Structural characterization of nano and micro-fractals using lacunarity analysis and small-angle scattering

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Abstract. The paper presents structural characterization of deterministic nano and micro-fractals using the lacunarity analysis and small-angle scattering technique. We show that for the considered mass-fractal models, the lacunarity spectrum reveals the main structural parameters of the fractal, such as overall size of the system, iteration number, scaling factor and the size of basic units.

1. Introduction

Fractals are known as the infinitively complex systems with self-similar spatial patterns across different scales [1]. Having such properties, fractals became very efficient mathematical models for describing a large number of natural formations from macro to micro scales [2] (galaxy clusters, clouds, trees, micro-molecules, nano-structures, etc).

Modern fractal research techniques usually focus on the calculation of the fractal dimension which, in the case of mass fractals, can be defined as the exponent that describes the distribution of mass $M(r)$ inside a spherical surface of radius $r$ centered on the fractal, through the relation $M(r) \propto r^{D_m}$, where $D_m$ is the fractal dimension [3, 4].

Despite that fractal dimension is considered as the main fractal property, it does not provide complete information about the fractal. The ambiguity of characterizing the spatial fractal pattern only by a fractal dimension is such that two fractals may share the same fractal dimension, but may differ in a distribution of mass. To overcome such uncertainty B. Mandelbrot [1] proposed an additional property, called lacunarity (from Latin "lacuna" meaning "gap") that shows the inhomogeneity (gappiness) of the fractal structure, describing the spatial distribution of elements (mass) inside the fractal.

In this paper we apply lacunarity analysis to digital images of the deterministic fractal sets for revealing their structural and fractal properties. The approach we use to determine lacunarity is the differential box counting method defined by Voss [5]. We show that the main morphological parameters of a fractal, such as the overall size, the size of basic units, iteration number and scaling factor can be extracted from the lacunarity spectrum. We compare our results with the ones obtained from the well-known small-angle scattering technique.
2. Theoretical background

2.1. Lacunarity

Several definitions and algorithms for estimating lacunarity have been proposed since B. Mandelbrot introduced the concept. For practical purposes, in our calculations we restrict ourselves with definition introduced by R. Voss based on the differential box-counting (DBC) algorithm [5]. The process starts with covering a fractal image with non-overlapping square boxes of the size $r$, then the number of occupied boxes, with $M$ number of pixels (mass) inside, is determined as $n(M, r)$. Dividing $n(M, r)$ by the total number of boxes $N$ that cover a fractal image, one obtains the probability function $P(M, r)$ that a box of size $r$ contains $M$ number of pixels. By introducing the statistical moments of $P(M, r)$, as

$$Z^{(q)}(r) = \sum_{M=1}^{N} M^q P(M, r), \quad (1)$$

the lacunarity can be defined as the fluctuations of mass-distributions over its mean

$$\Lambda(r) = \frac{Z^{(2)}(r) - (Z^{(1)}(r))^2}{(Z^{(1)}(r))^2}. \quad (2)$$

Obviously, the lacunarity has dependence on the size of boxes, the larger a box, the lesser the $\Lambda(r)$ due to the smaller variations of $M(r)$. On the scales of small $r$, lacunarity will depend on the distribution of mass inside the fractal. Clustered or inhomogeneous distribution of mass leads to higher values of lacunarity.

2.2. Small-angle scattering

The common used technique for structural analysis of nano and micro fractals is the small-angle scattering (SAS), which yields the differential elastic cross-section per unit solid angle as a function of the momentum transfer, and describes the spatial density-density correlations in the investigated sample [6, 7]. The main indicator of the fractal structure is the fractal dimension, and it can be obtained from the power-law behavior of the scattering intensity $I(q)$ given by [8, 9]

$$I(q) \sim q^{-\alpha} \quad (3)$$

where $q = (4\pi \sin 2\theta)/\lambda$, $\theta$ is the scattering angle and $\lambda$ is the wavelength of incident radiation. The exponent $\alpha$ shows the fractal dimension [10] of the fractal, $\alpha = D_m$ for mass fractals [8] and $\alpha = 6 - D_s$ for surface fractals [3], where $D_m$ is mass fractal dimension and $D_s$ is surface fractal dimension. Besides the fractal dimension, SAS can reveal additional structural parameters as: scaling factor, number of units composing the fractal, and the iteration number of regular mass and surface fractals [11, 12, 13, 14] and fat fractals [15, 16, 17, 18].

3. Deterministic mass-fractal models

In order to calculate lacunarity of the fractals of the same fractal dimension, but with different mass distribution we consider images (300x300 pixels) of four deterministic mass-fractal models. In Fig. 1 are represented fractals up to the third iteration.

One of the well-known algorithms for constructing the deterministic fractal is the following [13, 19]:

(i) Start with the disk with the diameter $a = 300$ pixels (initiator), represented by the iteration number $m = 0$.

(ii) Scale down the initiator by the factor of three ($\beta_s = 1/3$), and make four copies of it.
Figure 1. (Color online) Construction of the deterministic mass-fractals up to third iteration \( m = 3 \).

(iii) Shift each scaled copy of side length \( a_m = \beta_s a \) to four different vertices of a rectangle (for Fractal-a) into which the initiator is inscribed at \( m = 0 \) and obtain the fractal at \( m = 1 \).

(iv) Repeat the same procedure for each new disk in order to obtain the next iteration.

For an arbitrary \( m \)-th iteration, the number of units that compose the fractals is given by

\[
N_m = 4^m. \tag{4}
\]

For the fractals -b, -c and -d from Fig. 1, Step (iii) is modified, and the translation of one of the copies is performed arbitrarily. Please note that according to the proposed algorithm all fractals have the same fractal dimension

\[
D = \lim_{m \to \infty} \frac{\log N_m}{\log (a/a_m)} \approx 1.26, \tag{5}
\]

4. Results and discussion

For the considered deterministic mass-fractal models we calculated the lacunarity spectra according to Eq. 2 for iteration number \( m = 2, 3 \). The results are shown in Fig. 2(left side for \( m = 2 \) and right side for \( m = 3 \)).

From the construction of the models shown in the Fig. 1, it can be seen that fractals -b, -c and -d have a more clustered structure and the corresponding lacunarity curves from Fig. 2 have higher value in comparison with fractal-a. For iteration of higher order such correlation become more significant, allowing one to quantitatively differentiate a distribution of mass between fractals.

Spectra of lacunarity reveal main morphological features of fractals. Non-zero value of lacunarity appears when the size of boxes covering the image is less than half of the image size due to the mass-distribution fluctuations. In the case of the considered mass-fractal models, non-zero lacunarity starts from 150 pixels and shows that the overall size of the fractal is twice
this value, as expected. When we cover the fractal with boxes of exact size as the size of its elements of the particular iteration $m$, the number of empty boxes will take maximum value, increasing the lacunarity in this region. The number of the most pronounced local maxima shows the iteration number of the fractal, positions of this maxima reveal the size of the units at particular iteration and by taking the ratio between two consecutive maxima we can obtain the scaling factor.

Characterizing the structure of the fractal using the lacunarity is performed in a real space. On the contrary, small-angles scattering spectrum gives information in the reciprocal space. Fig. 3 represents the scattering structure factors of deterministic mass-fractals for $m = 2$ and $m = 3$.

In the SAS data, the region with a constant intensity at small values of $q$ is called Guinier region. The rightmost part of the region shows the overall size of the fractal as $q = 2\pi/a$, where $a$ is the side length of the fractal. The number and positions of the most pronounced minima (denoted by vertical dotted lines) indicates the iteration number, and respectively the sizes of
units at corresponding iteration. The scaling factor of the fractal can be calculated by the ratio of the values of two consecutive minima. Additionally, the asymptotic behavior of SAS spectrum at high values of $q$ provides the information about number of basic units $N_m$ at particular iteration.

5. Conclusions
We considered the deterministic mass-fractal models that are characterized by the same fractal dimension, but different spatial distribution of mass. Lacunarity spectrum of each model is calculated using differential box-counting algorithm proposed by Voss. The results obtained give the information about main morphological and fractal properties as overall size of fractal, iteration number and the scaling factor.

We confirm our results by comparing them with data from the simulation of the small-angle scattering from the considered mass fractal models. Corresponding structure factors are calculated using the algorithm developed by Pantos [21].

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