P452

Computational Physics

Project report

Event-driven Simulation of Freely Cooling Granular Gas

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1 Abstract

We are looking at binary collisions of particles of a granular gas in a square box with periodic boundary conditions. We have estimated the time taken by the system to thermalize for different packing fractions. We have also looked at density fluctuations within the system for different particle numbers and at different scales.

2 Introduction

We do an *Event-driven Simulation* whereby we look only at the instants when a collision takes place between two particles in the system. This method is suited for sparse systems like gases where the mean time between two successive collisions is much greater than the duration of a collision. This is because we save the computational time required to evolve the trajectories of all the particles over every time step. Instead, we compute how the velocities change when two particles collide. The rest of the particles simply follow their well-known Newtonian straight line trajectories and their positions can therefore be easily updated. The main assumption in this method is that at most one pair of particles can collide in a given time instant. If two or more pairs are colliding at the same time instant, then this method will miss all but one of them. Also, we ignore collisions of three or more particles. However, such events are rare and ignoring them should not make a significant difference to our calculations.

3 Methodology

The following is a step-by-step walkthrough of the algorithm followed:

1. Suppose we have N particles in an $L \times L$ box. We initialise the position and momentum of each particle using random variables.

2. We run a loop from $i = 1$ to 10000 to observe the first 10000 collisions in the system.

3. At every iteration, for every pair of particles, we compute the time t^* at which they will collide using the following formula:

$$| [\vec{r_i} + (t^* - t)\vec{v_i}] | - | [Vecr_j + (t^* - t)\vec{v_j}] | = 2R \tag{1}$$

where t is the present time from the beginning of the simulation and R is the radius of each particle. We choose the smaller solution if there are two.

4. We identify the pair of particles with minimum t^* and compute the post-collision velocities of those particles as follows:

$$\vec{v_1}' = \vec{v_1} - \frac{\mu}{m_1}\frac{\epsilon+1}{2}\vec{g} \tag{2}$$

$$\vec{v_2}' = \vec{v_2} - \frac{\mu}{m_2}\frac{\epsilon+1}{2}\vec{g} \tag{3}$$

where $g = (\vec{v_{12}}.\vec{e})\vec{e}$ where $\vec{e} \equiv \frac{\vec{r_1}-\vec{r_2}}{|\vec{r_1}-\vec{r_2}|}$ and $\mu = \frac{m_1 m_2}{m_1+m_2}$. For our case, the coefficient of restitution $\epsilon = 1$ as we consider the collisions to be perfectly elastic and $m_1 = m_2$ as all particles are identical.

5. We update the positions of the remaining particles as

$$\vec{r_i}' = \vec{r_i} + (t^8 - t)\vec{v_i} \tag{4}$$

6. We set the present time $t = t^*$ and repeat the above process.

Note: We observed a problem for the grazing incidence, i.e. when they have parallel velocities $\vec{r_{ij}}$ is perpendicular to the velocities and $|\vec{r_i} - \vec{r_j}| = 2R$. At this point, the simulation gets stuck and keeps picking up the same pair of particles over and over. For this, we added a check that if $t^* = t$, we ignore that pair of particles.

4 Results and Discussion

4.1 Thermalization

The first check we had to perform was to check that the particle velocities assume the Maxwell-Boltzmann distribution after a certain no. of collisions, Below, I have shared the histogram for the square of the norm of the velocities of a system having 1500 particles in a 50×50 box with periodic boundary conditions. Due to hardware limitations, we could not run the simulation with such a large no. of particles for more no. of collisions, although we know it would have produced a better histogram closer to the Maxwell-Boltzmann

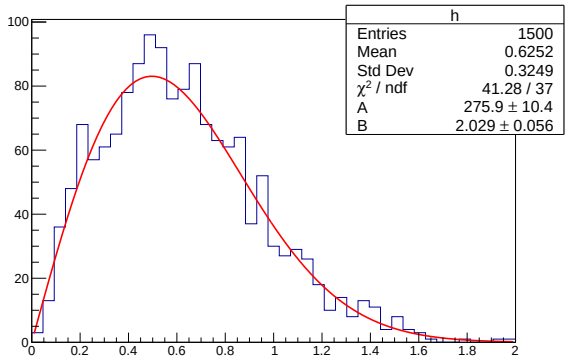

Figure 1: Histogram for 1500 particles in 50×50 periodic box after 500 collisions. Temperature equals 0.246 ± 0.007 i natural units where $m = k_B = 1$

distribution and would have allowed us to calculate the time taken for the system to thermalize by observing when the reduced chi-squared becomes nearly constant around unity. Alternatively, we can collect the velocity for a single particle in the system at several instants over a long period of time. Due to the Ergodic Principle, this should also give us a Maxwell-Boltzmann distribution. We have checked this by tracking a single particle in a 20×20 box containing 64 particles. However, this method too is computationally costly as we have to compute a very large no. of collisions and hence, perform a large no. of iterations. To get the best of both worlds, we combine both

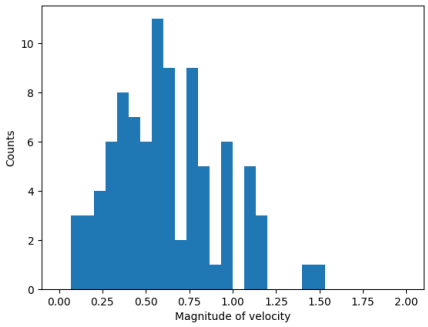

Figure 2: Histogram for the velocities of a single particle in a 20×20 system with 64 particles at 100 different instants

spatial and time averages. In the same 20×20 box containing 64 particles, we accummulate the data for all the particles after every 500 collisions. The main problem with a small system is that due to random fluctuations, we always have a few particles which lie outside the Maxwell-Boltzmann distribution which for a small system, creates a significant deviation from the expected value for one or more bin, thereby meddling with the plot. By adding up data from different instants, the effect of these random fluctuations on each bin decreases as the fluctuations occur in different bins at different instants. We

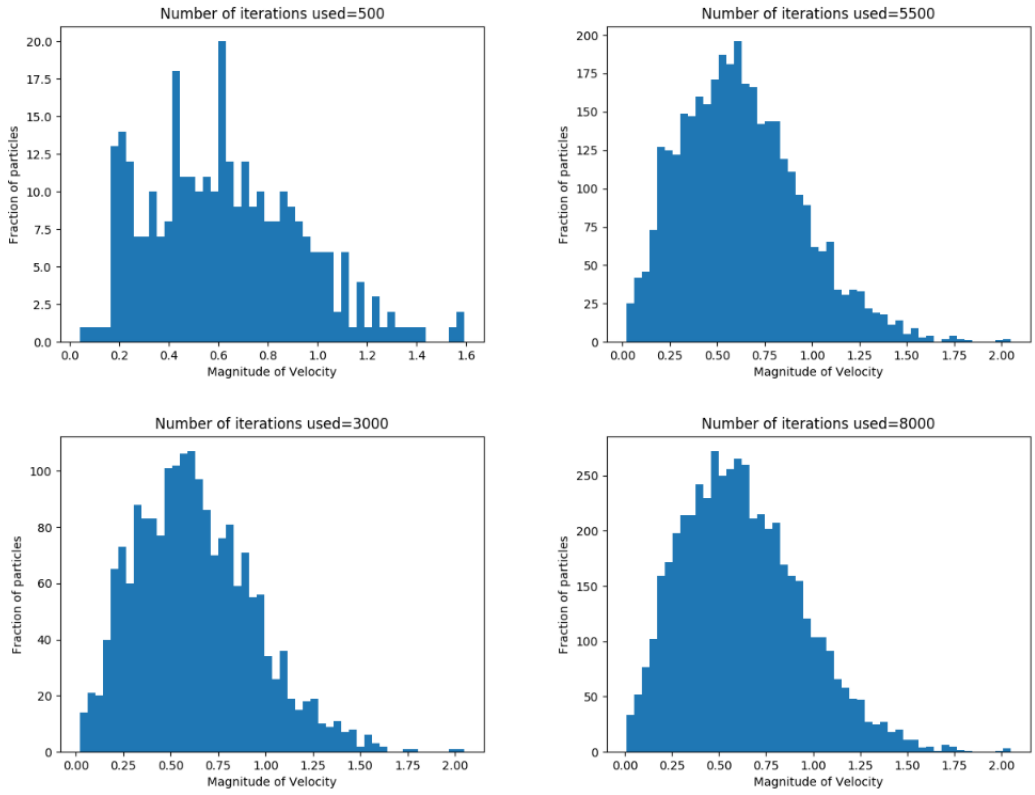

Figure 3: Cumulated histograms for the velocities of all particles in a 20×20 system with 64 particles after 1500, 4000, 6500 and 9000 iterations by accumulating the data after every 500th iteration

were able to fit the cumulated histogram after 3500 iterations with the 2D Maxwell-Boltzmann and get the temperature of the system to be 0.247 ± 0.082 in natural units where the mass of the partible and the Boltzmann constant

have been taken to be unity.

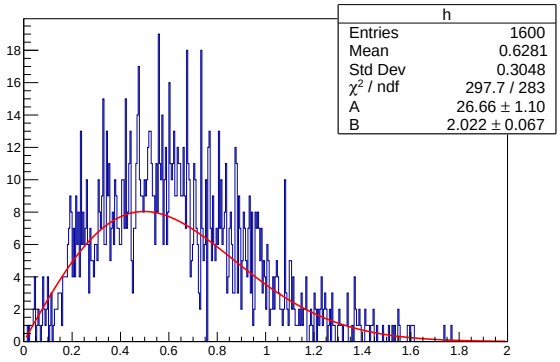

Figure 4: Cumulated histograms for the velocities of all particles in a 20×20 system with 64 particles after 3500 iterations by accumulating the data after every 500th iteration fitted with a 2D Boltzmann distribution

4.2 Fluctuations

We consider a smaller box at the centre of a 20×20 box with 60 particles and plot the fluctuation in the number of particles in the box against the simulation time. We see that the standard deviation in the no. of particles decreases as the box size increases. This is because the no. of particles inside the box is proportional to its area while the no. of particles leaving or entering the box is proportional to its perimeter. In the following plot, we plot the standard deviations in number density for different box sizes using the following formula:

$$\sigma = \frac{\sqrt{\sum_{i=1}^{1100}(x(t_i) - \bar{x})^2}}{\bar{x}} \tag{5}$$

where $\bar{x}$ is the time average of the no. of particles inside the box.

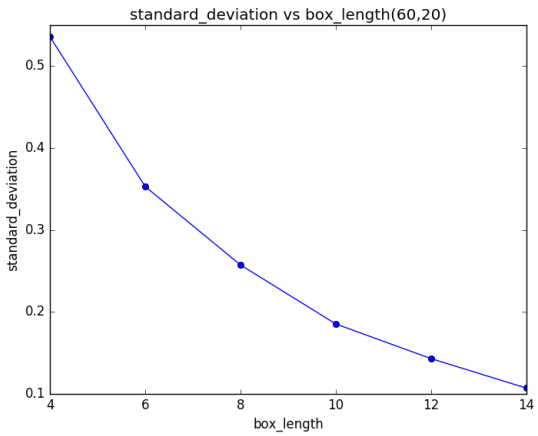

Figure 5: Standard deviation of particle no. density vs. box length