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Introducing a selective dynamics releasing frame algorithm to speed-up stochastic aggregation computer simulations

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Abstract

A faster algorithm, the selective dynamics releasing frame (SDRF), to computer-simulate the stochastic aggregation of diffusing particles is introduced. The SDRF is presented making reference to the DLA model of Witen & Sander, however it can be applied to any DLA-like model which simulates cluster growth by diffusion. Traditional DLA-like models use the longest radius of the growing aggregate to control the radius of a Circular Launching Frame from where the particles are released to diffusion. The SDRF uses the different radii of the regions of the growing cluster to fix a particular distance from where to release the particles to diffusion in every region. In bi-dimensional DLA simulations, a reduction in 30% of computer time was observed when the SDRF was used. The algorithm here introduced is for a bi-dimensional simulation, however its application to higher dimensions is straightforward.

Keywords: DLA; Simulation; Stochastic; Aggregation; Launching frame; SDRF.

Resumen

Se presenta un algoritmo más rápido, el de marco de lanzamiento de dinámica selectiva (SDRF), para simulaciones en computadora de la agregación estocástica de partículas que difunden. El SDRF se presenta haciendo referencia al modelo de DLA de Witten & Sander, sin embargo, el mismo puede ser aplicado a cualquier modelo tipo DLA que simule el crecimiento de racimos debido a la agregación de partículas que difunden. Los modelos tradicionales tipo DLA usan el radio mas largo del agregado que esta creciendo, para controlar el radio del Círculo de Lanzamiento, desde el cual se liberan las partículas que se difunden. El SDRF usa las diferentes regiones en los radios del agregado en crecimiento, para fijar distancias particulares desde las cuales se liberan -en cada región- las partículas que se difunden. Cuando se ha usado el SDRF en simulaciones DLA bi-dimensionales se ha observado una reducción en 30% del tiempo de maquina, con respecto al método tradicional de un solo radio. El algoritmo se presenta para el caso bi-dimensional, sin embargo su adaptación a casos de mayores dimensiones es inmediato.

Palabras clave: DLA; Simulación; Estocástica; Agregación; Marco de lanzamiento; SDRF.

1. Introduction

The stochastic non-reversible aggregation of diffusing particles to produce an aggregate (cluster), is an ubiquitous phenomenon in nature (dust, soot, ash, etc) and the study of this phenomenon is important because of its applications in technology (colloids, polymers, etc).

Since it is difficult to follow experimentally the displacement and clustering of tiny particles, it is indispensable to resort to computer simulation. The Diffusion-Limited Aggregation (DLA) model was created by Witten & Sander [1,2,3] to computer-simulate the

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growth of clusters that result from the irreversible stochastic aggregation of tiny particle that diffuse. This model has inspired many others, for this reason, the Selective Dynamics Releasing Frame (SDRF) will refer to the DLA model, however the reader will see that the SDRF can be applied to other models that simulate aggregation by diffusion.

The DLA model is a computer simulation algorithm that has stimulated –since its introduction in 1981- the study of particle clustering [6,7,8,9]. 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].

Each region in the stochastically growing aggregate has a radius, which measures the distance from the seed particle (around which diffusing particles agglomerate), to the most exterior particle radially located.

2. The DLA and the dynamics Releasing Circle

In the DLA model, a seed particle (the nucleation center) is placed in the origin of a coordinate system. 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 are used in the simulation[2,4,7], both centered in 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 2 Rmax or even more, is the Killing Circle, if 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, Ao = 5, that Ao means?, which units? (particle radius?) however this value is not definitive. The launching circle has a dynamic behavior because its radius R grows as the longest radius in the aggregate (Rmax) does. The same happens with the killing (outer) circle.

3. The effects of the launching circle controlled by Rmax

Due to the stochasticity inherent to the capture of diffusing particles, the aggregates by diffusion do not grow uniformly, they rather tend to develop protuberances and these, branches, thus some regions of the aggregates may have a much shorter radius than Rmax. 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 dynamics releasing circle (controlled by Rmax), may result too large for some regions of the aggregate. In this way the particles that stick in regions whose radius is shorter than Rmax, have to displace longer distances than those captured by regions neighbouring Rmax. Since the particles diffuse via random steps, many times the net displacement from releasing to sticking may take a very long (computer) time. The SDRF introduced next reduces this (computer) time.

4. The selective dynamics releasing frame, SDRF

In order to reduce computer time in aggregation by diffusion simulations, the SDRF algorithm is introduced. In SDRF the diffusion bi-dimensional XY-space is divided in a number regions, we use eight regions or octants, each one 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=1,2,3,..8). In this way the launching or releasing circle originally controlled only by Rmax has now been replaced by eight arc-segments, 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, the eight regions used here just set down a first degree of speed increment. However there arise some technical problems with the installation of more than eight regions, these will be discussed in a next paper.

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

If a particle is released to diffusion in octant m and sticks to the aggregate in a region being or lying on the same octant m, and if $R(m)_{max}$ increases, then Rm must be updated. If the particle released in octant m sticks to the aggregate in a region lying on octant 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. Outside the circle of radius Rmax + Ao, the diffusing particles are allowed to make large jumps in any randomly selected direction [11]. 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.

5. Results and discusions

In the nature when a stochastic aggregate develops the growing of a branch in a given direction does not affect the growing of branches in other directions, this effect is much better achieved with the SDRF than with the traditional Circular Launching Frame.

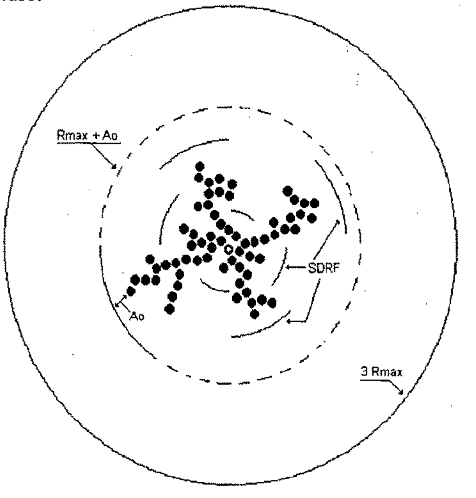
With respect to the parameter Ao which controls the radius $Rn = R(n)_{max} + Ao$, of each releasing arc-segment, its value may be adjusted by the researcher to the type of particle displacement and aggregation type to be simulated in each case.

In bi-dimensional square-lattice DLA simulations with the SDRF, a reduction in 30% of computer time with respect to the Launching Circle algorithm has been measured by this author.

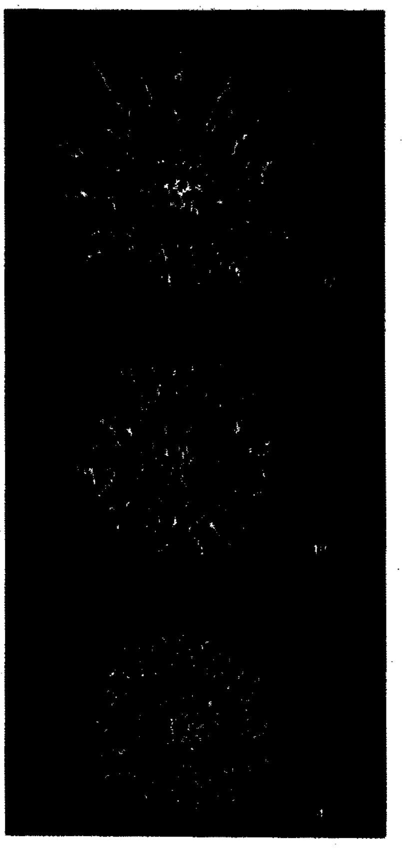
Since aggregates in three or higher dimensions will generate more radii than in two dimensions, the SDRF algorithm will result particularly useful when simulating in those spaces. An immediate application of the SDRF algorithm would be the stochastic growth simulation from a single seed with the FDL (Finite-Diffusion-Length) model [12], in cases like this the parameter Ao would play the main role.

Figure(1).displays the Circular Dynamic Launching Frame (inner dashed circle), the SDRF (eight arc-segments) and the killing circle (outer circle, not used with the SDRF). The seed particle appears as a hollowed dot in the center of the aggregate. Since the parameter Ao is being used in the SDRF, one of its arc-segments lies on the dashed circle. In the SDRF any diffusing particle going away the dashed circle is discarded, thus saving additional computer time.

Figure(2) shows three Equilibrium (stable) Square-Lattice Stochastic Aggregates made up of 6500 Random Walkers each, there the number of SDRF regions from top to bottom aggregate are 32, 48 and 64 respectively. It can be seen that the higher the number of SRDF regions, the better the resemblance with aggregates grown by diffusion in nature.



Figure(1). Circular Dynamic Launching Frame (inner dashed circle), SDRF (eight arc-segments) and the killing circle (outer circle, not used with the SDRF).



Figure(2). Random Walkers (6500) in an equilibrium (stable) square-lattice stochastic aggregate. In each case the number of the regions in the SDRF is shown.

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6. References

[1]. T.A. Witten & L.M. Sander, Phys. Rev. Lett., 47-19 (Nov 81)

[2]. T.A. Witten & L.M. Sander, Phys. Rev. B, 27-9 (May 83)

[3]. L.M. Sander, "Growth by Particle Aggregation" Scaling Phenomena in disordered systems (Pynn & Skjeltorp, Plenum Press, 1985)

[4]. P. Meakin, Faraday Discuss. Chem Soc. 83, paper 9, 1987

[5]. P. Meakin, "Fractal Aggregates and their fractal measures", pre-print, 1987

[6]. P. Meakin, CRC critical reviews in solid state and material Sc., Vol 13, issue 2, pag 143-189

[7]. P. Meakin, "The growth of fractal aggregates", pre-print.

[8]. P. Meakin, "Some recent advances in the simulation of DLA and related processes", pre-print.

[9]. P. Meakin, Phys. Rev A. 35-5, March 1987

[10]. Family-Viseck-Taggett, J. Phys. A: Math. Gen. 19 (1986) L727-L732

[11]. Family & Vicseck, "Simulating Fractal Aggregation", Computers in Physics, Jan/Feb 1990

[12]. R.L. Smith & S.D. Collins, Phys. Rev A, 39-10, May 15, 1989.