Chapter 5

Self-Gravitating Granular Gases

5.1 Introduction

In Sec. 1.4.4, we had mentioned that the freely-evolving granular gas was proposed as a possible model for aggregation of galaxies and planets from interstellar dust [1]. Clearly, self-gravity plays an important role in this evolution. However, to the best of our knowledge, there have been no studies of freely-evolving granular gases with gravity. Therefore, in this chapter, we study the free evolution of an inelastic granular gas with a gravitational attraction between the grains. Unfortunately, we can no longer use event-driven molecular dynamics (EDMD) to simulate a system with an inter-grain potential. Rather, we have to revert to the usual time-step-driven MD which was discussed in Sec. 1.3.1.

The simulation of long-ranged forces is a notoriously difficult problem, and there are problems associated with the definition of the thermodynamic limit [2, 3, 4, 5]. In this chapter, we use the recently-proposed hierarchical linked cell (HLC) algorithm [6]
to study the self-gravitating granular gas. We focus on the evolution morphology of this system, and calculate the time-dependent structure factor and the cluster growth law. In order to check if the dissipation is comparable to the one we have been using in our instantaneous collision model [cf. Eq. (2.10)], we use a dissipative particle dynamics (DPD) simulation [4]. The model for our DPD simulation is the commonly used linear-spring-dashpot (LSD) model [7, 8].

The organization of this chapter is as follows. In Sec. 5.2, we present a brief overview of the various integration schemes available to study a system interacting via long-range forces, and highlight the advantage of the HLC algorithm over the conventional methods. We introduce the LSD model in Sec. 5.3. The detailed numerical results from our MD simulations are presented in Sec. 5.4. We conclude this chapter with a summary and discussion in Sec. 5.5.

5.2 The Hierarchal Linked Cell Method

The aim of an MD technique is to calculate the pair-wise interaction between all the particles or molecules of a system and advance the system in small time-steps over which the calculated force can be assumed constant. For a small system ($N \sim 1000$), this method is reasonably efficient as contributions from a large fraction of $N$ are significant, and hence need to be calculated. Also, the computational effort required in making lists of particles is more or less compensated by the efficiency achieved. As $N$ increases, the method of calculating forces between each pair becomes computationally more expensive, so much so that any simulation with $N > 2500$ particles can not be run within a reasonable amount of time.
The effective range of interaction for most of the potentials used in MD simulations extends no more than a few particle diameters. The contribution from the rest of the system, though non-zero, does not affect properties of interest much. It is commonplace in MD simulations to look for contributions from within a certain cut-off radius. This procedure does not require scanning through the entire system to calculate the force on a particle. A significant reduction in computational effort is achieved this way, without having to compromise on the accuracy of the result. Moreover, the quadratic dependence of the computational time on $N$ is replaced by a linear dependence, if such a method is adopted. This means that if we increase $N$ by a factor of two, the computational time also increases two times and not four times as would happen in the pair-wise calculation of forces over the entire system.

Long-range forces (e.g., electrostatic or gravitational forces) are different in the sense that the effective range of forces extend through the system and the contribution from a distant set of particles is significant and, hence, needs to be calculated. The pair-wise summation of interactions can still be avoided, and a number of algorithms have been proposed to achieve this. For a long time, the hierarchical tree code method proposed by Hut and Barnes (HB)[9] has been used for such simulations. In the HB method, efficiency is achieved by clubbing the far-away particles together. The entire simulation region is recursively subdivided into smaller and smaller cells such that no cell contains more than one particle. Beginning from the entire box, the cells of smaller size are labelled as cells of lower and lower hierarchy. In order to calculate the contributions from the cells, the so-called opening-angle criterion is imposed on the larger cell. The opening angle is the ratio of the cell size to the distance from the particle. If the opening angle $\theta$ is less than a prespecified value $\theta_0$, the contribution
from the entire cell, with cells and particles contained therein, is clubbed together as
the cell is considered to be distant. Else, the cell is subdivided into daughter cells or
cells of lower hierarchy and the same procedure is applied again.

Muller and Luding [6] have recently proposed a novel technique for a hierarchical
calculation of force for a system of particles interacting through long-range forces.
The HLC method they have proposed has two advantages over the tree code of Hut
and Barnes:

(a) The HLC method is easy to code, whereas the tree code of HB uses extremely
complex data structures; and

(b) the condition of periodic boundaries is in-built in the HLC method.

The simulation domain is divided into $(3^r)^d$ cells of lowest hierarchy (H1). Here $r$ is
a number whose value depends on the size of the domain, and defines the range up
to which one would like to calculate interactions through direct summations; and $d$
is the dimensionality. The force on the particle of interest (or poi) is calculated as
follows. The 27 cells in the neighborhood of the cell of interest (or coi), with the coi
in the middle, constitute the linked-cell neighborhood of the coi. The contributions
from all particles within the linked-cell neighborhood are calculated directly, with
a suitable cut-off radius in order to maintain symmetry. The particles outside the
cut-off radius are grouped together in each cell to make a pseudo-particle located at
the center of mass of the constituent particles.

In order to take care of periodic boundary conditions, the cells around the coi are
rearranged such that it finds itself in the middle of the cell structure. In order to
calculate the contributions from distant particles, the following procedure is adopted.
27 cells of hierarchy one or H1 around coi are grouped together to make a cell of H2. 27 cells of H2 around coi are grouped together to make a cell of H3, and so on. The contributions from 26 neighboring cells of a particular hierarchy on poi is calculated by grouping the particles within the cell and positioning a pseudo-particle at the center of mass. This procedure is applied recursively until the contributions from all other members on the poi is calculated.

5.3 Model for a Self-Gravitating Granular Gas

The granular system considered in this chapter is one whose particles (a) evolve under the influence of long-range gravitational forces; and (b) continuously lose energy like any other granular gas due to dissipative collisions. The gravitational interaction is conservative and present even at large distances. However, the contact forces apply only when a pair of particles touch each other physically. The contact interactions or collisions in this case occur over a non-zero time interval, unlike in EDMD, where the contact was instantaneous. The reason for choosing an alternative method here is that, while we can manage particle collisions as before, the particle-particle interactions between collisions is no more constant. The long-range gravitational force is to be calculated at each time step and is given by

\[
\vec{F}_i^g = -G \frac{m_im_j}{r_{ij}^2} \hat{r}_{ij}.
\] (5.1)

Here G is a constant, and \(\hat{r}_{ij}\) is the unit vector along the line joining j to i. (We assume that the particles are identical with unit mass, \(m_i = m_j = m\), and unit diameter.) One can distinguish forces along the normal and the tangential directions during collision.
There are two basic ingredients of contact forces for the particular case of granular particles. The impenetrability of particles has to be considered, and dissipation of a fraction of the normal component of the relative velocity has to be accounted for. Two types of forces are commonly used in MD simulations to model the collision of two particles, a force of elastic restitution $\vec{F}^s$ and a viscous friction force $\vec{F}^d$. Due to its mechanical analogy with a system of a spring and dashpot, this type of modelling is often referred to as a spring dashpot model.

It has been observed experimentally that the relevant quantity for various contact forces is the penetration depth

$$\delta = \frac{1}{2} (\sigma_i + \sigma_j) - r_{ij}, \quad (5.2)$$

and its time-derivative. The restoring force is often modelled as depending linearly on $\delta$ like the Hooke's force,

$$\vec{F}^s = -\kappa \left[ \frac{1}{2} (\sigma_i + \sigma_j) - r_{ij} \right] \hat{r}_{ij}, \quad (5.3)$$

where $\kappa$ is a constant analogous to stiffness of a spring and $\sigma$'s are the diameters. More generally, the elastic restoring force depends non-linearly on the penetration depth and is given by $[7, 8]$

$$\vec{F}^s = -\kappa \left[ \frac{1}{2} (\sigma_i + \sigma_j) - r_{ij} \right]^{(1+\alpha)} \hat{r}_{ij}. \quad (5.4)$$

For the linear case $\alpha = 0$, whereas for the Hertz model $\alpha = 1/2$.

The dissipative friction force is given by

$$\vec{F}^d = -\beta (\vec{u}_{ij} \cdot \hat{r}_{ij}) \hat{r}_{ij}, \quad (5.5)$$

where $\beta$ is a constant determining the amount of dissipation in the interaction. Here also we can accommodate nonlinearity by introducing $\delta$-dependence of the dissipative
force in the following way:

\[ F^d = -\beta (\vec{v}_{ij} \cdot \vec{r}_{ij}) \left( \frac{1}{2} (\sigma_i + \sigma_j) - r_{ij} \right) \vec{r}_{ij}. \]  

(5.6)

Henceforth, we restrict ourselves to the model we have used in our simulation, i.e., the \textit{linear spring-dashpot} model, which is a combination of the linear spring in Eq. (5.3) and the linear dissipative force in Eq. (5.5).

\textbf{Coefficient Of Restitution}

We examine the collision of two identical spherical particles with radii \( \sigma_i = \sigma_j = \sigma \) and mass \( m_i = m_j = m \) so that the reduced mass is \( \mu = m/2 \). In the simplest case, the interaction is modelled by a linear spring acting as a restituting force, and a linear dashpot providing necessary energy dissipation for interaction between particles of a granular gas. The collision in one dimension, i.e., the normal direction, suffices for our purpose. The relative acceleration during contact is given by,

\[ \ddot{\delta} = \frac{f_j}{m_j} - \frac{f_i}{m_i}, \]  

(5.7)

with

\[ f_{i,j} = f^e_{i,j} + f^d_{i,j}. \]  

(5.8)

Using the condition \( f_j = -f_i \), we obtain the following differential equation for \( \delta \),

\[ \ddot{\delta} + 2\gamma \dot{\delta} + \omega_0^2 \delta = 0, \]  

(5.9)

where \( \omega_0^2 = \sqrt{\kappa/\mu} \) is the natural frequency of oscillation, and \( \gamma = \beta/(2\mu) \) is the damping factor. The solution of Eq. (5.9) is,

\[ \delta(t) = \frac{2\theta}{\omega} \exp(-\gamma t) \sin(\omega t). \]  

(5.10)
and the corresponding velocity is,

$$\delta(t) = \frac{\nu_0}{\omega} \exp(-\gamma t) \left[-\gamma \sin(\omega t) + \omega \cos(\omega t)\right]. \quad (5.11)$$

Here, $\nu_0 = \delta(0)$ is the relative velocity before collision and $\omega = \sqrt{\omega_0^2 - \gamma^2}$ is the damping frequency.

As long as $\omega_0^2 > \gamma^2$, the typical duration of contact of two particles is half the time period of oscillation and is given by,

$$t_c = \frac{T}{2} = \frac{\pi}{\omega}, \quad (5.12)$$

as the interaction ceases when $\delta(t) > 0$. The coefficient of restitution $e$ is defined as the ratio of velocity of separation to the velocity of approach, i.e.,

$$e = \frac{-\dot{\delta}(t_c)}{\delta(0)} = \exp\left(-\frac{\pi \gamma}{\omega}\right). \quad (5.13)$$

The maximum penetration corresponds to the condition $\dot{\delta}(t_{max}) = 0$, so that

$$\omega t_{max} = \arctan\left(\frac{\omega}{\gamma}\right) = \arcsin\left(\frac{\omega}{\omega_0}\right), \quad (5.14)$$

whence it follows that

$$\delta_{max} = \left(\frac{\nu_0}{\omega}\right) \exp(-\gamma t_{max}) \sin(\omega t_{max}). \quad (5.15)$$

### 5.4 Numerical Results

#### 5.4.1 Details of Simulations

We used the time-synchronous leap-frog algorithm (see Sec. 1.3.1) to simulate a system of dissipatively interacting particles which evolve under the influence of
self-gravity. The mass $m$ and diameter $\sigma$ were assigned the value unity. The gas consists of $N = 10^5$ particles distributed homogeneously over a 3-d box of dimension $64 \times 64 \times 64$ with periodic boundary conditions. The value of the spring constant is always kept to be $\kappa = 10^6$.

For reference purposes, it is convenient to first consider the case without gravity ($G = 0$). In Fig. 5.1, we compare simulations for energy decay in the DPD model with different values of $\beta$, and EDMD with $e$ determined by Eq. (5.13). The two cooling curves are numerically indistinguishable, demonstrating that the DPD model mimics the granular gas very well. The dissipation parameter $\beta$ has been so chosen that the $e$-values are closest to the typical values chosen in our ED simulation of Chapters 3 and 4, i.e., $e = 0.7, 0.8, 0.9$ and 0.95. The corresponding values are $\beta \approx 159, 100, 47, 23$.

Our simulations for the self-gravitating gas were done with $G = 0.1, 0.01, 0.001$. The initial condition for a run was obtained as follows. We allowed a random initial condition to evolve for some time using the DPD scheme with $G = 0$ and $\beta = 0$, corresponding to the elastic limit $e = 1$. The resultant initial condition has a homogeneous density field, and a Maxwell-Boltzmann (MB) distribution of velocities.

### 5.4.2 Clustering in a Granular Gas with Self-Gravity

In Fig. 5.1, we compared results from the DPD simulation (with different values of $\beta$) with ED simulation results (for comparable values of $e$). We used the expression for coefficient of restitution in Eq. (5.13) to find out the approximate values for the dissipation coefficient $\beta$. 

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Figure 5.1: Comparison of time-dependence of energy using dissipative particle dynamics (DPD) simulations and event-driven (ED) simulations. The symbols represent results obtained from DPD simulations with the specified values of $\beta$. The lines denote results from ED simulations with $e = 0.95$ ($\beta = 23$), 0.9 ($\beta = 47$), 0.8 ($\beta = 100$) and 0.7 ($\beta = 159$).
In Figs. 5.2, 5.3 and 5.4, we show the time-dependence of the growth of clusters. We fix the values of $\beta = 100$ (or $e = 0.8$) and vary the values of the gravitational constant $G$ in these three figures. In Fig. 5.2, we set $G = 0$ and examine clustering in the absence of gravity. Notice that there is no visible clustering on the time-scale of our simulation, i.e., up to $t = 40$. This figure will serve as a reference point to understand what happens when gravity is switched on in the system.

Figure 5.3 corresponds to the case where we have a strong gravitational potential with $G = 0.1$. The introduction of gravity increases the collision frequency. As a consequence, there is more dissipation and clustering. Figure 5.4 corresponds to the case of a weaker gravitational strength, $G = 0.01$. As expected, there is a delay in the onset of the clustering phase and the growth of domains is slower as well. Next, we consider the $\beta$-dependence of the clustering kinetics. We have seen in Chapter 3 that, for higher dissipation parameters, we observe more clustering. In Figs. 5.5 and 5.6 we show snapshots at the same time ($t = 20$) for different values of $\beta$. The snapshots in Figs. 5.5 and 5.6 correspond to $G = 0.1$ and $G = 0.01$, respectively.

Next, let us try to quantify the growth of domains. We will focus on the case $G = 0.1$, i.e., the clustering kinetics shown in Fig. 5.3. Figure 5.7 shows the time-dependence of the length scale calculated from the structure factor. For $G = 0.1$, the system quickly enters a time-regime where domains grow. These domains grow till the size of the clusters is comparable to the size of the system. In Fig. 5.7, we focus on the time-regime where finite-size effects can be neglected. Our MD data for the length scale is consistent with diffusive growth, $L(t) \sim t^{1/2}$, over the time scales of observation. For lesser values of $G$, the clustering process starts later but the asymptotic growth exponent is the same. Finally, Fig. 5.8 shows the scaled structure
Figure 5.2: Time evolution of the density field for a granular gas with $N = 10^5$, $\beta = 100$ in the absence of gravity ($G = 0$). The particles are contained in a box of size $64^3$ with periodic boundary conditions. We do not expect clusters to be visible at these times, from our past experience with event-driven simulations.
Figure 5.3: Analogous to Fig. 5.2, but for the case with $G = 0.1$. The gravitational strength is strong and hence the system quickly settles into a clustering regime.
Figure 5.4: Analogous to Fig. 5.2, but for the case with $G = 0.01$. Compared to the $G = 0.1$ case, the onset of the clustering regime is delayed, and the coarsening of the clusters is also slower.
Figure 5.5: Evolution snapshots taken at $t = 20$ for the specified $\beta$-values. The value of the gravitational constant is $G = 0.1$ for all the snapshots.
Figure 5.6: Analogous to Fig. 5.5, but for the case with $G = 0.01$. 

\[
\begin{align*}
\beta &= 23 \\
\beta &= 47 \\
\beta &= 100 \\
\beta &= 159
\end{align*}
\]
Figure 5.7: Time-dependence of cluster length scales for a granular gas with $G = 0.1$. We plot $L(t)$ vs. $t$ on a log-log scale for $\beta = 159$ and 100, as indicated. Our length-scale data is consistent with diffusive growth, $L \sim t^{1/2}$, in the late stages of simulation.
factor at some representative times for $G = 0.1$ and $\beta = 100$. We superpose data for $L^{-d}S(k, t)$ vs. $kL(t)$ at times $t = 20, 40, 60$. The data at different time collapse onto a master curve, demonstrating that the system exhibits dynamic scaling [10, 11]. The tail of the structure factor shows the Porod law, $S(k, t) \sim k^{-4}$, which is typical of scattering off sharp interfaces [12]. The system of self-gravitating particles is still being investigated by us, and we intend to publish comprehensive results on this system in the near future.

5.5 Summary and Discussion

We conclude this chapter with a summary and discussion of the results. The evolving morphology of a system of self-gravitating inelastic particles is studied using the hierarchical linked cell (HLC) method. The model for particle-particle interaction consists of a long-range gravitational interaction and a short-range linear-spring-dashpot (LSD) type interaction. The linear spring is the restituting force, whereas the dashpot provides the necessary dissipation for granular interactions. In order to compare our inelasticity values in the LSD model with those of event-driven-type instantaneous collisions, we used the dissipative dynamics simulation for values closest to $e = 0.7, 0.8, 0.9$ and 0.95 which are $\beta = 159, 100, 47$ and 23. The time-dependence of temperature in these two models displays nearly identical behavior.

Then we ran our HLC simulation for the same values of $\beta$. The evolving system shows an explicit dependence on time. The clustering of the particles is studied using the structure factor and the length scale of clusters calculated thereof. The length scale of clusters shows a power-law dependence on time. The clustering process is
Figure 5.8: Plot of scaled structure factor, $S(k,t)L^{-d} \text{ vs. } kL$, for $G = 0.1$, and $\beta = 100$. The data correspond to times $t = 20, 40, 60$ and $80$, as specified. The line of slope $-4$ denotes Porod's law, which characterizes scattering off sharp interfaces [12].
more pronounced in the case with greater gravitational strength and also for the case of larger dissipation. The gravitational potential promotes more collisions, therefore we should not expect Haff's law to be obeyed in this case. The self-gravitating system is still being investigated by us, and we intend to publish a comprehensive paper on this subject in the near future.
Bibliography


