Project 1: Monte Carlo simulations of Hard Disks

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Abstract

In this project, we first introduce the concept of Markov Chain Monte Carlo methods (MC-MC) and its implementation with the Metropolis algorithm. We then use this methods to simulate a system of hard disks in a box with periodic boundary conditions, we find power law dependencies of the Mean Square Displacement (MSD) and the diffusion coefficient (D). Next, we provide a qualitative analysis of the equilibrium behavior of the system at different densities with an ordered initial condition. And to finish, we explore the effects of gravity on the system when we also introduce hard walls; we explore the sedimentation of the disks as well as the equilibrium density profiles created.

1 Introduction

In this project, we aim to use Markov Chain Monte Carlo (MC-MC) methods to simulate the interaction of Hard Disks in a box. MC-MC methods work by proposing *trial moves* that take the system from microstate x to microstate y, and then, by either accepting or rejecting this proposed moves according to some probability.

Mathematically, the transition probability from state x to state y will be equal to the product of the independent probabilities of selecting that particular trial move, $T(y|x)$, and then to accept it, $A(y|x)$. Which is written as

$$W(y|x) = T(y|x)A(y|x). \tag{1}$$

If we denote by $P(x)$ the probability distribution of configurations of x. Given that we have a thermodynamical system in contact with a thermal bath, this probability follows a Boltzmann distribution $P(x) = \frac{e^{-\beta E_x}}{\mathcal{Z}}$, where $\beta = 1/K_B T$, $\mathcal{Z}$ is the canonical partition function, and E_x the energy of that particular state.

To ensure the relaxation of our Markov Chain to $P(x)$, this one has to be aperiodic and irreducible (it is). On top of that, we impose the *detailed balance* condition

$$W(y|x)P(x) = W(x|y)P(y). \tag{2}$$

We implemented the Metropolis algorithm, in which we choose our trial probability to be uniform and an acceptance probability

$$A(y|x) = \min\left[1, \frac{P(y)}{P(x)}\right]. \tag{3}$$

In practice, and since we are dealing with hard balls, we will consider that $P(y) = 0$ if there exists an overlap in between the balls in the proposed state y, and if not, we will have $P(y)/P(x) = 1$ meaning that the proposed move will always be accepted if there is no overlap.

In our simulation we have defined $\sigma = 1$ as the diameter of the disks, N the number of disks, and L the length of the side of our box. With those quantities, we define the packing fraction ϕ as

$$\phi = \frac{\pi\sigma^2 N}{4L^2}. \tag{4}$$

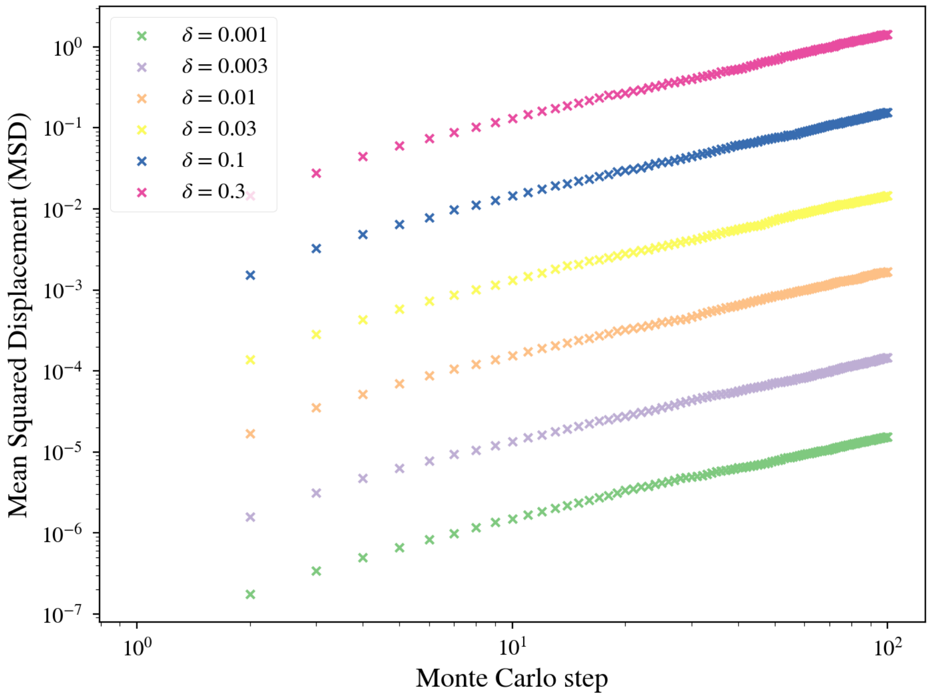


Figure 1: Mean Square Displacement as a function of the Monte Carlo step in log-log scale for values of $\delta = 0.3, 0.1, 0.03, 0.01, 0.003, 0.001$. Calculated averaging over $N = 1000$ disks.

1.1 Metropolis algorithm

Before presenting the results a quick summary of our implementation of the Metropolis algorithm.

Given all the positions of the N particles, we randomly select one of them.

Let that position be $\vec{r_i}(t) = (x_i, y_i)$, then, the new proposed move will be

$$x_i(t+1) = x_i(t) + \delta(\xi_x - 0.5),$$

$$y_i(t+1) = y_i(t) + \delta(\xi_y - 0.5),$$

where ξ_x and ξ_y are sampled from the uniform distribution $[0, 1]$, and δ is a parameter of our choosing.

This proposed move can be either accepted or rejected according to the criterion we described before. Nonetheless, after we have performed this operation N times, i.e. each particle has been selected on average once, we say that a Monte Carlo step has passed.

2 Mean Square Displacement (MSD)

In this first part we calculated the MSD for different values of δ. The outcome of this calculation is presented in Fig. 1, where we can observe that the MSD increases as a power law with the Monte Carlo step, and that a larger δ leads to higher Mean Square displacement for the same number of Monte Carlo steps.

We also asked ourselves about the relationship of D, the diffusivity, on the value of δ. In Fig. 2 we see that once again the relation between both parameters is a power law. If we fit this points to a power law function such as $D(\delta) = A\delta^B$, we obtain the coefficients

$$A = (4.1 \pm 0.2) \times 10^{-3},$$

$$B = 2.005 \pm 0.011.$$

All this is consistent with the theoretical predictions of the 2D Langevin equation. The diffusion relationship

$$\Delta^2(t) \equiv \mathrm{MSD}(t) = 4Dt, \tag{5}$$

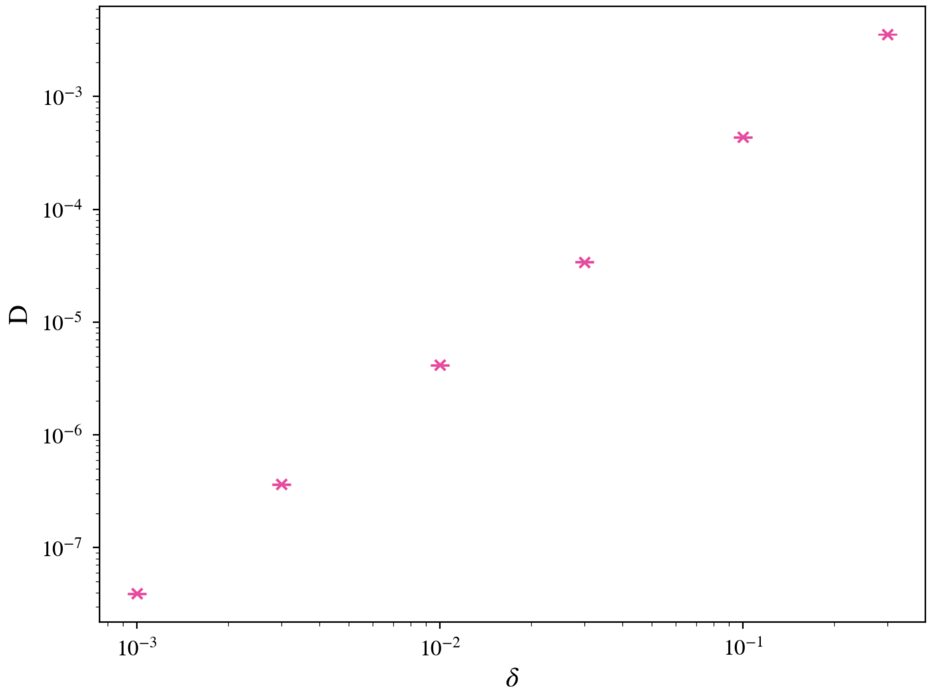


Figure 2: Diffusivity (D) as a function of δ in log-log scale with error bars.

$$\log(\Delta^2(t)) = \log(4D) + \log(t), \tag{6}$$

correctly predicts that we should expect straight lines of slope one in a log-log plot, with a different initial condition depending on the diffusion coefficient, as we see clearly in Fig. 1. On the other hand, since the square displacement is proportional to the delta squared, and linear in time, $\Delta^2(t) \propto \delta^2 t$, identifying terms with Eq. 5 we can also find the relationship $D \propto \delta^2$, consistent with our findings.

3 Equilibrium state

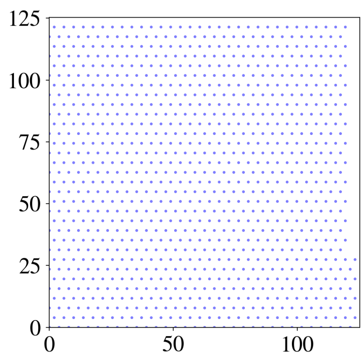
In this section we want to evaluate how the relaxation time changes as we change the density. We will approximate this visually, first we initialize the disks in a triangular lattice as it can be seen in Fig. 3. And then we let it evolve, we can get a clue for when the system has reached a steady state by looking at the MSD over time, in Fig. 4 we can see that all the systems start in a diffusive state, as the MSD trajectories are straight lines in log-log space. The first one to depart from this diffusive regime, around MC step 10, is the system with the highest density ($\phi = 0.5$). Then, around MC step 60, the system with $\phi = 0.2$ starts to also deviate from the diffusive regime. In contrast, the lowest density system ($\phi = 0.05$) appears to never leave the diffusive regime.

The explanation for this is simple, the higher the density the bigger the effect of the hard wall interactions. For a packing fraction as low as $\phi = 0.05$ the system almost does not experiment collisions, so it stays in the diffusive regime as an ideal gas with no collisions would. As we increase the density of our system the further we depart from this approximation. We could understand this as a phase transition, from a gas to a liquid, and then to a solid-like phase.

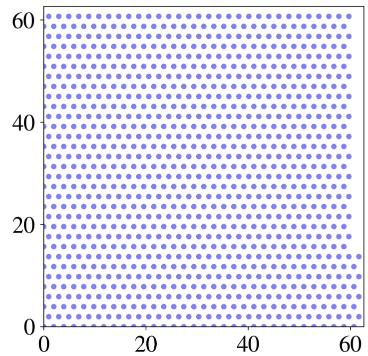
To close off this chapter, we have plotted the final configurations of our system for all packing fractions if Fig. 5.

4 Metropolis modification to include hard walls

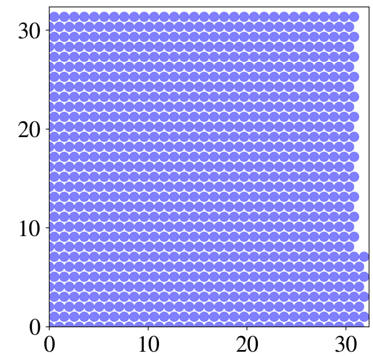
For the rest of this work, we are asked to make the particle-wall interactions hard core. Theoretically this means adding an infinite potential barrier at $\sigma/2$ from the walls, so that the probability of the



(a) $\phi = 0.05$



(b) $\phi = 0.2$



(c) $\phi = 0.5$

Figure 3: Initial condition for $N = 1000$ disks in different packing fractions $\phi = 0.05, 0.2, 0.5$.

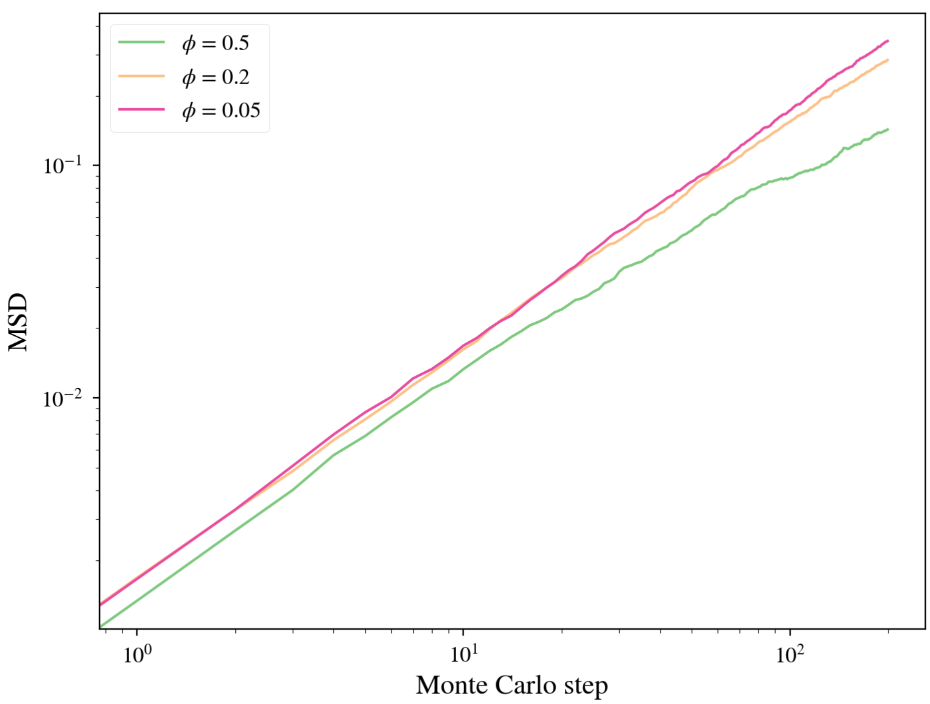
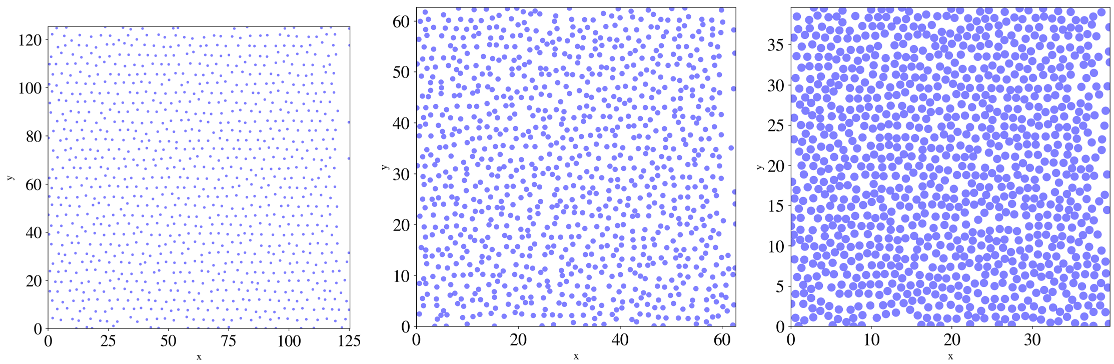


Figure 4: Mean Square Displacement as a function of the Monte Carlo step in log-log scale for three different packing fractions $\phi = 0.05, 0.2, 0.5$. Calculated averaging over $N = 1000$ particles and 200 MC steps.



(a) $\phi = 0.05$ (b) $\phi = 0.2$ (c) $\phi = 0.5$

Figure 5: Final configuration of $N = 1000$ disks after 200 MC steps in different packing fractions $\phi = 0.05, 0.2, 0.5$.

center of our disk getting closer than that is zero. In practice, we first ditch periodical boundary conditions, and add the condition that we reject every move that allows the center of the particle to get closer to the wall than its radius. The condition of no overlapping in between balls stays in place.

It is also important to also update our disk initialization method to fulfill the hard wall condition.

5 Metropolis modification to include gravity

Now that we have hard wall interactions, we want to study the sedimentation of hard disks in the presence of gravity. This gravitational effect will be added through modifying our Metropolis algorithm. If we recover Eq. 3, the acceptance probability of our algorithm, and substitute the Boltzmann probability distribution for $P(x)$ and $P(y)$ we get

$$A(y|x) = \min\left[1, e^{\beta(E_x - E_y)}\right], \tag{7}$$

where E_x and E_y are the energies assigned to each state x and y respectively.

Before, those energies E_i where either zero, if there was no overlap, or infinite if the disks overlapped in the virtual move. But now, if the move implies a displacement in y, we have an energy change like $\Delta E = mg\Delta y$. Substituting this in Eq. 7 we get

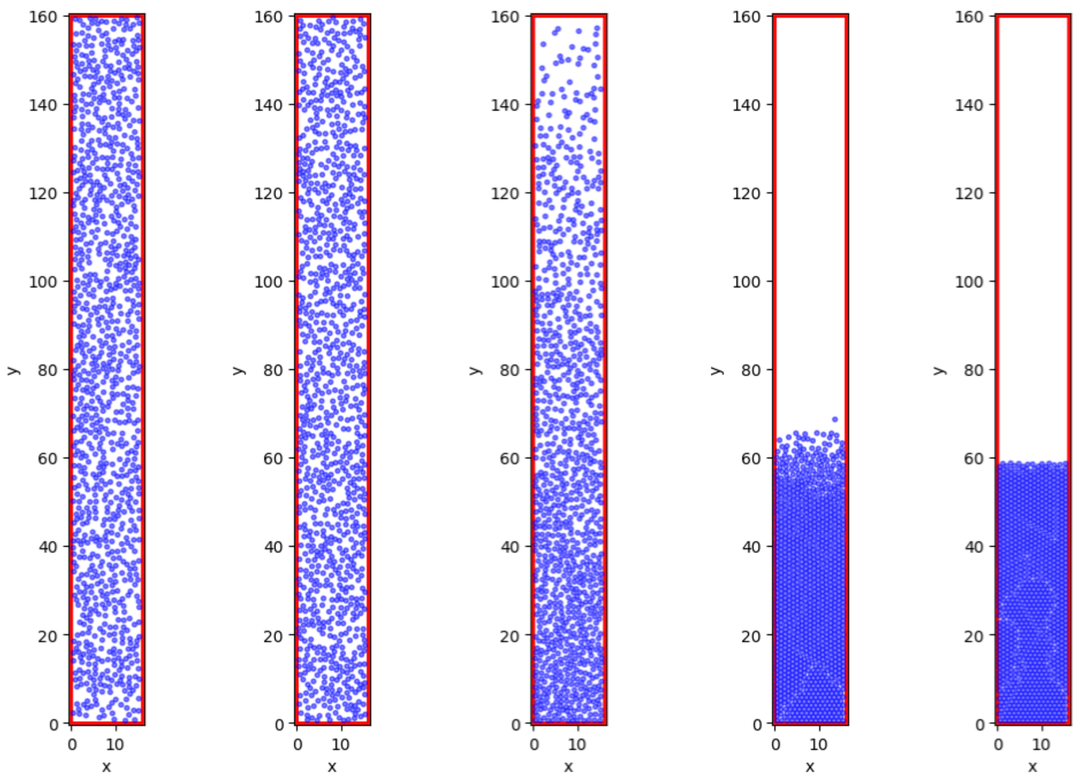
$$A(y|x) = \min\left[1, e^{-\beta mg\Delta y}\right]. \tag{8}$$

We can interpret this expression as follows. When the virtual random displacement is downwards ($\Delta y < 0$) it always is accepted, but if the virtual displacement takes the particle upwards ($\Delta y > 0$), the probability decays exponentially fast on Δy. We can also note that a temperature increase makes displacements against gravity more likely ($\beta = 1/K_B T$). Of course, the opposite happens at low temperatures.

6 Sedimentation

We can use our new methods to study the sedimentation of hard disks under gravity. For this, we created an elongated box, with hard walls, in a constant gravity field g along the y-axis. We let the box with the disks evolve until it reaches its steady state. In Fig. 6 we show snapshots of the system after 10^5 MC steps at $\delta = 0.1$, as we consider that after this time the steady state has been reached, for different values of g at $T = 1$, and in units where $m = K_B = 1$.

In this example, the dimensions of the elongated box are crucial. First, for sedimentation to occur we of course need the length of the base to be far greater than the particle size ($L_x \gg \sigma$), but we also need it not to be so large that we don't have enough particles to appropriately observe the density gradient.



(a) $g = 0$ (b) $g = 0.01$ (c) $g = 0.1$ (d) $g = 1$ (e) $g = 10$

Figure 6: Steady state configurations of $N = 1000$ disks in gravitational fields of different strength $g = 0, 0.01, 0.1, 1, 10$ after 10^5 MC steps. The box dimensions are $L_x = 16\sigma$, and $L_y = 10L_x$.

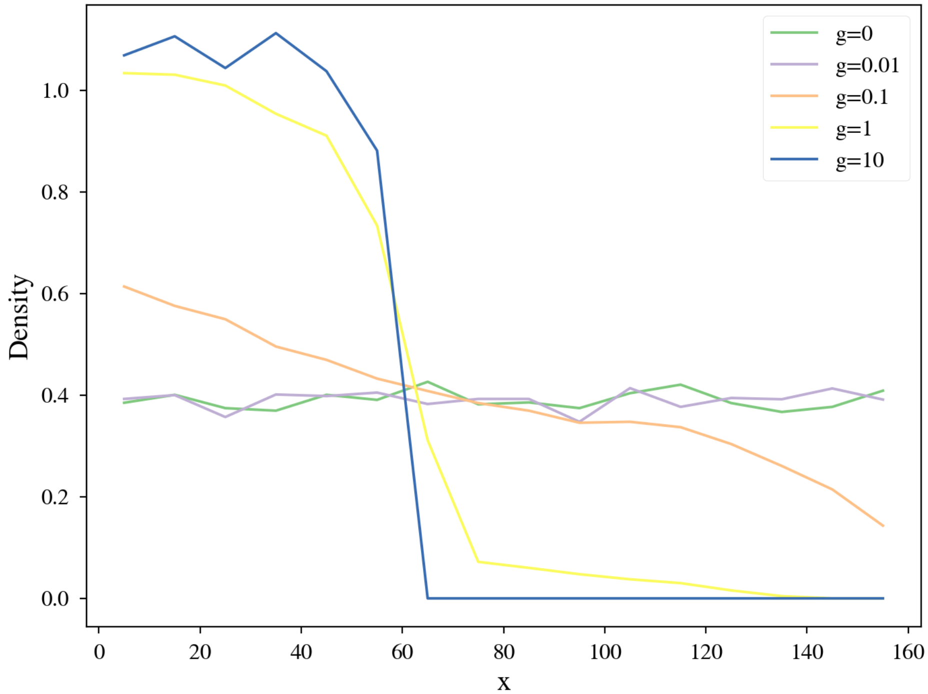


Figure 7: Density profiles averaged over 10 realizations, for a system of $N = 1000$ disks at $T = 1$ and values of gravity $g = 0, 0.01, 0.1, 1, 10$, after 10^5 MC steps, calculated using a bin size $b = 10$, and box dimensions $L_x = 16\sigma$, and $L_y = 10L_x$.

In equilibrium and in the presence of an external field, the density profile of the particles decreases exponentially with height as

$$\rho(y) = \rho_0 e^{-y/\lambda},$$

with λ some characteristic length, and ρ_0 the density at the bottom of the box. We identify this characteristic length of the system with that of the transition probabilities $\lambda = 1/\beta mg$. From this expression we can see that, increasing g makes the gradient steeper, as it also does decreasing the temperature, on the other hand, decreasing g, or increasing the temperature, result in a flatter density profile. In Fig 7 we present the density profiles after 10^5 MC steps for different values of g averaged over 10 realizations.

A Code availability

Code is available in the following GitHub repository Project 1 Francesc Bagur