Raúl Mañas Fernández 01/2022
Master in Complex Systems and Biophysics

Projects review

Project 1: Brownian Dynamics, Fluctuations and Response

1) The Gaussian white noise verifies:

$$< \eta_i^{\alpha}(t)\eta_j^{\beta}(t') >= 2\Gamma\delta(t-t')\delta^{\alpha\beta}\delta^{ij} \qquad < \eta_i^{\alpha}(t) >= 0\,, \forall t, i$$

If we make a change of variables:

$$\eta_i(t) = \sqrt{2\Gamma}\xi_i(t)$$

Now the new gaussian white noise verifies:

$$< \xi^2 >= 1\,, if\ t = t', i = j\ and\ \alpha = \beta \qquad < \xi >= 0$$

2) The Euler Maruyama algorithm is implemented in the file Project1.py.

3)

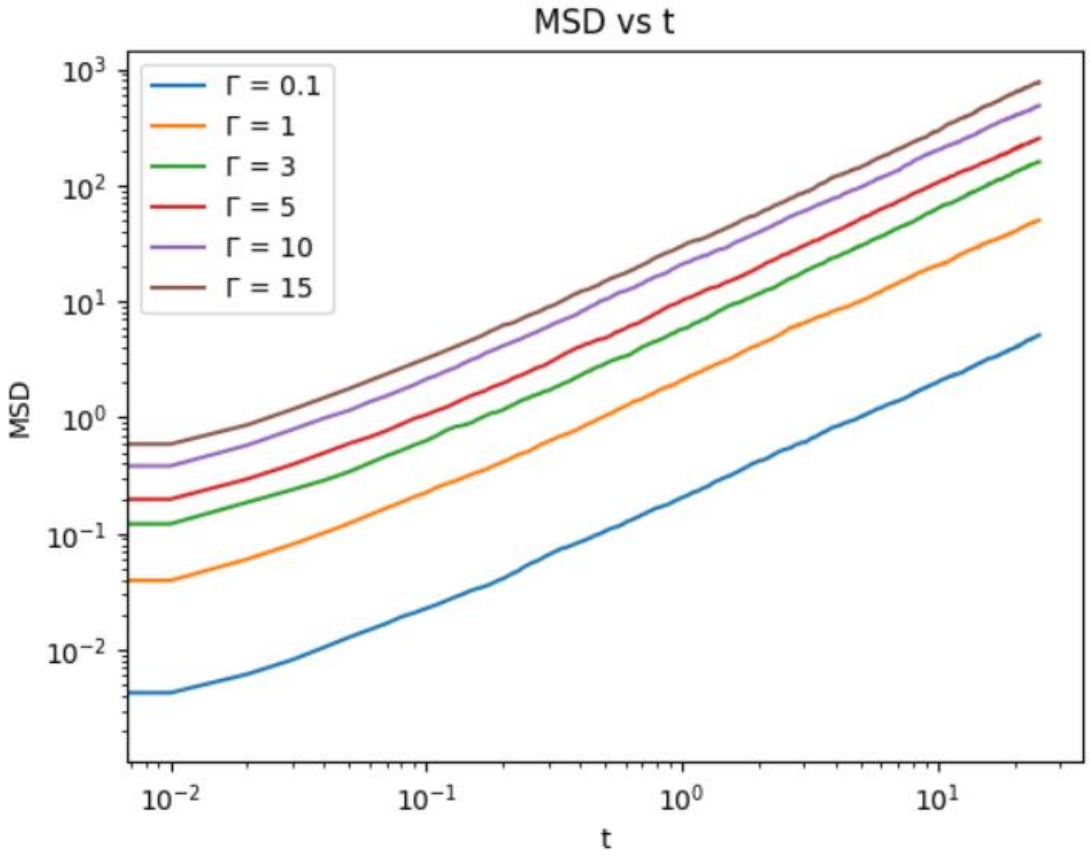

Figure 1. MSD vs t in log-log scale. We confirm a linear behaviour between the two variables.

As we expected, we obtain a Mean Square Displacement proportional to the time with exponent one, because the Wiener process exhibits a diffusion behaviour. For larger values of Γ, the MSD is larger, because each particle presents a greater diffusion (We can appreciate that fact in figure 2).

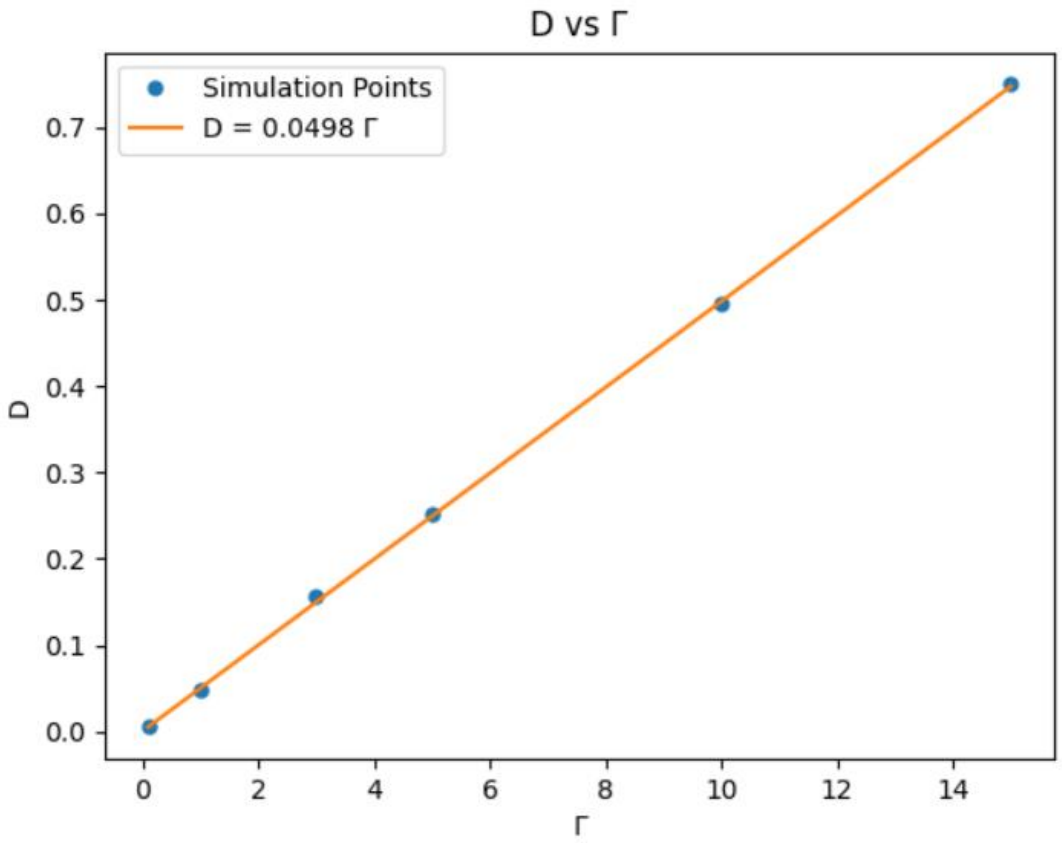

Figure 2. Diffusion coefficient vs Gamma

In figure 2 we can see a linear correlation between the diffusion coefficient extracted from the long term behaviour of Figure 1, and Γ , the strength of the Gaussian white noise.

This observation is due to the Fluctuation-Dissipation Theorem., which related the diffusion of the process with the strength of the noise.

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Project 2: Monte Carlo simulation of Hard Disks

1) The Montecarlo Metropolis Algorithm is implemented and commented in Project2.py

2) Random initial configuration with $\phi = 0.05, and\ N = 1000$:

I fix the length of the box at L = 50. With all this parameters the radius of the particle is:

$$\Phi = \frac{\pi a^2 N}{L^2} \rightarrow a \cong 0.4$$

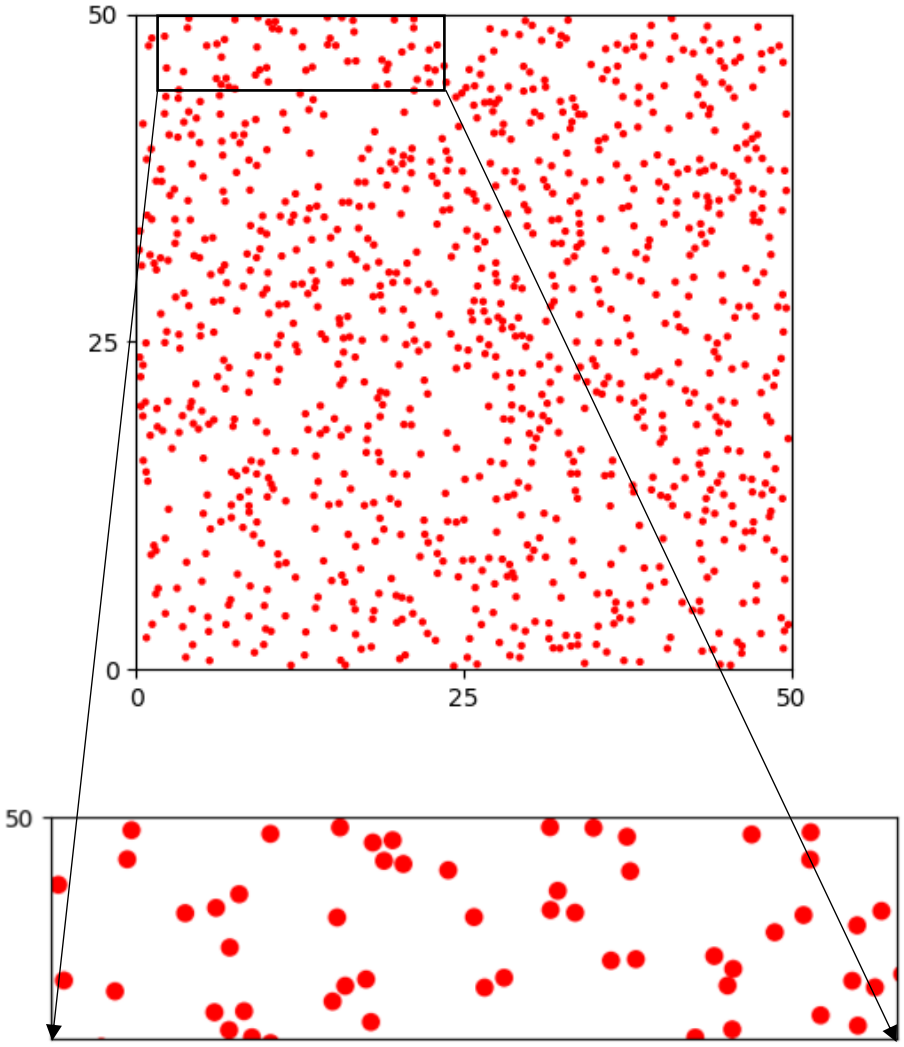


Figure 3. Initial random configuration. N particles are placed with uniform distribution. No overlap is allowed. Zoom of a part of the system to show no overlap with the boundaries either.

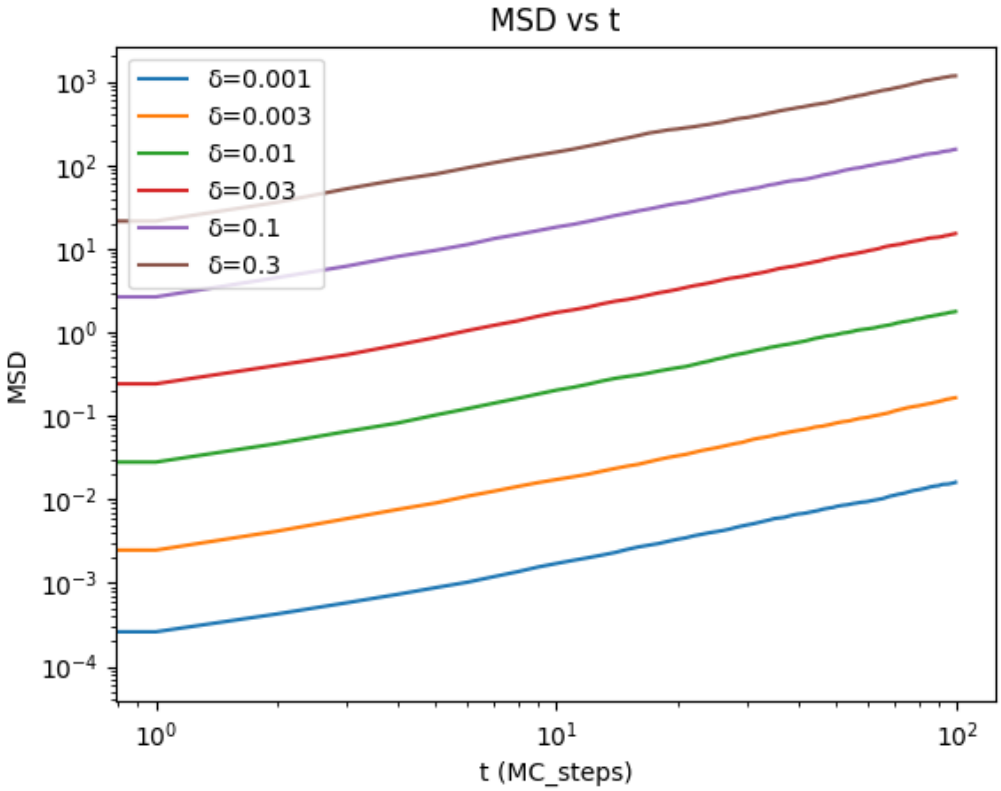


Figure 4. MSD vs t. We can appreciate a linear behaviour between the two variables.

Delta is the strength of the random kick. We can see that the higher the delta, the higher the MSD.

Here, we are using the Metropolis algorithm as follows:

If the change in position, overlaps another particle, the change is rejected, and if it doesn't overlap, the change is accepted. That way, the temperature has no role at all.

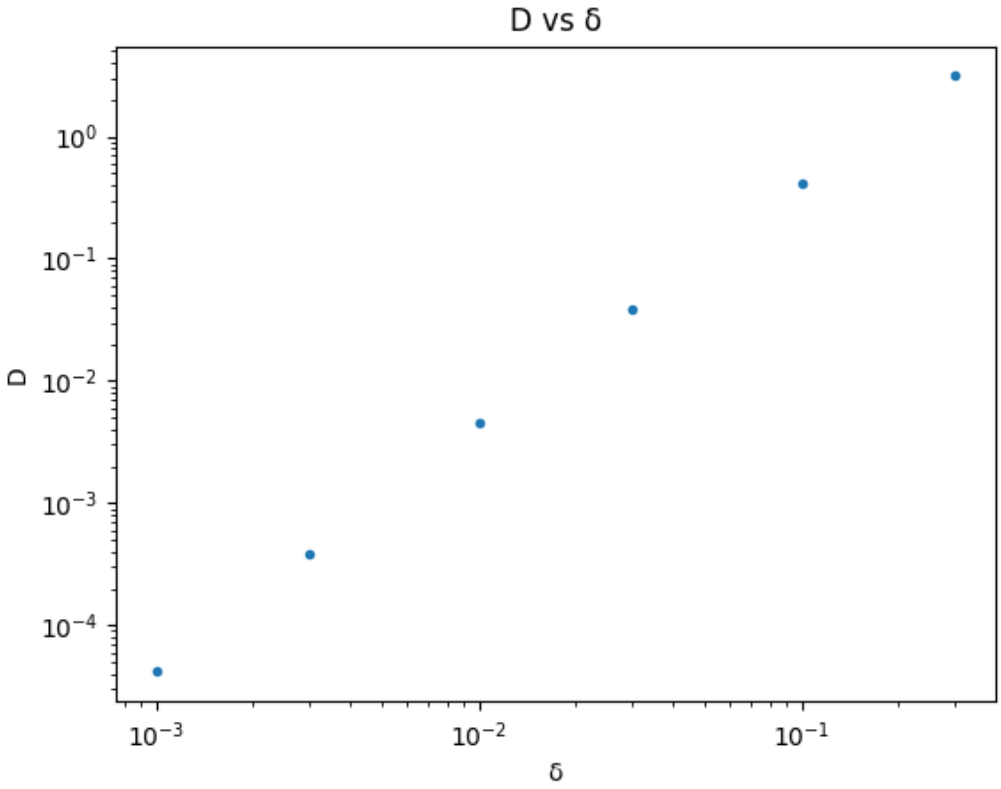


Figure 5. D vs delta.

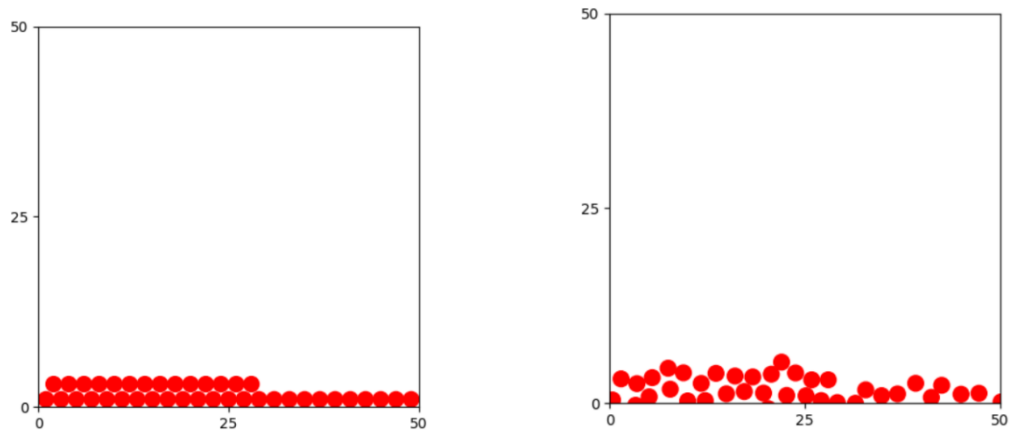
The higher the strength of the random kick, the higher the Diffusion Constant as we expected.

This is a log-log plot and we are observing a linear relation, so, Delta and D are related by a exponent law.

3) Relaxation from an ordered state

The particles are placed in the sites of a triangular lattice. From here, the MonteCarlo algorithm is applied to see how the particles can move. $\delta = 0.05$ in all the four cases.

$$\phi = 0.05 \ (N = 39)$$



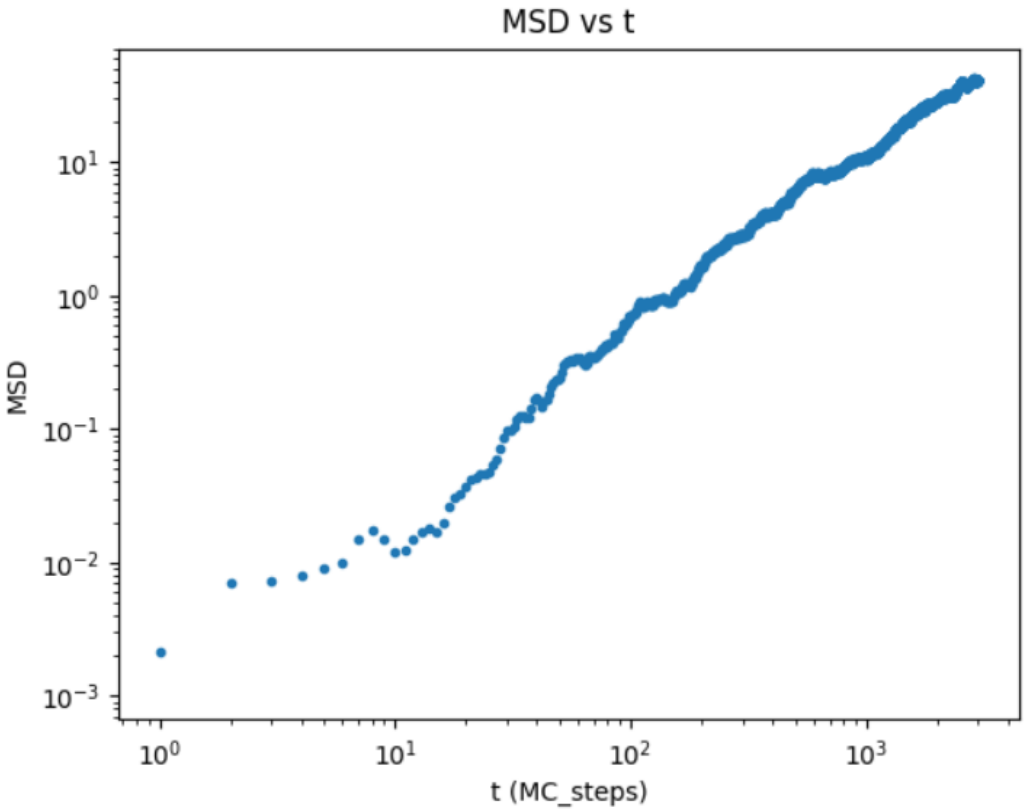
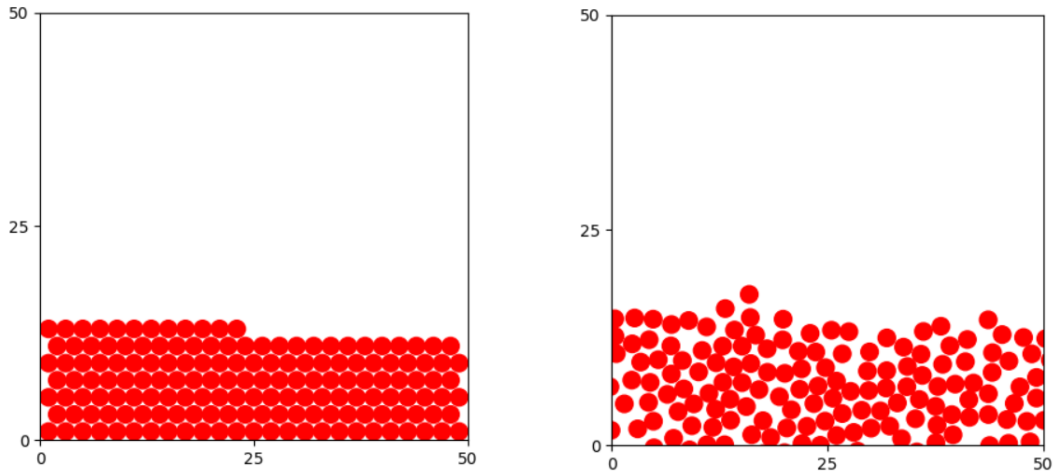


Figure 6. Simulation runned until 3000 MC steps at $\phi = 0.05$

Ordered state and disordered state after 3000 MonteCarlo steps. We can see that at such low density, the particles can move almost in a diffusive manner after around only 100 MC steps.

$$\phi = 0.2 \ (N = 159)$$



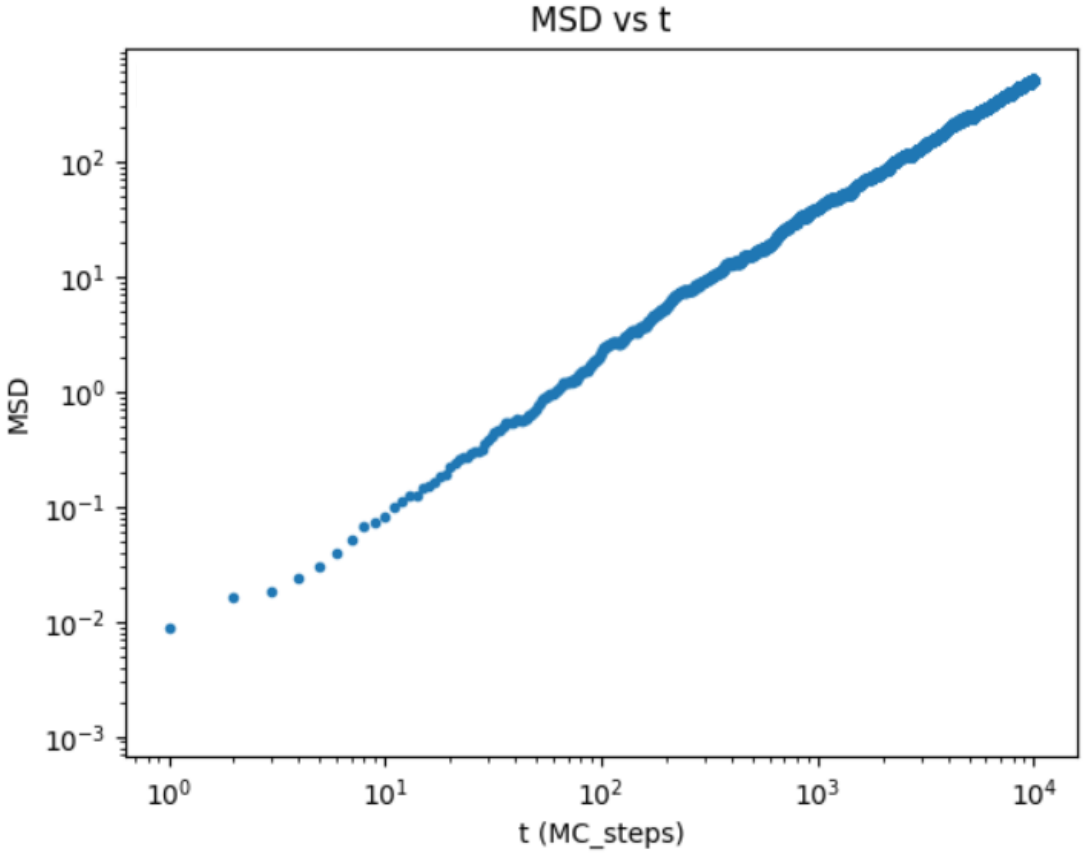
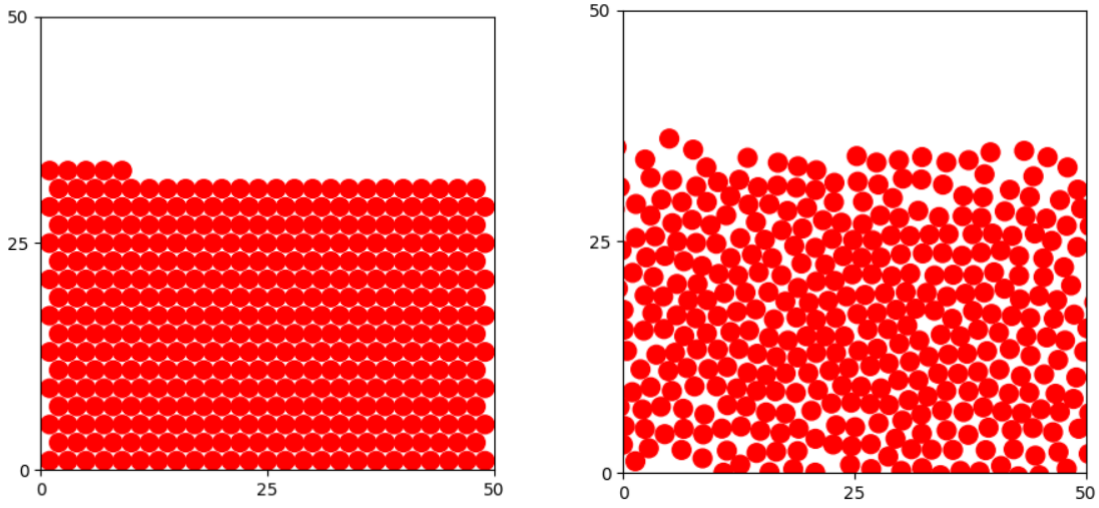


Figure 7. Simulation runned until 10000 MC steps at $\phi = 0.2$

In this density we can not appreciate if the system has reached equilibrium. Judging by the snapshots above, the particles are still very close. Maybe with more MC steps, we would observe an increase in the slope of the MSD, and therefore an approximation to equilibrium.

$$\phi = 0.5 \ (N = 397)$$



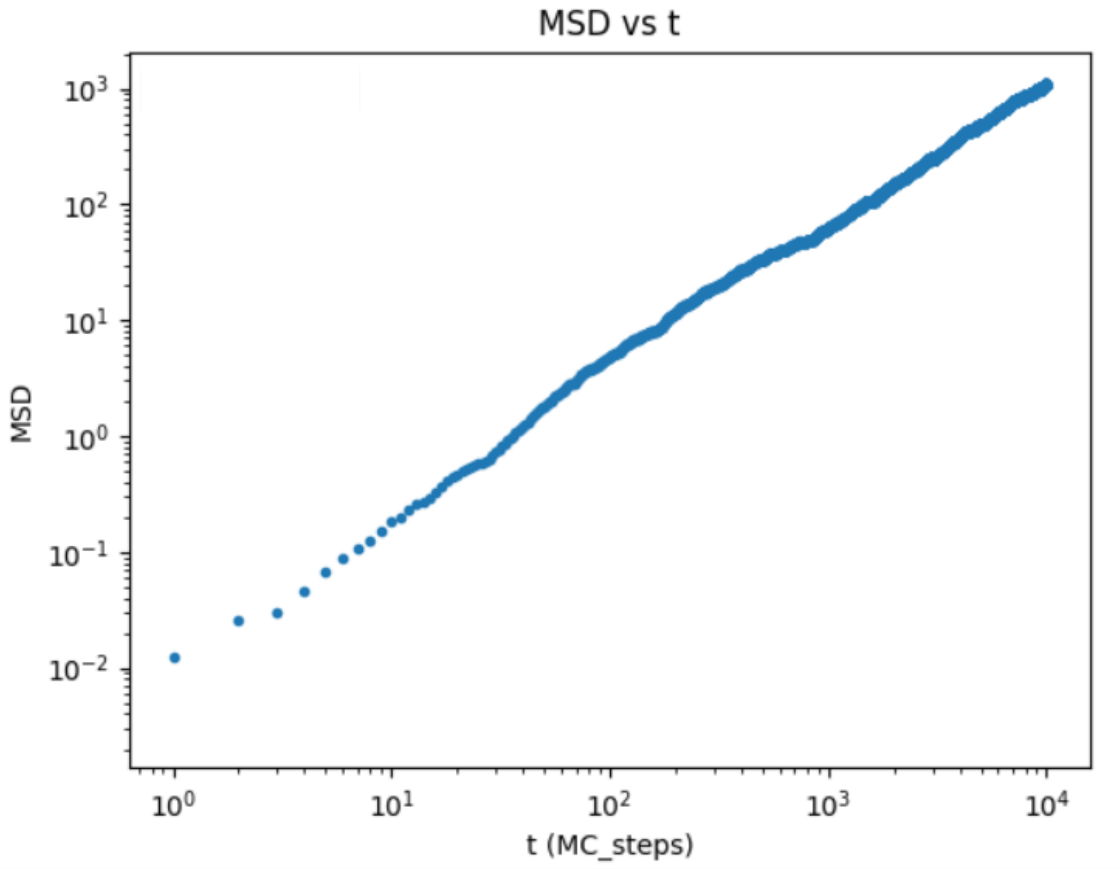
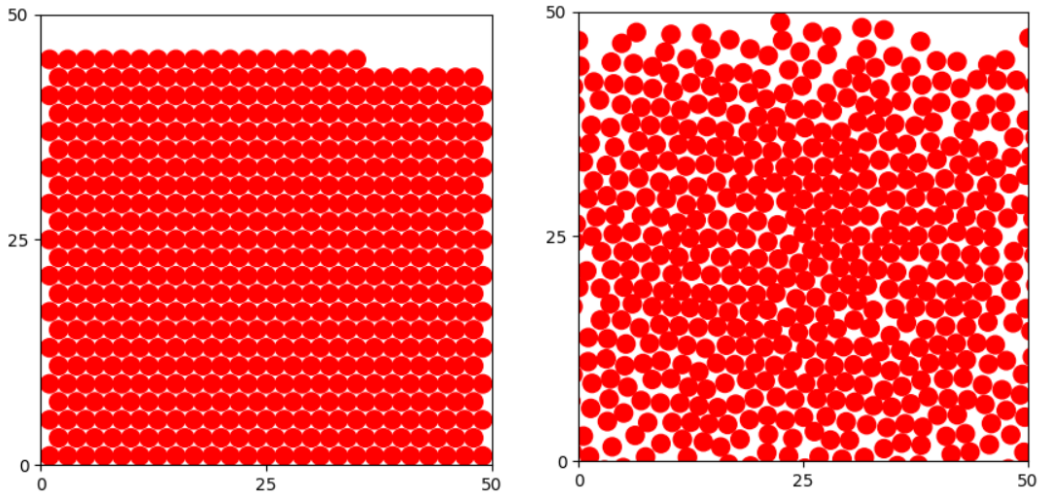


Figure 8. Simulation runned until 10000 MC steps at $\phi = 0.5$

Same reasoning that in the $\phi = 0.2$ case.

$$\phi = 0.7 \ (N = 557)$$



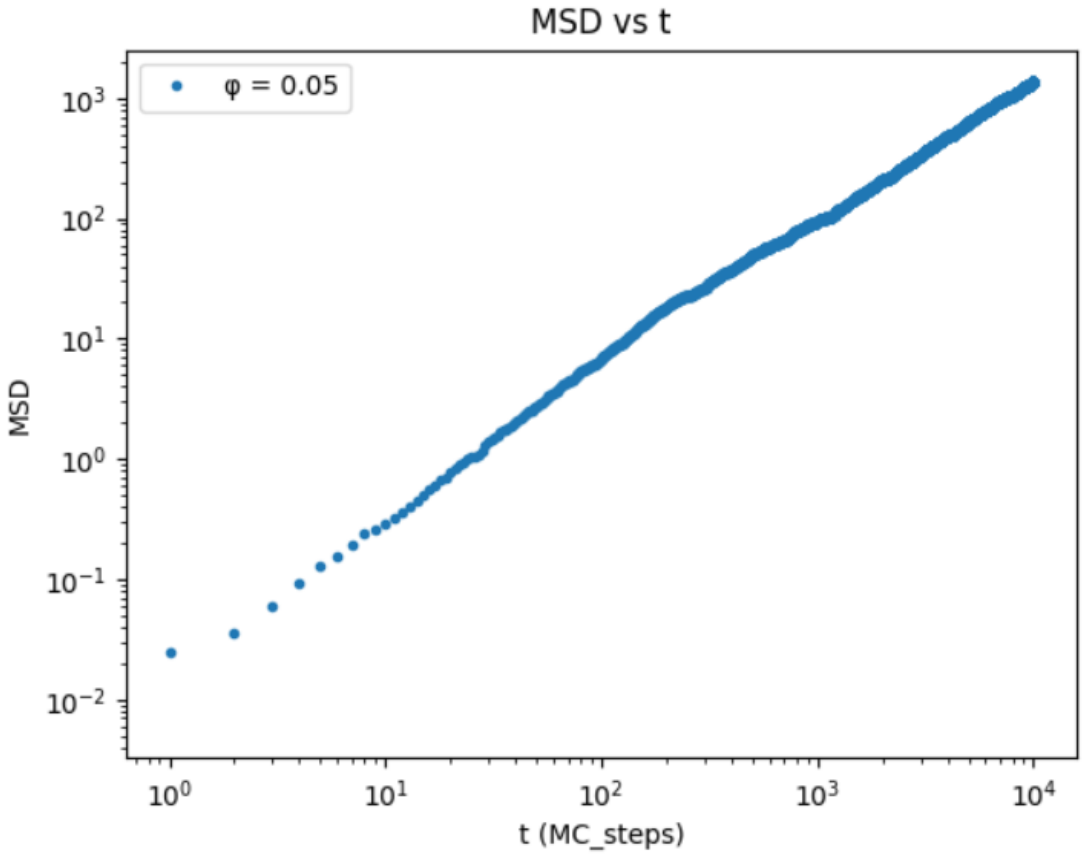


Figure 9. Simulation runned until 10000 MC steps at $\phi = 0.7$

Same reasoning that in the $\phi = 0.2$ and $\phi = 0.5$ case.

As the density is increased, we could expect a phase transition from state liquid-gas to solid. In solid states (can be appreciated at $\phi = 0.7$) the particles are well packed and cannot move well. Even after $N * MC_{steps} = 557 * 10000 = 5{,}57 \cdot 10^{6}$ changes, the original structure can be appreciated.

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Project 3: Kinetic Montecarlo Simulations in continuous time

1) Tables of energies:

Class l_i	$n_i \rightarrow n_f$	ΔE
0	$0 \rightarrow 6$	-12J
1	$1 \rightarrow 5$	-8J
2	$2 \rightarrow 4$	-4J
3	$3 \rightarrow 3$	0J
4	$4 \rightarrow 2$	4J
5	$5 \rightarrow 1$	8J
6	$6 \rightarrow 0$	12J

Table 1. Energy changes in the Ferromagnetic Version (J > 0)

Class l_i	$n_i \rightarrow n_f$	ΔE
0	$0 \rightarrow 6$	12J
1	$1 \rightarrow 5$	8J
2	$2 \rightarrow 4$	4J
3	$3 \rightarrow 3$	0J
4	$4 \rightarrow 2$	-4J
5	$5 \rightarrow 1$	-8J
6	$6 \rightarrow 0$	-12J

Table 2. Energy changes in the Antiferromagnetic Version (J < 0)

In Table 1 and 2 we can easily see all the possible changes in energy of the system at each time step. The system has short-range interactions, only with 6 Nearest Neighbours because is a triangular lattice. At each proposal of change in the Metropolis Algorithm, the system only has 7 configurations to go, depending on the value of the spin selected, and the value of the spin of the 6NN.

n_i is the number of spins correctly positioned before the change (Parallel if the interaction is Ferromagnetic and antiparallel if it's Antiferromagnetic).

n_f is the number of spins correctly positioned after the change (Parallel if the interaction is Ferromagnetic and antiparallel if it's Antiferromagnetic).

ΔE is the energy change in that spin change.

2) Disordered configuration:

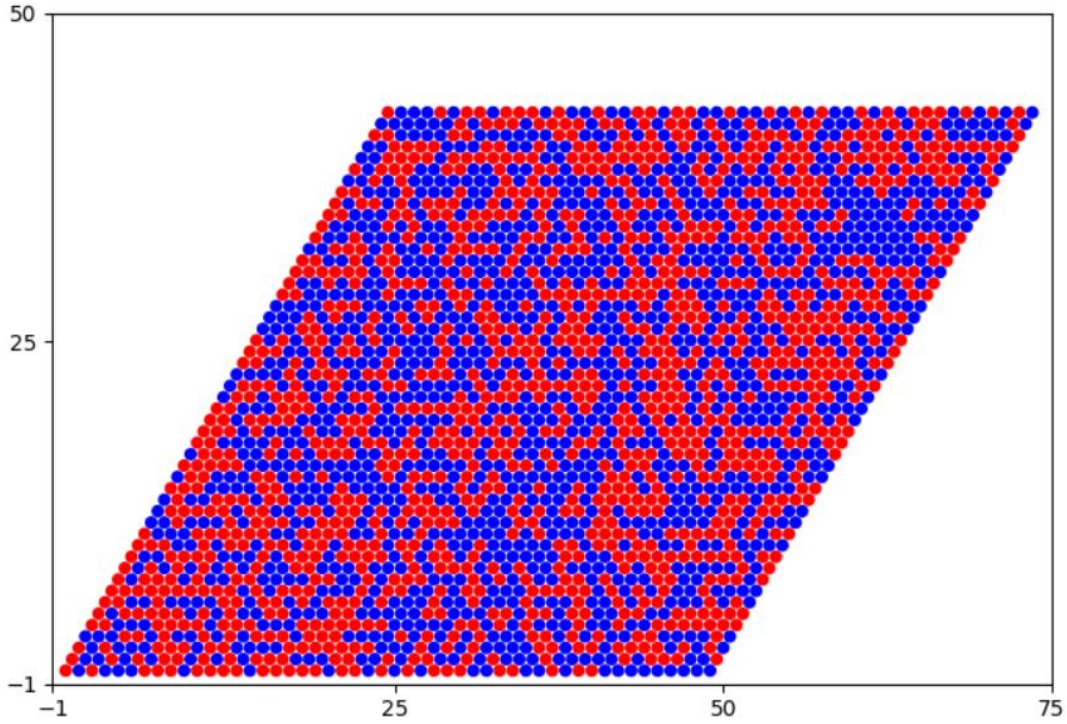

Figure 10. Initial random configuration of a triangular lattice with LxL (50x50) sizes and therefore 2500 spins. Blue ($\sigma = -1$). Red ($\sigma = +1$).

In the figure above we can appreciate a disordered configuration of the system. Each spin is equally probable of be in state +1 or -1

3) Fixed Time step Montecarlo (FSMC)

The system evolves from t=0, through 1000 Montecarlo Steps, at T=0. In the standard Metropolis algorithm, a virtual change of a particular spin is computed. If it lowers the energy, the change is accepted. If it raises the energy, the probability of the transition (where the Temperature takes a role) is compared with a random number between 0 and 1. In this simulation, because the Temperature is 0, the probability of the transition is 0 (because the exponent of $(-\beta)$.

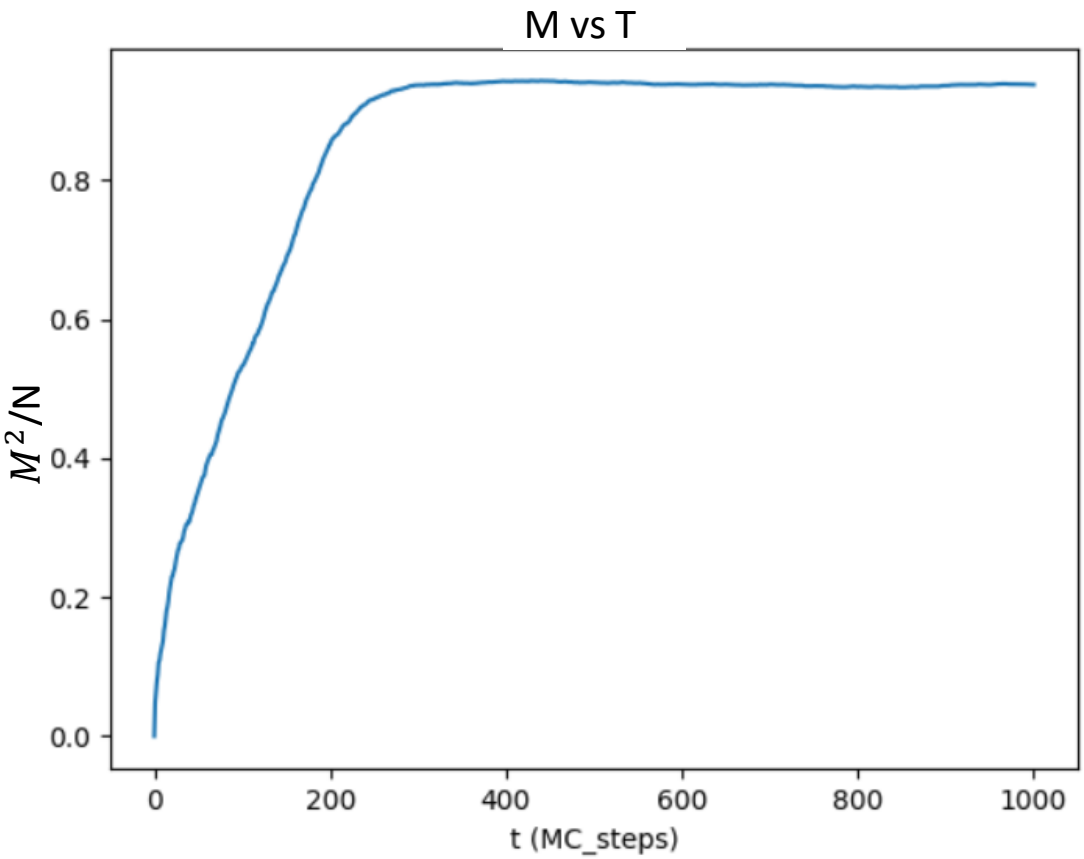

Figure 11. Absolute value of the Magnetization over the simulation time. Averaged over 10 different configurations.

As we can see in the figure above, the magnetization tends to increase as the time passes. Around t=400, almost all the spins are already in the same direction(M=1). Sometimes, due to the probabilistic nature of the algorithm, the system ends in an intermediate state (Figure of the right). If we let more time to pass, all the spins would end pointing in the same direction. That's why is an interesting option, to repeat the simulation a certain number of times, to take into the acount all the cases and compute the Magnetization average over the different Configurations rather than individual cases.

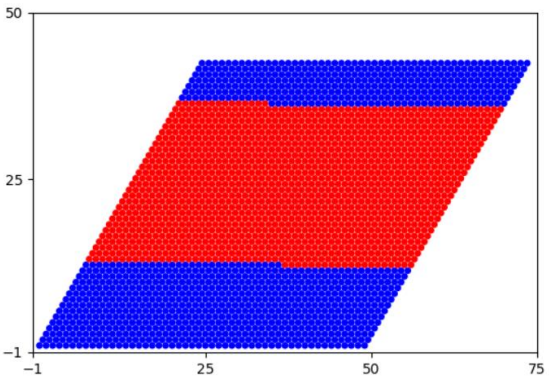

Figure 12. Intermediate State

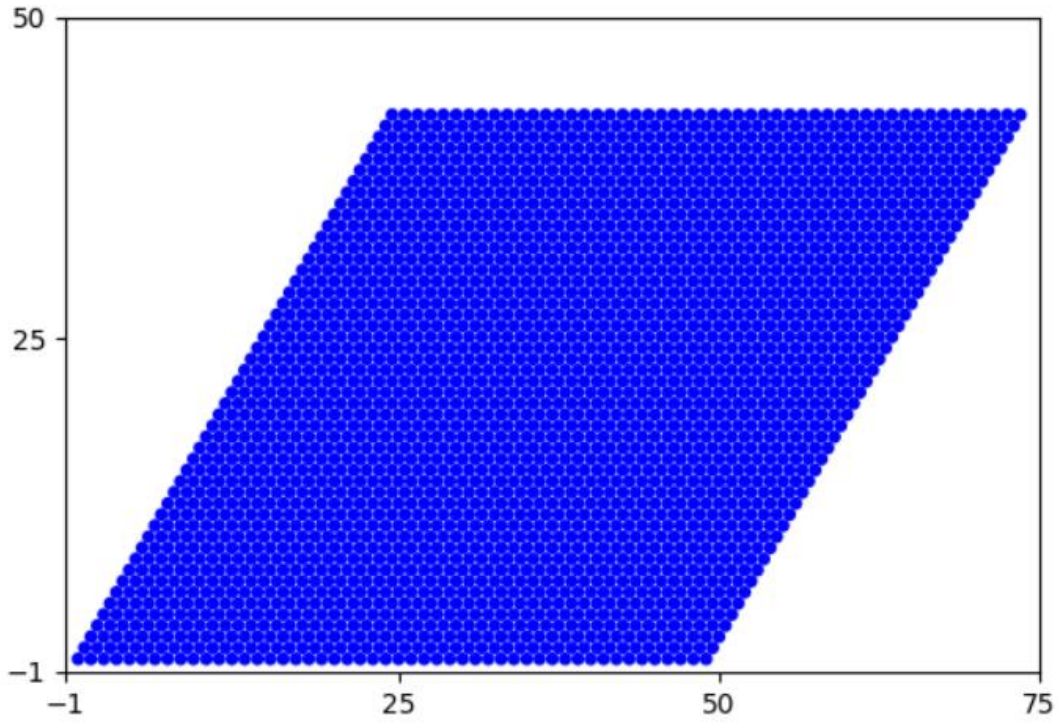

Figure 13. Final State of the system. Because is a ferromagnetic interaction, all the spins ends up pointing in the same direction. In this particular case, ended in -1. But could end in +1 too with the same probability.

4) Continuous Time Monte Carlo (CTMC)

Unlike FTMC, CTMC is rejection free. It's useful when the dynamics are very slow, for example, near the equilibrium.

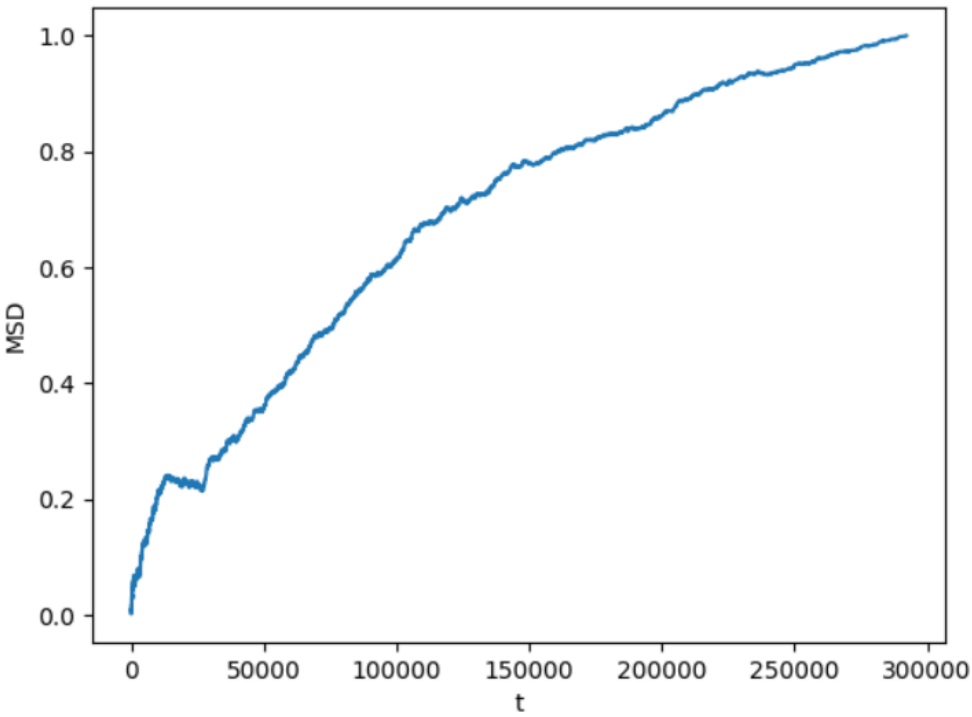

Figure 14. CTMC. An increase in the Magnetization is observed.

We can appreciate how, although the magnetization is increasing over time, it requires a lot more "real time" than the FSMC. My guess is that this system doesn't have a real slow dynamics near the equilibrium point, so the upgrade that CTMC could provide us is not being very exploited.

Project 4: Stochastic differential equations

1) 1D Brownian walker moving along a straight Line of length L In absence of disorder. The update of the position is implemented with the Euler-Maruyama scheme in the file Project4.py

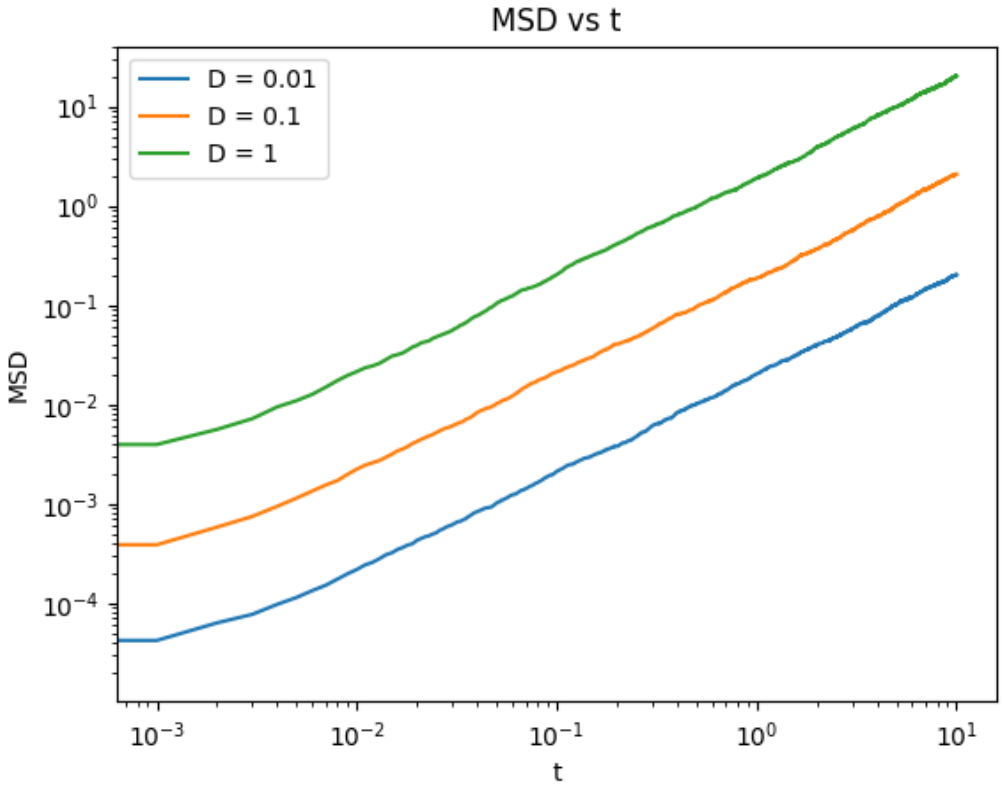

Figure 15. We can observe diffusion. Time-step $\delta t = 10^{-3}$.

As in Project 1, we have Brownian walkers, but this time in 1D. then, the mean square displacement is as follows:

$$< MSD >= 2 * Diff * t$$

Where Diff is the diffusion constant which we can extract from the long behaviour of the Brownian walker as follows:

$$Diff = lim_{t\to\infty} \frac{MSD(t)}{2t}$$

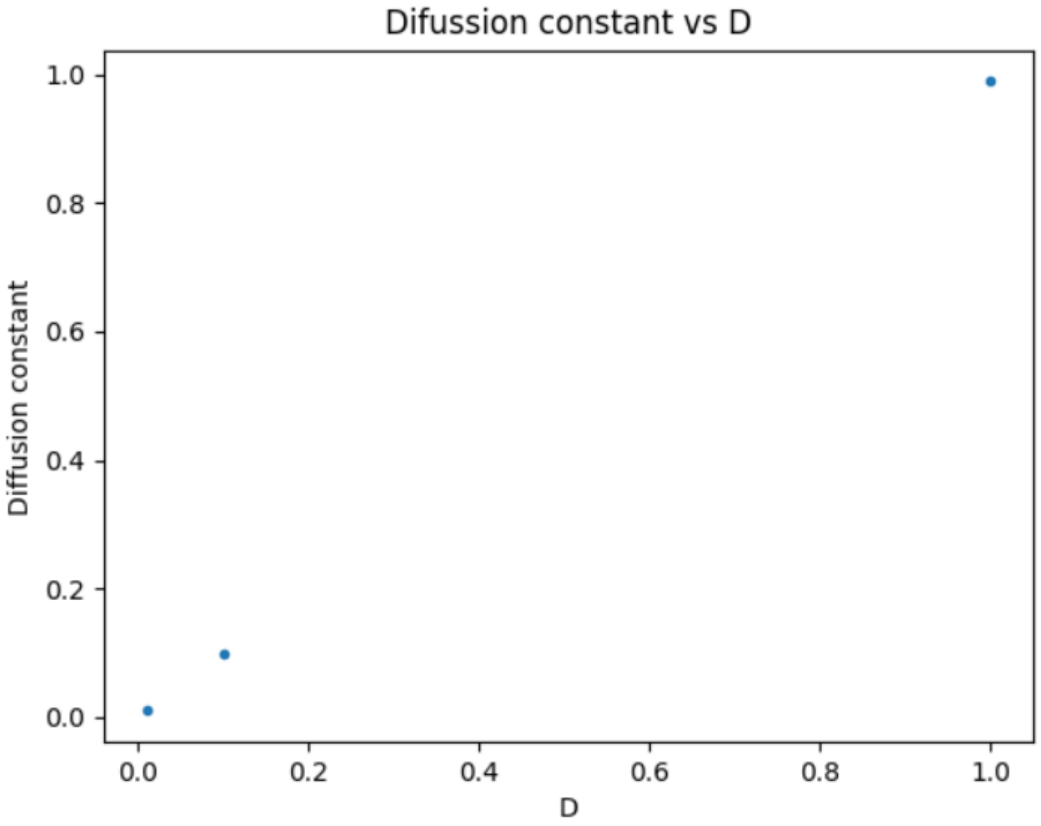

Figure 16. As we expected a linear relation holds between D and the diffusion constant.

2) Force profiles for the different strength of F(x).

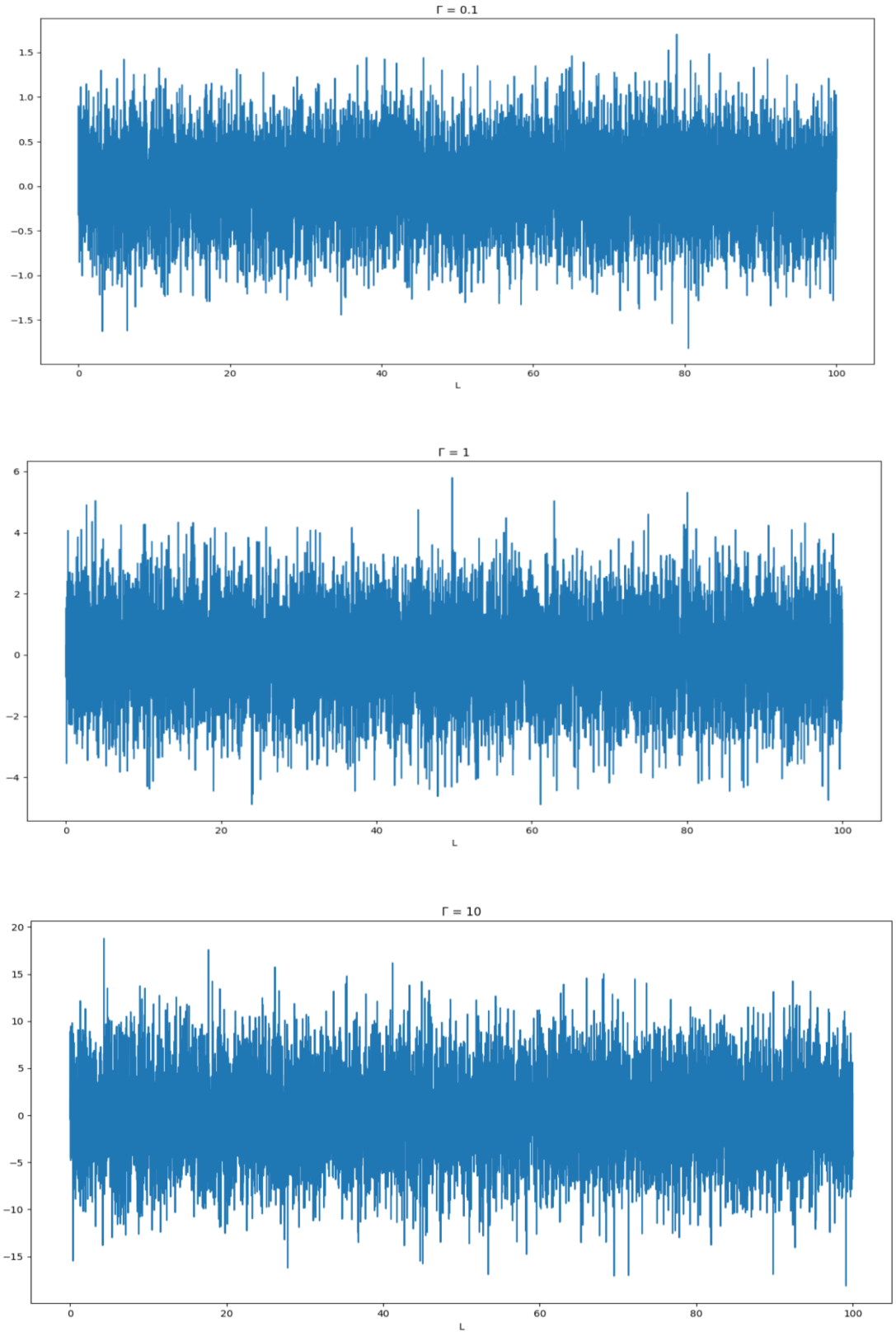

Figure 16. Force profiles for different values of Γ.

3) Brownian Walkers with noise and quenched disorder:

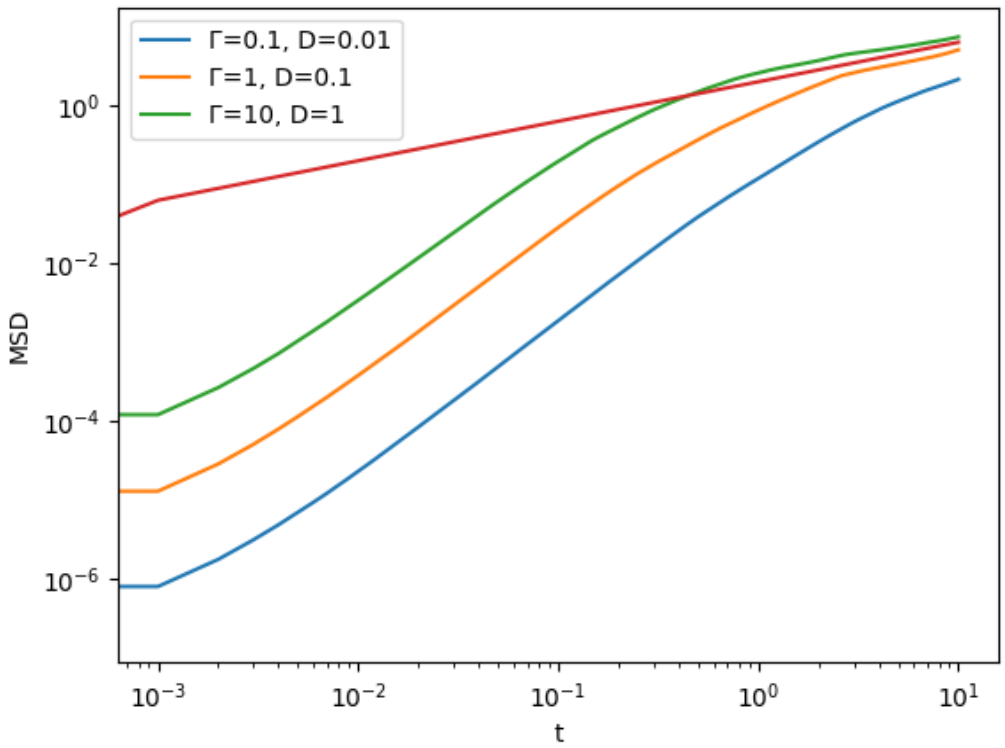

Figure 17. Initially, a diffusive process is observed, but as time goes on, the random walkers are slowed down. The red line is the function: $MSD = 2t^{\frac{1}{2}}$. It is a subdifusive behaviour because the exponent is less than 1.