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Corresponding Author: Mr. Sebastian Gonzalez,

Corresponding Author's Institution: UTwente

First Author: Sebastian Gonzalez

Order of Authors: Sebastian Gonzalez; Anthony R Thornton, PhD; Stefan Luding, Prof. Dr. rer.-nat.

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*Cover Letter

In this paper, we present our findings regarding
the fractal dimension and scaling behavior associated with
an event-driven simulation of irreversible agglomeration. We consider
this work of importance for two reasons: on the one hand, we are broadening the
posibilities of event-driven simulations of granular matter, and on the other hand, we have
studied the dynamics of a process, to our knolwedge, not studied before.

Corresponding Author:
Sebastian Gonzalez
Multi Scale Mechanics, Universiteit Twente (UT), CTW , TS, P.O. Box 217, 7500 AE Enschede,
Email: j.s.l.gonzalezbriones@utwente.nl
Phone: +31 53 489 3371

Potential Reviewers:

Rodrigo Soto

E-Mail: rsoto@dfi.uchile.cl
Phone: +56 2 9784520
http://www.dfi.uchile.cl/~rsoto

Sean McNamara

Institut de Physique de Rennes, Universite de Rennes 1, 35042 Rennes cedex, France
sean.mcnamara@univ-rennes1.fr

Prof. Dr. Hans Jürgen Herrmann
Institut für Baustoffe (IfB)
HIF E 12
Schafmattstr. 6
8093 Zürich

Phone: +41 44 633 27 01
E-Mail: hans@ifb.baug.ethz.ch

An Event-Driven Algorithm for Fractal Cluster Formation

S. González, A. R. Thornton, S. Luding

Multi Scale Mechanichs, TS, CTW, UTwente
P.O.Box 217, 7500 AE Enschede, Netherlands

Abstract

A new cluster based event-driven algorithm is developed to simulate the formation of clusters in a two dimensional gas: particles move freely until they collide and "stick" together irreversibly. These clusters aggregate into bigger structures in an isotropic (random) way, forming fractal structures whose fractal dimension depends on the initial density of the system.

Keywords: fractals, event-driven simulation, granular matter, agglomeration, cluster formation

1. Introduction

Cluster formation is an important subject in various areas of physics; for example, in astronomy, ice clusters are believed to aggregate into planetesimals [1], the base of todays planets. In granular materials, the main theme of this paper, tiny nano-Newton forces are responsible for macroscopic clusters in free falling jets [2]. These are similar to those that appear in nano jets from plasma physics [3]. Clusters are also found in granular avalanches [4], and air-driven granular beds [5].

Motivated by nanoaerosols [6], a cluster based event-driven algorithm is developed to simulate the formation of clusters in a $2D$ gas with periodic boundary conditions: particles move freely until they collide and "stick" together irreversibly, moving as one cluster. The dynamics of the clusters is utterly simplified in our model. Conserving only linear momentum during collisions, angular momentum is disregarded. These clusters evolve and aggregate into bigger fractal structures, whose dimension d_f is found to be in the range $1.4 < d_f < 2$; in contrast, to the case of diffusion-limited aggregation (DLA), where $d_f = 1.67$ [7]. Here, we keep track of the dynamics of the clusters instead of adding particles one by one like in DLA. This procedure can be seen as a mix between irreversible coalescence [8], and a lattice-free version of a cluster-cluster aggregation model [9].

Implementing clusters in an event-driven algorithm has two advantages: Firstly, defining clusters of particles avoids the need to predict the events between particles of the same cluster. Since particles in a cluster move together as a rigid solid, they cannot collide. This alone decreases the computational effort required to simulate the clusters, where in standard event-driven models most of the collisions occur [10]. Secondly, the concept of clusters appears in a wide range of particulate physics: granular structures develop long correlations in space and time; see for example, Keys *et. al.*, Ref. [5], where it is found that particles move in one-dimensional paths ("strings") that aggregate into clusters.

In the next section we explain the algorithm used and how it is related to the classical event-driven model. After that, we present a selection of numerical simulations. Finally, concluding remarks and plans for future work are discussed.

2. Algorithm

By event-driven we mean that the state of the system is evolved in time from one event to the next. After each event, the time of the next event is calculated and the system advances. For the details of the algorithm we refer the reader to standard papers and books, see e.g. Refs. [**?** 12]. In brief, the algorithm consists of:

1. Given the instantaneous positions and velocities of all particles in the system,
2. predict the time of the next collision,
3. advance the time of the system to that instant, and
4. update the velocities of the particles that collide with a given collision rule, and repeat from 1.

The event-driven algorithm presented here builds on previous work, where the static phase in dense granular systems was simulated with a different dynamics, also improving the performance [13]. This is a necessary step towards a multiple-scale event-driven simulation for granular matter, where each cluster can have its own dynamics and collision rules.

The kind of clusters we are interested in at the moment are, e.g., suspensions of nanoparticles in a gas, which stick together at contact due to Van der Waals forces (as in Ref. [14]). In reality, clusters of particles conserve angular momentum when they collide, which results in rotating clusters. For the sake of simplicity, and since (at the moment) we are mainly interested in the algorithm rather than in recovering the right physics, we will disregard rotations of the clusters and, hence, consider only translational motion. Note that, anyway, no considerable rotation of large clusters is expected in a gas.

In normal event-driven algorithms one has to predict the next collision between all two-particle pairs. In this version, we introduce a new object called cluster (which may consist of just

one particle or many), and only collisions between these objects have to be computed. Since a cluster consists of a finite number of particles, the position of a particle i within a cluster C, is given by

$$\vec{r}_{i,C}(t) = \vec{r}_0 + \vec{v}_C t,$$

where $\vec{v}_C$ is the linear velocity of the cluster. The time is measured since its last collision, and r_0 is the center of mass of the cluster at that instant.

Now that we have defined the evolution of particles within a cluster, collisions between particles in different clusters can be detected. This is a massive time saving as collision between particles within the same cluster do not have to be checked for, and as the size of the clusters increases the total number of checks decreases. Once the collision of two clusters has been carried out, the colliding particles "stick" together and the two clusters are combined into a single larger one. The velocity of the newly formed cluster is calculated by considering the conservation of linear momentum only. This process is repeated until the system consists only of a single cluster.

The classical event-driven model needs to deal with a quadratic equation, both in the case with or without gravity. Like in the classical case, here we have to find the time of collision between two particles i, j by (analytically) finding the first (smallest) positive root of

$$|\vec{r}_i(t) - \vec{r}_j(t)|^2 = d^2,$$

with d the diameter of a particle. The inclusion of rotating clusters in the simulation makes the equation to find the collision time highly nonlinear. Recently, methods have been developed to deal with these situations [15, 16], but the inclusion of rotation is beyond the scope of this paper.

Summarizing the simulation procedure, one has to:

1. Start with an initial configuration of particles,
2. find the time for the next collision in the system.
3. Advance the system to that instant and merge the two particles (clusters) into a single cluster,
4. predict the next event with the new configuration, and
5. repeat until all the energy is dissipated and a single cluster is present in the simulation (the simulations are run in the center of mass reference frame).

Three snapshots of a simulation are shown in Fig. 1. At the beginning of the simulation, (a) particles are arranged in a square lattice with random velocities (each component of the velocity is take from an uniform distribution with zero mean). The color code represents different clusters in the simulation. At this initial time, every cluster correspond to strictly one single particle. At a later time, (b) clusters of different size coexist in the simulation and aggregate as soon as they are in contact. Finally, (c) the system contains only two clusters that will collide in the next event of the simulation, form one cluster, and end the aggregation process.

3. Experiments

The simulation consists of a system of N particles in a $2D$ square box of size L with periodic boundary conditions. Particles are monodisperse with diameter d and mass m. The packing fraction of the system is given by $\nu = N\pi d^2/(4L^2)$. In order to start with a homogeneous configuration, we let the system equilibrate: starting from a square lattice, each particle collides at least 10 times elastically until a homogeneous regime is reached with average velocity v_0. Once thermalized, the clustering algorithm is switched on, and the simulation runs until one big cluster is formed.

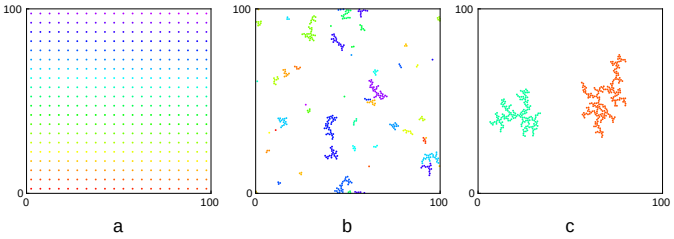

Figure 1: Three snapshots during the evolution of a system of $N = 400$ particles in a box of size $L = 100d$, a packing fraction of $\nu \simeq 0.03$. Each color represents a different cluster. Time increases from left to right.

3.1. Temporal Evolution

The natural time scale is the initial Boltzmann mean collision time (as defined in [8]), $\tau_0 = (4d\pi^2/v_0^2)^{1/2}/\nu$, with ν the packing fraction, and $g(\nu) \simeq 1$ for low densities.

The scaling behavior of the energy was studied. For dilute systems, the mean kinetic energy per particle follows a power law $\langle E_K\rangle/\langle E_K\rangle_0 \propto \tau^{-\delta}$, with $\delta = 1.3$ for almost four decades, as can be seen in figure 2. This results is similar to the one from Ref. [8], where a scaling with $\delta = 1.12$ was found. This scaling breaks down when the number of clusters is small and finite size effects become important, leading to bad statistics, since we did not employ ensemble averaging.

For these systems, the average cluster size also follows a power law scaling $\langle S_C\rangle \propto \tau^{\zeta}$ with $\zeta = 1$, which corresponds exactly to the mean field predictions in Ref. [17].

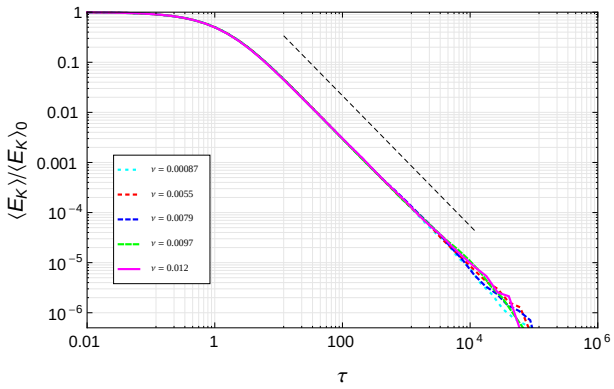

Figure 2: Energy as a function of the non-dimensional time $\tau = t/\tau_0$ for five systems with $N = 10^6$ and packing fractions in the range $0.0008 \leq \nu \leq 0.012$. The energy follows a power law $\langle E_K\rangle/\langle E_K\rangle_0 \propto \tau^{-\delta}$ with $\delta = 1.3$, as indicated by the dashed line

3.2. Cluster size distribution

As the simulation evolves, the distribution of clusters develops from N clusters of size one (free particles), to one cluster of size N. The change of the cluster size distribution as a function of time is plotted in figure 3. Since the raw probability density function (PDF) is noisy, see Fig. 4, we plot the cumulative distribution function (CDF) as a function of cluster size for different non-dimensional times. The data presented here correspond to $N = 10^6$ and a fairly dilute packing fraction of $\nu = 0.0097$. As time increases the number of clusters decreases and the distribution broadens, i.e. the difference between the biggest cluster and the smallest becomes larger, reaching a maximum around $\tau \sim 924$.

The resulting PDF cannot be fitted by an exponential function as in [8]. For intermediate times a fit of the form $P(s;\tau) = a(\tau)s^{-\gamma(\tau)}\exp(-w(\tau)s)$, with $a(\tau)$, $\gamma(\tau)$, and $w(\tau)$ are time dependent free parameters, while s is the cluster size. This can reproduce the qualitative behavior of the distribution: Fig. 4 shows the PDF for three intermediate times together with the best fit. The numerical values for the coefficients appear in the caption of the figure.

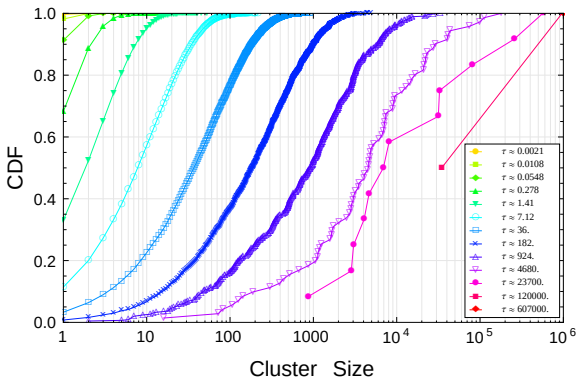

Figure 3: Cumulative distribution function for different non-dimensional times τ for a system of $N = 10^6$ and $\nu = 0.0097$. As time increases the number of cluster decreases and the distribution broadens, reaching a maximum around $\tau \sim 924$. Eventually, just two clusters are present: (red) squares. On the plot, each symbol (data point) represents one cluster, so we can see that as long as there are some free particles in the system, the distribution is smooth.

3.3. Fractal dimension and density

With the final configuration from each simulation, we count the number of particles present in a circle of radius r around ten randomly chosen particles of the cluster. We do this to obtain the number distribution $n(r)$, whose exponent is the fractal dimension of the system. We confirmed that the fractal dimension was almost independent of the points selected, by choosing points in the inner third, and in the outer third of the fractal: both measurements lead to practically the same results; here, we present data for d_f based on inner points.

The fractal dimension we obtain is strongly dependent on the density of the system. If we start with a very dense system, there is no re-arrangement possible and the final state will practically coincide with the initial state. Due to this, an integer

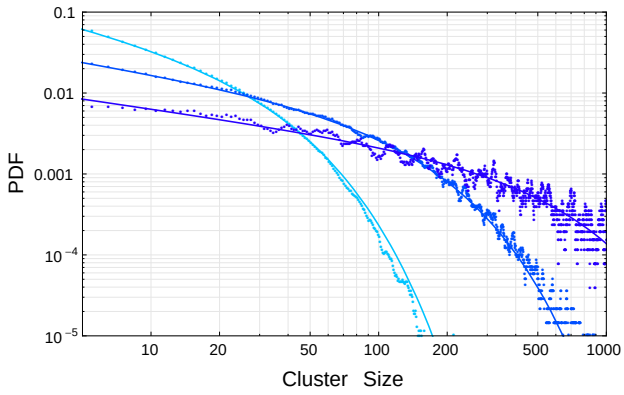

Figure 4: Probability distribution function for $\tau = 7.12, 36$, and 182 and the same system of Fig. 3. The distribution flattens and becomes more noisy as time passes. The solid lines correspond to the fit, while points correspond to the data. The functions plotted are $P(s;7.12) = 0.2(1)s^{-0.63(1)}e^{-0.038(1)s}$; $P(s;36) = 0.052(1)s^{-0.46(1)}e^{-0.0086(1)s}$; and $P(s;182) = 0.016(1)s^{-0.40(1)}e^{-0.0020(1)s}$ from top to bottom.

dimension of $d_f = 2$ is expected for dense systems. For vanishing density, we expect an asymptotic lower fractal dimension, since after some point the mean free path is much larger than the cluster size, i.e., the system is so dilute that molecular chaos holds.

Figure 5 shows the fractal dimension plotted against the density for different systems. To measure the effect of the density, we vary the size of the system for a given number of particles $N = 10^6$. The system sizes chosen are in the range $40000d \geq L \geq 1000d$, corresponding to densities between $0.0005 \leq \nu \leq 0.78$. We have realized one simulation for each system size, but gather statics by choosing different central particles.

The error bars correspond to the fluctuations in the measurement of the fractal dimension on a single simulation, and not to different realizations for the same system. As expected, for high densities the fractal dimension approaches 2, namely for $d_f(0.78) = 1.97 \pm 0.01$, that is, the cluster approaches a two dimensional structure. For vanishing densities it is found that $d_f(\nu \to 0)$ does not reach a clear asymptotic value and decreases with density, at least for the few values studied here. This fractal dimension is considerably smaller than the one found, by Witten et al. for the diffusion-limited aggregation process [7], where the fractal dimension is $d_{\mathrm{DLA}} = 1.67$.

4. Conclusions

In this paper we have presented event-driven simulations of irreversibly aggregating clusters in $2D$ systems of various densities. These clusters have non-physical dynamics but represent a "toy" model that permits us to understand how to make cluster simulations in an event-driven algorithm. The formation of fractals was studied, and the exponent found depends strongly on the initial density of the system, with dimensions in the range $1.4 \leq d_f \leq 2$. The denser the system, the closer to a two dimensional structure the fractal is. There remains the open question of what the smallest fractal dimension is that can be achieved

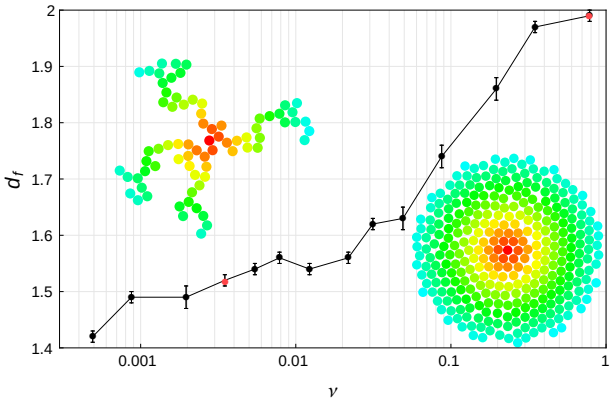

Figure 5: Fractal dimension as a function of packing fraction for systems with $N = 10^6$ particles. The dots are the simulation results while the solid line is just a guide to the eye. The error bars correspond to the fluctuations associated with the measurement of d_f and not to ensemble averages. In the inset, two examples of the structures obtained for two different densities $\nu_{\text{dilute}} = 0.0035$ and $\nu_{\text{dense}} = 0.784$, marked as red points on the plot. The structures are colorized from red to blue depending on the distance to the central particle.

with this algorithm. Besides the accumulation of better statistics, the inclusion of more realistic dynamics and collision rules for the clusters is currently being investigated.

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