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LETTER TO THE EDITOR

Position space renormalisation group for aggregation fractals

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Abstract. A simple position space renormalisation group scheme is used to find the fractal dimension of Sutherland type aggregation clusters grown in low-dimensional space. Clusters which move along paths of fractal dimension $d_w = 0, 1, 2$ are considered and a systematic variation in cluster fractal dimension matching that of recent computer simulations is found.

Meakin (1983) and independently Kolb *et al* (1983) introduced a model of 'kinetic clustering of clusters' to describe the flocculation of colloids and aerosols. Thus far three different kinetics have been studied: clusters moving diffusively (Kolb *et al* 1983, Meakin 1983 and the experiments of Weitz and Oliveria 1984), clusters moving ballistically (P Meakin, to be published) and the kinetics of chemically limited aggregation (CLA) (Schaeffer *et al* 1984, D A Weitz and M Oliveria, private communication). CLA may be realised as a computer simulation in which a pair of clusters is collided by positioning them repeatedly at random in a box until they are adjacent but not intersecting (W D Brown and R C Ball, to be published). These three kinetics correspond to requiring that clusters move along paths having fractal dimensions $d_w = 2, 1, 0$ respectively (Mandelbrot 1982).

A particularly simple cluster-cluster aggregation model is the hierarchical model due originally to Sutherland (1967, 1970) which has been studied numerically in low dimensions (Botet *et al* 1984, Jullien *et al* 1984a, b, W D Brown, private communication) and theoretically in high dimensions (Ball 1984, Ball and Witten 1984). In this model one starts with $N_0 = 2^k$ independent seed particles and constructs clusters iteratively. The $(q+1)$th iteration consists of forming $N_0/2^{q+1}$ clusters each of 2^{q+1} particles. This is done by grouping the clusters formed in the qth iteration into pairs and colliding each pair of clusters. This process continues until one cluster of N_0 particles is formed. We call a cluster of 2^q particles a q cluster. All three kinetics, $d_w = 2, 1, 0$ have been considered for this model (Jullien *et al* 1984b, R Jullien and M Kolb, to be published, W D Brown, private communication). For ballistically moving clusters we consider only the case in which the impact parameter b is chosen randomly. We do not consider the case in which two clusters are always collided along a line through their centres of mass, i.e. $b \equiv 0$ (Jullien 1984).

Aggregation clusters can be partly characterised by how the number of particles in the cluster, N, scales with the cluster radius of gyration, R, $N \sim R^{D(d)}$, in the limit $N \to \infty$. Here $D(d)$ is the cluster fractal dimension and d is the dimension of Euclidean space in which the clusters form. Hentschel and Deutch (1984) suggested for Sutherland

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clusters that

$$D(d) = d(4d+3)/(9d-2) \qquad d < d_c = 8 \tag{1}$$

$$D(d) = d/2 \qquad d > d_c \tag{2}$$

independent of kinetics. This result was found using an argument which required two lengths, the cluster radius of gyration and the distance two clusters interpenetrate before a collision. It is presumably wrong: for low d computer simulations show a systematic variation of $D(d)$ with kinetics (see table 1) and for high d it has been shown (Ball and Witten 1984) that the exact answer is

$$D(d) = D^* = \ln 4/\ln (3/2) \qquad \text{for } d > d_c = 2D^* + d_w.$$

Table 1. Comparison of simulation results (Jullien *et al* 1984b[a], R Jullien and M Kolb[b], to be published, W D Brown[c], private communication) with position space renormalisation group (PSRG) results for fractal dimension $D(d)$ of Sutherland clusters moving with $d_w = 0, 1, 2$. PSRG results for $D(d_c)$ where $d_c = 2D^* + d_w$ are given. These should be compared with the exact result $D(d_c) = D^*$ for $d_w = 0, 1, 2$ where $D^* = \ln 4/\ln(3/2) \simeq 3.42$ (Ball and Witten 1984).

	$d_w = 0$ $D(d)$		$d_w = 1$ $D(d)$		$d_2 = 2$ $D(d)$	
d	Simulation	PSRG	Simulation	PSRG	Simulation	PSRG
1		1.00		0.89		
2	1.53 ± 0.04[b]	1.56	1.56 ± 0.03[a]	1.41	1.42 ± 0.03[a]	1.43
	1.60 ± 0.05[c]					
3	1.98 ± 0.04[b]	2.06	1.98 ± 0.05[a]	1.87	1.78 ± 0.05[a]	1.79
4	2.32 ± 0.04[b]	2.53	2.35 ± 0.08[a]	2.31	2.04 ± 0.08[a]	2.13
5		3.03	2.5 ± 0.2[a]	2.75	2.3 ± 0.2[a]	2.46
6		3.44	2.7 ± 0.2[a]	3.14		2.80
7		3.89		3.61		3.15
8				4.04		3.51
9						3.90
d_c		3.82		3.97		3.84

To evaluate $D(d)$ for Sutherland clusters we use a simple position space renormalisation group scheme which requires only one length, the cluster radius of gyration. We first note that for Sutherland clusters $D(d)$ can be written (Botet *et al* 1984)

$$D(d) = \lim_{q\to\infty} \frac{\ln(N_{q+1}/N_q)}{\ln(R_{q+1}/R_q)}$$

$$= \lim_{q\to\infty} \frac{\ln 2}{\ln \lambda_q}$$

where R_q is the radius of gyration of a q cluster, $N_q = 2^q$ is the number of particles in a q cluster and $\lambda_q = R_{q+1}/R_q$. The method we use for finding λ_q is sufficiently simple to be independent of q. Thus we are forced to assume the method is valid for large q and so gives a good approximation to $\lambda = \lim_{q\to\infty} \lambda_q$. We now write λ in place of λ_q.

To find λ we represent a q cluster in d dimensions by a sphere of radius r_q. This radius is determined by the requirement that the sphere must have the correct kinetic cross-section for hitting another q cluster, itself represented by a sphere. In principle

we could model r_q on any characteristic radius of the cluster which scales with the radius of gyration, but if a sphere is to be a good representation of a q cluster we must choose the definition of r_q which is most pertinent to the aggregation. We assume that for $d < d_c$ there exists for a q cluster a 'hitching radius' $R_h(q)$ (Botet and Jullien 1984). This radius is defined to be the maximum radius that has the property that there is zero probability that the centres of mass of two collided q clusters are less than $2R_h(q)$ apart. Thus $R_h(q)$ defines an impenetrable hard sphere inside a q cluster. As a low-dimensional approximation (exact in one dimension) we assume that the centres of two collided q clusters are precisely $2R_h(q)$ apart. Of course actually the centres of mass of two collided q clusters are at least $2R_h(q)$ apart from the definition of $R_h(q)$. $R_h(q)$ is the radius that we use for r_q. Using this approximation a $q+1$ cluster is represented as two touching spheres each of radius r_q. To find r_{q+1}, i.e. to find the correct radius for approximating (renormalising) two touching spheres of radius r_q by a single sphere of radius r_{q+1}, we require that both the unrenormalised and renormalised representations of a $q+1$ cluster have the same cross-section to another $q+1$ cluster. The latter $q+1$ cluster is represented as a sphere of radius r_{q+1} for simplicity. We write $\sigma_1(r_q, r_{+1})$ for the cross-section of two touching spheres of radius r_q to a single sphere of radius r_{q+1} and we write $\sigma_2(r_q+1)$ for the cross-section of one sphere of radius r_{q+1} to another sphere of radius r_{q+1}. Thus we require

$$\sigma_1(r_q, r_{q+1}) = \sigma_2(r_{q+1})$$

or equivalently

$$\sigma_1(1, \lambda) = \sigma_2(\lambda). \tag{3}$$

It is in the definitions of the cross-sections that cluster kinetics appear. Since solving (3) for λ gives $D(d)$, the Sutherland cluster fractal dimension does depend on cluster kinetics in this approach in contrast to the earlier result of Hentschel and Deutch (1984) given by (1) and (2).

For the kinetics of CLA excluded volume is used as the cross-section. That is, the cross-section of one cluster to another is taken to be the volume about one cluster in which the other cluster cannot sit without the two clusters intersecting. Thus $\sigma_1(1, \lambda)$ is the mutually excluded volume of two touching d-dimensional spheres of radius 1 (one $q+1$ cluster) and a sphere of radius λ (the other, renormalised, $q+1$ cluster). This is the volume in d dimensions of two intersecting spheres of radius $1+\lambda$ with centres 2 apart. Similarly $\sigma_2(\lambda)$ is the mutually excluded volume of two spheres of radius λ which is the volume of a sphere of radius 2λ. With these definitions of $\sigma_1(1, \lambda)$ and $\sigma_2(\lambda)$ for the kinetics of CLA equation (3) reduces to (see figure 1)

$$\left(\frac{2\lambda}{1+\lambda}\right)^d = 1 + \left(\int_0^{\theta_0} \cos^{d-1}\theta \, \mathrm{d}(\sin\theta) \Big/ \int_0^{\pi/2} \cos^{d-1}\theta \, \mathrm{d}(\sin\theta)\right) \tag{4}$$

where

$$\sin\theta_0 = 1/(1+\lambda).$$

The values obtained for $D(d)$ by solving (4) numerically are given in table 1.

For Sutherland clusters which move linearly, the average ballistic cross-section is used for σ_1 and σ_2. Thus $\sigma_1(1, \lambda)$ is the average ballistic cross-section of two touching d-dimensional spheres of radius 1 to a sphere of radius λ. This is the isotropically averaged projected 'area' of two d-dimensional spheres of radius $1+\lambda$ with centres 2 apart. Similarly $\sigma_2(\lambda)$ is the average ballistic cross-section of one sphere of radius λ

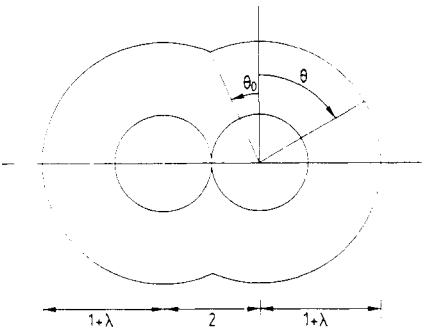

Figure 1.

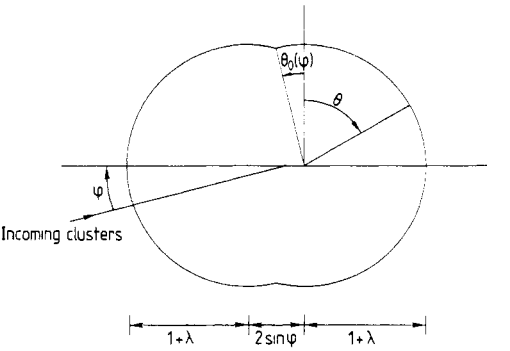

Figure 2.

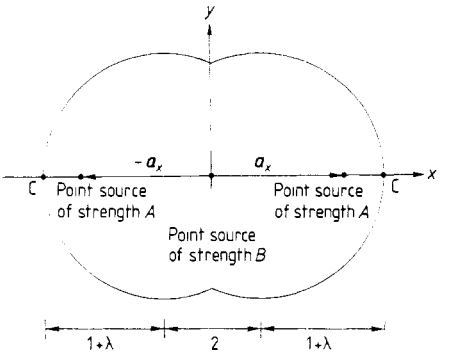

Figure 3.

Figure 1. Geometry of excluded volume cross-section.

Figure 2. Geometry of average ballistic cross-section.

Figure 3. Geometry of diffusive cross-section.

to another sphere of radius λ which is the isotropically averaged projected 'area' of a d-dimensional sphere of radius 2λ. This is of course the volume of a $(d-1)$-dimensional sphere of radius 2λ. With these definitions of $\sigma_1(1,\lambda)$ and $\sigma_2(\lambda)$ for ballistically moving clusters equation (3) reduces to (see figure 2)

$$\left(\frac{2\lambda}{1+\lambda}\right)^{d-1} = 1+\left[\left(\int_0^{\pi/2}\sin^{d-2}\phi\int_0^{\theta_0(\phi)}\cos^{d-2}\theta\,\mathrm{d}(\sin\theta)\,\mathrm{d}\phi\right)\times\left(\int_0^{\pi/2}\sin^{d-2}\phi\int_0^{\pi/2}\cos^{d-2}\theta\,\mathrm{d}(\sin\theta)\,\mathrm{d}\phi\right)^{-1}\right] \tag{5}$$

where

$$\sin\theta_0(\phi) = (\sin\phi)/(1+\lambda).$$

The values obtained for $D(d)$ by solving (5) numerically are given in table 1. The value $D(1)$ was obtained by solving (5) in the limit $d \to 1_+$.

For Sutherland clusters which move diffusively, σ_1 and σ_2 are diffusive cross-sections. σ_1 is the steady state absorption rate by two touching spheres of radius 1, of spheres of radius λ, from a field of unit concentration at infinity. That is,

$$\sigma_1(1,\lambda) = \int_{S_1}\nabla\phi_1\cdot\mathrm{d}\boldsymbol{S}; \qquad \nabla^2\phi_1 = 0; \qquad \phi_1|_{S_1} = 0; \qquad \lim_{r\to\infty}\phi_1(\boldsymbol{r}) = 1.$$

Here S_1 is the surface of two intersecting spheres of radius $1+\lambda$ with centres 2 apart. Similarly σ_2 is the steady state absorption rate by a sphere of radius λ of spheres of

radius λ from a field of unit concentration at infinity. Thus we have

$$\sigma_2(\lambda) = \int_{S_2} \nabla\phi_2 \cdot \mathrm{d}\boldsymbol{S}; \qquad \nabla^2\phi_2 = 0; \qquad \phi_2|_{S_2} = 0; \qquad \lim_{r\to\infty} \phi_2(\boldsymbol{r}) = 1$$

where S_2 is the surface of a sphere of radius 2λ. To find λ we use a crude approximation to ϕ_1 to calculate σ_1. This is because we could not find an exact, tractable solution ϕ_1 to Laplace's equation with the boundary conditions described above. The approximation used also has the advantage that it makes sense for non-integral dimensions. We set (see figure 3)

$$\phi_1(\boldsymbol{r}) = A/|\boldsymbol{r}+\boldsymbol{a}_x|^{d-2} + A/|\boldsymbol{r}-\boldsymbol{a}_x|^{d-2} + B/|\boldsymbol{r}|^{d-2} + 1.$$

We also set

$$\phi_2(\boldsymbol{r}) = (2A+B)/|\boldsymbol{r}|^{d-2} + 1$$

where

$$(2A+B) = -1/(2\lambda)^{d-2} \tag{6}$$

so the requirements that the total steady state flux through S_1 and S_2 be equal and that $\phi_2|_{S_2} = 0$ are automatically satisfied. We have also satisfied $\nabla^2\phi_1 = 0$, $\lim_{r\to\infty} \phi_1(\boldsymbol{r}) = 1$, $\nabla^2\phi_2 = 0$ and $\lim_{r\to\infty} \phi_2(\boldsymbol{r}) = 1$. However, the requirement that $\phi_1|_{S_1} = 0$ can only be approximately met. We determine the four unknowns A, B, $\boldsymbol{a}_x$ and λ by requiring (6) be satisfied, the zero potential surface of ϕ_1 pass through the extremities of S_1 (points C on figure 3) and that this surface has the same values of $\partial^2 x/\partial y^2$ and $\partial^4 x/\partial y^4$ at points C as S_1. This criterion is used as, for low d, most diffusing clusters hit the cluster tips. Thus we require at points C

$$-\frac{\partial^2\phi/\partial y^2}{\partial\phi/\partial x} = -(1+\lambda)^{-1},$$

$$-\frac{\partial^4\phi/\partial y^4}{\partial\phi/\partial x} + \frac{6(\partial^2\phi/\partial y^2)(\partial^3\phi/\partial x\partial y^2)}{(\partial\phi/\partial x)^2} - \frac{3(\partial^2\phi/\partial y^2)^2(\partial^2\phi/\partial x^2)}{(\partial\phi/\partial x)^3}$$

$$= -3(1+\lambda)^{-3},$$

$\phi_1|_C = 0$ and that (6) is satisfied. The values for $D(d)$ obtained by solving these equations numerically are given in table 1. The value for $D(2)$ was obtained by solving them in the limit $d \to 2_+$.

We see from table 1 that for each d the values for $D(d)$ obtained from simulations (Jullien *et al* 1984b, R Jullien and M Kolb, to be published, W D Brown, private communication) decrease as d_w increases as do the values for $D(d)$ obtained from the above position space renormalisation group approach. This systematic variation in the simulation values of $D(d)$ is expected since as d_w increases clusters interpenetrate less before colliding and thus form more open structures. We also see that for each of $d_w = 0$, 1, 2 the agreement between values for $D(d)$ obtained using this approach and those obtained from computer simulations worsens as d increases. This is expected as we have used the low-dimensional approximation that q clusters collide when their centres are precisely $2r_q$ apart. The close agreement for low d for $d_w = 2$ is no doubt a coincidence due to the rather *ad hoc* approximation used for ϕ_1. However it should be noted that as $d \to \infty$ this approximation becomes an exact solution (with $B = 0$). It can be shown analytically that as $d \to \infty$, $D(d)$ slowly approaches from above the

asymptote $(d-d_w)/2$ rather than the correct asymptote $D(d)=\ln 4/\ln(3/2)$. This shows the method is self consistent; we made the low-dimensional approximation that Sutherland q clusters interpenetrate only to r_q and for all values of d we find that $D(d)>(d-d_w)/2$ i.e. that Sutherland clusters are indeed opaque to each other for each of the three kinetics considered.

Work is continuing on the application of the above position space renormalisation group approach to polydispersed models of cluster-cluster aggregation (P Meakin, to be published) and to diffusion limited aggregation (Witten and Sander 1981).

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