Project 2. Monte Carlo simulations of Hard Disks

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1 Mean-square displacement different δ

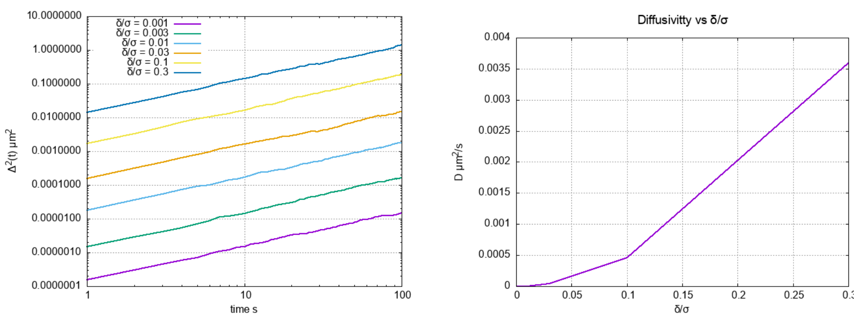

Figure 1: It is shown how the MSD behaves in time for different maximum particles displacement δ/σ, on the right side we can observe the diffusivity dependence also on the maximum displacement.

2 System relaxation from a triangular initial configuration

For the following plots X and Y axis represent X and Y coordinates in μm. As we can see there is a clear difference for the different ϕ parameter values, the need a different number of MC steps

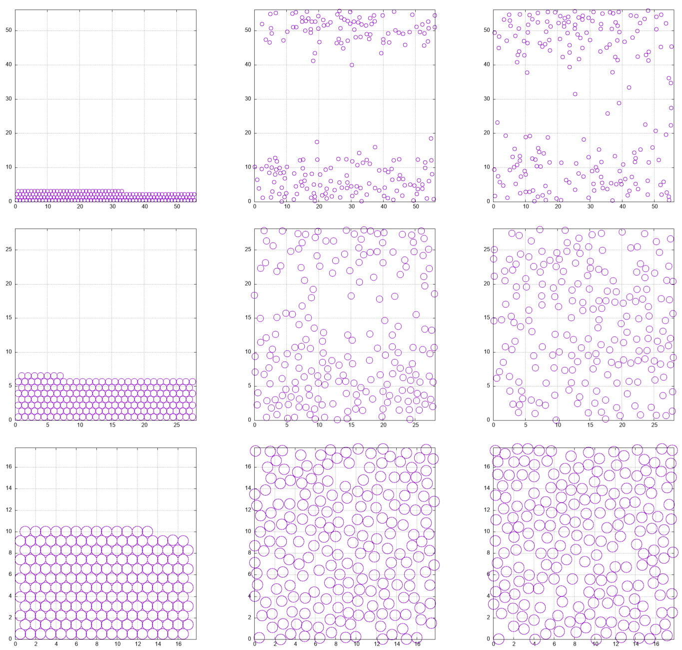

Figure 2: The first row corresponds to $\phi = 0.05$: initial condition, 50.000 and 100.000 MC steps respectively. The second row corresponds to $\phi = 0.2$: initial condition, 40.000 and 80.000 MC steps. Third row is the configuration for $\phi = 0.5$: initial condition, 20.000 and 40.000 MC steps.

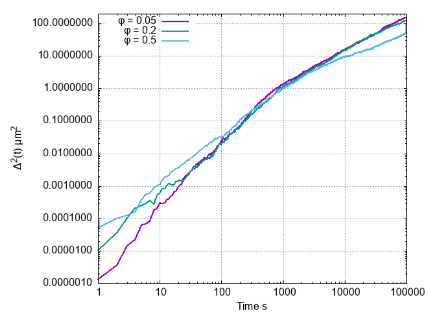

Figure 3: MSD versus MC steps (measured in time, seconds) for different ϕ values.

As it is seen in Figure 2 and 3 a ordered system relaxes from an ordered initial configuration but it takes different MC steps for the different densities ϕ. We can expect a qualitative state change from an ordered configuration to a disordered, but the bigger the density the hardest the phase transition, exist a critical density which the disks won't be able to move. It is seen in Figure 3 the MSD for the biggest density grows slower than the other two. The temperature will affect disordering the system faster as it increases.

3 Closed box $L_x \times L_y$

We must consider the walls as the same interaction disk-disk. The disks cannot enter the wall either cross it.

4 The influence of gravity

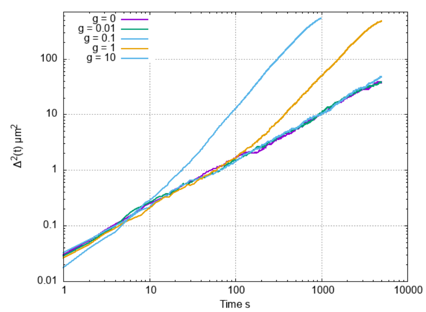

Figure 4: MSD versus MC steps (measured in time, seconds) for different g values.

Now we must have into account another condition to accept the trial movement. We have to compare the Boltzmann factor $e^{-\beta E_i}$ (known $E_i = mgh$) with a random number uniformly distributed between 1 and 0. This algorithm makes favorable the particles to fall (sedimentation). Then the Boltzmann factor has a $\beta = \frac{1}{K_B T}$ the bigger the temperature the bigger the exponential so it would be easier to reach the random number, this physically means it exists more acceptance for both up and down movements so it would difficult the sedimentation. As we can see in Figure 4 MSD saturates at 5000 MCS for $g = 1$ and at 1000 MCS for $g = 10$ so we will take the probabilities transitions at each MCS.

Gravity	0	0.01	0.1	1	10
Trans prob	0.7343	0.7353	0.7284	0.5118	0.3284

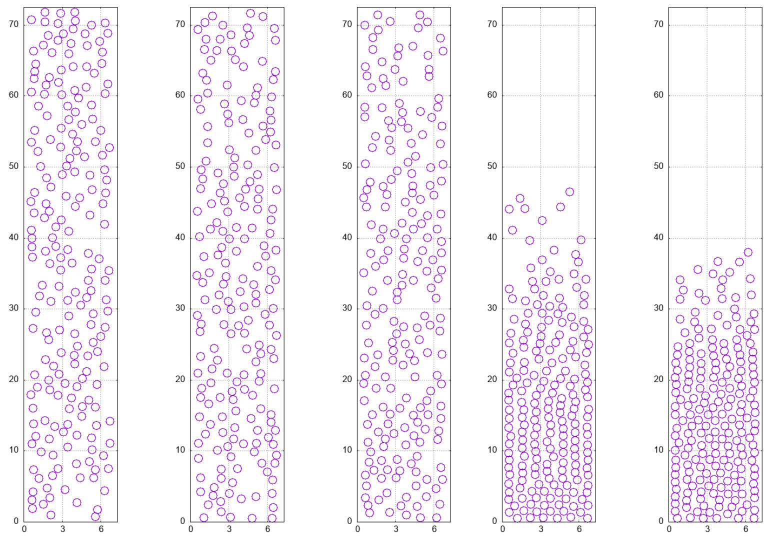

Figure 5: They are shown the equilibrium configurations for $g = 0, 0.01, 0.1, 1, 10$, according to the MSD shown in Figure 4, the first 4 snapshots are taken at MCS = 5000 and the last one is taken at MCS = 1000.

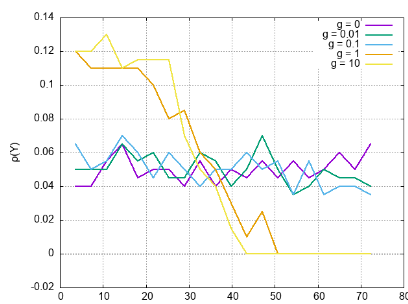

Figure 6: Here appears the density profile for the Y coordinate in the presence of different gravity values. The value chosen for testing this phenomena is $\phi = 0.3, \delta = 0.5$ and $\sigma = 1$.