ON MODELLING OF DIFFUSION LIMITED AGGREGATION PROCESSES ON TRIANGULATION NET

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Abstract

The implementations of diffusion-limited aggregation algorithms both on the plane lattice and a surface approximated by irregular triangulation net are described. The optimization of the method based on the a priori estimation of the sticking probability of a particle to the aggregation (joining coefficient) has been proposed and realized. The algorithm complexity estimation and results of numerical experiments are described.

1. INTRODUCTION

Many processes both in nature and society have chaotic dynamics resulting in appearance of complex fractal structures characterized by statistical (noncomplete) recurrence.

These objects are often called by chaotic fractals. Fractal clusters are the class of chaotic fractals such that their density decreasing when the cluster grows.

The investigation of fractal clusters began with a theoretical model of Diffusion Limited Aggregation (DLA) process that describes the aggregation of particles in conditions of their random walking. Later the models of Cluster-Cluster Aggregation (CCA) and Reaction-Limited Cluster Aggregation (RLCA) were proposed. One can find their detail description in [5].

The DLA model describes the growth of groups of particles (called aggregates) when the particles perform random (Brownian) walks on the sides of rectangle lattice on the plane. This model was considered in [4] by Witten and Sander and by Pinski in [7]. It seemed to be widely applicable for simulation such processes as metal deposition in electrolysis, propagation of electric discharge in dielectric breakdown, diffusion in liquids and gases.

Implementation of algorithms for DLA modelling is rather time-consuming. There are variants of optimization for the Pinski algorithm that result in a reducing run-time for aggregates containing a large number of particles. Some of them are given in [6]. One way of optimization is to allow walking for one step on the distance more than 1. Another way is to specify an initial vector of translational motion for a particle and add this vector to the particle free movement on every step of walking.

In [1] we implemented the optimization of basic algorithm for DLA model on the plane, which was based on the calculation of a priori estimations of the probabilities of a particle joins to boundary points of the aggregate. That reduced run-time more than 10 times in average.

A natural generalization of the algorithm DLA on the plane is to consider a surface in R^3. Such an algorithm was proposed and implemented in [2], where the surface was approximated by irregular triangular net. The implementation of the algorithm shows that, as in case of the plane, the construction of an aggregate from a large number of particles requires a great deal of time.

In this work we propose an optimization method for DLA on irregular triangular net by using a priori estimation of joining probability. As in [2] we assume that transitions between triangles of the net have different probabilities. Experiments show that we obtain considerable run-time reducing for repeated construction of aggregate.

2. DLA MODEL ON THE PLANE

In accordance with basic DLA model particles walk on sides of rectangular lattice. Particles join to the aggregate one by one. The aggregate formation starts with a particle being in the lattice coordinate

origin. The initial position of the following particle is defined in a random way. This particle starts walking on the lattice sides, in doing so on every step it may move with the probability $^1/_4$ to one of points which are one the distance 1 from it. The process continues for as long as the particle became adjacent with a particle from the aggregate. Then it connected with the aggregate by a segment and is considered as the aggregate part. This process is repeated.

In practice one should consider additional restrictions: a particle is thrown in a given neighbourhood of the aggregate, being the number of walking steps is supposed not greater than N. If the particle does not join to the aggregate for N steps, we consider the following one.

3. OPTIMIZATION OF DLA MODEL ON THE PLANE

In [1] we describe an implementation of the based algorithm which used a priori estimation of joining coefficients. This estimation depends on the initial distance between points: if two points are on the distance *a* on X and *b* on Y then the joining coefficient for them is $\frac{1}{4^{a+b}}$.

For each particle throwing on the plane with using of its initial coordinates we calculate all the joining coefficients to the boundary points of the aggregate. Then according to the coefficients we construct a distribution function ["numerical distribution function", 3] and chose randomly a number from the function value area. The proimage of the number determines the point of the aggregate which the particle joins to.

Hence, we do not consider all the possible paths by which a particle can join to the aggregate and lost an information. But experiments show that such an approach leads to the considerable run time reducing, in doing so the structure of the cluster practically does not differ from the results given by the classical model.

Given M points on the rectangle lattice we calculate joining coefficients for all pairs of points and form of them matrix G with size MxM such that G(i,j) is the a transition probability for a particle to move from the point i to j. It is easy to understand that for the pairs of points that have the same values $s = a + b$ joining coefficients are also the same and equal to $^1/_{4^s}$. Hence it is not necessary to use a matrix to save obtained values. However such a matrix will be useful in the sequel.

4. ADAPTATION OF DLA MODEL FOR TRIANGULAR NET

In [2] authors described an implementation of DLA algorithm on irregular triangular net. The initial particle is in a given triangle. Next, a new particle initiates its random walk on the net. On every step the particle can move to one of adjoining triangle with a probability depending on lengths of sides, providing that one particle only can occupy each triangle. For any adjoining triangles 1 and 2 the particle transition probability to move from 1 to 2 is calculated by the formula,

$$P(1 \to 2) = \frac{^1/_a}{^1/_a + {}^1/_b + {}^1/_c} \qquad (1)$$

where a, b, c – are lenths of sides for the triangle 1 (Fig.1).

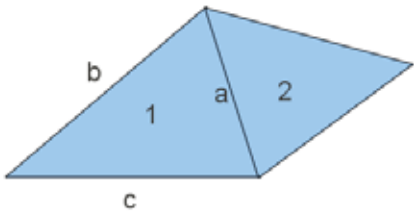

Fig. 1. Calculation of the transition probability

As the example of the application of the described algorithm the process of a matter distribution on bone surface was modelled. As in the case of the plane, to computer aggregation consisting from a large number of particles we need a considerable time.

5. OPTIMIZATION OF DLA MODEL FOR TRIANGULAR NET

Construct on a given area of the surface an irregular triangular net. Let the number of triangles to be M.

Consider an oriented graph $\square_{\square}$ with M vertices. To every triangle M_i we match a vertex i in $\square_{\square}$. There is the edge (i,j) iff M_i и M_j have a common side. Every edge (i,j) has a weight $\square(i, \square)$ calculated in accordance to (1).

Consider all the paths on $\square_{\square}$ that have the length not greater than N. The weight of a path between i and j is a production of weights of all the edges.

Choice coefficient for vertex i and j we define as the sum of weights of all the paths by length not greater than N between the vertices. The obtained coefficients save in a matrix G with size MxM.

To obtain the choice coefficients we use the following algorithm. Let on the initial step $\square = \square_{\square}$, where $\square_{\square}$ consists of weights of all the paths by length 1, i.e $\square(i, \square) = \square(i, \square)$. Form $\square_2$ containing weights of all the paths by length 2 by the following way. For a given pair (i,j) consider all the edges starting from j: $\square(\square, \square)$. There are not greater than 3 such edges because every triangle has not greater than 3 adjoining ones. Then we calculate length of the path by length 2 as $\square(i, \square) = \square(i, \square)\square(\square, \square)$ and set $\square_2(i, \square) = \square(i, \square)$. Hence, given $\square_{\square}$ we construct $\square_{\square+\square}$ by above way. Summing up all $\square_{\square}$ for k=1,…N we obtain G.

Time complexity for the algorithm of G construction is $O(NM^2)$. By the definition on the path weight (transition between vertices are independent) we do not need to save all the $\square_i$ obtained to the step k, but only G_1, G_k and G. Thus the memory size is proportional to M^2.

The modelling of particles throwing is performed in accordance with choice coefficients by the same way as for the plane. For T particles time complexity is $O(TM)$.

We see that as opposed to the case of the plane, for the modelling on a surface the matrix structure is essential. In fact this matrix saves an information about the triangulation structure.

The calculation of G for M large enough is time-consuming and when computing the aggregate one time we do not obtain a considerable advantage. But, as a rule, the studying of dynamics of processes on a surface to collect statistical data requires repeated experiments. Hence it is the great advantage that G is calculated one time and reused in what follows without changing.

We implemented two algorithms to construct an aggregate on irregular triangle net: proposed in [2] and based on a priori estimation and choice coefficients. The experiments were performed for the surface $\frac{x^2}{4} + \frac{y^2}{4} - z^2 = 1$ and the following parameter values: NA (the number of aggregate) is equal to 1 and 10, N = 300, M = 5000, T = 1000. Run times are shown in the table.

NA	Basic algorithm	Optimized algorithm
1	26 m. 12 s.	29 m. 43 s.
10	4 h. 47 m. 33 s.	31 m. 58 s.

6. CONCLUSION

The optimization of the algorithm of the construction of aggregate in accordance with DLA model on irregular triangle net has been designed and implemented. It is efficient when repeating experiments. Such an optimization may be applicable to other models of cluster forming.

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