Project 4. Stochastic differential equations with memory

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1 Langevin equation's discretization

Here appears the Langevin equation, then the discretization using the Euler-Mayurama scheme:

$$\begin{aligned}
&\gamma\dot{\mathbf{r_i}}(t) = \mathbf{F_i} + \boldsymbol{\xi}_\mathbf{i} \\
&\mathbf{r_i}(t+\delta t) = \mathbf{r_i}(t) + \delta t\frac{\mathbf{F_i}}{\gamma}(t) + \delta t\frac{\boldsymbol{\xi}_\mathbf{i}(t)}{\gamma}
\end{aligned} \tag{1}$$

The $\boldsymbol{\xi}_\mathbf{i}$ is a Non-Markovian noise. Its behaviour and its corresponding discretization appears below:

$$\begin{aligned}
&\dot{\boldsymbol{\xi}}_i(t) = -\frac{\boldsymbol{\xi}_i}{\tau} + \sqrt{\frac{2D}{\tau^2}}\boldsymbol{\eta_i}(t) \\
&\boldsymbol{\xi_i}(t+\delta t) = \boldsymbol{\xi_i}(t) - \delta t\frac{\boldsymbol{\xi_i}}{\tau} + \sqrt{\frac{2D\delta t}{\tau^2}}\boldsymbol{\eta_i}(t)
\end{aligned} \tag{2}$$

So we can compute the $\boldsymbol{\xi}(t)$ in order to find the position in 3. For now on we are about to consider $\gamma = 1$, the problem parameter will be: N = 200 particles, L = 20 (size of the system), D = 1.0 (diffusion coefficient), δt = 0.1 s (time step) and t = 100 s (total time).
It is important to give a time step small enough in order not to accumulate a big error and of course letting the system evolve like a continuous dynamic. The number of particles must be big enough to have real statistics but low enough to run the simulation.

2 MSD

For $\mathbf{F_i}$ we obtain the three curves for three different values of τ (correlation time). Besides it is shown each analytic case:

$$\Delta^2(t) = 4D\left(1 + \tau\left(e^{-\tau/t} - 1\right)\right) \tag{3}$$

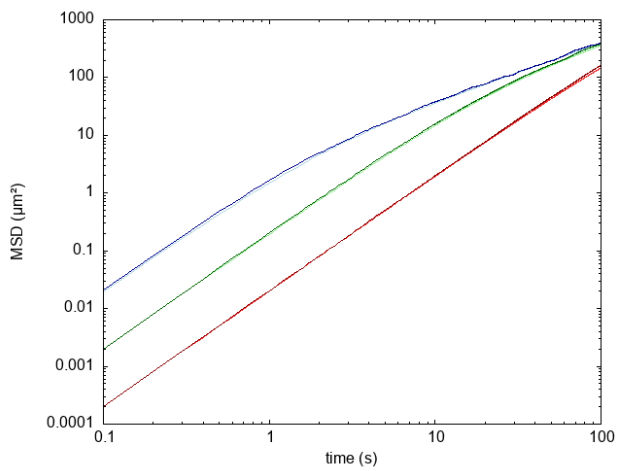

Figure 1: It is shown blue for $\tau = 1s$, green $\tau = 10s$ and red $\tau = 100s$ the dark colors are for experimental and the light colors represent the analytic expression

Down here they are shown a representative trajectory for each τ:

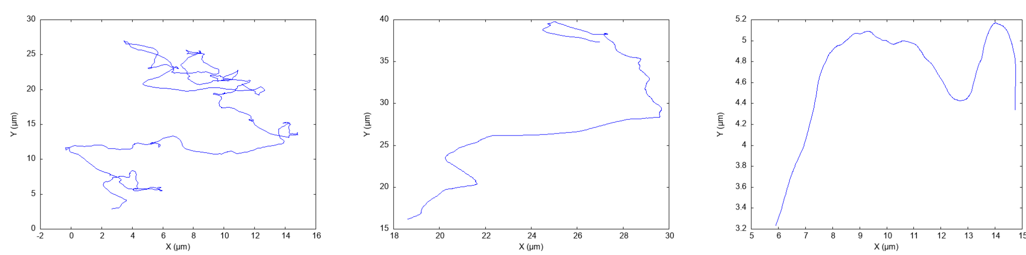

Figure 2: Random particle trajectory for $\tau = 1s$, $\tau = 10s$ and $\tau = 100s$ respectively

3 Correlation Function

The correlation functions has this behaviour for the different tau. The color criteria is the same as 1:

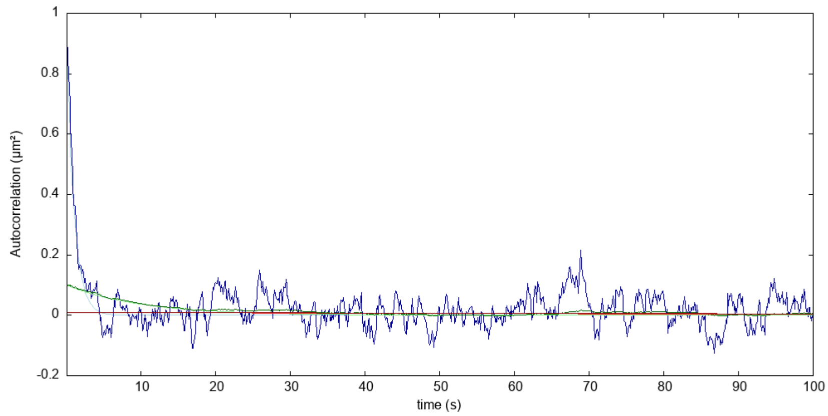

Figure 3: It was fixed $t' = 0$. We can appreciate the bigger the correlatien time the lower the autocorrelation at any time.

4 Applying a force

We now apply a force on the X direction. $Ox : \boldsymbol{f}_i = \epsilon_i f \boldsymbol{u}_x$ and measure the MSD and the displacement on the X direction:

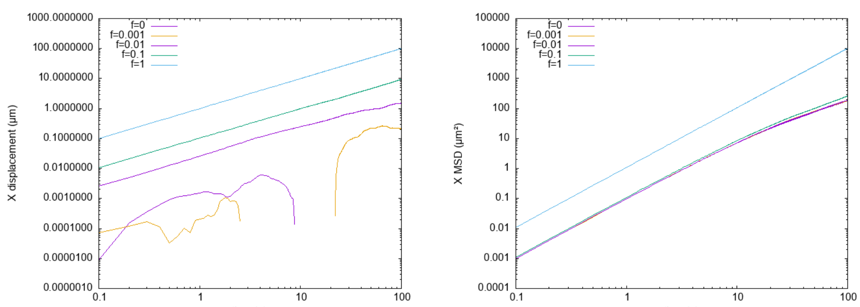

Figure 4: On the left side we can see the particle mean displacement along the x direction. On the right side we can see the same for the MSD.

As we can see for $\boldsymbol{f}_i = 0.1$ the noise is no longer a driven force but a perturbation. So we can assume the linear regime for this f value.

5 Mobility and diffusion coefficient

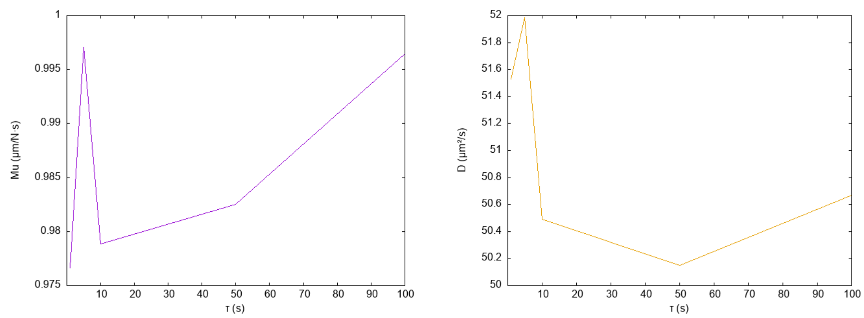

Figure 5: On the left side we can see the mobility coefficient versus the τ value. On the right side we can see the same for the diffusion coefficient.

6 Fluctuation-Dissipation Theorem (FDT)

As we can see in Figure 5 the relation is no lineal as it is expected in order to fulfill the FDT. This fluctuation measures the particles memory so for τ big enough we won't have the behaviour expected. We would find the linearity at low correlation time values.