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SELECTIVE DYNAMICS RELEASING FRAME KNOW HOW & WHY

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Abstract

The Selective Dynamics Releasing Frame (SDRF) algorithm was created some time ago by the author of this paper to speed-up the computer simulations of stochastic aggregation of diffusing particles and to reduce the number of preferred directions of growth anomaly resulting when these simulations are executed with the traditional DLA algorithm.

In this paper a detailed study of the SDRF, carried out to become acquainted thoroughly with the effects of its number of arc-segments (frames) on the morphology of the resulting aggregates, is reported. The reduction power of the SRDF concerning the number of preferred directions of growth in the resulting aggregates is investigated. Simulations of 250 stochastic aggregations of diffusing particles were carried out varying the number of frames in the SDRF. The resulting average fractal dimensions, densities and radii of the aggregates are analysed and reported. Also the observed fluctuations and general evolution of the aggregates is discussed. The use of a Seminal Group of particles instead of a single seed is introduced to improve the growth simulations.

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Keywords: DLA, SDRF, Monte Carlo, Computer Simulation, Stochastic, Aggregation, Diffusing particles, Launching frame, Seminal Group.

Resumen

El algoritmo Sectores Circulares de Dinámica Selectiva, SDRF, fue creado hace algún tiempo por el autor de este reporte, para acelerar la simulación computarizada de la agregación estocástica de partículas en difusión, y para reducir el número de las direcciones preferenciales de crecimiento que anómalamente resultan cuando la simulación se ejecuta con el algoritmo DLA tradicional.

En este trabajo se reporta un escrupuloso estudio del SDRF, ejecutado para conocer cabalmente los efectos del número de segmentos de arco del SDRF sobre la morfología de los agregados resultantes. Se investiga el poder de reducción del SDRF con respecto al número de direcciones preferenciales de crecimiento en los agregados resultantes de las simulaciones. Se simuló el crecimiento de 250 agregados estocásticos a partir de partículas en difusión, variando el número de arcos en el SDRF. Las densidades, dimensiones fractales y los radios de los agregados son estudiados y analizados. También se discuten las fluctuaciones observadas y la evolución de los agregados en general. Se introduce el uso de un Grupo Seminal en lugar de una sola semilla inicial en las simulaciones.

Palabras claves: DLA, SDRF, Monte Carlo, Simulación computarizada, Agregación estocástica, difusión, Marco de lanzamiento, Grupo Seminal.

1. Introduction

The stochastic non-reversible aggregation of diffusing particles to produce a cluster or aggregate is an ubiquitous phenomenon in nature, it can be found in dust, soot, ash, etc, and the study of this phenomenon is important because of its applications in colloid and polymer science and technology.

Being it impossible to follow experimentally the displacement and clustering of tiny particles and, at

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the same time collect the corresponding data, it is indispensable to resort to Monte Carlo computer simulations. The Diffusion-Limited Aggregation (DLA) model was created by Witten & Sander[1,2,3] to computer-simulate the growth of clusters that result from the irreversible stochastic aggregation of tiny particles that diffuse. This DLA model inspired many others, among them, the Selective Dynamics Releasing Frame (SDRF)[13,14], which can also be applied to other models that simulate stochastic aggregation of diffusing particles.

The DLA model is a computer simulation algorithm that has stimulated –since its introduction in 1981- the study of particle clustering[6,8,9,10]. Some variations of the basic DLA model have been developed to study non-equilibrium growth[5]. The resulting aggregate in a DLA-like simulation is a tenuous ramified (branched) structure, which branches prevent diffusing particles from penetrating in the interior of the aggregate, thus favoring the growth in the peripheric (exterior) region of the branches[3,7].

Regions in the stochastically growing aggregate have particular radii, which measure the distance from the seed particle (around which diffusing particles agglomerate), to the most exterior particles radially located. This is true for nature-made and computer-simulated aggregates. The SDRF resembles more realistically than the original DLA algorithm what takes place in nature.

This paper is organized as follows: Next a description of the original DLA algorithm is presented, it is followed by a description of the anomaly introduced by the DLA algorithm, next a description of the SDRF algorithm is presented, subsequently the equations to compute the fractal dimension and density are deduced. An introduction to the use of a Seminal Group instead of a single seed particle in the simulations comes next, then the parameters of the investigation carried-out are presented so that any one desiring to repeat or go beyond this research is fully instructed. The work concludes with a presentation of the computer simulation results, including some graphs and a table and its corresponding interpretations, and finally, the general conclusions are exposed.

2. The Original DLA Model

2.1 The DLA and the Dynamic Releasing Frame

In the DLA model, a single seed particle (the nucleation center) is placed at the origin of a system of coordinates. Far away from this seed, random walking particles are released to diffusion, one at a time. When a random walker meets the seed, it sticks irreversibly to it, then a new random walker is released far away, and the story repeats until an aggregate of as many particles as desired is grown.

Two concentric circles (see Fig.1) are used in the simulation[2,4,7], both centered at the seed particle. The inner circle whose radius R is slightly longer than the longest radius Rmax in the aggregate, is the Launching Circle, all diffusing particles are released from this circle. The outer circle whose radius is 3 Rmax or even more, is the Killing Circle. When a diffusing particle reaches this killing circle, it is killed (discarded) and a new particle is released in the launching (inner) circle. While a particle is in the region between the two concentric circles, it is allowed to displace by large jumps[11], eventually it may return to the inner circle, at any point of it, with the same probability. The releasing (launching) circle just depicted has a radius R = Rmax + Ao, which is controlled by the longest radius of the growing aggregate. In a typical[4] square-lattice DLA simulation, A_o=5, however this value is not definitive. The launching circle has a dynamic behavior because its radius R must be increased as the longest radius in the aggregate (Rmax) does. The same happens with the killing (outer) circle.

2.2 *Anomaly and Deficiency Introduced by the DLA Algorithm*

Real life stochastic aggregates of diffusing particles grow stochastically but uniformly (isotropically) in all directions about the nucleation center, in natural conditions there is no preferred radial direction of growth. However, during the computer simulations the aggregates by diffusion do not grow uniformly, they rather tend to develop preferred radial directions of growth, this results in some regions of the aggregates artificially having much shorter radii than Rmax (the longest radius in the aggregate). This branching effect is increased by the fact that the diffusing particles have a greater probability of being captured by the extending branches than by the central part of the aggregate. In this way the largest branch tend to grow every time larger and longer, and since Rmax is the radius of the longest branch, then the radius R = Rmax + Ao of the dynamic releasing circle (controlled by Rmax), may result too large for some regions of the aggregate. On the other hand, the particles in a DLA-like computer simulation have a pre-fixed Life-time, which allows a particle to execute a pre fixed number of steps given by its Life-time. The pre fixed Life-time together with the low opportunities of reaching the inner parts of the aggregate produce aggregates artificially empty in their inner regions, this effect is not present in real life stochastic aggregates (because there is no pre fixed life time) and it is rather an anomaly and deficiency introduced by the simulation algorithm, which is in strong disagreement with real life behavior.

2.3 *The Selective Dynamics Releasing Frame, SDRF Algorithm*

The SDRF introduced by this author[13,14], besides reducing computer time it also overcomes the anomaly of the preferred growth directions[15] during computer simulations of stochastic aggregates by diffusion.

In the SDRF the diffusion bi-dimensional XY-space is divided in a number No of regions about the seed particle, each region having its own control radius Rn, whose length is determined by $Rn = R(n)_{max} + Ao$, where $R(n)_{max}$ is the largest radius of the growing aggregate in region n (n = 1, 2, ..., No). In this way the launching or releasing circle originally controlled by the largest aggregate radius Rmax has now been replaced by No arc-segments (see Fig.1), each one with its own radius and own dynamics.

Obviously and ideally, the number of regions in which the diffusing XY-space is divided must be as large as possible.

In montecarlo computer simulations with the SDRF every diffusing particle is released from a randomly selected arc-segment. At the beginning of the simulation the radii of the arc-segments measure all the same, this is, we have a releasing circle of some radius Ao. As the aggregate grows every arc-segment or region will develop its own radius Rn.

If a particle is released to diffusion in arc-segment m and sticks to the aggregate in a region belonging to the same arc-segment m, and if $R(m)_{max}$ increases, then Rm must be updated.

If the particle released in arc-segment m sticks to the aggregate in a region associated to arc-segment k, and $R(k)_{max}$ increases, then Rk must be updated, keeping Rm and $R(m)_{max}$ their original values in this case.

Concerning the Killing Circle (whose radius is larger than Rmax + Ao), the SDRF algoritm does not make use of it. Since outside the circle of radius Rmax + Ao, the diffusing particles are allowed to make large jumps in any randomly selected direction[11] then in SDRF if a diffusing particle goes farther than Rmax + Ao, it is discarded and a new particle is released randomly from any arc-segment, this because beyond Rmax + Ao the particles can make large jumps and thus may return to the circle Rmax + Ao at any point.

2.4 *Using a Seminal Group in the Simulations*

From real-time visualizations of step-by-step computer simulations of a very large number of stochastic aggregates it is concluded that in order to avoid the almost always present artificial preferred directions of growth, it is necessary to make use of a Seminal Group of particles.

Depending on the particle-particle aggregation type, it seems better to this investigator to start a growth simulation with a single circular launching frame around a solitary seed particle, then once this seed has gathered a by-experience prefixed number of particles -the Seminal Group- trigger the SDRF, in this way the resulting aggregates resemble more realistically those found in nature. Since the seminal group is a rather small number of particles (from 2 to 25), its statistical influence is negligible but it adds isotropy to the grown aggregate reducing the preferred directions of growth. In this research the particles attached to the aggregate followed an out-of-equilibrium sticking protocol and the seminal group was fixed in 15 particles.

2. 5 *Calculating Fractal Dimension and Density of Stochastic aggregates*

For an stochastic aggregate the relationship between its Radius of Gyration Rg, its total number of particles N and its Fractal Dimension D, is given by[16].

$$R_g = C\, N^{1/D} \tag{1}$$

where C is a normalization constant. In interference-free conditions the aggregate must grow isotropically around its seed cell and it can be assumed that if fully filled by particles, it will be a circle centered in the seed, in these conditions it may be taken into account the fact that the Rg of a circle of radius R, around its center is given by

$$R_g = R/\sqrt{2} \tag{2}$$

To deduce the value of C, it must be considered that the number No of particles in a circle of radius R is given by

$$N_o = \pi R^2 \tag{3}$$

When the circle becomes fully covered by particles, its fractal dimension becomes equal to its area dimension 2, hence replacing (2) and (3) in (1), for D = 2:

$$C = 1/\sqrt{2\pi} \tag{4}$$

after replacing (4) in (1), the fractal dimension D is calculated by means of

$$D = \frac{\ln N}{\ln\left(R_g \sqrt{2\pi}\right)} \tag{5}$$

The DLA Circular Launching Frame and the Selective Dynamics Releasing Frame (SDRF)

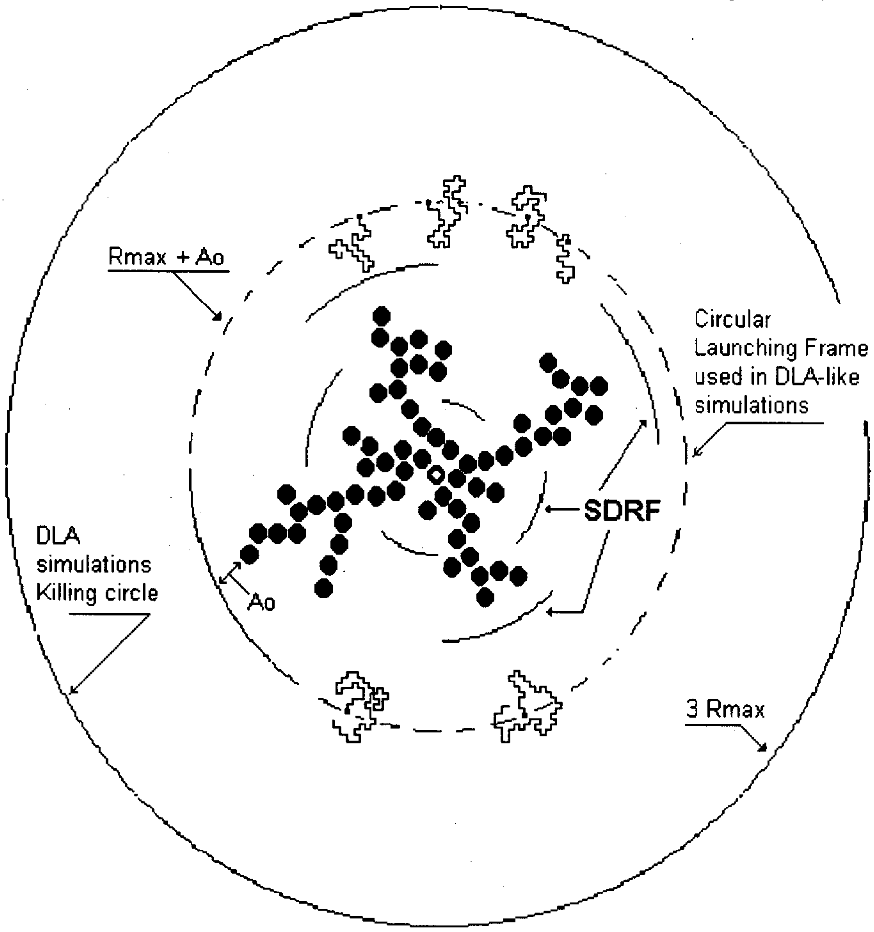

Fig 1. The circular Launching Frame used in DLA-like simulations and the SDRF used in this research are displayed. Some Random Walkers released in the Launching Frame are shown, it can be seen that random walkers keep moving in the neighborhood of their starting points, thus very hardly reaching the aggregate, hence the need of releasing them as close as possible to the aggregate branches, a mission successfully achieved by the SDRF.

To calculate Rg its already popular equation is used:

$$R_g = \left[\frac{1}{N} \sum_{i=1}^{N} r_i^2 \right]^{1/2} \qquad (6)$$

Concerning the Density of an aggregate of N particles and largest radius Rmax, it may be computed by means of

$$\rho = \frac{N}{N_o} = \frac{N}{\pi R_{max}^2} \qquad 0 \le \rho \le 1 \qquad (7)$$

where No according to eq.(3), is the number of particles in a fully filled aggregate of radius Rmax, in this way the density is zero when the aggregate is empty and is 1 when it is fully filled, otherwise its value is intermediate.

2.6 *The Parameters of the Investigation*

The research supporting this paper was strictly a set of computer simulations with the SRDF, a variation of the DLA algorithm, it has had the following parameters:

Random Walkers: Bearing in mind that the discretized solution of the Laplace diffusion equation is given by random walkers[16,17], in this research diffusing particles displace as unit random walkers in a square lattice, this means that the particles displace North, South, East or West and the length of the displacement is always one unit. This is, from one cell to its next neighbor in a bidimensional Euclidian space.

Not Stable Aggregation: The aggregation takes place in a square lattice and it is not stable (out-of-equilibrium sticking protocol), which means that the particles attach to the aggregate as soon as they meet it. In an stable (equilibrium) aggregation, before sticking to the aggregate, the particles check the energy of that particle they are going to stick to, if the energy is low, they stick, otherwise they continue their Brownian diffusion until they detect a low energy particle in the aggregate, to stick to.

Life Time: A diffusing particle is enabled to as many random walk steps, as it s life-time, before sticking to the aggregate or dying (being discarded) and thus allowing to release a new particle to diffusion. In this work, the life-time of the diffusing particles is 1000 units.

Number of Particles: During simulations the growth of an aggregate is finished, (1) when all the available particles have been released to diffusion, (2) when the aggregate collected a prefixed number of particles or (3) when one of its branches reaches the borders of the simulation space. For every simulation in this research it was assumed that 50000 particles would be released to diffusion. However, the resulting aggregates reached the frontiers of the simulation space before aggregating that number of particles, this was mainly due to the rather small simulation space (a squared 501 x 501 matrix) and not so strong computing power, with more powerful computers and with larger memories this number may be also larger. As usual the seed particle was placed in (0,0) at the center of the matrix.

Number of Circular Sectors: This is precisely the objective of this research, the study of the aggregation varying the number of circular sectors in the SDRF, each one having its own particular launching frame (circular segment). A Seminal Group of 15 particles was used. Fifty aggregates were grown using in each case a SDRF with 8, 16, 32, 64 and 128 circular sectors, this makes a total of 250 aggregates for the whole research. Averages were taken for every SRDF investigated.

Aggregate to Launching-Frame distance: throughout all the research the distance Ao between the aggregate and the arc segment of every circular sector, was fixed in 10 units.

3. Results and Discussion

Despite the fact that in general the averages show the global results, during the simulations there were no large fluctuations in the values observed. All the developed aggregates shared the same behavior.

As it can be seen in Table 1, the higher the number of arc-segments (frames) in the SDRF, the higher the Number of cells in the aggregates, the higher their Fractal Dimensions and also the higher their Density. This effects are due to the fact that with more frames in the SDRF, the number of preferred directions of growth is reduced, consequently the aggregate expansion diminishes and the diffusing particles have more chances of being captured by the inner regions of the aggregate, as it takes place in perturbation-free grown aggregates of real life. It is necessary at this point to recognize that the radius of the launching frames constitute a perturbation that introduces anomalies to the stochastic aggregation simulation, taking it far from what happens with aggregates grown in the nature. It was observed that the lower the number of frames in the SDRF, the thinner and more ramified the aggregates and conversely, the higher the number of SDRF, the fatter and more natural the aggregates.

According to Vicsek[16] the reported fractal dimensions of DLA clusters grown using modified versions of the DLA model fall within $D=1,72\pm0,06$, though that author does not mention the algorithms. Aggregates grown in this research produce fractal dimensions D in agreement with those values, also within the expected $d-1<D<d$, and not so far from those predicted by the Mean-Field theory $D=(d^2+1)/(d+1)=1,667$, where d is the embedding dimension (d=2).

Despite the fact that a special research to investigate the relationship between the Life-time and the morphology of the aggregates has not been carried-out with the SDRF, it is expected that a short life time favors the development of aggregates with rather long and thin arms (preferred directions of growth), this because with a short life time the only diffusing particles allowed to find where to stick are those very close to the tips of the branches, those diffusing far from the arms will die before finding where to add to.

4. General Conclusions

In nature, when a stochastic aggregate grows a branch in a given direction, its radius does not affect the growing of branches in other directions, this because diffusing particles in nature have infinite lifetimes, an effect much better simulated with the SDRF than with the traditional single Circular Launching Frame.

In this research simulation spaces with (a) 8, (b) 16, (c) 32, (d) 64 and (e) 128 circular sectors (frames in the SDRF) have been used. In simulations with 8 circular sectors or less, the growth of the aggregates does not follow a definite and regular behavior, the fluctuations observed are rather large[15], sometimes

Table I. Average results obtained from the simulations

Averages of 50 aggregates for every SDRF investigated				
Number of frames in SDRF	**N, Number of attached cells**	**Radius of Gyration, Rg**	**Fractal Dimension, D**	**Aggregate Density**
8	21680	147,70	1,68	0,11
16	27285	149,33	1,72	0,15
32	30428	149,32	1,74	0,16
64	35452	151,79	1,76	0,19
128	41483	154,66	1,78	0,22

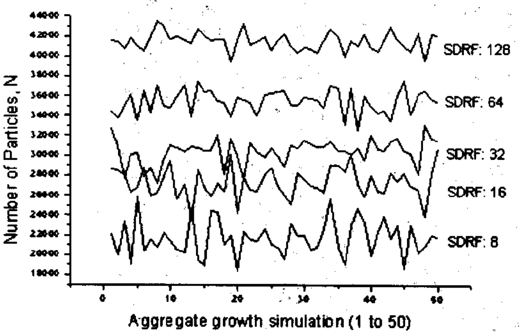

Fig 2 *Number of Particles, N.-* The fluctuations in the number N of particles reduce as the number of frames in the SDRF is increased. The higher the number of frames, the more uniform the number of particles captured by the aggregate. As expected, the higher the number of frames in the SDRF, the higher the particle population in the aggregates.

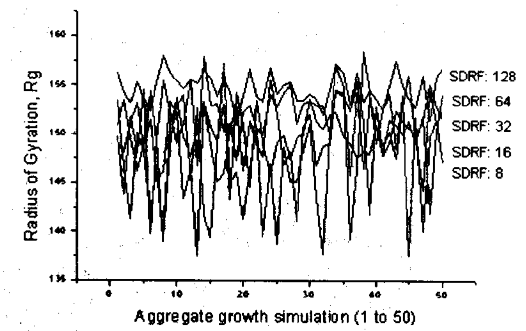

Fig 3 *Radius of Gyration, Rg.-*The magnitude of the fluctuations in the radii of gyration of the aggregates decreases as the number of frames in the SDRF increases, this may be due to the fact that as the number of frames is increased, the aggregates become more isotropic because a higher number of frames reduces the number of directions of preferential growth.

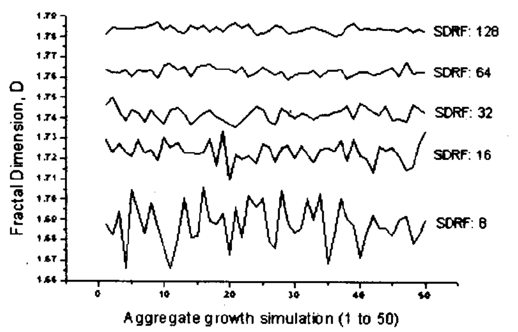

Fig 4 *Fractal Dimension.-* As the number of frames in the SDRF increases, the aggregate fractal dimension D, raise, because with a higher number of frames the likelihood of capturing more particles is higher than with few frames. This is, the number of frames contribute to the development of fat aggregates. The fractal dimension fluctuations reduce with higher numbers of frames, this is, aggregates show a tendency to grow more isotropic when large numbers of frames are used in the SDRF.

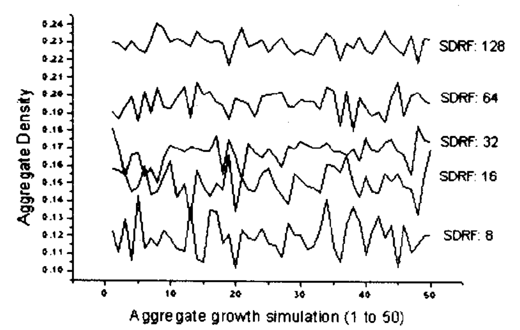

Fig 5 *Aggregate Density.-* As the number of frames in the SDRF increases, the aggregate density does too, because with a higher number of frames the likelihood of capturing more particles is higher than with few frames. Density fluctuations reduce with higher numbers of frames. As may be expected the density of the aggregates never reached 1,00; they never became 100% massive, they are plenty of cavities, however those cavities turn out to be smaller and smaller as the number of frames raises (compare aggregates in Fig 6).

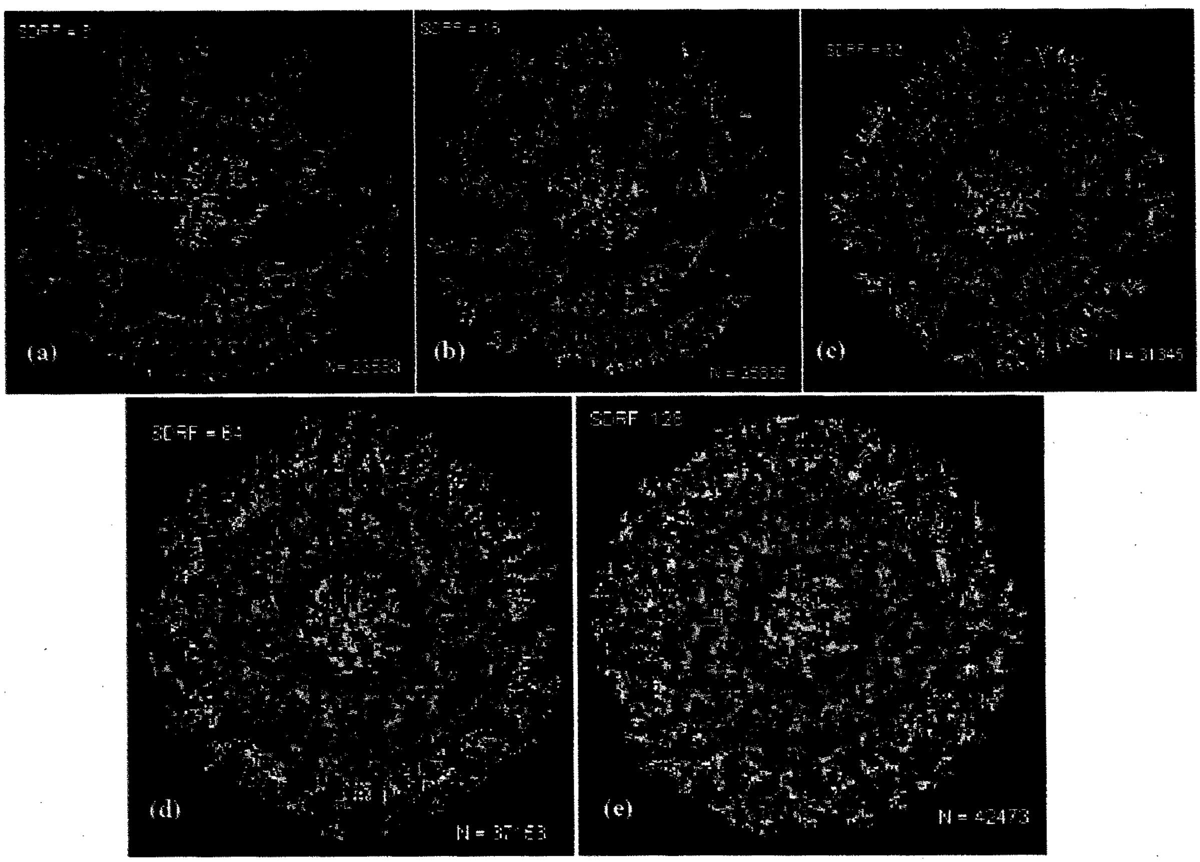

Fig 6. Five randomly taken images of aggregates developed with (a) 8, (b) 16, (c) 32, (d) 64 and (e) 128 frames respectively, every image displays the number of frames used in the SDRF and the number N of captured particles. In general, aggregates grown with the SDRF resemble more realistically those produced by nature under unperturbed conditions, than those produced with the DLA algorithm, which produce aggregates containing artificial cavities due to a deficiency of the algorithm.

the resulting aggregates are isotropic and some other times strongly favored branches result in the aggregates, for this reason these cases do not represent the situations found in real life, where it is expected that aggregates grown from diffusing particles are stochastic but isotropic, with no preferred directions of growth.

Within the parameters of the simulations reported here, 16 or more frames in the SDRF must be preferred when carrying out stochastic growth simulations, because the fluctuations inherent to the algorithm are reduced, which contribute to more accurate statistics.

When the number of circular sectors is small, the resulting aggregates present longer arms, and hence a lower number of particles in the aggregates when one of its branches reaches the borders of the simulation space and the growth of the aggregate is finished.

The higher the number of circular sectors, the higher the number of branches developed by the aggregates, the smaller their radii and the larger the number of captured particles. Hence the compactness and fractal dimensions of the aggregates will maintain a direct relationship with the number of circular sectors used in the growth simulation[15].

The spatial distribution of an stochastic aggregate developed with many circular sectors, resemble more realistically the geometric structure of those found in nature. The interesting point is that for aggregates with very large radii, even 128 frames in the SRDF might not be enough at some moment, because as the aggregates develop their radii, the arc of influence of the frames (arc-segments) becomes too large to be effectively nourished with diffusing particles. It may be necessary in this cases to develop an algorithm with an adaptable number of arc-segments as the aggregate radii get larger.

With respect to the parameter Ao (distance from the aggregate branch tip to the releasing frame) which controls the radius $Rn = R(n)_{max} + Ao$, of each releasing arc-segment, its value may be adjusted by the researcher to the type of particle displacement and aggregation type to be simulated in each case, Ao might play an interesting role in stochastic aggregation simulations with the Finite-Diffusion-Length, FDL algorithm[12].

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