Stochastic differential equations with memory - FENE

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1 Exercise 1:

The following coupled system of overdamped Langevin equations governs the dynamics of this simulation:

$$\gamma\dot{\mathbf{r}}(t) = \mathbf{F}(\mathbf{r}) + \boldsymbol{\xi}(t) \tag{1.1}$$

with ξ Gaussian noise verifying: $\langle\boldsymbol{\xi}\rangle_n = 0, \quad \langle\xi_\alpha(t)\xi_\beta(t')\rangle_n \; = \Gamma(t-t')\delta_{\alpha\beta}$

$$\dot{\boldsymbol{\xi}}_i(t) = -\frac{\xi_i}{\tau} + \sqrt{\frac{2D}{\tau^2}}\boldsymbol{\eta}_i(t) \tag{1.2}$$

We discretize both of them using the Euler-Mayurama scheme and introduce the evolution of noise into the position Equation (1.1):

$$\boldsymbol{\xi}_i(t+\delta\, t) = \left(1 - \frac{\delta\, t}{\tau}\right)\boldsymbol{\xi}_i(t) + \frac{\sqrt{2D\delta\, t}}{\tau}\boldsymbol{\eta}_i(t) \tag{1.3}$$

$$\gamma\mathbf{r}(t+\delta\, t) = \gamma\mathbf{r}(t) + \mathbf{F}(\mathbf{r})\,\delta\, t + \left(\left(1 - \frac{\delta\, t}{\tau}\right)\boldsymbol{\xi}_i(t) + \frac{\sqrt{2\Gamma\delta\, t}}{\tau}\boldsymbol{\eta}_i(t)\right)\delta\, t \tag{1.4}$$

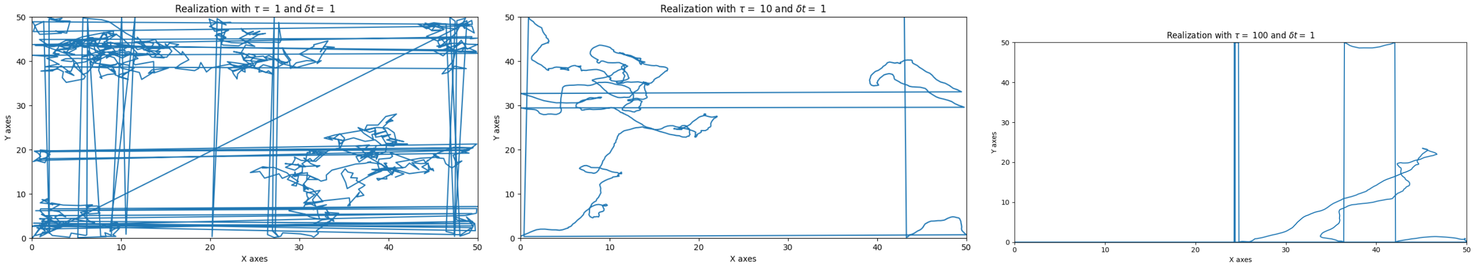
$$\tag{1.5}$$

In Equation (1.5) the variable $\boldsymbol{\eta}_i(t)$ is a Gaussian noise N(0,1).

The simulation has been run with the following value for the variables:

- Number of particles, N: 1000 particles. Good amount in order to obtain averaged values in the behaviour of the system
- Size of box, L: 50 units. Because the diffusion constant is small.
- Diffusion constant, D: $\frac{1}{2}$. Chosen at random but small so that the particles take a little time in reaching the outer box limits
- Time step, $\delta\, t$, and total simulation time: $\delta\, t = 1$ chosen at random and the simulation time is $1500\delta\, t$ steps.
- Correlation time, τ: 1,10,100, 1000.
- Damping coefficient, $\gamma = 1$

If the correlation time is equal to the time step, the model will behave like a random walk. If it is higher, the system displays a ballistic behaviour because it has a certain memory given by parameter τ.



(a) (b) (c)

Figure 1: Different relizations with different memory times. The lines crossing each plot mean that the particle has exited through a side and come back by the opposite one.

Plot a) defines a pure random walk and plot c) depicts ballistic behaviour, that is why its trajectory is almost a straight liene, because the particle remembers its previous positions, up to t-τ, at any time given.

2 Exercise 2: MSD without force

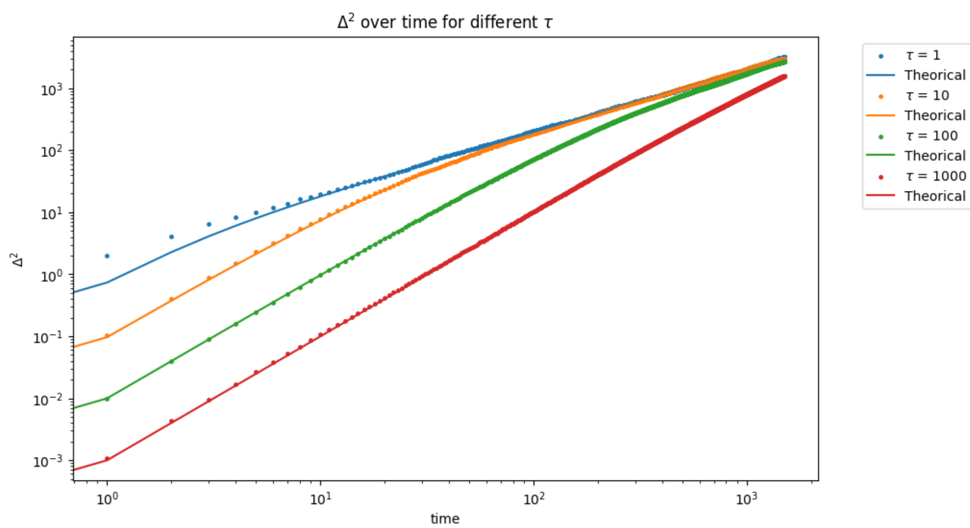


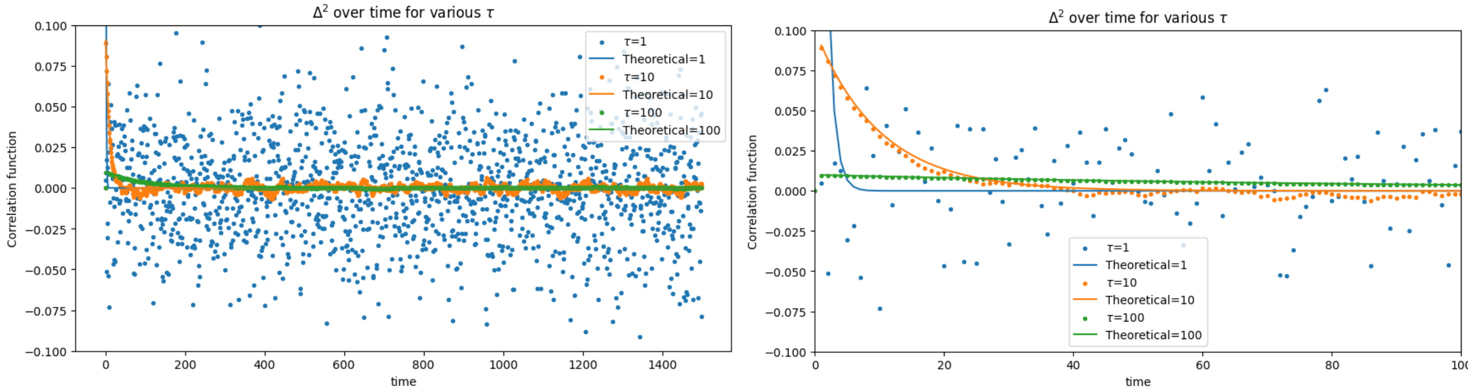
Figure 2: The average MSD value for N particles with their correspondent theoretical function, Equation (2.6), plotted together.

The mean square displacement, $\Delta^2(t)$, for a particle with memory and without an outside interacting force is given by equation:

$$\Delta^2(t) = 4D(t + \tau(e^{-t/\tau} - 1)) \tag{2.6}$$

We expect the MSD have different behaviours depending on the correlation time. If t<τ we will observe ballistic behaviour, which corresponds with $\Delta^2 \propto t$ (in logarithmic scale). We can perfectly observe this specially in the system with memory $\tau = 1000$. However, if we look at the blue line, corresponding to the random walk system, we can observe a change in this behaviour.
For t<τ we lose temporal correlation and start to display random walk behaviour, where $\Delta^2 \propto 4D\,t$. That is why all MSD are the same in a long enough timeline.

3 Exercise 3: Correlation function



(a) (b)

Figure 3: Correlation function of the noise for different memory times. Plot b) has a closeup depiction of their behaviour at small times.

We know the correlation function is:

$$\langle \xi_i(t)\xi_j(t') \rangle = \frac{D}{\tau} e^{-|t-t'|/\tau} \delta_{ij} \mathbf{1} \tag{3.7}$$

This equation has been plotted for each memory time, labeled as 'Theoretical' in the figures. We can see for $\tau \neq 1$ an exponential decay with a characteristic time given by τ. For the pure Brownian motion movement, we can see its correlation does not follow this function as it is only correlated with itself at each point in time.

4 Exercise 4: Applying a constant force

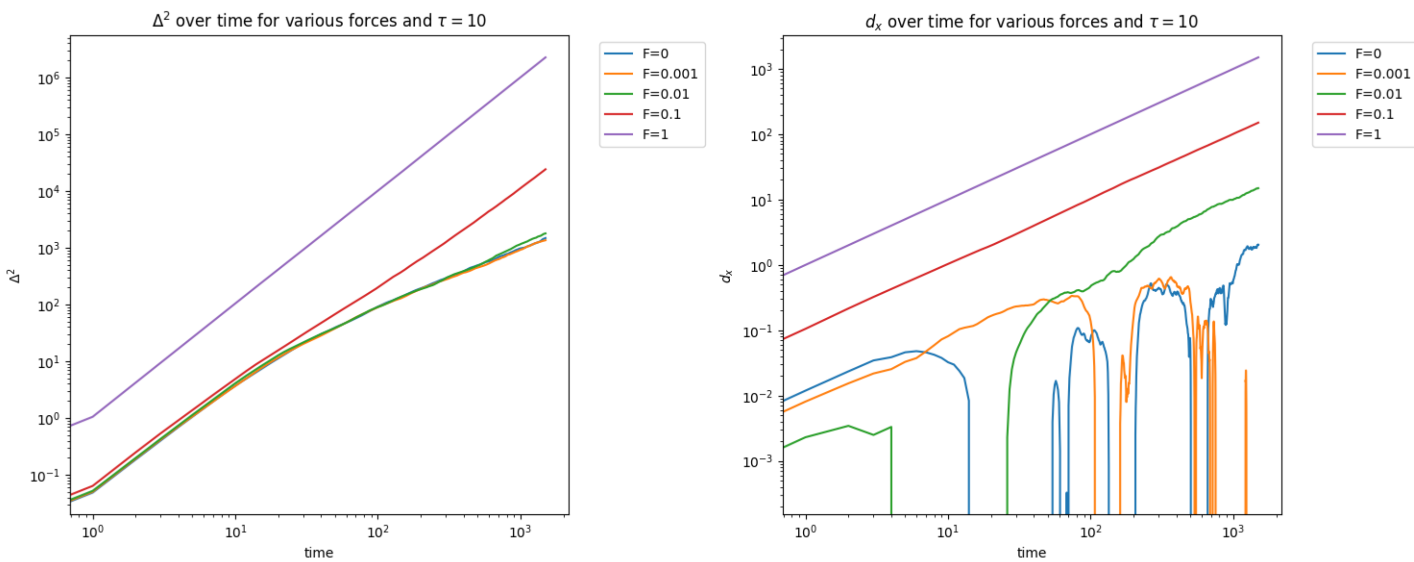


Figure 4: Figure 4.a): The average MSD value for N particles with their correspondent theoretical function, Equation (2.6), plotted together. Ballistic behaviour is acchieved on higher forces. Figure 4.b): Averaged displacement on the x axes. We can see for small forces a random walk behaviour from t=τ onwards.

We know the MSD must follow Equation (2.6) for $\tau = 10$ up to a scaling factor, because its half its value. When the force is strong enough we reproduce purely ballistic behaviour because the diffusive state associated with a the random walk regime is surpressed, that is why for t=10 onwards the MSD and d_x are linear in time. For f<0.1 we can consider the force a perturbation and the linear response regime is acchieved.

5 Exercise 5 and 6: Linear response function and the fluctuation dissipation theorem

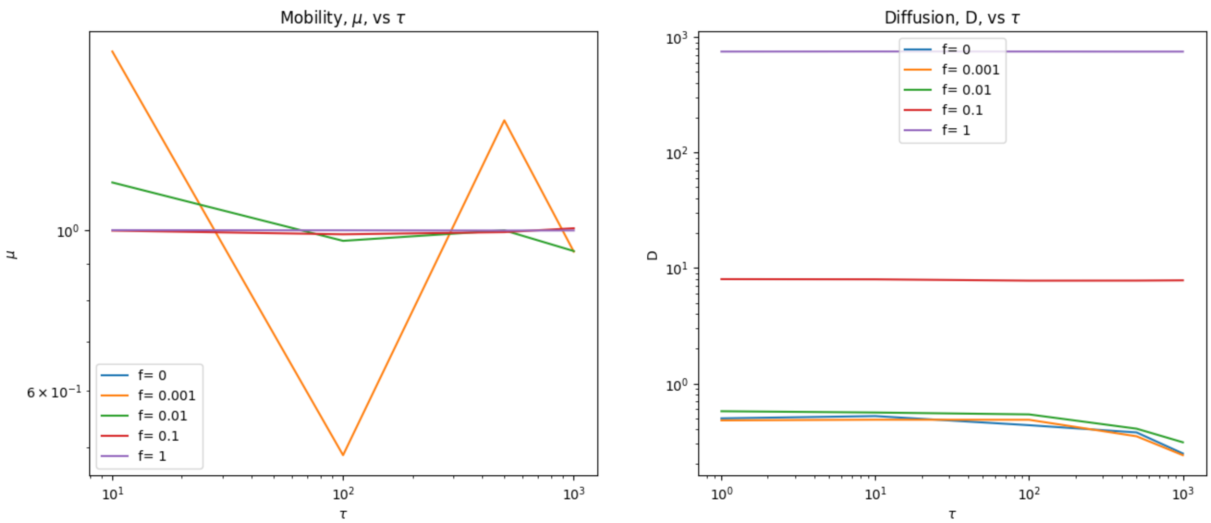


Figure 5: Mobility, μ, and diffusion constant, D, for different values of memory time, $\tau = [1, 10, 100, 500, 1000]$, for 1000 realizations and set diffusion D=$\frac{1}{2}$.

About diffusion, for small forces we can see the particles diffuse, with the same value, as long as the force is small. If f>0.01 then they will not diffuse and behave ballistically even for larger times. So memory does not affect the result.

About mobility, except for the case f=0, its value stabilizes in 1, so it does not change with the loss of memory or the force applied.

We can see only if the applied force is small and the memory is equal to the time step, we conserve the fluctuation-dissipation thorem. Otherwise, the force is too strong and there is no random walk behaviour on the particle, so this theorem can not apply.