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RAPID COMMUNICATION

On obtaining the fractal dimension of a 3D cluster from its projection on a plane—application to smoke agglomerates

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Abstract. The finite size of a fractal cluster of dimension D causes a reduction in the dimension of its projection to D^* on any finite observation scale. A theoretical argument is presented which relates the apparent dimension D^* to D and to the observation scale as a fraction of the outer fractal scale. The theory is tested for computer-generated fractal clusters. When applied to a sample of electron micrographs of diesel soot particles whose apparent dimension is 1.83 ± 0.06, the theory gives 1.90 ± 0.07 as the true fractal dimension of the soot.

A number of materials, such as soot, occur naturally as sparse random aggregates which possess dilation symmetry over a range of length scales. Such structures are characterised by a fractal dimension D which is less than 3. Their fractality is manifest in the limiting behaviour of the density correlation function $C(r)$ which varies like r^{D-3} for small r; and also in the scaling of cluster characteristic radius R with mass M: $M \propto R^D$.

It is often necessary to measure the dimensionality of a structure in three-dimensional space from its plane projection. In the case of a perfect, infinite fractal the projection has the dimension D of the parent fractal if $D < 2$, but is compact with dimension 2, if $D \geqslant 2$. Real fractals, however, are limited by an inner and an outer scale, arising from the finite size of the component particles and of the cluster. The effect of those limits on the apparent fractal dimension of the projection is the subject of this article.

Consider a cluster containing N sites with R being the RMS separation of two sites. Self-similarity in a cluster means that the density correlation function $C(r)$, normalised to N, satisfies

$$p(r/R) = 4\pi R^3 C(r)/N \tag{1}$$

where $p(x)$ is a scale invariant function since R is a characteristic length of the cluster (Berry and Percival 1986). It then readily follows from the definition of R and N that $p(x)$ satisfies the normalisation relation

$$\int_0^\infty x^2 p(x)\,\mathrm{d}x = 1 = \int_0^\infty x^4 p(x)\,\mathrm{d}x. \tag{2}$$

For a fractal cluster $p(x)$ behaves as x^{D-3} for small x, and we can therefore let

$$p(x) = Ax^{D-3}f(x) \tag{3}$$

where $f(x)$ is some cut-off function which tends to 1 as x tends to 0, and which vanishes more rapidly than $x^{-(D+2)}$ as x tends to ∞.

Let the cluster be projected on the x–y plane. Now the scaled distribution of pairs of projected sites is

$$q(X) = \int_{-\infty}^{\infty} p[(X^2 + z^2)^{1/2}]\,\mathrm{d}z. \tag{4}$$

Using (3)

$$\begin{aligned} q(X) &= 2AX^{D-2}\int_0^{\pi/2} (\cos\varphi)^{1-D} f(X/\cos\varphi)\,\mathrm{d}\varphi \\ &= 2AX^{D-2} I(X, D) \end{aligned} \tag{5}$$

where

$$I(X, D) = \int_1^\infty [s^{D-2}/(s^2-1)^{1/2}] f(Xs)\, ds. \tag{6}$$

Thus the two-dimensional distribution will scale with dimension D when $I(X, D)$ is a constant.

For geometrically opaque fractals $D \geqslant 2$ and the limiting form of (6) for small X varies like X^{2-D} giving, through (5), a compact projection.

When $D < 2$ the principal contribution to the integral in (6) is from small s. The value of $I(X, D)$ is then determined by the choice of cut-off function $f(x)$, but since all $f(Xs)$ tend to unity for small s the exact form used is of secondary importance. We will use the convenient general form

$$f(x) = \exp[-(x/x_c)^\alpha] \tag{7}$$

where the cut-off x_c is determined from the normalisation conditions (2)

$$x_c = [\Gamma(D/\alpha)/\Gamma((D+2)/\alpha)]^{1/2} \tag{8}$$

and α is a constant whose value determines the rate of decay of $f(x)$ as x approaches the outer fractal scale. Analysis of models of soot aggregates generated by Brownian processes by Mountain and Mulholland (1988) and Nelson (1989) shows that the cut-off function decays faster than a Gaussian, i.e. $\alpha > 2$. Mountain and Mulholland in fact suggest the value $\alpha = 2.5$ for their Langevin dynamics-simulated smoke agglomerates. In the application of our method to soot given below we use this value as typical of soot, but consider the effect of varying $f(x)$ between the bounds of the Gaussian decay function ($\alpha = 2$) and the step function ($\alpha = \infty$).

Then, using (7)

$$I(X, D<2) = \int_1^\infty \frac{s^{D-2}}{(s^2-1)^{1/2}}\, ds - \int_1^\infty \frac{s^{D-2}\{1-\exp[-(Xs/x_c)^\alpha]\}}{(s^2-1)^{1/2}}\, ds. \tag{9}$$

The first term will be written as $C(D)$ and is given exactly by

$$C(D) = \int_0^{\pi/2} (\cos\varphi)^{1-D}\, d\varphi = 2^{-D}\frac{[\Gamma(1-\tfrac{1}{2}D)]^2}{\Gamma(2-D)}. \tag{10}$$

Expanding the denominator of the second term in powers of s and integrating each term in the resulting series by parts, we obtain, to leading order in (X/x_c)

$$I(X, D<2) = C(D) - \frac{(X/x_c)^{2-D}}{(2-D)} \times \Gamma\left(\frac{D-2}{\alpha}+1\right) + O((X/x_c)^\alpha). \tag{11}$$

In the limit of large clusters where $X/x_c \to 0$, $I(X, D)$ is effectively constant and the two-dimensional distribution has the dimensionality of the parent cluster.

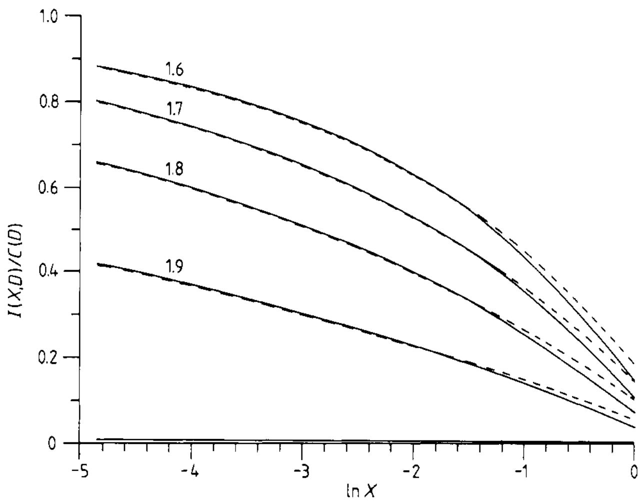

Figure 1. $I(X, D)/C(D)$ as a function of $\ln X$ for $D = 1.6$, 1.7, 1.8 and 1.9. The full curves correspond to the exact value of $I(X, D)$ as given by equation (9) while the broken curves correspond to the approximate form for $I(X, D)$ as given by equation (11), taken to leading order in X.

This is illustrated in figure 1 where $I(X, D)$ is plotted as a function of X for $D = 1.6$, 1.7, 1.8 and 1.9. Note how $I(X, D)$ approaches its small X limit more slowly for higher values of D. The approximate form (11) to leading order in X is plotted for comparison. The cut-off with $\alpha = 2.5$ is used in this figure. The effect of varying α is considered later.

The fractal dimension of an image is usually measured from its density correlation function behaviour assuming fractality. That is, an apparent dimension D^* is measured, on some observation scale X, as

$$D^* = \frac{\partial \ln q(X)}{\partial \ln X} + 2 \tag{12}$$

where $q(x)$, as defined in (4), is proportional to the projected density correlation function. Equation (5) with (11) to leading order in X yields the approximation

$$D^* = D - (X/x_c)^{2-D}\Gamma\left(\frac{D-2}{\alpha}+1\right)\Big/C(D). \tag{13}$$

In figure 2, D^* from (13) is plotted against X over a range of values of D for $\alpha = 2.5$. D^* approaches D in the limits where $X \to 0$ and $D \to 2$.

Let us now consider the sensitivity of our expression (13) to the choice of cut-off function. The discrepancy $(D - D^*)$ between true and apparent dimensions depends on α through a factor

$$[\Gamma(D/\alpha)/\Gamma((D+2)/\alpha)]^{D/2-1}\Gamma\left(\frac{D-2}{\alpha}+1\right). \tag{14}$$

While for D close to 1 this factor depends strongly on α, as D approaches 2 the effect of choice of α diminishes. For instance, when $D = 1.8$—a typical value for agglomerates produced by diffusion-limited aggregation and, as shown below, for soot—the factor (14) for $\alpha = 2.5$ differs from the slow cut-off limit ($\alpha = 2$)

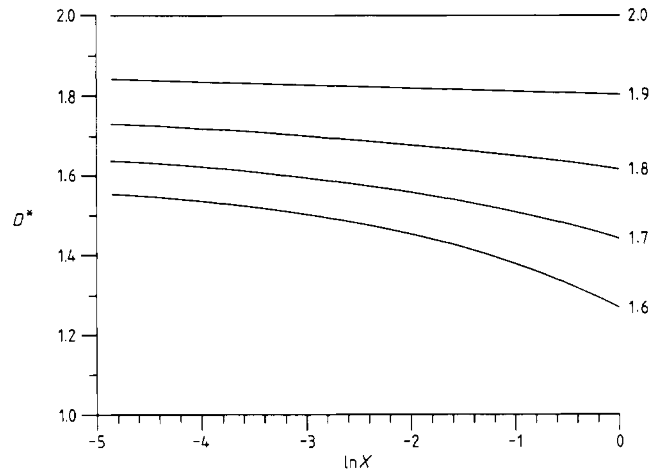

Figure 2. D^* as a function of $\ln X$ for $D = 1.6, 1.7, 1.8, 1.9$ and 2.0—see equation (13).

by only 4% and from the fast cut-off limit ($\alpha = \infty$) by 8%. Indeed, for all cases illustrated ($1.6 \leqslant D < 2$) uncertainty in α introduces an error in $(D - D^*)$ of $\leqslant$15%. This error may be substantially reduced by closer determination of the cut-off function arising from a particular aggregation process. However, a merit of this approach is the relative insensitivity of $(D - D^*)$ to α, even when very little is known about the form of the cut-off.

The above deals with finite cluster size. As regards finite component size, this imparts finite area to the cluster projection. However, component size merely fixes the inner fractal scale of the projection but does not affect the apparent dimension. This follows from the definition of fractality which states that the number of d-dimensional units of side L required to completely cover a fractal set of dimension D in d-dimensional Euclidean space varies like L^{-D} (Mandelbrot 1982). The number of circles of radius L required to cover the projection of a fractal aggregate of spheres of radius a will be independent of a provided that a is considerably smaller than L.

As a test of the validity of equation (13) between the fractal dimension of a cluster and the apparent dimension of its projection we analysed the projections of a set of well characterised, computer-generated fractal clusters. A hierarchical version of cluster–cluster diffusion-limited aggregation, due to Botet *et al* (1984), was implemented to generate a set of 10 random clusters, each of 2048 sites. Analysis of the clusters in terms of their density correlation function and the variation of cluster radius R with number of sites N verified that the clusters were fractal with $D = 1.80 \pm 0.05$.

A digitised projection of each cluster was prepared by calculating the positions of its 2048 sites projected on to a square lattice at some randomly chosen orientation, and filling each lattice site into which the image of one or more cluster sites fell. The apparent dimension of the projection was estimated from its density correlation function in the following manner.

The image was enclosed in the smallest rectangular box that would just contain it, and an inner margin drawn at l_{max} lattice units from each side, leaving a rectangular window. Then for each occupied site within the window the number of occupied sites $n(l)$ lying on the square of side $2l$ centred on that site was counted for values of l between some lower cut-off l_{min} and l_{max}. l_{min} and l_{max} were taken as 3 and 12 lattice units respectively, to eliminate the effects of the lattice and the cluster edges. Finally the $n(l)$ were averaged over all sites in the window and over the ensemble of cluster projections. As $n(l)$ is related to the density correlation function $C(l)$ by $n(l) \simeq lC(l)$, it should vary like l^{D^*-1} for a fractal projection of dimension D^*.

Fitting an analytic function of the form

$$n(l) = Al^{D^*-1} \exp(-Bl^2) \tag{15}$$

to the data returned an apparent dimension of $D^* = 1.71 \pm 0.05$. The observation scale X for this measurement is given by l_{min}/R and is about 0.05 for a cluster–cluster DLA aggregate of 2048 sites. Substituting into (13) for D and X and using $\alpha = 2.5$ as suggested above, we find $D^* = 1.70$, which is in very good agreement with the measured value.

Finally we consider the application of our theory to experimental measurements on soot agglomerates. A comprehensive study by Samson *et al* (1987) of the structure of such agglomerates has shown that the aggregates are fractal, in projection, with an apparent dimension of 1.7–1.9. The fractal dimension of soot influences its optical properties (Berry and Percival 1986) and so it is important to relate the apparent dimension of soot agglomerates to their true fractal dimension.

In order to apply our technique to this situation, samples of soot were produced by the combustion of carbon-containing fuels and an examination of particulate chains in these samples was performed by means of transmission electron microscopy. The samples were collected on 3 mm diameter 'Formvar' carbon coated (300 mesh) copper grids from the exhaust of a running diesel engine and from the high-pressure combustion chamber of a continuous oil spray burner. Electron micrographs (enlarged to 300 mm × 210 mm photographs) were produced at a magnification of 100000 times using a JEOL JEM-200 CX electron microscope. Soot agglomerates with some 100 primary particles of diameter around 50 nm were obtained from diesel and vegetable oil fuels and from oil: water emulsions burning at equivalence ratios (fuel: air ratio/stoichiometric fuel: air ratio) in the range 0.8–1.1.

Digitised images of twelve of these agglomerates were analysed by the method described above and were found to have an apparent dimension D^* of 1.83 ± 0.06, which is consistent with the result of Samson *et al*. The measurement was made at an observation scale X of about 0.1. (The soot agglomerates were smaller than the fractal clusters considered earlier.) Finally, inversion of the theoretical relation (13) for

D^* with $2 \leqslant \alpha < \infty$ implies that the fractal dimension of soot in three-dimensional space is 1.90 ± 0.07. This result agrees with the value of D obtained for simulated smoke clusters produced by the Langevin dynamics technique (Mountain and Mulholland 1988) while being greater than, though not inconsistent with, the value of D arising from diffusion-limited cluster aggregation. It therefore supports diffusive aggregation as a possible mechanism of soot particle formation.

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