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MODELING OF BROWNIAN MOTION OF COMPACT CLUSTERS

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ABSTRACT

A model for simulating kinetics of centre of mass (CM) of a constant mass cluster (i.e. cluster with fixed number of particles N) is proposed. Here, a case of two dimensional compact cluster is considered. In this model, clusters consisting of fixed number of particles N, are grown on a two dimensional square lattice. Diffusion limited aggregation (DLA) process is modified to grow compact clusters. After the basic cluster is grown, a fixed number of particles (depending upon the mass of the cluster) are removed from periphery of the cluster and same number of new particles are deposited by random walker in every time step, and the motion of CM is studied with time t. It has been seen that mean square displacement (MSD) of CM is changing with time t as t^{α} for whole time span. The value of exponent α is 1.000 ± 0.005 for compact cluster of any mass. Hence, it concludes that the compact cluster is performing a normal diffusion. It can also be concluded that α is nearly equal to the ratio of embedded dimension and actual dimension of the cluster. In case of compact cluster it is 1.0 (as embedded dimension is same as actual dimension).

Keywords: Compact clusters, Diffusion Limited Aggregation, Mean Square Displacement, Centre of Mass

I. INTRODUCTION

1.1 Theoretical Background

Brownian motion is a well-known problem and has been useful in modeling of many fundamental as well as applied phenomena in physical, chemical and biological sciences. In biological systems, modern video imaging techniques [1] have shown many interesting characteristics of the diffusion process. The clusters of aggregate particles like nano-gels, micro gel, polymer etc. are always considered as a rigid spherical body with radius *R*. The molecules of fluid are constantly hitting the macromolecules at surface of the aggregates. In this study the random walk of a compact cluster is simulated to study the diffusion process. It is seen that the compact aggregate shows normal diffusive behavior.

1.2 Diffusion Limited Aggregation (DLA) Model

DLA model is very well known for simulating the growth of fractal clusters. In this model particles undergo random walk due to Brownian motion and cluster together to form aggregated of particles. For cluster growth in two dimensions, this model exhibit fractal nature with dimensions nearly equal to 1.7. In this model, a seed is placed at the centre of the square lattice. Then a circle of very large diameter is considered to start a random walk. When the random walk reaches a vacant site whose neighboring sites are filled then a random number is used to take a decision of filling the vacant site. The probability of filling is inversely proportional to the number of neighboring filled sites [2].

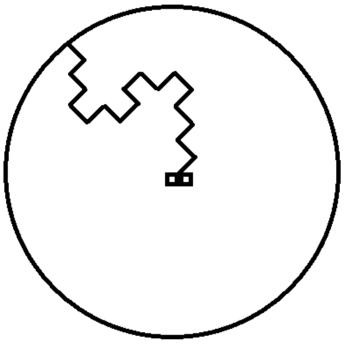

Figure 1. Basic Random Walk for Aggregation in DLA

This model was proposed by T. A. Witten Jr. and L. M. Sander in 1981. It is applicable to many systems where diffusion causes the aggregation of particles. Examples of such systems are dielectric breakdown, electrodeposition, mineral deposits etc

II. MODELING AND SIMULATION

2.1 Basic Methodology

In this study, the Diffusion Limited Aggregation (DLA) model is modified to simulate growth of compact clusters instead of fractal clusters [3]. Compact clusters of different number of particles (mass) varying from N = 500, 1000, 5000, 10000, 50000 are grown on a two dimensional square lattice. The modification that is introduced in this model is that the sticking probability is reversed for particles so that the cluster will become compact. In our model, the probability of filling vacant site is directly proportional to the number of neighboring filled sites. After the growth of a compact cluster of particular number of particles N, a fixed number of particles (scaled as N/5000) are added into peripheral sites of the cluster selected by a random walker. Number of particles in the cluster (N) was kept constant by removing equal number of particles from peripheral sites of the cluster selected by another random walker. This process is repeated for 1×10^5 iterations. In this process it is assured that the structure of the cluster is not changed even for large number of iterations. Thus, with this modified model, the Brownian motion of a compact cluster is studied with this continuous addition and removal of particles from peripheral sites of the cluster [4]. Figure 2 shows a growth of the compact cluster.

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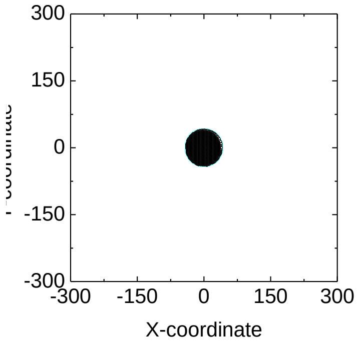

Figure 2. Compact Cluster of N = 5000

III. RESULTS AND DISCUSSION

Figure 3 shows a plot of motion of center of mass (CM) coordinate of a compact cluster of mass number N = 5000 and 1×10^5 number of iterations [5].

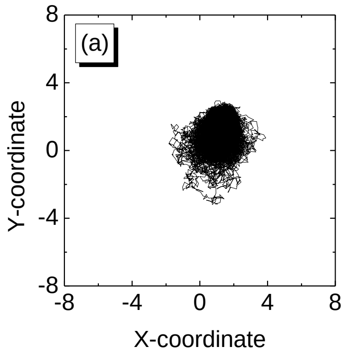

Figure 3. Motion of CM of Compact Cluster

Langevin equation for spherical compact particle can be solved to get a functional relation between mean square displacement (MSD) and time t as $\langle x^2 \rangle \propto t^{\alpha}$. From the analysis of graphs shown in Fig. 4 and Fig. 5, it is seen that the value of exponent α for compact clusters is around 1.0. This shows that the compact clusters exhibit normal diffusion [5]. It is found that the exponent of time α depends upon dimensions of cluster and the embedded dimensions.

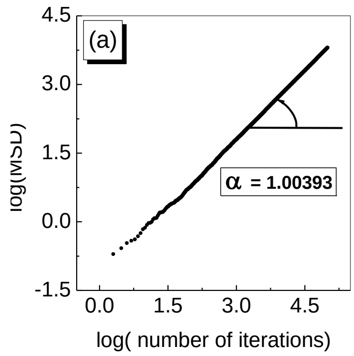

Figure 4. Plot of MSD vs *t* for Compact Clusters plotted on log-log scale.

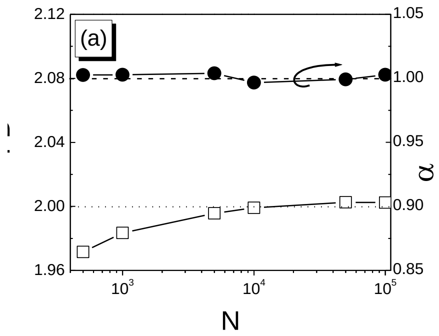

Figure 5. Plot shows the variation of FD and α against *N* particle number for a compact cluster From Fig. 5 it is clear that the value of exponent α depends on cluster dimension (FD) and not on the size (*N*) of the cluster.

IV. CONCLUSION AND FUTURE ASPECTS

Finally, it is concluded that successful demonstration of the Brownian motion of compact clusters of different sizes using the modified DLA model is given. In this study it is found that the time exponent α is approximately 1.0 for compact clusters. This indicates that the compact clusters perform normal diffusion. It is also proved that the value of this exponent depends on cluster dimensions and it is independent of mass of the cluster. In many experimental studies it has been shown that the fractal objects exhibit non-Brownian motion [1]. This model can be used to simulate this experimental finding and validate it. Therefore, in future one can extend this methodology to fractal clusters as well which will validate the conclusion of this work with more certainty [4], [6]. Also one can extend this model to one and three dimensions as well.

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