MODELS OF DIFFUSION PROCESSES ON TRIANGULATED SURFACES

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Abstract

Diffusion processes occur in many scientific areas, they are especially important in chemistry, biology and medicine. The most part of mathematical models for a description of diffusion are nonlinear Partial Differential Equations which do not have analytical solutions, and numerical methods require large computing resources. As scientific interest to the structures (fractal clusters) generated in the result of diffusion processes grows, the search of new models is intensified. The important method complementary to mathematical models is imitation modeling in which 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 we implement based on random walk algorithms for the modeling of the growth of fractal clusters on triangulated surfaces. We use classical variants of Diffusion Limited Aggregation (DLA) and Reaction Limited Aggregation (RLA) models. It is shown that for Cluster Aggregation (CCA) model fractal cluster cannot be constructed correctly without additional assumptions about the cluster restructuring. The software is implemented on Python language and may be used by both researchers and students as a tool for modeling complex processes.

1. INTRODUCTION

Diffusion is one of main processes when two substance interact. Hence the mathematical and imitation modelling are common tool for research. Mathematical models are often do not have analytical solutions and we need to apply numerical methods. In additional to these methods one may use imitation modelling in which a mobility of particles is modelled directly. Such an approach allows obtaining visual representation of the objects which appear in the 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. Really, aggregates may be not only fractals but multifractals as well.

The active studying of such structures began in 1970 and continues successfully up to now. Imitation modelling of the growth of fractal clusters in an environment having given physical properties may help in the forecasting the process under study. Fractal aggregates appear in the process of crystallization [8], and hemagglutination [14]. Imitation modelling was applied to the study of the spread of cancer cells in blood [16].

The models of the construction of fractal clusters may be divided into following groups [13]:

- by a method of cluster formation (cluster-particle or cluster-cluster)
- by a method of the motion of particles or clusters (chaotic or directional)
- by a method of sticking of particles or clusters depending on a coefficient.

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

The second approach to the diffusion modeling is based on a widened notion of cellular automata. In this notion any alphabet, any transition functions and any 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 character including the processes with self-organisation ([1], [4])

In practical application it is important to use the modelling both on surfaces and in the space. An implementation of DLA algorithm on the bone surface and based on cellular automata approach was proposed in [4]. In [2] the optimized DLA algorithm on triangulated surface based on random walk was designed and implemented. CCA model was applied to study

processes in colloidal solutions and aerogels, the implementation was made in space configuration [10,11].

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

The software implemented on Python includes the following algorithms

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

The paper is organized by the following way. In sections 2 and 3 DLA model and its optimization both on the plane and a triangulated surface are described. The CCA model is discussed in the next section. In 5 we describe 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 equiprobably in 4 directions – up, down, left, right – on the lattice lines or cells. A particle joins to the cluster if it is a neighbour for 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 on the visualization results.

2.2. DLA on triangular lattice

In this case we should define the directions of the particle transitions. For a particle being in a triangular with sides a, b, c define the probabilities to move in neighbour triangulars through corresponding sides as follows

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

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

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

Divide the segment [0,1] on intervals proportionally these probabilities. Choose a random number and depending on the interval in which it lies take the neighbour cell.

For example in the triangular 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 neighbour triangular through side a, etc.

3. OPTIMIZATION OF 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 parts of surfaces the number of steps which are required to join to a cluster grows indefinitely. Thus for the large number of particles the run time may be unpredictably large.
2. In real experiments one usually model several clusters on the same surface. But this fact is not taken into account, that also results in the run time growth.

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

3.1. Optimization on square lattice

The optimization proposed in [2], defines the position of joining of a particle to 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 will be used to define the particle position.

When a particle is thrown on a lattice the choice coefficients are calculated for each boundary points 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

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

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 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 edges of the path. 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 the joining to 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 triangular 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 the both algorithms on the surface $x^3 + y^2 + z = 0$ are given. The number of triangles is 4000, the number of particles in 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

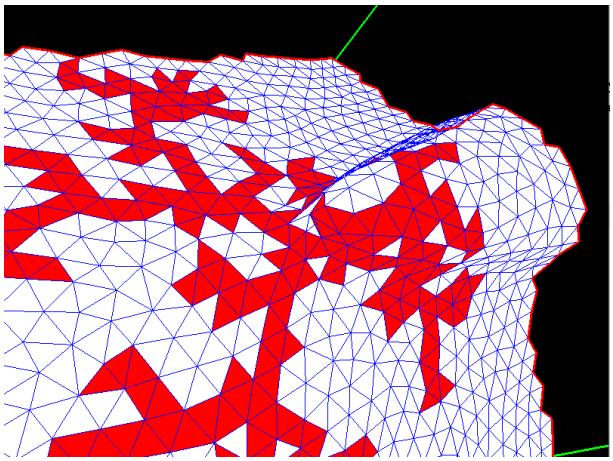

Figure 1. The result obtained by optimized DLA on the surface $\boldsymbol{x^3 + y^2 + z = 0}$

4. CCA MODEL

4.1. CCA on square lattice

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

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

The movement of a cluster on 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 equiprobably. Clusters are considered to be sticky if at least one particle of the first cluster is on the cell which is neighbor of a particle of the second one. In such a situation due to the square lattice, a cluster moves as a single whole and saves his structure.

4.2. Problems of CCA on triangular lattice

On a triangular lattice we not always can 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 that 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 has to turn. In other words we cannot move the cluster as a single whole. Such a situation is explained by the structure of triangular lattice.

On Fig.2 the red cluster on the left part of the picture moves in the direction marked the black arrow on 1 cell. 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. We see that the cluster makes 1 step, but to do it possible the particles should pass different number of cells. According to our definition the movement is semi-correct, because 1) does not hold. Note that this situation is possible only for regular triangular grid on the plane.

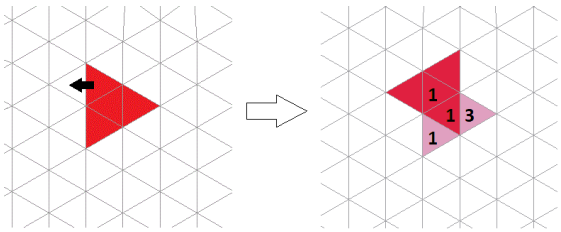

Figure 2. The example of the motion of a cluster on regular triangular grid: particles of the cluster make different number of steps

For non-regular triangular lattice the nodes of the lattice may have different number of neighbors and it does not allow preserving the structure of a cluster. This situation is illustrated on Fig.3. Blue cluster consists of 5 particles, every particle has 2 neighbors. We cannot move it into red area without changing the structure.

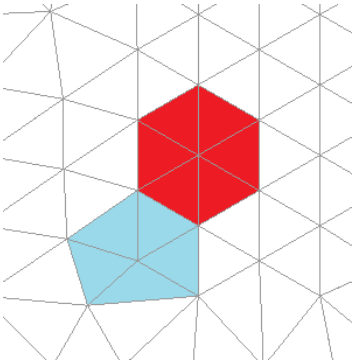

Figure 3. Restructuring on non-regular grid: blue cluster cannot be moved to the red area without changing its structure

Thus, it is impossible to implement CCA algorithm on a non-regular lattice without modifications allowing the cluster restructuring. For example in [17] the authors assumed that a cluster may spin, and 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 modelling of CCA on a surface has a limited scope of application, and the modelling 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 cluster collides with boundaries it moves in opposite direction. This model may be applied to the modelling 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 together 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 dynamical.

We implemented RLA on a triangulated surface and used a 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 continue to walk. Denote the number of walks by *N* and the number of walks which lead a particle to a cluster by N_w. One may assume that the less p_s the more N_w. For example if $p_s = 0.2$ we may take $N_w \leq 10$, and for $p_s = 0.5$ take $N_w \leq 6$. 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 on Fig. 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 $p_s = 1$.

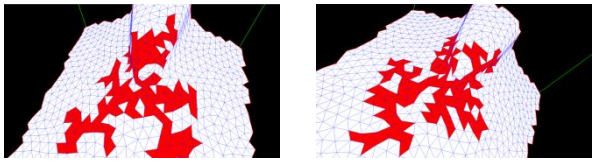

Figure 4. RLA model on the surface

$$\boldsymbol{x^3 + y^2 + z = 0}$$

$$\boldsymbol{p_s = 0.1}\ \text{(left)} \quad \boldsymbol{p_s = 1}\ \textbf{(right)}$$

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 may be defined 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 modelling. In this work we present a program system for the imitation modelling 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 grid without a restructuring of a cluster. The program may be useful both for researchers and students.

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