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Fractal geometries in decay models

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Abstract. Results of computer studies of the geometries produced by two distinct decay models are present. While one of the models (diffusion-limited decay) results in compact clusters, the other (random-walk decay) produces ramified clusters with the Hausdorf dimension (d_f) equal to 1.75 ± 0.03 and 2.34 ± 0.03 in two and three dimensions respectively. The spectral dimension (d_s) is found to be 1.68 ± 0.13 and 1.31 ± 0.04 for $d = 2$ and 3.

There have been many recent studies of universal geometries following the pioneering work of Mandelbrot (1977). Examples include clusters at the percolation threshold in ordinary percolation (static) (see, e.g., McKenzie 1976, Stauffer 1979, Stanley 1977) and invasion percolation (dynamic) (Chandler *et al* 1982, Wilkinson and Willemsen 1983). More recently considerable attention has been focused on growth models. It has been demonstrated that diffusion-limited aggregation (Witten and Sander 1981, Meakin 1983a, b, Kolb *et al* 1983, Muthukumar 1983, Gould *et al* 1983) leads to ramified clusters in contrast to the compact structures obtained by the Eden growth process (Eden 1961, Peters *et al* 1979). The reserve process of the decay of a given structure is of considerable interest in such diverse fields as biology and corrosion chemistry. In this paper we report the results of the first studies of the decay of compact clusters.

Our numerical studies have been carried out on a two-dimensional lattice for two decay models namely random-walk decay (RWD) and diffusion-limited decay (DLD). The starting point for the modelling is a regular two-dimensional compact lattice of L^2 particles (A) placed on a larger lattice with the same lattice spacing. We now consider the annihilation of the A particles by a diffusing reagent B introduced at some site of the larger lattice far away from A. The fundamental difference between the RWD and the DLD models is in the annihilation potency of the reagent B. In the first case we model the decomposition of structures by autocatalytic enzyme reactions (Wold 1971), corrosion etc, by postulating that a single B particle is capable of annihilating an infinite number of A particles. In contrast, the DLD model assumes that any B particle can annihilate only one A particle.

The DLD model can be thought of as a model for the reverse process of diffusion-limited aggregation (DLA). B particles are introduced, one at a time, far away from A. The particle undergoes diffusion until it encounters one of the A particles. The A and B particles annihilate each other and the next B particle is now introduced into the system. The DLD is followed as a function of the number of A particles remaining on the lattice. During the decay process, the radius of gyration, R_g, defined by

$$R_g^2 = \frac{1}{N_l} \sum_i r_i^2 \tag{1}$$

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of the largest connected cluster is computed. Here, N_l is the total number of particles in the cluster and $\boldsymbol{r}_i$ is the position vector of the ith particle measured from the centre of mass of the cluster.

Our DLD simulations have been carried out on a square lattice for $L = 128$, 96, 64 and 32. For each of these L values, the root-mean-square radius of gyration of the largest cluster has been computed as an average over 10 realisations for $\Phi = 0.875$, 0.75, 0.625, 0.5, 0.375, 0.25 and 0.125. Φ is the coverage defined as the fraction of the remaining A particles. We find that in all of the above cases this unreacted cluster is compact within the statistical error with the Hausdorf dimension $d_f \approx 2$.

It is not unexpected that the original compact A cluster does not become ramified due to this decay process. The reagent particles B are effectively screened from entering the interior of the cluster and almost entirely react at the surface. It is interesting to ask what the DLD model would yield if the original cluster were not compact. In particular, if the original cluster were one obtained by the process of DLA, one might speculate that the process of DLD would lead to the DLA process running in reverse.

We now turn to the RWD model. Operationally, the simulation is identical to the DLD model described above with the following important differences. (1) Since a single B particle is capable of annihilating an infinite number of A particles, only *one B* particle is introduced into the lattice. (2) Once the B particle encounters the A cluster, it is assumed that for the motion of the B particle the lattice has L^2 sites, corresponding to the sites originally occupied by the A particles, with *periodic boundary conditions.* (3) The B particle then undergoes a random walk annihilating all the A particles it encounters. The walk of B is taken to be purely random so that no restriction is placed on B returning to sites it has already visited. (4) This procedure is continued until the decay threshold is reached at which point the A particles form a connected cluster which barely pervades to all the boundaries. (5) Discarding all smaller clusters, we analyse the geometry of the barely pervading cluster. We compute the density-density correlation function of the N_t particles in the cluster

$$C(r) = \frac{1}{N_t} \sum_{r'} \rho(r')\rho(r'+r) \tag{2}$$

$\rho(r)$ is defined to be 1 for the occupied site and 0 otherwise.

Figure 1 shows $\langle C(r) \rangle$ averaged over 50 such simulations starting with a compact object of 96×96 particles on a square lattice. The data are consistent with an algebraic decay of $\langle C(r) \rangle$ for r greater than a few lattice spacings. $\langle C(r) \rangle$ levels off for r comparable to the size of the compact cluster because of the periodic boundary conditions. To estimate the statical error due to the averaging over 50 realisations, we have carried out three other batches of 50 realisations for $L = 96$. Similar decay studies for a compact object of 63×63 particles have been carried out to study the effects of finite sizes. We have carried out identical studies to that described above for a triangular lattice, as well. A summary of our results is shown in figure 2. The data of the various batches of different sizes and lattices shown in the figure have been shifted by an arbitrary amount with respect to each other along the log $C(r)$ axis so that they all overlap for one particular value of r. All the results are consistent with a power law decay of $\langle C(r) \rangle$

$$\langle C(r) \rangle \sim r^{-0.25 \pm 0.03}. \tag{3}$$

Since the dependence of $\langle C(r) \rangle$ on the Hausdorf dimension d_f describing the geometry

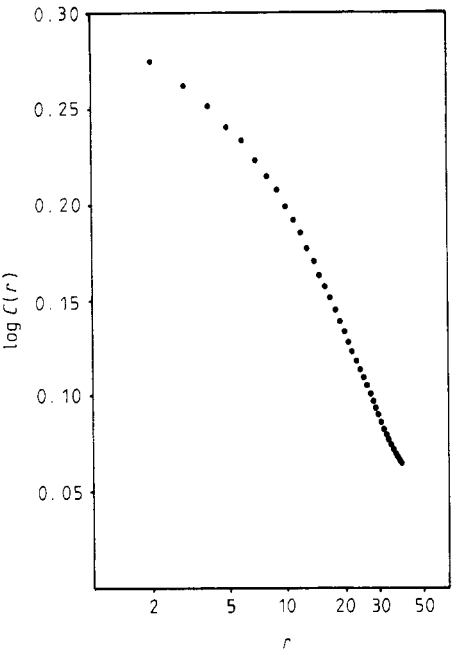

Figure 1. Plot of $\log_{10}\langle C(r)\rangle$ against r for RWD on a 96×96 square lattice. The average as been taken over 50 realisations.

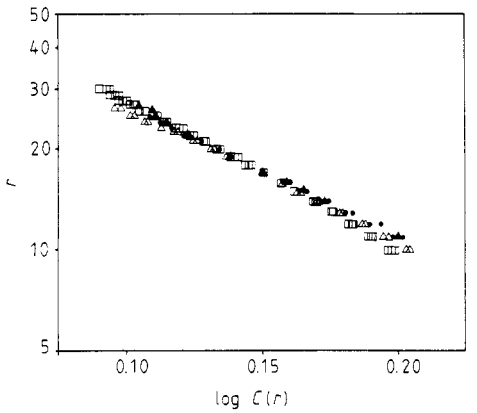

Figure 2. Plot of r against $\log_{10}\langle C(r)\rangle$ for RWD for different lattices and different sizes. □ = square lattice, $L=96$; △ = triangular lattice, $L=96$; ● = square lattice, $L=63$; ▲ = triangular lattice, $L=63$. To facilitate easy comparison, the curves corresponding to the different symbols have been shifted with respect to each other in the $\log\langle C(r)\rangle$ direction.

of the pervading cluster is $\langle C(r)\rangle \sim r^{d_f-d}$

$$d_f = 1.75 \pm 0.03. \tag{4}$$

Within the accuracy of the simulations, d_f appears to be universal with respect to the lattice details and the size of the compact cluster. Figure 3 shows a typical decay cluster obtained on a square lattice with $L=148$.

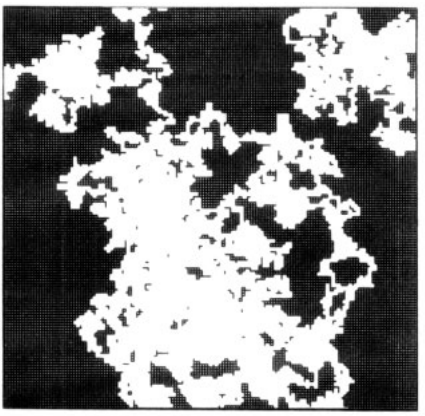

Figure 3. RWD clusters (in black) on a 148×148 square lattice at the decay threshold. Our analyses have been carried out only on the pervading cluster.

We have carried out similar studies in $d = 3$ on a simple cubic lattice containing up tc $50 \times 50 \times 50$ sites. Our results are summarised in table 1. We have also carried out calculations of the spectral dimension (Alexander and Orbach 1982, Rammal and Toulouse 1983) $d_s = 2d_f/d_w$ in both $d = 2$ and 3. d_w is the dimension of a random walk on the fractal, defined by $N_w \sim (\xi_w)^{d_w}$ where ξ_w is the RMS displacement of a random walker after N_w steps. d_s may also be directly calculated using the relationship $N_c \sim (N_w)^{d_s/2}$ where N_c is the mean number of sites visited in N_w steps (Rammal and Toulouse 1983). It has been suggested that homogeneous fractals (Leyvraz and Stanley 1983) such as percolation clusters (Alexander and Orbach 1982) and Witten-Sander aggregates (Meakin and Stanley 1983) may possess a superuniversality in that d_s is independent of d. Our calculations show that the RWD clusters do not have this property. Curiously, d_s is found to decrease on increasing d from 2 to 3.

Our results were obtained by taking ten clusters each in $d = 2$ and 3 each containing $\sim 10\,000$ sites. 2000 walks of 400 steps each were carried out on each of the clusters. For example, figure 4 shows double logarithmic plots of ξ_w^2 against N_w and N_c against N_w in $d = 2$. Table 1 lists the values of d_s obtained directly from the decay of the correlation function and by using the formula $d_s = 2d_f/d_w$. Both methods yield consistent results.

In summary, we have carried out numerical studies of the geometries produced by two distinct decay models. In the case of the DLD model, compact clusters were obtained whereas the RWD model produces ramified clusters. The superuniversality hypothesis does not seem to hold for these clusters. Further, the fractal dimensionality is different from those obtained in percolation/invasion percolation or in any of the growth models leading to yet another universality class of model geometries.

Table 1. Summary of exponents obtained for RWD fractals in $d = 2$ and 3.

d	d_f	d_w	d_s (Measured directly)	d_s $(=2d_f/d_w)$
2	1.75 ± 0.03	2.17 ± 0.11	1.68 ± 0.13	1.61 ± 0.12
3	2.34 ± 0.03	3.56 ± 0.28	1.31 ± 0.04	1.31 ± 0.11

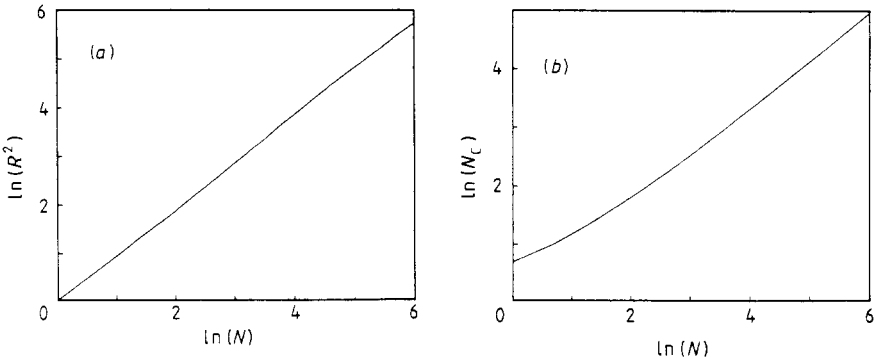

Figure 4. Double logarithmic plots of (*a*) mean-square end-to-end distance R^2, and (*b*) the mean number of sites visited, N_c, against the number of steps in the walk, N, for random walks on $d = 2$ RWD fractals.

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Note added in proof. B Mandelbrot has kindly pointed out that the RWD cluster formation process resembles the Brown hull constructions (Mandelbrot 1977, pp 242-3). However, RWD, unlike the Brown hull, stops at the decay threshold. Nevertheless, it is possible that despite this difference, the interior of the RWD cluster becomes compact as the sample size is increased, with only the boundary remaining fractal.

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