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LETTER TO THE EDITOR

Exact enumeration method for diffusion-limited aggregation

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Abstract. We present a new method for growing and analysing diffusion-limited aggregates (DLA). The method is based on the exact enumeration approach which enables us to calculate exactly the probability density of a random walker starting from an outer circle (at $r = r_1$). The method yields the exact growth probabilities, p_i, of the perimeter sites, i, for a given configuration as a *function of time*. We study the histogram, $n(p)$, i.e. the number of perimeter sites having growth probability p, as a function of time, for several different boundary conditions. Our results suggest that the fluctuations in the survival times of the particle are very small compared with the large fluctuations in the growth probabilities. We find that at times of the order of r_1^2 *all* growth probabilities are essentially converged. Very long survival particles have only a negligible effect on the histogram $n(p)$ and thus on the DLA structure.

The study of growth processes and aggregation has been a subject of considerable interest in recent years [1–5]. Much effort has been invested to study the diffusion-limited aggregate (DLA) model introduced by Witten and Sander [6]. This is because the DLA model provides a simple example for a variety of phenomena in which the diffusion process is the dominant mechanism in the growth. The model is easy to formulate and shows the essential surprising features of fractal growth [3].

In this letter we present a new method for growing and studying DLA-type aggregates. The method is based on the exact enumeration method which was found useful in the study of diffusion in disordered media (for a recent review see [7]). The method enables us to enumerate exactly the probability density as a function of *time* of a random walker starting from an outer circle. In this method the growth probabilities for a given cluster configuration are determined *exactly*. The method is used to study several growth properties such as the *time-dependent* growth probability, the effect of the size of the outer circle, and the effect of different boundary conditions on the outer circle (absorbing or reflecting). Our results show that the fluctuations in the convergence times of the growth probabilities to their stationary values (characteristic survival times) are very small compared with the large fluctuations in the values of the growth probabilities.

The usual growth process is based on an external source of diffusing particles that aggregate on the cluster when they touch it. At the beginning one particle (a seed) is placed at the origin. Then particles are released one after the other from random positions on an outer circle or radius r_1 enclosing the seed (cluster). Each particle moves in a random walk fashion until it reaches a neighbouring site of the aggregate and becomes part of the growing cluster. At $r = r_2 > r_1$ an absorbing boundary is set and if a particle visits a site at distance $r > r_2 > r_1$ from the seed it is absorbed.

Our growth method is based on simulating the above process using the exact enumeration method for diffusion [7]. The key of the exact enumeration procedure is that the probability of a random walker being at site i at time t is determined solely by the probabilities of being at the nearest neighbours of site i at time $t-1$. At $t=0$ a seed particle is fixed at the origin and at sites in the outer circle of radius r_1 numbers equal to 1 are uniformly distributed. The value 1 represents the probability of a random walker to be at r_1 in $t=0$, i.e. $P(r_1, 0)=1$ (see figure 1). For a square lattice we use iteratively the equation

$$P(x, y, t)=\tfrac{1}{4}[P(x-1, y, t-1)+P(x+1, y, t-1)+P(x, y-1, t-1)+P(x, y+1, t-1)] \tag{1}$$

to find $P(\mathbf{r}, t)$ for any position $\mathbf{r}$ and time t. Equation (1) is used subject to the boundary conditions: (i) $P(\mathbf{r}_2, t)=0$ and (ii) each site on the perimeter $r=\mathbf{r}$ of the cluster is absorbing and thus $P(\mathbf{r}, t)$ is regarded as zero in the right-hand side of (1). The quantity $P(\mathbf{r}, t)$ is accumulated and represents the growth probabilities up to time t of the perimeter sites located at $\mathbf{r}$. A new site is chosen to grow randomly according to these probabilities and the process starts from the beginning, $t=0$, as illustrated in figure 1. We choose the time t for growing a new site such that $P(\mathbf{r}, t)$ reaches a plateau for all $\mathbf{r}$. In figure 2 we compare the time-dependence growth probabilities of several tip sites and fjord sites. It is seen that the large probability at the tip and the small probability at the fjords reach the plateau essentially at the same relatively short times. An interesting feature of our results which is also seen in figure 2 is the fact that, although there is a factor of 10^6 between the growth probabilities, the ratio between the convergence times to the asymptotic values (survival times) is less than two. Indeed we find that for times of the order of r_1^2 essentially all growth-sites probabilities reach

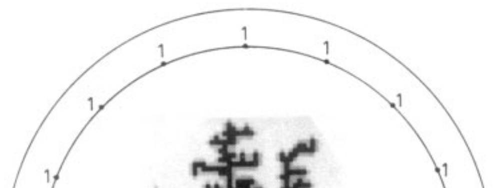

Figure 1. The DLA cluster (500 sites) grown using the exact enumeration method described in the text. The circles represent the boundary conditions used for the iterations of equation (1). The outer circle at $r=\mathbf{r}_2$, as well as the perimeter sites of the DLA cluster, are absorbing boundaries. The inner circle at $r=\mathbf{r}_1$ is under the condition that $P(\mathbf{r}_1, 0)=1$. For our numerical simulations we used a square lattice and the actual position of the 'ones' could not be taken exactly on the inner circle $\mathbf{r}_1$. We therefore chose lattice sites which are closest to $\mathbf{r}_1$. The larger is the cluster so the radius $\mathbf{r}_1$ is taken larger and the deviation from an exact circle becomes smaller.

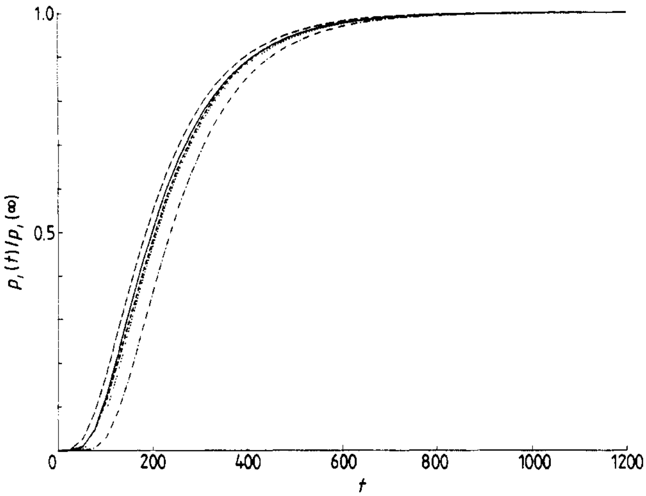

Figure 2. Plot of $p_i(t)/p_i(\infty)$ as a function of time for several fjord and tip sites. The $\cdots$ and —·—·— curves represent fjord sites with growth probabilities: $p_i(\infty) = 1.1\times10^{-6}$ and 5.2×10^{-8} respectively. The - - - - - and — — — curves represent tip sites with growth probabilities 1.1×10^{-2} and 4.9×10^{-2} respectively. The full curve represents a site with growth probability, 2.6×10^{-3}. The accuracy of the values found for $p_i(\infty)$ is determined only by the round-off errors in the calculations. We estimate these errors to be less than 10^{-40} thus not affecting our numerical results. Note the very small fluctuations in the convergence time compared with the large fluctuations in the growth probabilities.

a plateau. This justifies the use of our growth method at relatively short times, thus saving computing time. An example of a cluster grown up to 500 sites by this method is shown in figure 1.

An important measure [8-10] of an aggregate is the set of growth probabilities $\{p_i\}$, where i runs over all perimeter sites of the DLA cluster. This set is calculated here more generally as a function of time, i.e. the set of $P(\boldsymbol{r}, t)$. The limit $t\to\infty$ of $P(\boldsymbol{r}, t)$ represents the stationary set of growth probabilities. In figure 3 we show the histogram $n(p)$, i.e. the number of growing sites having the growth probabilities $p = P(\boldsymbol{r}, t)$, for several time values and for the aggregate shown in figure 1. We see that most of the changes occur at very small times and $n(p)$ converges quite rapidly.

This growth method can be easily applied to study different cases of boundary conditions. We studied the effect of changing the radius r_1 and r_2 ($r_2 - r_1 = 5$ was chosen constant). Our results for $n(p)$ suggest that increasing the outer radius has only a negligible effect on $n(p)$ and thus on the aggregate structure. We also compared the cases of absorbing and reflecting boundary conditions at $r = r_2$. We find that the histograms $n(p)$ are very similar in both cases, see figure 4. This indicates that growing DLA using absorbing or reflecting boundary conditions at r_2 have essentially the same effect on the cluster structure.

In summary we have presented a new growth method for DLA-type aggregates. The main advantage of the method is that it yields exactly the *time-dependent* growth probabilities in addition to the *stationary* ($t\to\infty$) probabilities obtained by other techniques [11]. Our method yields a clear criterion for the time needed to stop the diffusion process and to let the growth process occur. We find that the fluctuations in the convergence time of $p_i(t)$ are very small when compared with the huge fluctuations in their values.

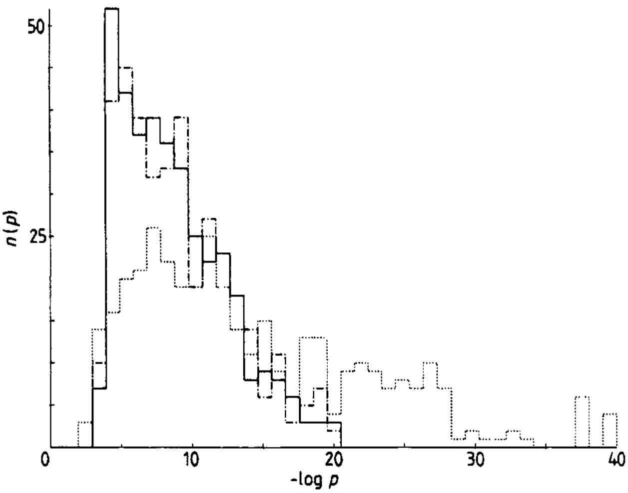

Figure 3. Plot of the histogram, $n(p)$ for several values of times. The dotted line represents the short-time data $t = 50$. The chain line represents $t = 300$ and the full line $t = 1600$. It is seen that small changes occur between $t = 300$ and $t = 1600$, indicating the convergence of our method in relatively short timees.

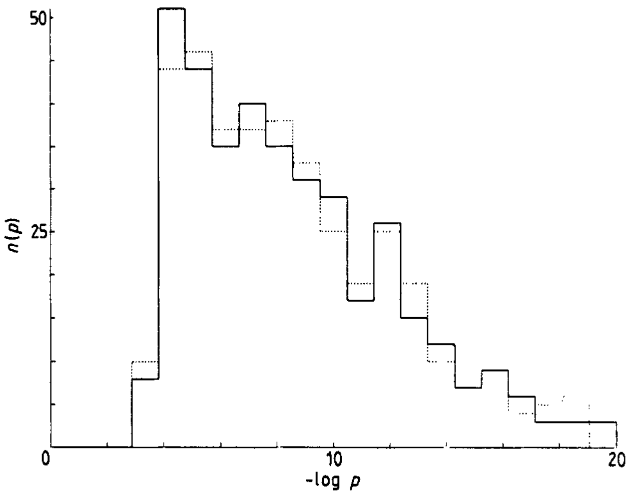

Figure 4. Comparison of $n(p)$ for absorbing (dotted line) and reflecting (full line) boundary conditions.

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