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LETTER TO THE EDITOR

Static and dynamic scaling for chain–chain aggregation in two dimensions

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Abstract. Chain-chain aggregation is studied on the square lattice by Monte Carlo simulations. The fractal dimension of the aggregates is found to be $D = 1.32 \pm 0.04$. The results support the dynamic scaling relation $n_s(t) \sim s^{-2} f(s/t^z)$ with $z = 0.72 \pm 0.02$.

A rich variety of physical phenomena such as aggregation, coagulation or polymerisation lead to the formation of branched random clusters (Friedlander 1977). A non-equilibrium growth model based on aggregation of clusters, proposed to describe the formation of such aggregates (Meakin 1983, Kolb *et al* 1983), displays interesting dynamic features in 2D (Vicsek and Family 1984, Kolb 1984, Botet and Jullien 1984, Meakin *et al* 1985, Jullien 1986 and references therein): the cluster size distribution function $n_s(t)$ varies with s (cluster size) and t (time), according to

$$n_s(t) \sim s^{-2} f(s/t^z) \tag{1}$$

where the scaling function $f(x) \sim x^{\delta}$ when $x \ll 1$ and $f(x) \ll 1$ when $x \gg 1$.

Besides these branched clusters, natural phenomena may also lead to the formation of unramified aggregates (chains). A model of linear diffusion-limited aggregation has recently been proposed (Debierre and Turban 1986, Bradley and Kung 1986) as a first attempt to simulate these phenomena. In this letter we introduce a new dynamic aggregation process in which longer chains are grown by chain-chain aggregation.

At $t = 0$, N_0 monomers are randomly distributed on a $L \times L$ square lattice with periodic boundary conditions. They are then allowed to perform random walks on the lattice. When two monomers meet (i.e. arrive at first-neighbour positions) they stick to form a dimer. The process is continued and the chains may stick at both ends to form longer chains. The chains move rigidly as in the cluster-cluster aggregation model. As a consequence, inactive configurations may appear. In particular, closed loops which necessarily contain an even number of monomers remain inactive.

At each Monte Carlo step a chain (active or inactive) is chosen at random, independent of its size s, a one lattice unit move is attempted in a randomly chosen direction and the time is increased by an amount $\Delta t = s/N_0$ (Vicsek and Family 1984). To simulate the steric effects, we use reflecting boundary conditions (i.e. no part of the diffusing chain may visit an already occupied site). We have performed 100

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simulations on a 256×256 lattice for the density $\rho_1 = N_0/L^2 = 1/32 \simeq 0.03$ and 50 simulations on a 400×400 lattice for two values of the density, ρ_1 and $\rho_2 = \rho_1/2$. The time development of the chain–chain aggregation is illustrated in figure 1.

The first quantity of interest is the mean radius of gyration R_s of a s-site chain which is related to its fractal dimension D by

$$R_s \sim s^{1/D}. \tag{2}$$

Using equation (1), it is easy to show that, at a given time t, we have in the same way

$$\bar{R} \sim S^{1/D} \tag{3}$$

where

$$\bar{R} = \sum_s s n_s R_s \left(\sum_s s n_s \right)^{-1} \tag{4}$$

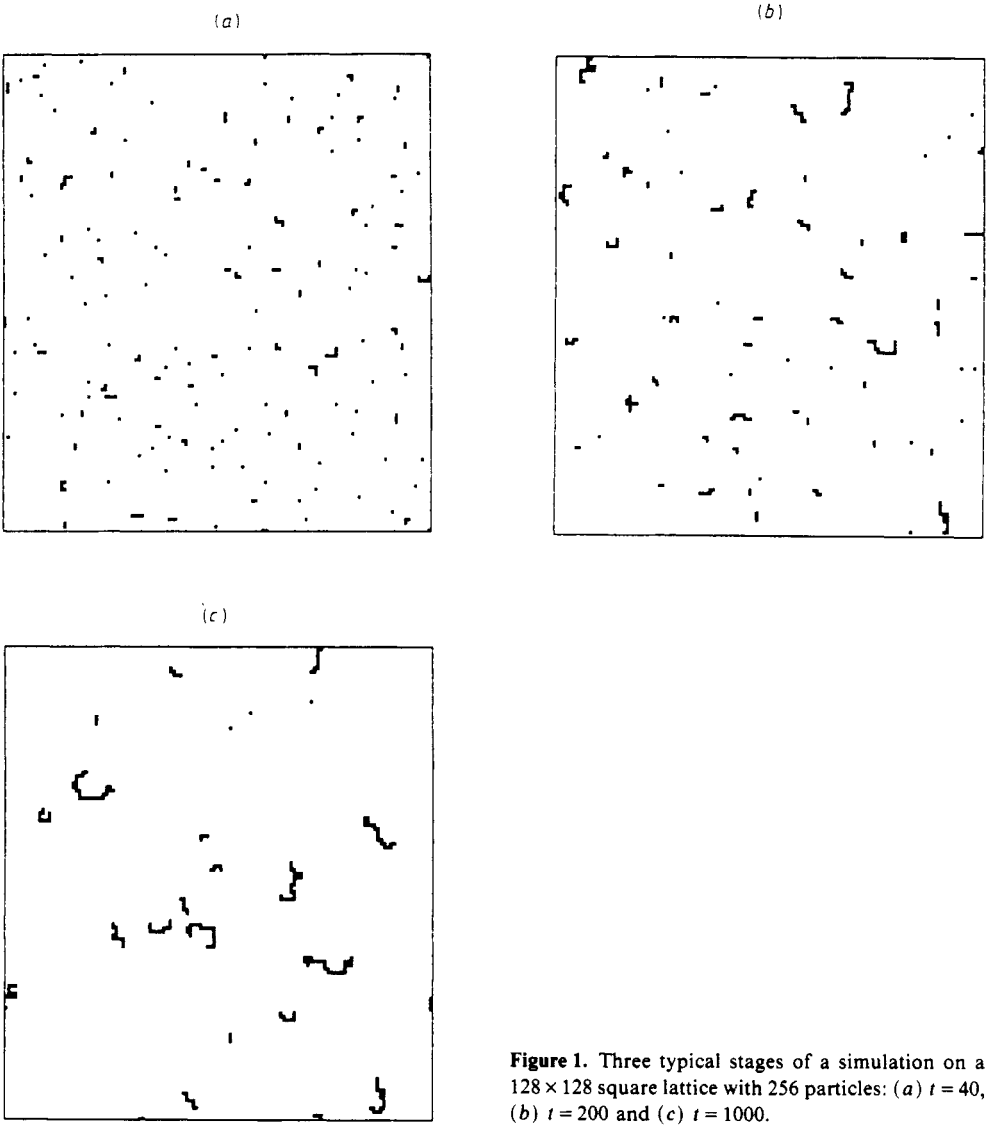

Figure 1. Three typical stages of a simulation on a 128×128 square lattice with 256 particles: (*a*) $t = 40$, (*b*) $t = 200$ and (*c*) $t = 1000$.

is the mean R_s value for all the chains present at time t and

$$S = \sum_s s^2 n_s \left(\sum_s s n_s \right)^{-1} \tag{5}$$

is the mean cluster size. The three D values obtained from the log-log plot of $\bar{R}$ against S (figure 2) for $L = 256$ and $L = 400$ with a density ρ_1 and $L = 400$ with ρ_2 are very close, suggesting no appreciable size or density effects. They lead to the following estimate:

$$D = 1.32 \pm 0.04 \tag{6}$$

near to the SAW value $D = \frac{4}{3}$.

We have also calculated the chain size distribution function given by

$$n_s(t) = N_s(t)/L^2 \tag{7}$$

where $N_s(t)$ is the number of chains of size s at time t and the mean cluster size $S(t)$.

For large t values, $S(t) \sim t^z$, and a fit of $\ln S(t)$ against $\ln t$ gives (figure 3)

$$z = 0.72 \pm 0.02. \tag{8}$$

At the higher density ρ_1, this curve saturates. For long times, large chains appear which prevent each other to move, freezing the time evolution.

According to equation (1), in the limit $x \ll 1$

$$n_s(t) \sim s^{-\tau} \qquad \tau = 2 - \delta \tag{9}$$

$$n_s(t) \sim t^{-w} \qquad w = \delta z = (2 - \tau) z. \tag{10}$$

The curves $\ln N_s(t)$ against $\ln t$ for different s values are displayed in figure 4. From the slope one gets

$$w = 1.5 \pm 0.2 \tag{11}$$

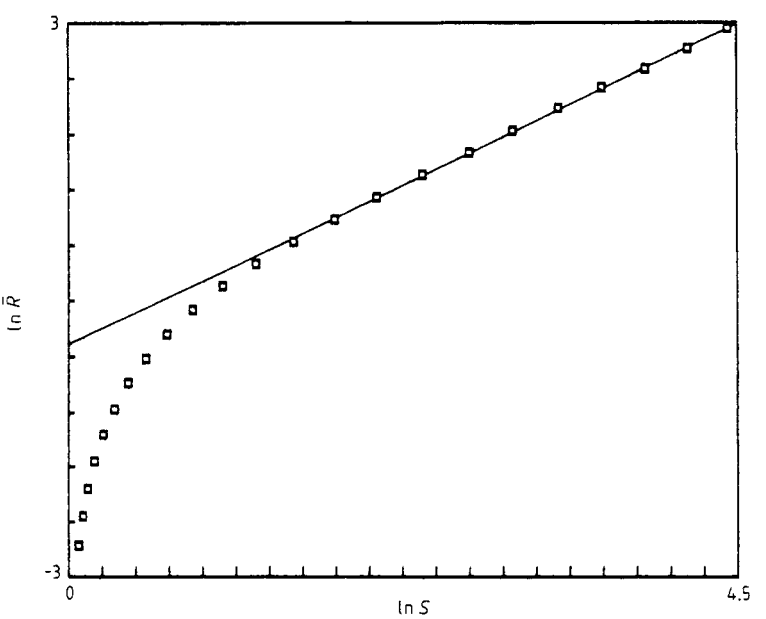

Figure 2. $\ln \bar{R}$ plotted against $\ln S$ for $L = 400$ and $\rho_2 = \frac{1}{64}$. The slope of the straight line gives $1/D = 0.76 \pm 0.02$.

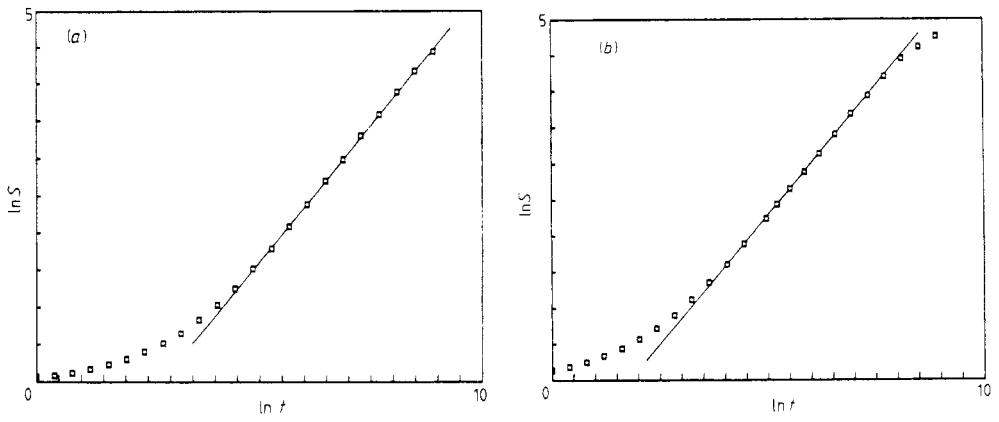

Figure 3. ln S plotted against ln t for $L = 400$: (a) $\rho_2 = \frac{1}{64}$ and (b) $\rho_1 = \frac{1}{32}$. The slope gives the exponent $z = 0.72 \pm 0.02$. Notice the saturation effect for long times at the larger density.

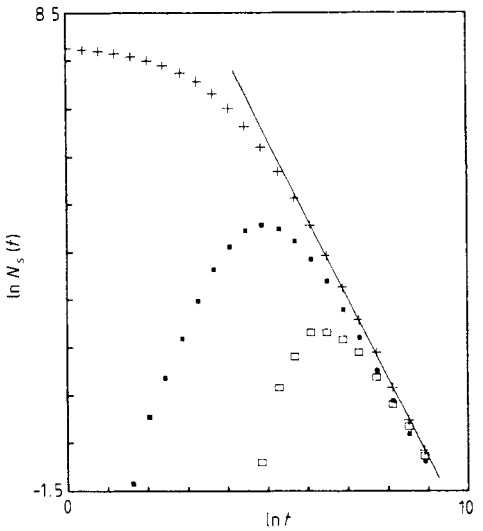

Figure 4. ln $N_s(t)$ plotted against ln t ($L = 400$, $\rho_2 = \frac{1}{64}$) for (+) $s = 1$, (■) $s = 5$ and (□) $s = 15$. From the slope one gets $w = 1.5 \pm 0.2$. Notice that the curves coalesce for long times.

The curves ln $N_s(t)$ against ln s are shown in figure 5 at different times. Even s values have been discarded since they contain the contribution of inactive closed loops. The envelope of the curves is a straight line with a slope close to 2, in agreement with (1) (Meakin *et al* 1985). This value results from the time independence of the density $\rho = \Sigma_s s n_s$. The slope of the linear part at large time gives

$$\tau \simeq 0. \tag{12}$$

These results support the Vicsek-Family scaling law (10).

The dynamics of cluster-cluster aggregation has been studied with a size-dependent cluster diffusion coefficient:

$$D_s \sim s^{\gamma}. \tag{13}$$

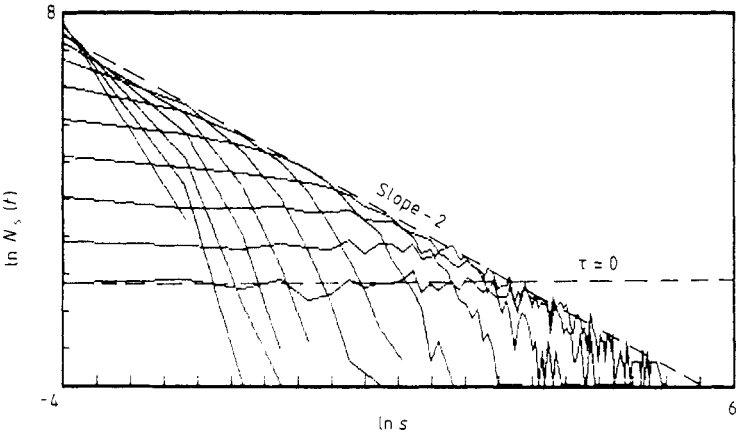

Figure 5. ln $N_s(t)$ plotted against ln s ($L = 400$, $p_2 = \frac{1}{64}$ for different values of the time ranging from $t = 1$ to $t = 7500$. The slope of the envelope is near to -2 as indicated by the broken line. For large values of t the curves have a wide horizontal part and $\tau \simeq 0$.

When $\gamma \gg 0$ the large clusters move faster, leaving a lot of small clusters unaffected and then $N_s(t)$ is a monotonic decreasing function of s. On the other hand, when $\gamma \ll 0$ the small clusters diffuse rapidly and join together to build larger clusters; then one gets a bell-shaped size distribution. At a critical value γ_c the transition between the two regimes is characterised by a plateau in the size distribution leading to $\tau = 0$. This transition is observed for $\gamma_c = -\frac{1}{4}$ in 2D and $\gamma_c = -\frac{1}{2}$ in 3D (Meakin *et al* 1985). In our simulations where the diffusivity is size independent we get $\tau \simeq 0$ so that $\gamma_c \simeq 0$ for the chain-chain aggregation in 2D.

Assuming the scaling relation

$$K(\lambda s_i, \lambda s_j) = \lambda^{2\omega} K(s_i, s_j) \tag{14}$$

for the kernel in the Smoluchowski equation (Smoluchowski 1917) the exponent z may be related to ω through (Botet and Jullien 1984)

$$z = (1 - 2\omega)^{-1}. \tag{15}$$

Our value $z \simeq 0{\cdot}72$ corresponds to $\omega \simeq -0.2$ so that we are in the flocculation regime ($\omega < \frac{1}{2}$).

When the aggregation is diffusion-limited a scaling argument (Kolb 1984, Botet and Jullien 1984) leads to

$$z = [1 - \gamma - (d-2)/D]^{-1}. \tag{16}$$

This relation gives $z = 1$ in 2D when $\gamma = 0$, to be compared to $z \simeq 0.72$ in our simulations. It follows that chain-chain aggregation is not simply diffusion-limited. A systematic study of the influence of the diffusivity is required to clarify the aggregation process.

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