AN INFLUENCE OF VARIOUS FIELDS ON DIFFUSION LIMITED AGGREGATION PROCESS

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SUMMARY

A computer simulation of Diffusion Limited Aggregation (DLA) processes on a square lattice by Monte-Carlo technique has been done. An influence of various fields (external directional fields, attracting interface fields) on the DLA clusters has been investigated and expressed in terms of scaling laws and fractal geometry.

INTRODUCTION

Monte-Carlo simulation of various kinetic processes reached quite a new level since the easy access to the fast computers [1,2]. DLA processes are ones of the most intensively studied aggregation phenomena within the wide class of treated by this way [3,4]. The resulting aggregates frequently have a complex random structure with a low average density [3], and are often described in such rough terms as fine, ramified, wispy or tenuous, i.e. the structures are suspected to have their noninteger (fractal) dimensions [4] significantly less than dimension of the respective Euclidean space in which they are allowed to grow.

The lack of a quantitative description of random clusters has inhibited the development of systematic studies of their properties. Recently, it has been recognized that some properties of these structures can be described in terms of the fractal geometry [5].

The fractal geometry does not provide a complete description of the structure of the ramified aggregates. However, it does provide a theoretical tool for developing a better understanding of many from the important properties of, at least, some types of clusters such as DLA aggregates [6]. DLA has originally been proposed to describe the formation of soot particles in the air or the flocculation in colloidal aggregates [7]. Later it was realized that in these experimental situations larger clusters are not only formed by the aggregation of dust but also essentially through the coagulation of aggregates of comparable size and so a model of cluster-cluster aggregation for description of DLA phenomena has also been used [8]. In the meantime much better experimental realizations for DLA emerged and a good agreement in the critical exponents between the model and the measurements has been generally reached [9,10].

In this paper we focus on fingering the DLA structures produced by so called Eden-cluster-producing algorithm [11], and investigate, mainly qualitatively, the typical DLA structure (Witten and Sander [7]) and its modifications caused by different additional fields.

RANDOM WALK ON A SQUARE LATTICE

In general, the random walk on the square lattice may be described by a discretized form of the Fokker-Planck (or generalized diffusion) equation [12]

$$\mathbb{P}_k(x) = \sum_{i=1}^{2d} \mathbb{P}_{k-1}(y_i)\, W_{k-1}(x/y_i) \qquad (1)$$

where

$\mathbb{P}_k(x)$ is the probability of finding a walker at the point x after k steps,

$\mathbb{P}_{k-1}(y_i)$ is the probability of finding a walker at the point y_i after k-1 steps,

and

$W_{k-1}(x/y_i)$ represents the transition probability (from y_i to x in one of each four possible directions).

It is obvious that d stands for dimension of Euclidean space, and is equal 2 in this case.

Note that the process represented by eq.(1) is nonstationary one, and therefore, there exist the indexes k and k-1 .

The situation described by eq.(1) can also be schematically shown in Fig.1.

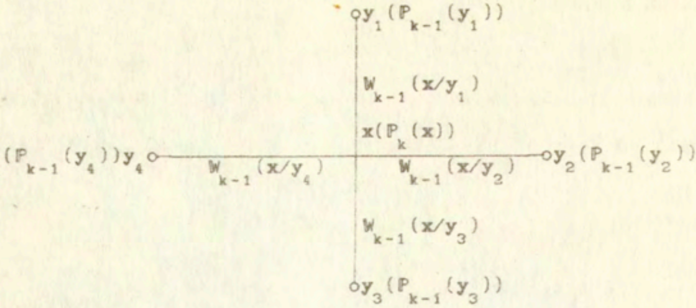

Fig. 1.

The random walk on a square lattice by means of probability diagram.

DIFFERENCE SCHEME

It can be easily verified that the simplest nontrivial case that is included in eq. (1) is as follows

$$\mathbb{P}(x) = \frac{1}{4} \sum_{i=1}^{4} \mathbb{P}(y_i) \qquad (2)$$

what holds when

(i) $d = 2$

(ii) k and $k-1$ do not exist

(iii) $\forall_i \ \mathbb{P}(x/y_i) = \frac{1}{4}$.

The above is true when the random walk is stationary, i.e. independent of time (lack of k and k-1 indexes), and transition probability is time-independent and equal to $\frac{1}{4}$ for each of four possible directions.

The random walk of this type is said to be stationary (SRW) or

Laplacian (LRW).

Let us define the LRW in terms of difference schemes [13]

$$u_{i,j} = \frac{1}{4}\,[u_{i,j+1} + u_{i+1,j} + u_{i,j-1} + u_{i-1,j}] \qquad (3)$$

what is valid when

$$\frac{h_x}{h_y} = 1 \qquad (4)$$

where

h_x - constant step (lattice unit) along x-direction

h_y - " " " " y-direction,

and

$u_{x,y}$ - probability of finding a walker in (x,y)-discrete point.

The computational implementation of difference scheme (3) is based on utilizing a [0,1]-random number generator and its ability to produce the numbers, homogeneously distributed between 0 and 1, e.g. if the generator produces a number $x_s \in [0,\frac{1}{4}]$ then the walker is allowed to go into the positive values of y-direction, etc.

CONTINUOUS VERSION OF DIFFERENCE SCHEME

The continuous version of difference scheme (3) is represented by Laplace's equation, namely

$$\Delta u = 0 \tag{5}$$

where

Δ - Laplace's operator

and

$u = u(x,y)$,

with appropriate BCs (absorbing boundary condition at the internal boundary and constant nonzero boundary condition at the external boundary).

We have shown recently [14,15] how to treat the stationary DLA process for various boundary conditions.

WITTEN-SANDER MODEL

In the DLA model of Witten and Sander [7] particles are added, one at a time, to a growing cluster of particles via stationary random walk. The particles are supposed to come from infinity but are actually launched from a random position on a circle which just encloses the cluster (in this case the launching circle has a radius of $r_{max} + 5$ lattice units, where r_{max} is the maximum radius of the cluster measured from the original "seed" or growth site). Two typical random trajectories exist in this process. One of those eventually brings the random walker into an unoccupied perimeter site. At this stage growth occurs and, then, a new walker is launched from the launching circle (whose radius increases as the cluster grows). The second of two typical trajectories moves the particle a long distance away from the cluster and this is terminated after reaching the killing circle, i.e. a radius of $3r_{max}$ in this simulation.

The procedure described above is repeated many times until a large aggregate is formed. The aggregate obtained by means of afore described procedure can be named the typical (or Witten-Sander) cluster (t-DLA cluster).

It is also quite interesting to examine how an external (nondiffusional) field or specific field alterations connected with the cluster interface, or, both these things together, may change properties of the t-DLA cluster. Therefore, we decided to simulate and investigate the following:

- DLA cluster in regular diffusion field (t-DLA cluster),
- DLA cluster influenced by external field (ef-DLA cluster),
- DLA cluster with attracting interface (ai-DLA cluster) and, finally
- DLA cluster influenced by an external field and with attracting interface, i.e. the combined DLA cluster (com-DLA cluster).

GEOMETRICAL CATEGORIZATION OF THE FRACTAL DIMENSION

There are a few ways of defining the dimension of a given geometrical object. We use here so called all purpose fractal dimension d_F [4] which tells us how many (with respect to the whole number of sites in the space) of unoccupied sites in the space in which the aggregate is embedded, will be occupied until it stops to grow (the limit $N \Rightarrow \infty$ is expected in this case; N - number of particles in the cluster).
There is always

$$d_F \le d \tag{6}$$

but the equality holds only in the case of compact aggregates as in case of Eden clusters or ballistic aggregates [16].
For deterministic fractals such as Sierpiński-gasket or Cantor-set [17] d_F can be easily obtained in the exact form [18].
For statistical fractals, like DLA aggregates, d_F may be estimated from the scaling laws [19] given mostly in the form of [4,20]

$$R \propto N^{\nu} \tag{7}$$

or

$$\rho(r) \propto r^{-a} \tag{8}$$

where

- R - average radius of the cluster,
- ρ - density-density correlation function,
- r - current radius of the cluster,
- ν,a - characteristic exponents.

The fractal dimension d_F is hidden in the critical exponents ν and α, namely

$$d_F = \frac{1}{\nu} \qquad (9)$$

or

$$d_F = d - a \quad . \qquad (10)$$

It is also worth to notice that recently another approach to critical exponents describing the cluster structure has been proposed. The concept is based on so called $f(\alpha)$ spectrum (multifractality). In this case the fractal dimension d_F can be obtained directly from $f(\alpha)$ which plays the role of generalized fractal dimension [21,22].

RESULTS AND DISCUSSION

The modifications of the classical Witten-Sander DLA simulations have been started by Meakin in 1983 who showed effects of particle drift on DLA structure [23]. Vicsek, in turn, has investigated the influence of curvature of growing DLA clusters on their further evolution [24].

In this paper we tried to develop these ideas further. We have started our simulation with classical (typical) DLA process (Fig.2)

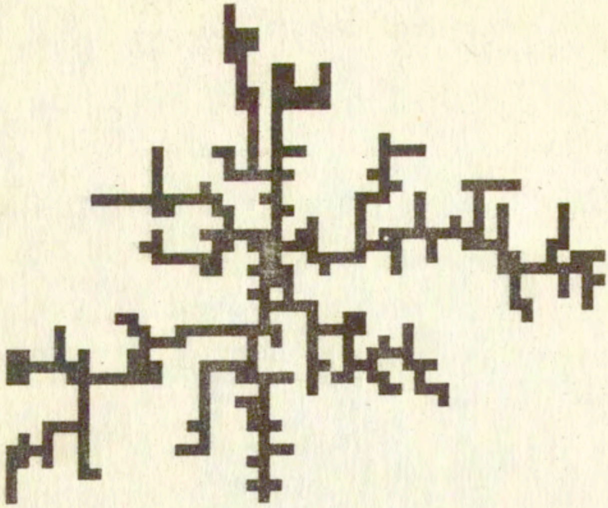

Fig.2

A typical (or classical) DLA cluster.

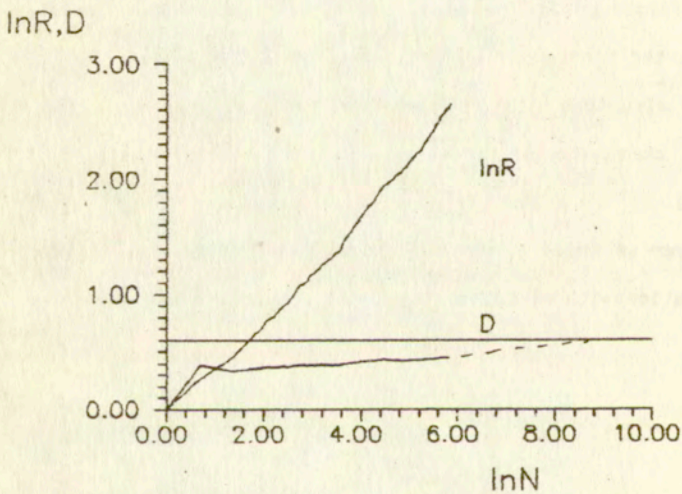

Fig.3

Average radius of t-DLA cluster and its derivative vs number of particles in the cluster (see eq.7).

Some of the quantitative measures of the aggregate from Fig.2 are presented in Fig.3

As can be seen from Fig.3 the derivative (curve D) has not reached its final asymptotic value yet. Constant, asymptotic value of this curve can be directly used to get the fractal dimension of a given cluster (see eq.9). It needs, however, much more computer time (so far one run consumed ca.16 hours), what can be roughly estimated from the ratio of solid and doted lines.

An influence of an external field (x-directional field) on DLA process can be seen in Fig.4.

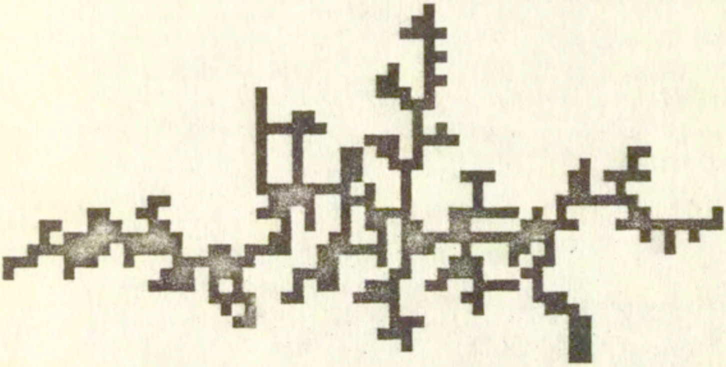

Fig.4.

DLA cluster with x-directional external field.

Analogically to the previous case we plot in Fig.5 some physical characteristics of the structure from Fig.4

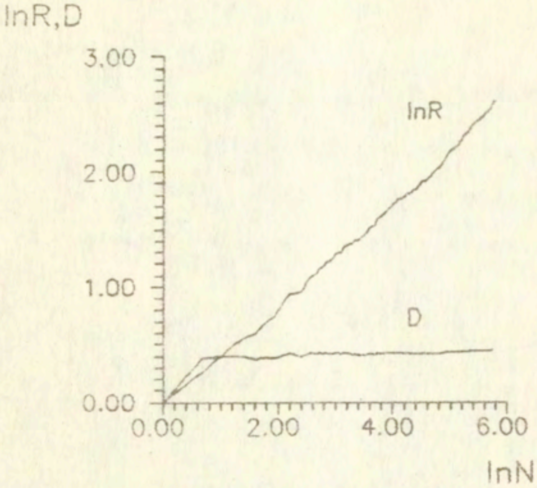

Fig.5.

Average radius of ef-DLA cluster and its derivative vs number of particles in the cluster.

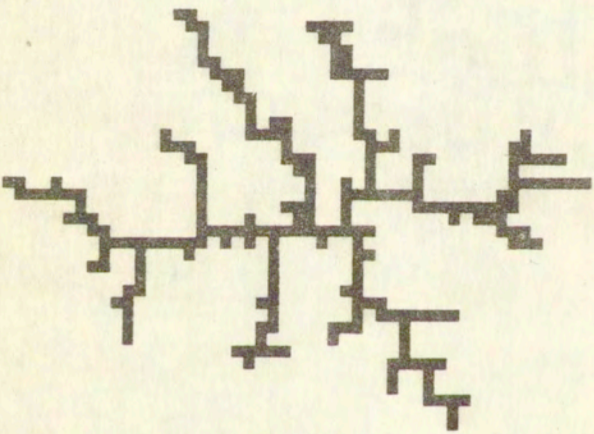

Fig.6.

DLA cluster with attracting interface.

When an effect of capturing the particles by the interface of a given cluster is taken into account the structure looks like that presented in Fig.6

The quantitative characteristics of the process are plotted in Fig.7

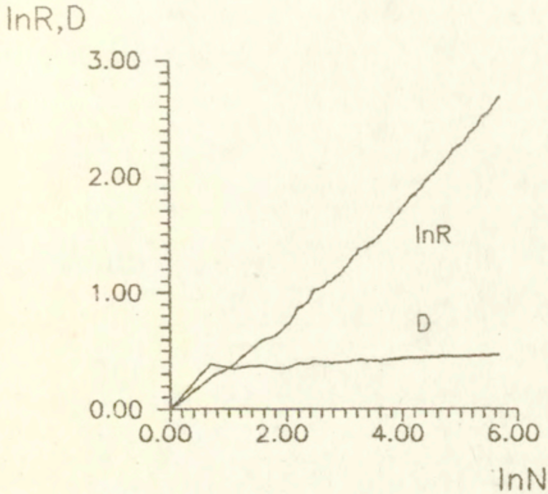

Fig.7.

Average radius of ai-DLA cluster and its derivative versus number of particles in the cluster.

The picture presented below shows how these two aforementioned fields together modify the structure of a given aggregate

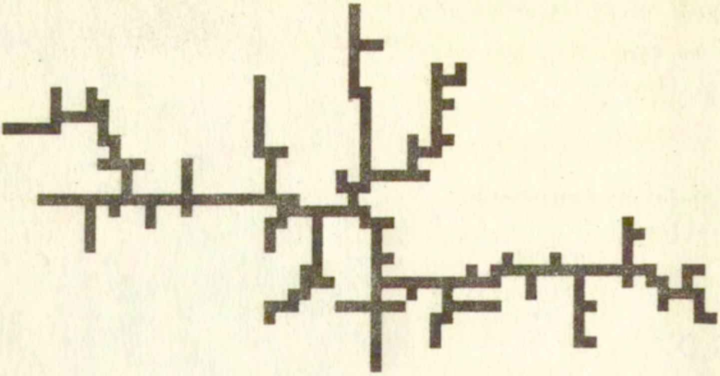

Fig.8.

"Two fields" DLA cluster.

As before, the main quantitative characteristics are shown in Fig.9

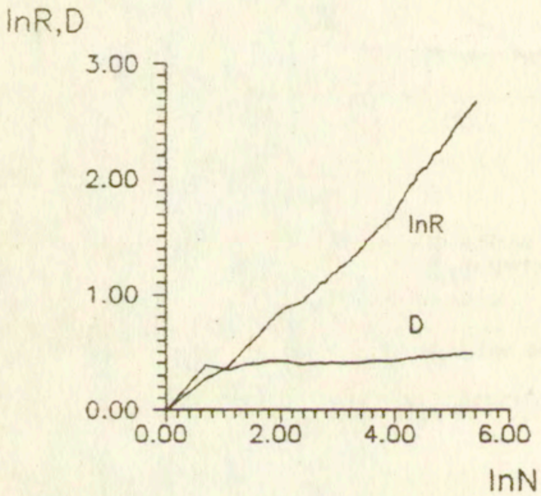

Fig.9. Average radius of com-DLA cluster and its derivative vs number of particles in the cluster.

One of the aims of our paper was to check whether some modifications of the growth rules, i.e. influence of an external field or presence of an attracting interface, or both these things together, may change the geometrical properties of the aggregate.
Bearing in mind the preliminary character of our results and being aware that the simulation have to be performed for larger clusters, we can see that, at least in case of DLA influenced by external field (see Fig.5), that the fractal dimension can differ from the classical case.
Finally, we can conclude as follows

- the results obtained in this work have rather preliminary character,
- full simulations are going to be performed in the nearest future with necessary optimization of existing program,
- the fractal dimension of t-DLA and com-DLA clusters is equal to ca. 1.7, i.e. has a value estimated by Witten and Sander,
- the "fractal dimension " of ef-DLA and ai-DLA clusters is equal to ca. 2.2, what violates basic inequality (6).

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