Homework 3

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1 Parameters

For the following exercises we took into account the values below as the parameters of the simulated system:

N_p	L	ρ	a	dt
13	20	0.03	2 Å	1 ns
80	20	0.2	2 Å	1 ns

Moreover we simulated 1000 timesteps (some of the plots show a smaller number of steps for clarity), and for each run we measured physical quantities at each timestep.

2 Exercise (a)

In Figure 1 it's quite clear that the theoretical expectation $\langle \Delta R^2(t) \rangle = a^2 N$ is well respected up to the theoretical limit. After the limit is surpassed, the

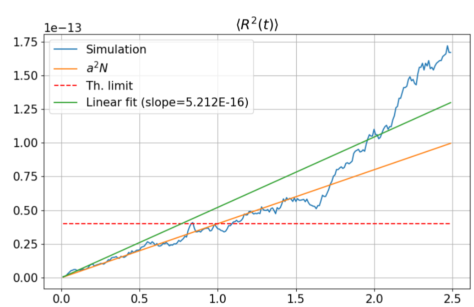

Figure 1: Value of $\Delta R^2(t) \rangle$ measured during the simulation, compared with theoretical expectations ($\rho = 0.035$).

empirically measured quantity $\langle \Delta R^2(t) \rangle$ starts to drift, and we cannot predict it anymore. We tried a linear fit against the whole time window, and obtained the slope written in the legend, which is quite accurate compared to the expected slope from the theory (i.e. a^2). We could expect more accuracy in this sense if the fit was performed only on the region where we're sure the theoretical expectation is well respected.

3 Exercise (c)

As expected the fluctuations in the measured value of $D(t)$ show up even after the equilibration phase. In Figure 2 we observe the relative amplitude of the fluctuations of $D(t)$ with respect to the value of D averaged on the whole time window after equilibration (we skipped the first 400 time instants). It's also quite clear that the fluctuations do not disappear or decrease as time passes.

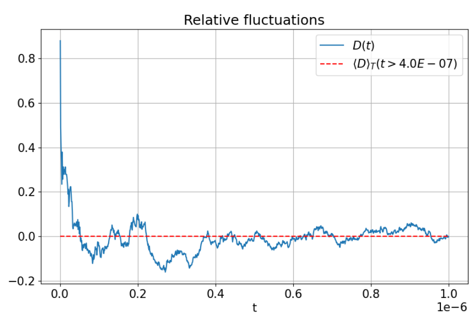

Figure 2: Relative fluctuations of $D(t)$ with respect to the temporal mean (excluding the equilibration phase) with $\rho = 0.2$.

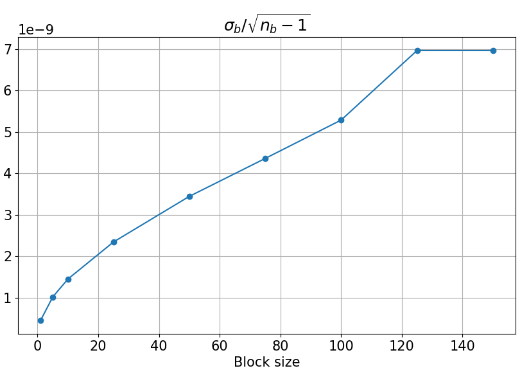

Figure 3: Statistical analysis of the standard deviation among the mean of blocks of the temporal dataset $D(t)$ increasing the size of such blocks.

4 Exercise (d)

First of all we carried out a preliminary examination on the temporal evolution of $D(t)$ in order to find the most appropriate value of the block size for the *block average*. Such analysis is summarized in Figure 3. After finding a plateau in the standard deviation of the means of the blocks for $b \geq 125$, we decided to divide the dataset in blocks comprising $b = 125$ timesteps for all further temporal averages. In Figure 4 we leverage such information to compute the value of $\langle D(t) \rangle_T$ from the measured evolution of $D(t)$, for several runs with random seeds, keeping all the parameters fixed. As we did in the previous exercise, we dropped the first 400 time instants to skip the equilibration phase. Finally, we use the estimations of D we computed (one for each run) to find a more accurate estimation of D, aggregating the samples by averaging. In Figure 5 we observe that averaging an increasing number of samples we eventually reach a plateau, but such plateau misses the theoretical expecation $D_{th} = a^2/4dt$ by 10% approximately.

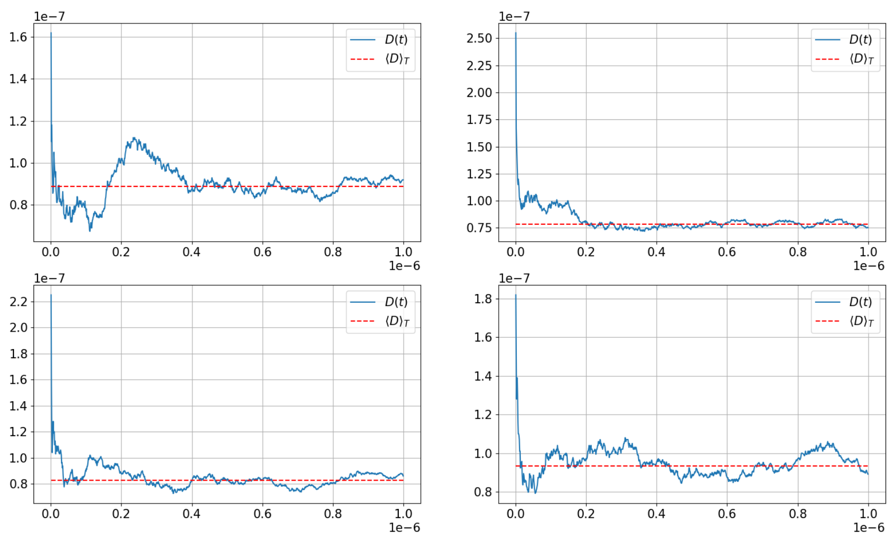

Figure 4: $D(t)$ compared with the block average (400 time instants for equilibration and $b = 125$) for several runs with random seeds at $\rho = 0.2$.

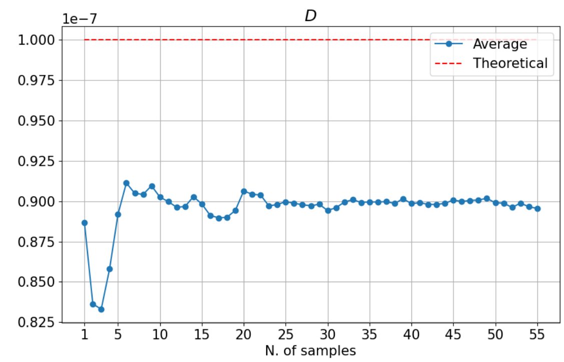

Figure 5: Accurate estimation of D by averaging the measured value for many independent runs with random seeds. The estimate is compared against the theoretical expectation $a^2/4dt$.

5 Exercise (f)

We now look into the dependency of D on the density ρ. By keeping the lattice dimension unchanged ($L = 20$) we vary the number of particles to obtain the desired densities, and we estimate the diffusion coefficient D by simulation for each ρ. We average 20 samples of D for each ρ, where each sample is obtained by block averages as we showed in the previous exercises. The results are plotted in Figure 6. Its quite clear that the expectation of decreasing monotonicity of $D(\rho)$ is respected. Such expectation is sound since as we increase the density an increasing number of particles will populate the lattice, thus resulting in a decreased number of free spots to move in. As the number of free spots

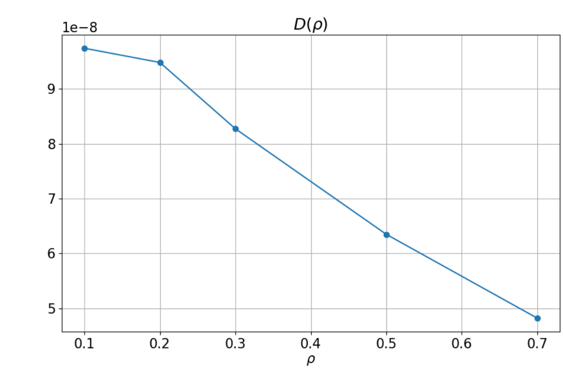

Figure 6: Dependency of D on the density ρ. Each measurement is the result of an average of 20 independent runs.

decreases, the number of particles which do not move during a given timestep is going to increase (this quantity is measured in `nfail` in the Fortran code), thus resulting in less diffusivity overall.

6 Software

All the simulations in this report were carried out using Fortran 90. Data analysis and visualization were carried out using Python 3 together with the libraries NumPy (for data collection and aggregation when necessary), Matplotlib and scikit-learn. All script files not provided with the delivered homework are available on my GitHub repository for the course *Computational Physics Lab*.