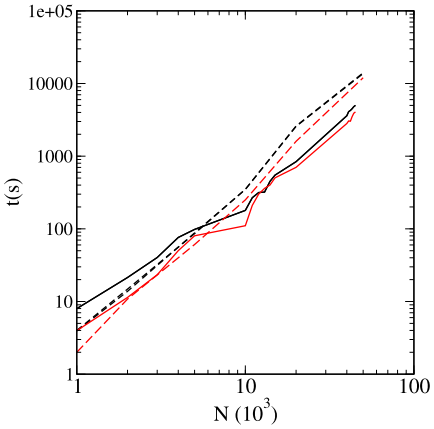


Fig. 6. Efficiency of the proposed algorithm compared with Alves et al. for large number of particle deposited. The black curves are the results made using a Pentium with an AMD Athlon 3400+ and the red curves were made in Xeon core 2 quadi. The dashed lines were obtained using the S.G. Alves method, and continuous lines were obtained using the proposed method. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

3. Numerical results

In addition with this optimization, we used the first and second optimization implemented in the work developed by Alves et al. [17] for the aggregation test. The simulations developed are restricted to the 2-dimensional case, because just this model can be compared to the results obtained by Alves et al. [17].

All the simulations were done using a Pentium with a AMD Athlon 3400+ processor and 1.0 Gb of RAM memory and a Xeon core 2 quadi with 2.21 GHz frequency processor and 2.0 Gb of RAM memory. The operational system used was a Linux distributed with a Debian kernel, and the softwares were developed using FORTRAN90.

As shown in Table 1, and Fig. 6 for a large number of particles deposited, the present algorithm is more efficient, but notice that the difference between the two algorithms increases proportionally with the size of the aggregate.

As can be seen in Fig. 7(a), the aggregates generated have a typical morphology of DLA.

In order to characterize this kind of aggregate we determine its fractal dimension, using the Mass–Radius [10] method and found $D_f \approx 1.71$, as shown in Fig. 7(b). This fractal dimension value is in agreement with the one proposed in the literature [10,16].

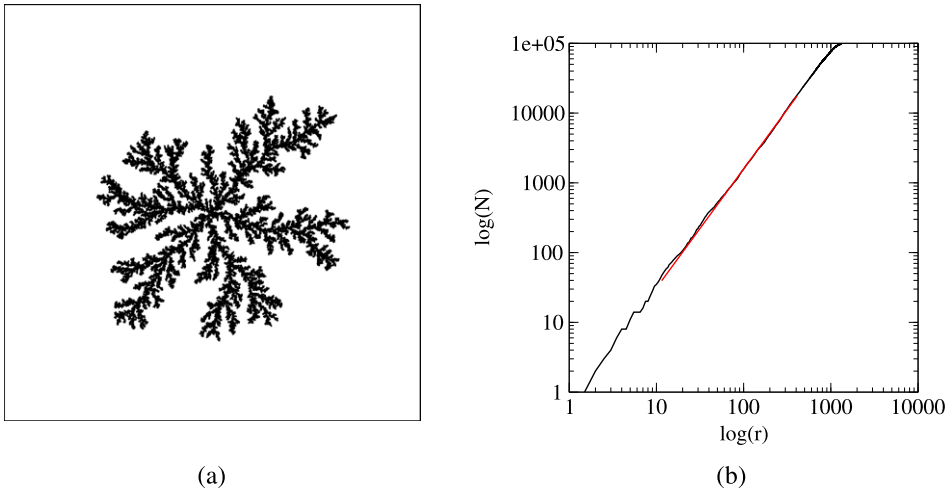


Fig. 7. (a) Aggregate with 10^5 particles grew using the proposed algorithm. (b) Fractal dimension for a DLA aggregate generated by the proposed method with 10^5 particles using the Mass–Radius method. The black curve is the numerical result and the red curve is the fit in the active region of the DLA, and its expression is $\log N \sim 1.708 \log r$. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

4. Conclusion

In conclusion, we have briefly described the main characteristics of the DLA model and demonstrate that the proposed method is more efficient to determine the aggregation of a particle in an off-lattice DLA simulation. And this effectiveness is achieved by a reduction of the number of logical tests made during the aggregation test. Although we only present here results for 2d Winter–Sander DLA we believe that this optimization can be more effective in a 3d model, since one more distance (z-dimension) has not to be calculated. Some future studies can be done for another DLA based models that could be implemented off-lattice and needing biggest aggregate.

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