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LETTER TO THE EDITOR

A Monte Carlo renormalisation group for aggregation processes

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Abstract. A general Monte Carlo renormalisation group transformation for the static as well as the kinetic properties of aggregates is formulated and applied to different growth models: particle aggregation (DLA), cluster aggregation (CICI) and invasion percolation(IP). The leading critical exponent is determined numerically. For DLA, the first correction to scaling exponent has been estimated as well.

Recently, scaling ideas have been applied successfully to disordered structures that result from aggregation and growth processes. Both theoretical [1-4] and experimental [5-8] results were analysed systematically using this approach. With a few exceptions [9-13], the theoretical investigations have so far been limited to direct simulations of the growth process.

The renormalisation group transformation (RG) [14-16] provides a general framework for concepts such as universality and scaling in critical phenomena. The Monte Carlo RG (MCRG) [17-20] is a powerful method for calculating critical properties and it has been applied extensively to spin systems. Here I propose to use the MCRG for growth processes, exploring the fact that this approach does not require the Hamiltonian to be known explicitly.

First, let us define a MCRG for single-particle aggregation processes such as diffusion-limited particle aggregation [1] (DLA). Consider a square lattice and associate with it a coarse grained block lattice. With every four neighbouring sites on the original lattice, one associates a block site (figure 1(*a*)). A cluster is grown on the original lattice by adding particles one by one and—through the RG—a cluster is grown on the coarse grained lattice in parallel. The rule for generating the block cluster is a modified majority rule (figures 1(*b*)-1(*d*)): (i) if no two neighbouring sites in a cell on the original lattice are occupied its block site is empty (figure 1(*b*)); (ii) if two neighbouring sites are occupied the block site is occupied for the first RG studied (RG1) and empty for the second RG considered (RG2) (figure 1(*c*)) and (iii) if three or four sites of a cell are occupied its block site is always occupied (figure 1(*d*)). An additional rule ensures that every newly occupied block site is a nearest neighbour of the block cluster‡; this is illustrated in figures 1(*e*) and (*f*). The order of growth on the original lattice imposes the order of growth on the block lattice (along the arrows in figures 1(*e*) and

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‡ Without this rule the RG is defined in an extended configuration space. Numerical results indicate that this RG does not have a stable non-trivial fixed point for the models considered here.

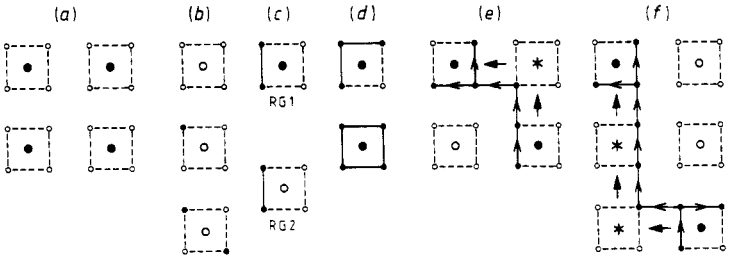

Figure 1. Definition of the RG on a square lattice. (*a*) The original lattice (○), the block lattice (●) and the cells associated with each block site. (*b*)-(*d*) The modified majority rule defining the RG. The two RG studied occupy a block site if its cell is spanned in one (RG1) or in both (RG2) directions. In (*e*) and (*f*) the growth on the original lattice (small arrows) and the corresponding growth on the new lattice (large arrows) are shown. The intermediate blocks (*) are occupied (even if the corresponding cells are not spanned) to assure that every site occupied is always a nearest neighbour of the cluster.

(*f*)). The RG defined in this way maps a single-particle growth process on exactly the same type of process on the coarse grained lattice. Analogous to the MCRG in critical phenomena [17], this statically defined RG also renormalises the dynamics. As a result, the growth rule on the block lattice is more complicated than the original one (and is not known explicitly).

To calculate the critical properties without knowing the Hamiltonian explicitly, the chain rule proposed in [18] is used. This assumes implicitly that the aggregate can be described in terms of short-range interactions, i.e. $H = K_{nn} \Sigma_{nn} \rho_i \rho_j + \ldots$ where $\rho_i = 0, 1$ is the particle density at site i. To characterise the RG one studies the behaviour of short-range correlations ($\langle \rho_i \rho_j \rangle_{nn}$, etc) under the transformation. Figure 2 shows the different interactions used in this study. 'Time-ordered' correlations (8-12 in figure 2) provide information on the growth aspect of the model.

An alternative way of calculating the leading (fractal) exponent is to use the renormalisation of the total number of particles†. The fractal dimension D is extracted

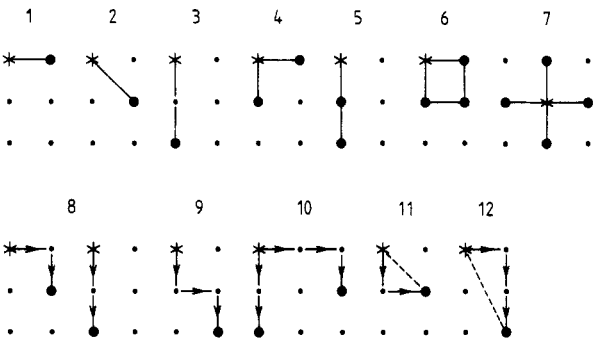

Figure 2. Short-range interactions used to monitor the RG flow. Interactions 1-7 determine the static properties: interaction 1 measures the probability that a first neighbour (●) of a particle on the cluster (*) is occupied (the nearest-neighbour correlation), etc. Interactions 8-12 characterise the dynamics (the time-ordered correlations): interaction 8 determines the probability that a second neighbour (●) along the bonds (chemical distance) is occupied after a given particle (*), etc. Similarly, interaction 11 is the average distance of the second neighbour (●) along the bonds added after a given particle (*).

† This can be viewed as an RG with a single interaction S_0.

from $N/N' = (R/R')^D = b^D$ (here $b = 2$), analogous to the usual determination of D from the scaling relation $N \sim R^D$.

For DLA 20 clusters were generated, each with a fixed radius of gyration $R = 100$ ($N \simeq 9000$) and six consecutive renormalisation transformations were applied to them. The short-range correlations of figure 2 were measured at each iteration (averaged over the whole cluster). The results of four iterations are shown in figure 3 for RG2 and they clearly show the trend towards a fixed point (RG2 converges bettter than RG1 for this model). Because of finite-size effects the correlations decrease rapidly for iterations 5 and 6, when the clusters have less than 50 particles. The results suggest that iteration $n = 3$ is closest to the fixed point. The dynamic correlations also converge but more slowly than the static ones and they are more sensitive to finite-size effects. To verify the RG flow, results from clusters with $R = 50$ are superposed in figure 3; they approach the $R = 100$ results rapidly.

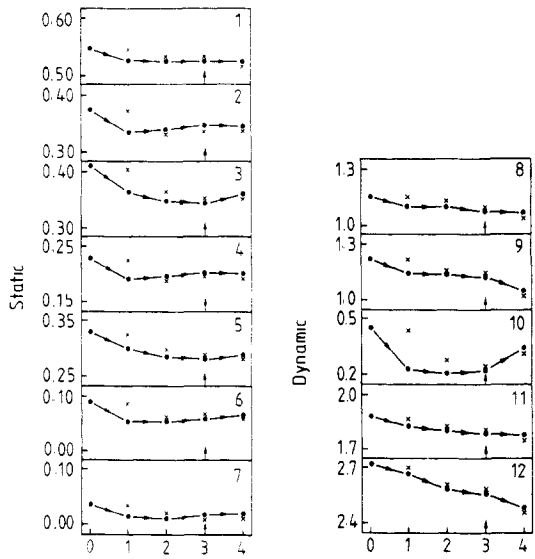

Figure 3. The static (1-7) and the dynamic (8-12) correlations of figure 2 (normalised by the total number of particles) for $n = 0$-4 iterations of the RG. Clusters with $R = 100$ (●) are compared with clusters with $R = 50$ (×), shifted to the right. The correlations stabilise (arrows) indicating that $n = 3$ is closest to the fixed point. The statistical errors are 0.002 (0.01) for statics (dynamics).

The critical exponents are calculated using the equation

$$\frac{\mathrm{d}}{\mathrm{d}K_\beta}\langle \hat{K}'_\alpha \rangle = \sum_\gamma \left(\langle K'_\alpha K'_\gamma \rangle - \langle K'_\alpha \rangle \langle K'_\gamma \rangle\right) \frac{\mathrm{d}K'_\gamma}{\mathrm{d}K_\beta}$$

$$= \left(\langle K'_\alpha K_\beta \rangle - \langle K'_\alpha \rangle \langle K_\beta \rangle\right) \tag{1}$$

where K_α are operators of the type defined in figure 2, primes refer to the renormalised system and the averages are both other unrenormalised and renormalised states. Table 1 shows the eigenvalues of the transformation matrix $\mathrm{d}K_\alpha^{(n+1)}/\mathrm{d}K_\beta^{(n)}$ calculated from equation (1). For this calculation, the chemical potential $K_0 = 0.000\,08$ ($N = 12\,000$) is fixed, instead of the number of particles N or the radius R. The size of the parameter space was varied using the interactions $S_0, S_1, S_2 \ldots$ (figure 2). The largest eigenvalue

increases both with the number of iterations and with the number of interactions, and near the fixed point it yields a fractal dimension to within 5% of the value $D = 1.70$ from direct simulations. The second eigenvalue λ_2 is also shown in table 1. It converges slower than λ_1. The estimate for the dominant correction is $y_2 = -0.38 \pm 0.18$ and hence there is only a single relevant eigenvalue. The second method of calculating D, $N/N' = b^D$, has been applied to clusters of fixed radius $R = 100$ and $R = 50$ and for RG1 and RG2. The results are presented in table 2. With increasing n, D converges from below

Table 1. The largest two eigenvalues λ_1 and λ_2 of RG2 (iterations n and $n+1$) applied to the Witten-Sander model. 20 clusters with $N = 12\,000$ on average (constant chemical potential) were analysed according to equation (1). The interactions used are $S_0 = \Sigma_i \rho_i$ and $S_1, S_2 \ldots$, from figure 2. The first eigenvalue determines the fractal dimension D, $\lambda_1 = b^D$, in good agreement with direct simulations. The second eigenvalue determines the leading corrections $\lambda_2 = b^{y_2}$. From this one estimates $y_2 = 0.38 \pm 0.18$. The statistical errors are 0.1 for λ_1 and 0.3 for λ_2. The * indicates a complex eigenvalue.

	λ_1					λ_2			
	Number of interactions					Number of interactions			
n	1	2	3	4	5	2	3	4	5
0	2.74	2.90	2.88	2.85	3.03	1.32	1.40	1.64	*
1	2.84	2.89	2.92	2.91	2.87	0.01	0.38	0.49	0.51
2	2.96	2.97	2.97	2.99	2.97	0.59	0.81	0.82	0.74
3	3.00	3.01	3.03	3.02	2.99	0.41	0.80	0.64	*
4	2.96	3.11	3.16	3.17	3.13	0.78	0.89	0.88	*

Table 2. Fractal dimension $D(n+1, n)$ using $N/N' = (R/R')^D = b^D$ for RG1 and RG2 and for $n = 0$–3 for DLA, CICI and IP. Clusters of radius $R = 100$ and $R = 50$ are compared for DLA and IP, clusters of 4096 and 2048 particles for CICI. The fixed point is indicated by (*). The statistical errors are 0.02. The values for D from direct simulations [1–4] are 1.70 (DLA), 1.89 (IP) and 1.43 (CICI).

	DLA			IP			CICI		
RG	1	2	2	1	2	2	1	2	2
Size	100	100	50	82	98	50	4096	4096	2048
$n0$	1.46	1.87		1.64	1.96		1.08	1.69	1.69
1	1.52	1.75	1.87	1.69	1.94	1.95	1.22	1.53	1.53
2	1.58	1.74*	1.79*	1.75	1.92	1.93	1.31	1.51*	1.50
3	1.61*	1.79	1.82	1.78*	1.89*	1.91*	1.36	1.52	1.51*

for RG1 and from above for RG2. For $n > 4$ finite-size effects become important. The $R = 100$ calculation gives slightly better results than the $R = 50$ calculation. All these results give a consistent picture in terms of a RG analysis.

The same method has been applied to invasion percolation [3] (IP). The convergence of the RG flow towards the fixed point is slower and using equation (1) one estimates $D = 1.80 \pm 0.13$ from 200 clusters with $K_n = 0.000\,06$ ($N = 17\,000$). The precision is not

sufficient to estimate the second eigenvalue for this process. The values of D from $N/N' = b^D$ for clusters with $R = 98$ and $R = 50$ and for RG1 and RG2 are shown in table 2 and agree well with direct simulations.

Finally, this MCRG has been applied to CICI [2]. 20 clusters were grown hierarchically ($N^{(n+1)} = 2N^{(n)}$) with 2048 (resp 4096) particles and analysed with RG1 and RG2. The renormalised clusters are not exactly monodisperse any more and only static properties have been considered. The growth rule for clusters which are not properly connected is slightly modified to take into account that the growth is hierarchical. The analysis of the correlations shows a flow towards a fixed point as for the other models and the value for D from $N/N' = b^D$ is listed in table 2.

The MCRG introduced here provides a systematic way of studying both static and kinetic aspects of aggregation processes. It gives accurate estimates for the fractal dimension and a fair estimate for the correction to scaling exponent for DLA.

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