DIFFUSION MODELS ON TRIANGULATED SURFACES

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Abstract

Diffusion processes occur in many scientific areas; they are especially important in chemistry, biology and medicine. Most of the mathematical models that describe diffusion are nonlinear Partial Differential Equations, which do not have analytical solutions and numerical methods require large computing resources. There is a growing interest in the structures (fractal clusters) generated by diffusion processes, and the search for new models has intensified. The important method complementary to mathematical models is imitation modeling in which the space mobility of the particles of a substance is directly modeled.

There are two directions in such an approach: an imitation of random walks of particles; and cellular automata modeling. In this work, for the modeling of the fractal cluster growth on triangulated surfaces, we implement algorithms based on random walk. We use classical variants of Diffusion Limited Aggregation (DLA) and Reaction Limited Aggregation (RLA) models. It is shown that, in the framework of the classical Cluster Aggregation (CCA) model, fractal cluster on a triangulated surface cannot be correctly constructed without additional assumptions about the cluster restructuring.

The software is written in Python; it may be used by both researchers and students as a tool for the modeling of complex processes.

1. INTRODUCTION

Diffusion is one of main processes when two substances interact. Hence mathematical and imitation modeling are common tools for research. Mathematical models often do not have analytical solutions. We need therefore to apply numerical methods and imitation modeling in which a mobility of particles is simulated directly. Such an approach allows visual representation to be obtained of the objects which appear as a result of diffusion both on surfaces and in the space. Complex structures generated by various diffusion processes are called aggregates, or fractal clusters, due to their similarity with well-known objects. In reality, aggregates may be not only fractals but multifractals as well.

The active studying of such structures began in 1970 and has continued successfully up to now. Fractal aggregates appear in the process of crystallization [8] and hemagglutination [14]. Imitation modeling of the growth of fractal clusters in an environment that has given physical properties may help in forecasting results of the process under study. This technique was efficiently applied to the study of the spread of cancer cells in blood [16].

The models of the construction of fractal clusters can be divided into the following properties [13]:

- The nature of a process (cluster-particle or cluster-cluster).
- The nature of the association of particles or clusters depending on the probability of sticking.
- The nature of the motion of particles or clusters (chaotic or directional).

In 1981 W. Witten and L. Sander proposed the first computer model (DLA) [15] which constructs a fractal cluster on the plane as a result of random walks of particles which are thrown one by one. This model was then widened and modified, which resulted in: the description of RLA, which allowed the addition of a physical parameter of a given environment; and the CCA model, which considered the motion of clusters not particles.

Another approach to diffusion modeling is based on a widened notion of cellular automata. In this notion any alphabet, transition functions and regimes of the change of cell states are possible. Such a wide interpretation of cellular automata allows us to construct mathematical descriptions of space-time processes of various nature including the processes with self-organization ([1],[4]).

In practical applications, it is important to use modeling both on surfaces and in the space. The approach based on cellular automata implementation of DLA on the bone surface was proposed in [4]. In [2] the author designed and implemented the optimized DLA algorithm on a triangulated surface, which is based on the random walk method. The CCA model was applied to study processes in colloidal solutions and aerogels; the implementation was made in space configuration [10,11,17].

This work is based on random walk imitation modeling for DLA, RLA, and CCA models. Optimized DLA and RLA are realized on a triangulated surface. For CCA it is shown that, in the framework of the classical model, a correct implementation on a triangulated surface is impossible without an assumption about the cluster restructuring.

The software written in Python includes :

- Triangulation of a surface by the marching method.
- Implementation of both base and optimized DLA for a triangulated surface.
- Implementation of RLA for a triangulated surface.
- Implementation of CCA on a square lattice.
- Visualization of results in 3D.

The paper is organized in the following way. In sections 2 and 3 there is a description of the DLA model and its optimization both on the plane and a triangulated surface. The CCA model is discussed in section 4. In section 5 we describe the RLA model. The results of numerical experiments are given.

2. DLA MODEL

2.1. Witten-Sander base model

In this variant, particles are thrown on the plane randomly and walk by random way on a square lattice. The initial particle is considered as a cluster. Every next particle may move with equal probability in 4 directions – up, down, left, right – on the lattice lines or cells. A particle joins the cluster if it is a neighbor of a particle in the cluster. The choice of a way of moving depends on the representation of a particle – it may be presented by a vertex of the lattice or by a cell. The representation naturally influences the visualization results.

2.2. DLA on triangular lattice

In this case, we should define the directions of the particle transitions. For a particle in a triangle with sides a, b, c, define the probabilities *p(a), p(b), p(c)* to move in neighboring triangles through corresponding sides as follows:

$$p(a) = \frac{1/a}{1/a + 1/b + 1/c}$$
$$p(b) = \frac{1/b}{1/a + 1/b + 1/c} \quad (1)$$
$$p(c) = \frac{1/c}{1/a + 1/b + 1/c}$$

For example, in the triangle with sides 3, 4, 5 we have p(a)=20/47, p(b)=15/47, p(c)=12/47. The unit segment is divided as [0, 20/47, 35/47, 1]. If the random number is in the first interval, we go to the neighboring triangle through side a, etc.

3. OPTIMIZATION OF THE DLA ALGORITHM

In applications, the base DLA model has some disadvantages:

1. Every particle moves on a lattice chaotically and the number of steps is unbounded. Hence for large surfaces the number of steps which are required to join to a cluster grows indefinitely. Thus, for a large number of particles the run time may be unpredictably large.
2. In real experiments one usually models several clusters on the same surface. But this fact is not taken into account, which also results in the run time growth.

It follows that in real modeling we have to use some restrictions on the number of particles, size of the surface, and the number of particles in the cluster. Moreover, we consider a variant of optimization based on a reduction of the number of random walking.

3.1. Optimization on square lattice

The optimization proposed in [2] defines a particle's position when it joins a cluster in advance – at the moment when the particle is thrown on the lattice. For a square lattice with M cells we compute a matrix of choice of coefficients G [M, M] which is used to define the particle position.

When a particle is thrown on a lattice the choice coefficients are calculated for each boundary point of the cluster. It is known [2] that these coefficients depend on only the sum of coordinate distances (a on abscissa and b on ordinate) between a new particle and boundary points of the cluster and may be calculated as:

$$p(a,b) = \frac{1}{4(a+b)} \tag{2}$$

We consider the obtained coefficients as values of a distribution function, choose a value randomly, and the preimage of this value defines the position of joining.

3.2. Optimization on a surface

For a triangulated surface we present the structure of a lattice by a graph, such that triangles correspond to the graph vertices, and edges between vertices mean that these triangles are adjacent. Define on edges (paths by length 1) weights (choice coefficients) which are calculated by (1). Write these weights in a matrix G_1. Then construct a sequence of matrices $\{G_k\}$, such that G_k contains choice coefficients for k-length paths. The weight of a path equals the product of weights of edges.

In G_1 denote by $p(i,j)$ the weight of the edge (i,j). Let $p(i,j) = y$, and $p(j,j_1) = y_1$, $p(j,j_2) = y_2, p(j,j_3) = y_3$ for neighbors of j. Then in G_2 in elements with indices (i,j_1), (i, j_2), (i, j_3) the coefficients $p(i,j_1) = yy_1, p(i,j_2) = yy_2$, $p(i,j_3) = yy_3$ will be written. Thus (i,j_1) corresponds to the 2-length path from i to j_1 and its weight is the product of the weights of the path edges. The matrices of higher order are constructed by analogy.

The common matrix of the choice coefficients is calculated as the sum of G_k, where k is from 1 to a given N. The position of the place of joining the cluster is defined by the analogy with the case 3.1. The optimized algorithm may require more or equal time than the base one. The optimization results in considerable time gain when we conduct a series of experiments, because the matrix G is calculated one time for a given surface.

Summing up one may say that:

1. When modeling one cluster, the base and optimized algorithms show close results. The optimized variant may be slower if the number of triangles is large.
2. When modeling the large number of clusters, the optimized algorithm reduces run-time considerably.

The optimized algorithm for a triangulated surface was implemented in [3]. In the next table the results of both algorithms on the surface $\boldsymbol{x^3 + y^2 + z = 0}$ are given. The number of triangles is 4000, the number of particles in the cluster is 500.

Table 1. The comparison of base and optimized DLA algorithms

The number of clusters	Base DLA	Optimized DLA
1	5m 56s	6m 59s
5	53m 11s	11m 41s

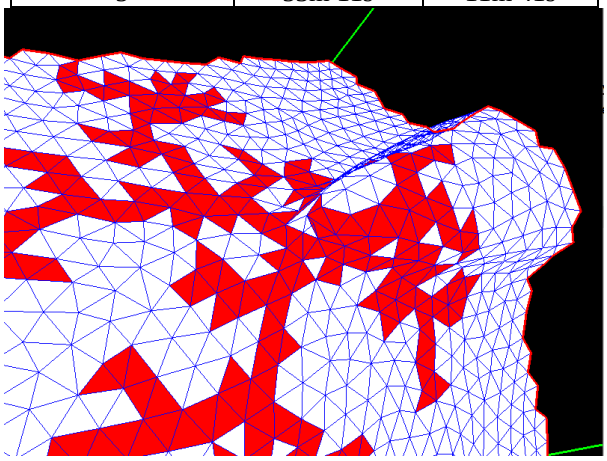

Figure 1. The result obtained by optimized DLA on the surface $\boldsymbol{x^3 + y^2 + z = 0}$

4. CCA MODEL

4.1. CCA on square lattice

This model was proposed in [9]. Compared with a particle-cluster model, in this model the common number of particles is known and all of them are on a surface (or plane).

The particles randomly walk on the lattice. When 2 particles collide they join into a cluster, and this cluster continues to walk. It is assumed that the probability of collision of 3 or more clusters is very small. At the end of the modeling, we have a final aggregate.

The movement of a cluster on a square lattice is similar to the movement of a particle – on every step the cluster may move one cell left or right or up or down with equal probability. Clusters are considered to be sticky if at least one particle of the first cluster is on the cell which is the neighbor of a particle of the second one. In such a situation, due to the structure of square lattice, a cluster moves as a single whole and saves its structure.

4.2. Problems of CCA on triangular lattice

On a triangular lattice we cannot always model the cluster movement to save its structure. To explain the situation, we give the following definitions. We call the movement of a cluster ***correct*** if :

(1) Every particle of the cluster passes through the same number of the cells of the lattice.

(2) The number of particles does not change, i.e. the structure is preserved.

The movement of a cluster is ***semi-correct*** if only (1) or (2) holds. The movement is ***incorrect*** if it is not correct or semi-correct.

It is easy to note when the movement of a cluster on square grid is correct, because all the particles pass the same distance in a chosen direction and the structure is preserved.

On a regular triangular grid, the movement of a cluster may be only semi-correct. In this case different particles may pass different distances and move in different directions. Hence, to save the structure, the cluster must turn. In other words, we cannot move the cluster as a single whole. Such a situation is explained by the structure of triangular lattice.

In Figure 2 the red cluster in the left part of the picture moves on 1 cell in the direction marked by the black arrow. On the right side its initial position (blue color) and the result of the movement (red color) are shown. We see that some particles pass 1 cell, and one particle should pass 3. The cluster makes 1 step, but to make it possible the particles should pass a different number of cells. According to our definition, the

movement is semi-correct because condition 1) does not hold. Note that this situation is possible only or regular triangular lattice on the plane.

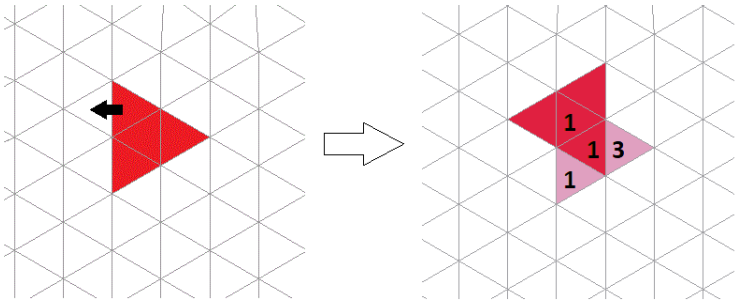

Figure 2. The example of the motion of a cluster on a regular triangular grid: particles of the cluster make a different number of steps

For non-regular triangular lattice, the nodes of the lattice may have a different number of neighbors; it does not allow the structure of a cluster to be preserved. This situation is illustrated in Figure 3. The blue cluster consists of 5 particles; every particle has 2 neighbors. We cannot move it into the red area without changing the structure.

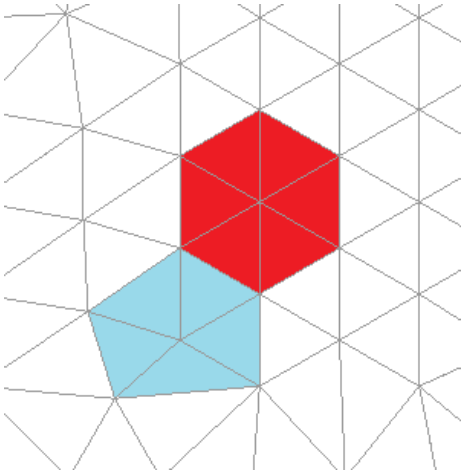

Figure 3. Restructuring on non-regular grid: blue cluster cannot be moved to the red area without changing its structure

Thus, it is impossible to implement the CCA algorithm on a non-regular lattice without modifications that allow the cluster restructuring. For example, in [17] the authors assumed that a cluster may spin; when 2 clusters stick together, they can spin in

the point of contact. They also proposed that there is a tension between particles, hence particles may influence each other in the process of the cluster growth. It may lead to a change of the cluster structure.

In real tasks the modeling of CCA on a surface has a limited scope of application, and the modeling in the space is more important. In this case some problems appearing for non-regular lattice on a surface may be solved and a cluster may be admitted to turn or change a structure. Such a model may be used when studying colloid solution or aerogels. In [16] an interesting variant of CCA space model in a boundary area was implemented: when a cluster collides with boundaries it moves in the opposite direction. This model may be applied to the modeling of nanoscale medicinal products [10], catalytic reactions [11] and physical properties of materials.

5. RLA MODEL

To take into account physical properties of a real environment, we should introduce some parameters. In this model the probability of joining a particle to a cluster is considered.

Proposed in [7] RLA (Reaction Limited Aggregation) model describes the growth of a fractal cluster when the probability of sticking is small. In [12] the authors merged CCA and RLA models, introduced the binding energy between particles, and assumed that the probability of sticking depends on the time of random walking and the time of breaking binds. Thus, the probability of sticking is a dynamical parameter.

We implemented RLA on a triangulated surface and used the probability of sticking as a parameter. This is a modification of DLA and may be performed both for base and optimized variants.

If a particle is near a cluster and the probability of sticking p_s is small, it continues to walk. Denote the number of walks by N and the number of walks which lead a particle to a cluster by N_w. Choose N, N_w such that $\frac{N_w}{N} = p_s$. If after N walking $N_w = 0$ (the particle did not get closer to the cluster) we delete the particle and throw a new one.

The example of the construction of the aggregate on the surface $x^3 + y^2 + z = 0$ for $p_s = 0.1$ (left) and $p_s = 1$ (right) is shown in Figure 4. The number of triangles is 1419, the number of particles is 200.

The run-time for $p_s = 0.1$ is 1m 3s, and 19s for $p_s = 1$.

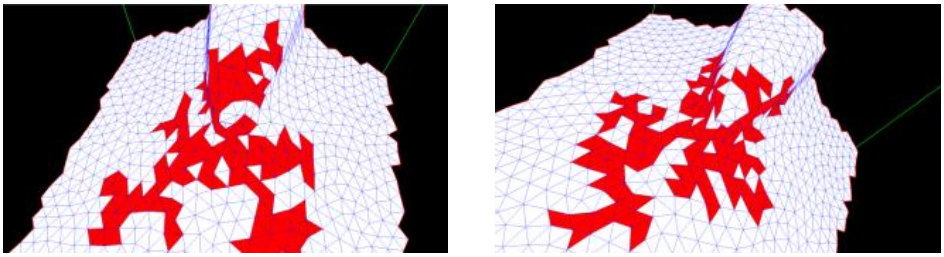

Figure 4. RLA model on the surface $x^3 + y^2 + z = 0$
$p_s = 0.1$(left) $p_s = 1$(right)

The triangulation was performed by the marching method proposed by E. Hartmann [5]. It is quite simple to implement and may be applied to any type of a surface. The size of the lattice is given by a parameter.

6. CONCLUSION

Mathematical models of diffusion are rather complex and as a rule do not have analytical solutions. For a successful study of diffusion processes, one should combine mathematical and numerical methods and imitation modeling. In this work, we present a program system for the imitation modeling of the growth of fractal clusters on a triangulated surface by DLA and RLA models. It is shown that CCA model cannot be implemented on a triangular lattice without a restructuring of a cluster. The program may be useful both for researchers and students.

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