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Pair-Pair Angular Correlation Function

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Additional information is available at the end of the chapter

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Abstract

In addition to the Hausdorff dimension used as fractal characterization parameter, in general, correlation functions can also be employed for this purpose. Given the approximately pure random spatial dispersion of big part of natural fractals, with respect to the center of a reference frame, the most common use of the pair-to-pair correlation function has as main variable the radial distance between two elements of the fractal. Such an approach is extremely practical, since the fractal basic structure statistically presents some kind of isotropy. For the cases where the fractal growth is not isotropic, the use of a pair-to-pair angular correlation function can detect a fractal pattern may be worthy. This will be the topic that is going to be discussed in this chapter, how to implement, discuss and visualize a pair-to-pair angular correlation function.

Keywords: characterization, correlation functions, fractal growth

1. Introduction

Several fractal structures show morphological properties that can be mapped and studied by means of a great amount of geometric parameters. Such definitions generally seek to directly and precisely evidence some physical and structural properties of the object. The Hausdorff dimension [1], recognized as the fractal dimension of a given object, represents a characteristically stationary information of the fractals, that is, it returns an image about the morphology after its formation. In general, this type of parameter becomes very effective in the characterization of several fractal types or different samples, where the process of formation of the same is well-known, such as the case for the deterministic fractals.

However, the most interesting fractals to be analyzed are those found in nature where the growth processes are not well known. In order to investigate and determine the main

phenomena involved in the formation of these fractals, it is vitally important to characterize the growth process of these objects. In this context, we can introduce the pair-pair correlation functions [2].

Statistically speaking, the pair-pair correlation functions return probabilistic information related to the dispersion of the constituent parts, taken as fractal singularity elements, to be found by a given characteristic separation. This statistical tool has applications within the analysis of fractal structures and is also commonly used in studies of Molecular Physics, in the analysis and interpretation of simulations of classical molecular dynamics (CMD). Using the taxonomy appropriate to this large area of knowledge, this function is called radial distribution function (RDF) [2]. As structurally CMD simulations require radial information, the most relevant spatial data retrieval takes into account that the dispersion of the particles to be investigated follows a spherical symmetry, hence only analyzing the radial dispersion of the particles.

In fractals with dendritic structures, such as diffusion limited aggregation (DLA) [1], which is a good representation of several physical and biological phenomena in nature, such as crystal growth, formation of polymers, sedimentation processes, among others or deterministic fractals of the group of Julia [3], this type of analysis, through the functions of pair-pair correlation, can elucidate the process of branching for the obtained structures.

Knowing how this process develops can help the scientists to predict the behavior of the Hausdorff dimension of the fractals analyzed, and the fractal morphologies. In the next session, we will present the basic definition of a DLA fractal in a 2D (two dimensional) perspective, which will be the basic archetype for the formal presentation of radial and angular correlation analysis, which will have a basic explanation of the implementation and subsequent analysis of the results obtained.

2. DLA and radial correlation function

Formally, the diffusion limited aggregation (DLA) was initially studied by Witten and Sander in 1970 [4], and consists of a process of simple aggregate formation that emulates processes of dendritic structures that grow through diffusion, as is the case with electrodeposition phenomena of solid materials in homogeneous solutions or polymerization process. From a computational modeling point of view, DLA aggregates can be obtained on-lattice and off-lattice, two dimensions (2D) and in three dimensions (3D) both initialized with a single deposited particle, called the seed. Given the diffusive characteristics of the system, all particles are taken as identical and run random walks, until they come into contact with the aggregate when they stop moving and are permanently added to it.

There are several variants of the DLA model, and several ways to obtain a DLA-type aggregate [5]. However, given the statistical properties of the random walk, the simplest way to perform such a simulation is to individually draw each particle and perform several steps of a random walk until one of two events may occur: First, if the particle comes into contact with some particle of the aggregate, the path is terminated and another particle is thrown at a fixed

distance from the seed, called the radius of launch R_{lau} , or second, particle reaches a position far from the seed, this distance called death ray R_{kill} , the probability of the particle to return by means of a random-walk and contact with the aggregate becomes very low, hence the walk is finished and another particle is thrown. In general, the launching radius is equal to the sum of the radius of the aggregate R_{agg} with a sufficiently large distance, to avoid a trend in aggregate growth. Since the particles are all identical, the rays of the particles are taken to be the basic unit (arbitrary unit). In general, $R_{\text{kill}} \gg R_{\text{lan}}$. The position of the walking particle launched is determined randomly at the launch circle. A schematic diagram of the basic structure of a DLA can be seen in **Figure 1**.

The most delicate part of a DLA simulation is the aggregation test. In the on-lattice cases, the test consists of the investigation of the elements of a regular network in the surroundings of the aggregated particles, if any element in the vicinity of the walking particle is occupied, it means that the particle has reached the aggregate and must be glued to it, see **Figure 2**. In the off-lattice cases, the aggregation is more complicate, since it must be checked at every step if the distance from the center of the walking particle to the center of all the aggregated particles is not less than twice the radius of the particles, if this occurs, the aggregation must be performed. However, double caution must be taken because in these configurations the overlap of particles must be avoided, see **Figure 2(b)**. Several works in the literature have explored algorithms that talk about this problem [6, 7].

As observed by the dendritic growth exposed at **Figure 2(a)** and **(b)**, the on-lattice simulations have typical different features when compared to the off-lattice simulations, and one special form to quantify this difference is the angular pair-pair correlation function that is discussed in Section 3.

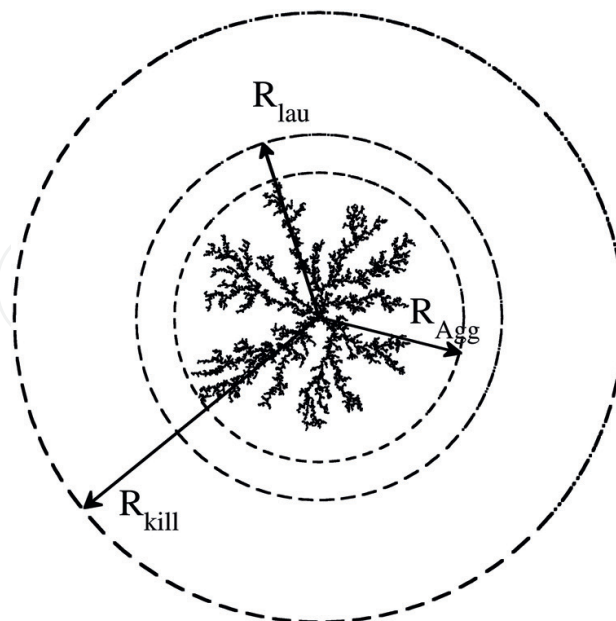


Figure 1. 2D DLA off-lattice containing 10^3 identical particles, showing the respective radii of the aggregates used during the simulation.

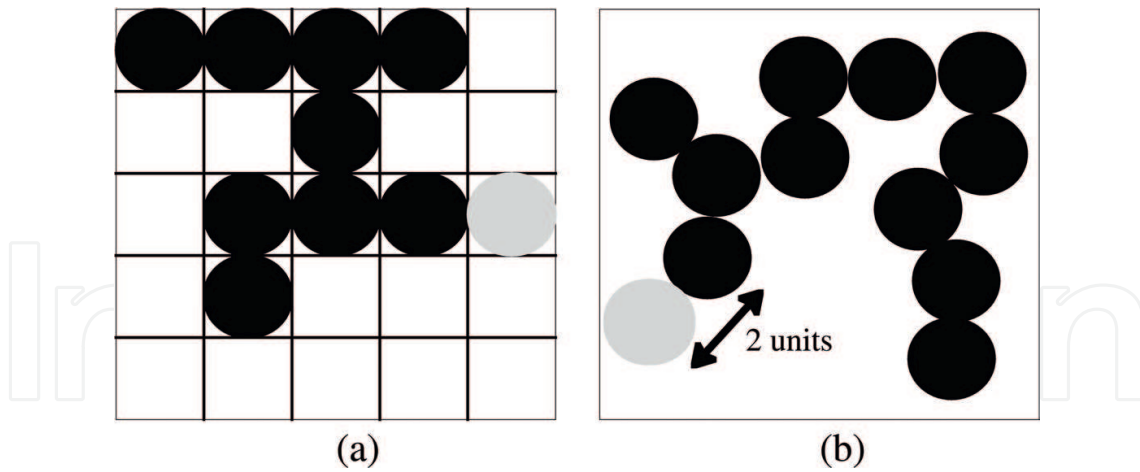


Figure 2. (a) Aggregation test in a 2D on-lattice DLA, white sites represent empty space, black sites represents spaces occupied by aggregate particles and gray site represents the walking particle. (b) DLA 2D off-lattice aggregation test, black circles are aggregate particles and the gray circle is the walking particle.

There are some types of DLAs that, instead of using a radial configuration for the launch of particles, they use a line (2D) or a plane (3D) and limitate the walk of the particles between the launching line/plane and parallel line/plane that contains the seed particle. see **Figure 3**. Although visually the two DLAs, planar-based growth and radial growth, are very different, both typically have a fractal dimension of approximately 1.71 for 2D cases [7].

The typical pair-pair correlation function $c(r)$ directly measures the probability of finding two particles separated by a given radial distance. In classical molecular dynamics simulations, this type of function is called radial distribution function $g(r)$ [2], and may characterize, among other things, the formation of micelles, clusters, and in some cases chemical bonds.

Mathematically, in the case of fractals, this radial function can be calculated as

$$c(r) = \frac{1}{N} \sum \sum \left(\vec{r} - \left| \vec{r}_i - \vec{r}_j \right| \right) \quad (1)$$

where $\delta(\vec{r} - \left| \vec{r}_i - \vec{r}_j \right|)$ is equal to the unit for the case of particles separated by a given radial separation r and zero otherwise. N is exactly the total number of particles added.

The radial feature of this distribution does not prevent it from being used in fractals that do not present radial symmetry, as is the case of planar-based DLA, but its analysis must be performed with more cautious. From the computational point of view, it is very rare for the particles to be perfectly separated by the distance r . Effectively, an average histogram-like calculation is made for the above summation as follows: every aggregate particle is taken as the center of a spherical/circular shell/ring in the surroundings of this particle. The thickness of this shell/ring is δr . It is counted how many particles have their centers within this ring of radius r and thickness δr , - see **Figure 4**. At the end of the calculation, the summation is divided the value by N .

When this calculation is performed for different values of r , going from 1 unit to R_{Agg} which is the characteristic size of the aggregate, we can determine a continuous curve, and to denote characteristics of probability distribution to this function. In general, this function is normalized

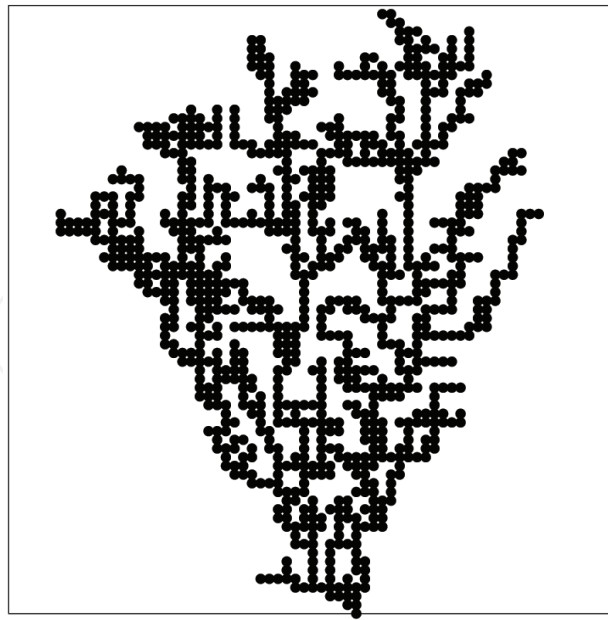


Figure 3. (a) DLA 2D with 10^3 particles deposited on-lattice for the case where the seed is deposited in a plane and the particles are thrown on top a plane.

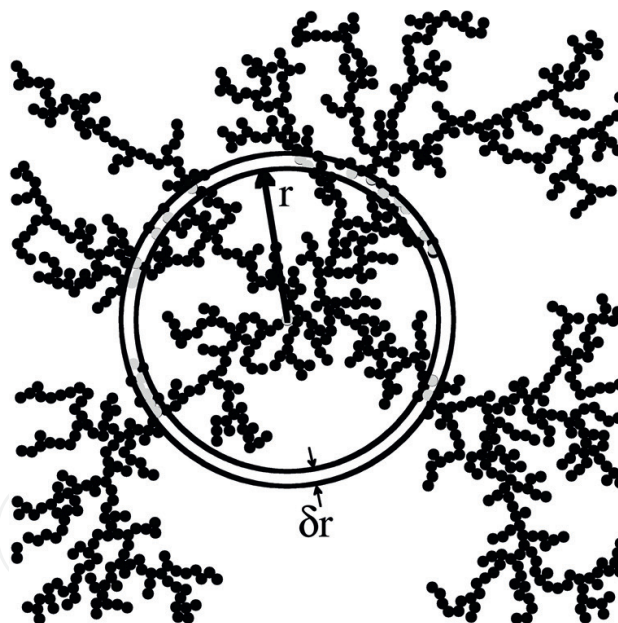


Figure 4. Schematic diagram of the calculation of $c(r)$ by accounting for a histogram of the radial correlation function for a 2D DLA particle. Black circles are aggregate circles, the centered gray circle is the center of the circular ring, and gray circles are the circles accounted due to their centers are within the circular ring of thickness δr .

with the integral of the function obtained in the domain of the function, or it is rescaled based on the maximum value $\text{Max}(c(r))$ of the function.

In the case of a typical DLA, $c(r)$ behaves similarly to that shown in **Figure 5**. Note that there is a global maximum and no other intermediate peaks. This value of r for which $c(r)$ reaches

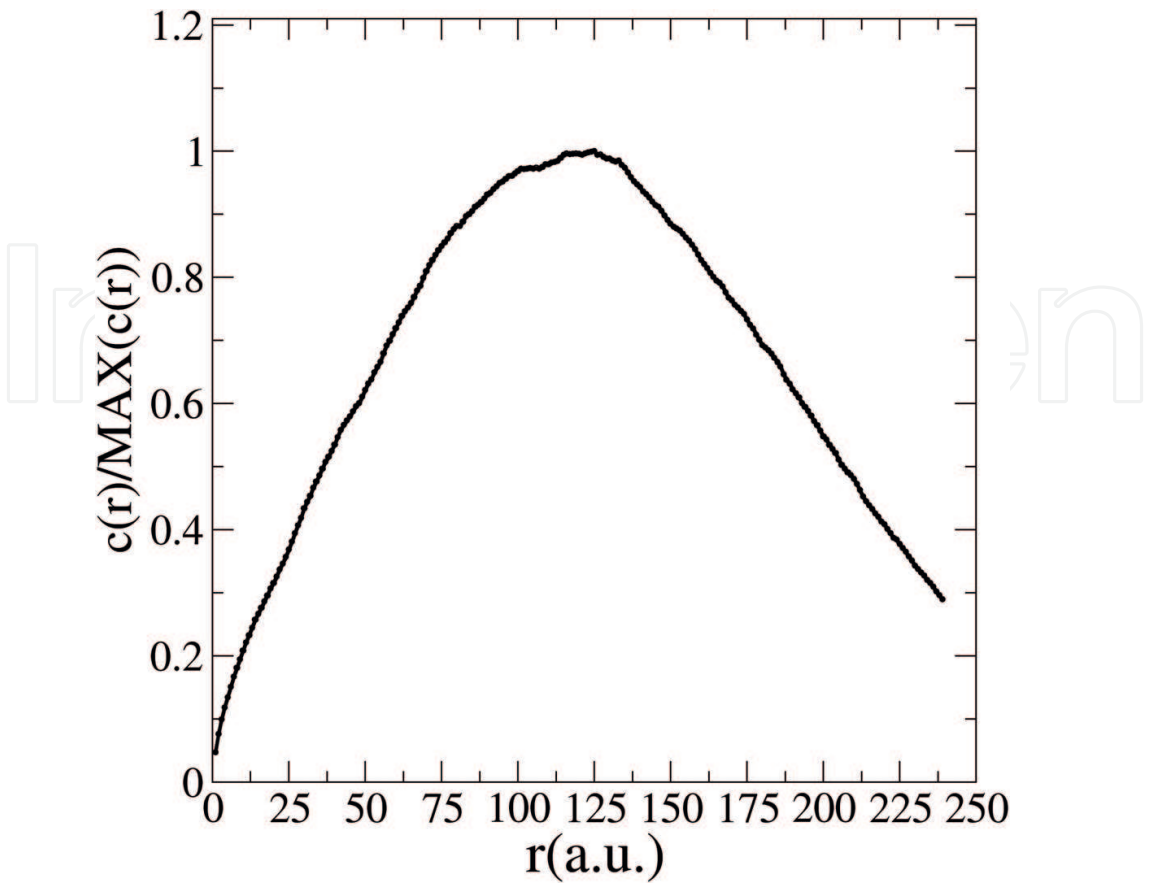


Figure 5. Radial distribution function for the 2D off-lattice DLA containing 10^4 particles of **Figure 1**.

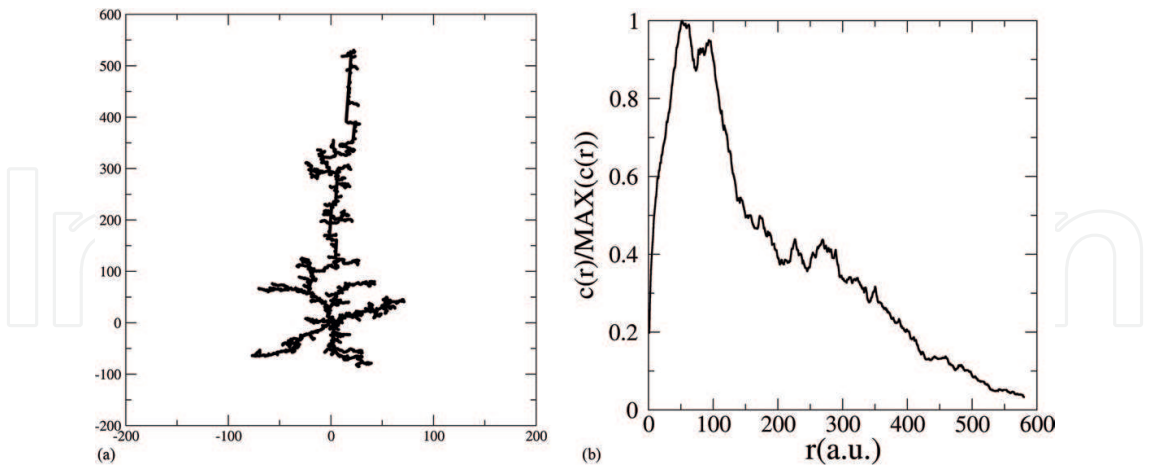


Figure 6. (a) DLA 2D off-lattice containing 2×10^3 particles containing one of the branches more developed than the other branches and (b) pair-pair radial distribution function referring to DLA of item (a) of this figure.

a maximum value means the most likely average separation between the particles. As there is only this peak, the aggregate is expected to exhibit isotropy in its morphology, or there is no trend in aggregate growth. In cases where the aggregate has one of the branches more

developed than the others, there is a change in this distance, and one of the peaks ends up becoming a peaked function, see **Figure 6**. The maximum of the function is shifted from its original position, making evident that exist an anisotropy at the aggregate, but cannot be the finally proven to be a signature of the anomalous growth of the fractal.

3. Angular pair-pair correlation function

The manner in which the dendrites of a DLA-type aggregate or other branched fractal are formed may be extremely relevant in their characterization. One way to characterize such branching is by calculating the angular pair correlation function $c(\theta)$.

Using the primitive ideas of $c(r)$, the pair-pair angular correlation function is nothing more than a probabilistic measure that we can find two aggregated particles, or two infinitesimal parts of the fractal, separated by an angular aperture (θ) one of the others. That is, we indirectly measure which angles of openings are more or less likely to be of branch bifurcations.

Mathematically, the correlation function $c(\theta)$ is

$$c(\theta) = \frac{1}{N} \sum \sum \delta(\theta - |\theta_i - \theta_j|) \quad (2)$$

where $\delta(\theta - |\theta_i - \theta_j|)$ is equal to unity since particles i and j are separated by an angular separation θ . N remains the total number of particles added to the aggregate.

Computationally speaking, it is also very complicated to determine θ angle, for this, we again perform the calculation of $c(\theta)$ by means of a histogram, which is executed as follows: all aggregated particles are taken as the center of circular sectors with angular opening $\delta(\theta)$, centered on (θ) , with (θ) being calculated as the angle based on the polar axis created on the particle analyzed, see **Figure 7**.

The aggregate particles that have their center inside the circular sector are accounted for in the histogram. After the calculation is performed for all aggregated particles, the sum is divided by the total number of particles added.

Similarly to the case of $c(r)$, one can normalize the function $c(\theta)$ or simply rescale it with its maximum value for a better visualization of it.

In the case of a typical 2D DLA, such a function can be seen in **Figure 8**. Note that again DLA growth isotropy returns us a function that is periodic with respect to the angle π and all dendrites grew at a periodic aperture, with multiple peaked angles at this interval. In cases where $c(\theta)$ presents more than one direction of growth, such a phenomenon may be associated with some anisotropy in fractal growth, similar to that presented in Ref. [8]. In general, these anisotropies are associated with symmetry breaks in the process of aggregate formation [8]. And such a mathematical tool is extremely useful and effective in the process of quantification of this phenomenology. As can be observed on the $c(\theta)$ function shown in **Figure 9**, for

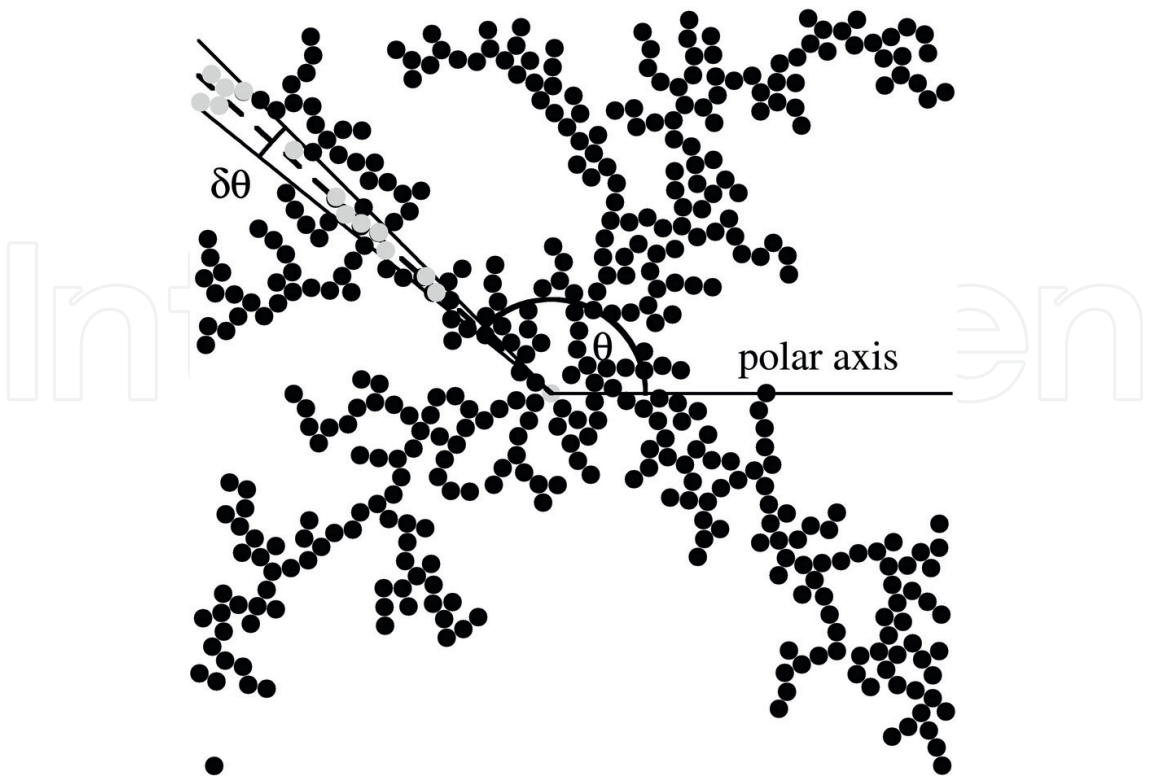


Figure 7. Schematic diagram of $c(\theta)$ calculation, for the 2D case the centered gray is the particle selected to be the center of the circular sector, the black circles are the aggregate particles and the gray circles are the particles that will be accounted for in the histogram. The black filled line is the polar axis associated with the selected particle, the black dotted lines is the centerline of the circular sector with opening $\delta\theta$ centered in angular position (θ).

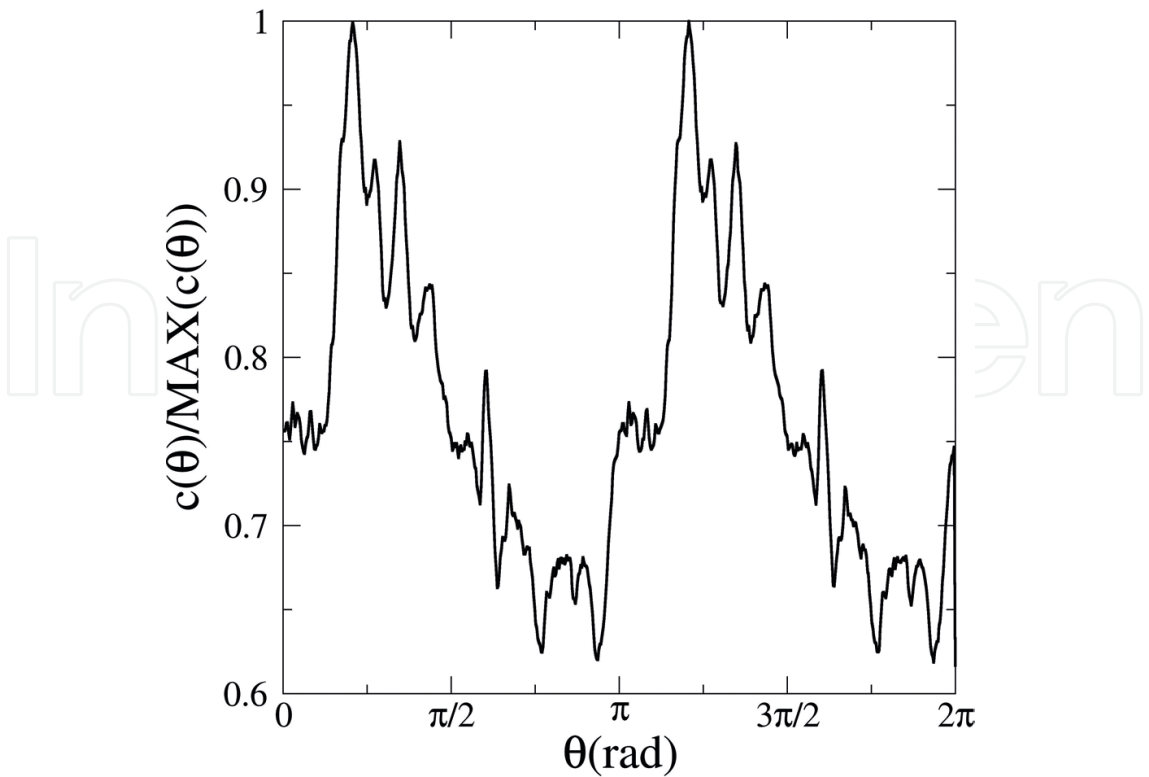


Figure 8. Rescaled $c(\theta)$ for the typical 2D DLA shown in Figure 1 performed as described in Section 3.

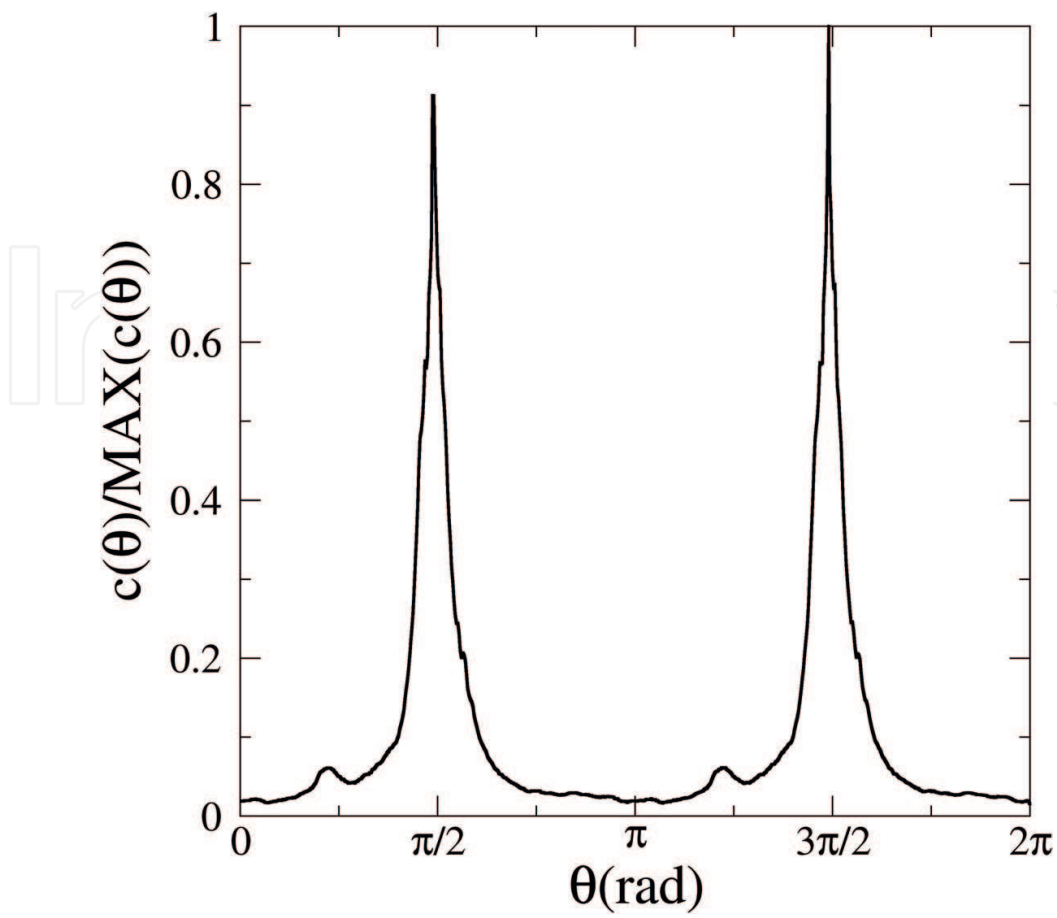


Figure 9. Rescaled $c(\theta)$ for the typical 2D DLA shown in **Figure 6(a)** performed as described in Section 3.

the anisotropic DLA, presented in **Figure 6(a)**, is visible that the peaked functions at the specific angle of approximately $\{\pi/2, 3\pi/2\}$ radians are associated with the anomalous branches that grew bigger than the rest of the aggregate.

Obviously, the Hausdorff dimension of these anisotropic structures also change, but meanwhile, the calculations of $c(r)$ and $c(\theta)$ end up corroborating the morphological changes advocated by a primary fractal dimension calculation.

There are cases in which the constituent species of the fractal/aggregate end up being different from each other, as was discussed in the paper [9]. In this case, it was necessary to create a correlation function for each of the species of particles involved in the aggregation growth process. This example proves the malleability of this type of function in the determination of morphological characteristics of the aggregates.

4. Conclusion

As observed throughout this chapter, the determination of the main characteristics associated with the morphological structures of two-dimensional fractals, especially those with dendritic properties and radial dispersion, involves the determination of angular correlation functions

$c(\theta)$ that may be useful at the capture of this characteristics. Investigations associated with diffusive processes such as crystal growth, neuronal formation, some types of tumoral growth, polymerization processes, deposition of materials, electric discharges, the formation of percolation networks among others are some of the examples that can be approached quantitatively by this mathematical tool.

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