Brownian Dynamics, Fluctuations and Response - FENE

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1 Exercise 1: Langevin equation

The dynamics of each particle in the system is given by the following overdamped Langevin equation:

$$\gamma \dot{\mathbf{r}}_i(t) = \boldsymbol{\eta}_i(t) \tag{1.1}$$

$$\text{with } \eta \text{ Gaussian noise verifying: } \langle \eta_i^\alpha(t) \rangle = 0, \forall\, i,\, t\,; \quad \langle \eta_i^\alpha(t)\eta_j^\beta(t') \rangle = 2\Gamma\delta(t-t')\delta^{\alpha\beta}\delta_{ij} \tag{1.2}$$

If we redefine write this gaussian noise using a Wiener process and check if this process reproduces the conditions given in Equation (1.2):

$$\mathbf{W}_i(t) = \int_0^t dt' \boldsymbol{\eta}_i(t') \tag{1.3}$$

$$\langle W_i^\alpha(t) \rangle = \left\langle \int_0^t dt' \eta_i^\alpha(t)(t') \right\rangle = \langle \eta_i^\alpha(t) \rangle = 0 \quad \text{and} \left\langle {}_i^\alpha(t)_j^\beta(t') \right\rangle = 2\Gamma\delta_{ij}\text{min(t,t')} \tag{1.4}$$

$$\text{The infinitesimal increment of a Wiener process can be redefined, [1], as: } \frac{d\mathbf{W}_i}{dt} \rightarrow \sqrt{2\Gamma}\boldsymbol{\xi}_i \tag{1.5}$$

Then we can rewrite Equation (1.1) as: $\gamma \dot{\mathbf{r}}_i(t) = \sqrt{2\Gamma}\boldsymbol{\xi}_i(t)$.

2 Exercise 2: Gaussian random number

Using the Box-Muller algorithm we can obtain a Gaussian distribution from two uniform distributions. The results have been normalized and plotted with a N(0,1) function in order to show their similarity.

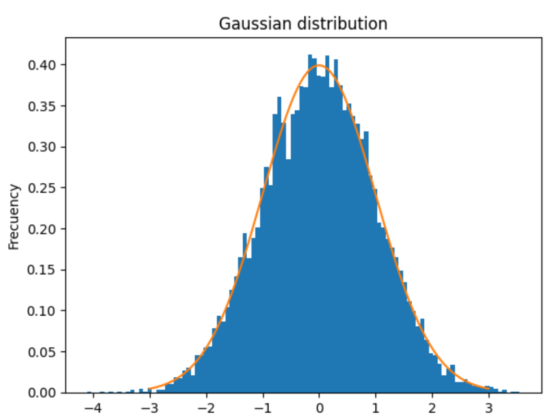


Figure 1: Histogram of data. In orange, a Gaussian function

Gaussian data's statistics: μ= 0.004, σ^2= 0.98. Therefore we obtained a proper gaussian distribution of cero mean and unit variance.

3 Exercise 3: Euler-Mayurama algorithm

In the following sections the amplitude of the noise is set to $\Gamma = 1$.

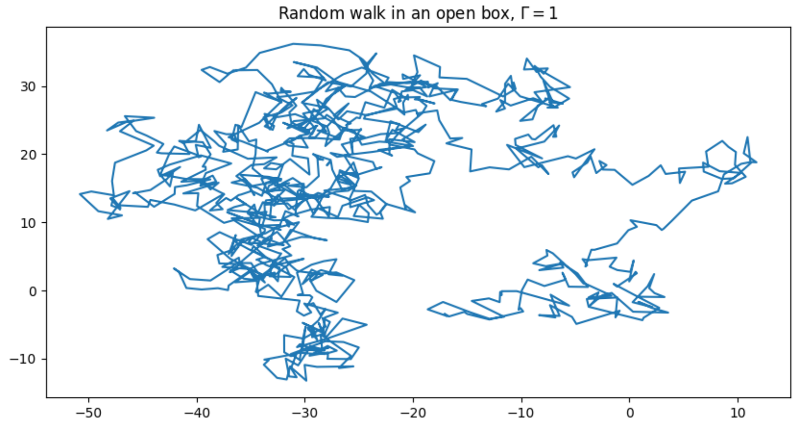


Figure 2: Random walk simulation for a particle in an open box after 1000 steps

4 Exercise 4: Particles in a box

Periodic Boundary Conditions have been implemented and there can be overlaps due to these particles not interacting with each other.

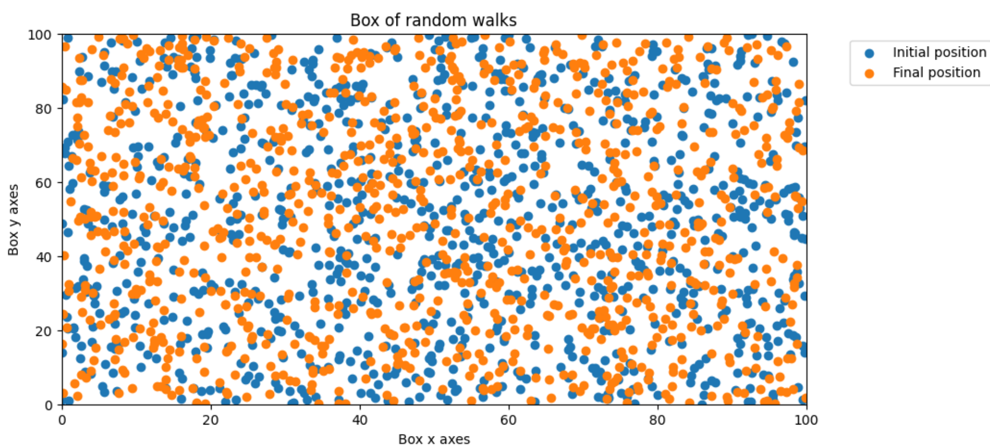


Figure 3: Figure
Random walk simulation of N=1000 particles in a closed box of 100x100 dimentions

5 Exercise 5: Mean Square Displacement

We know that $\Delta^2 = 4\Gamma t$, so if we define the diffusivity as $D = \lim_{t\to\infty} \frac{\Delta^2(t)}{4t}$ we can see $D = \Gamma$. The right plot shows on a log-log plot the validity of this calculation.

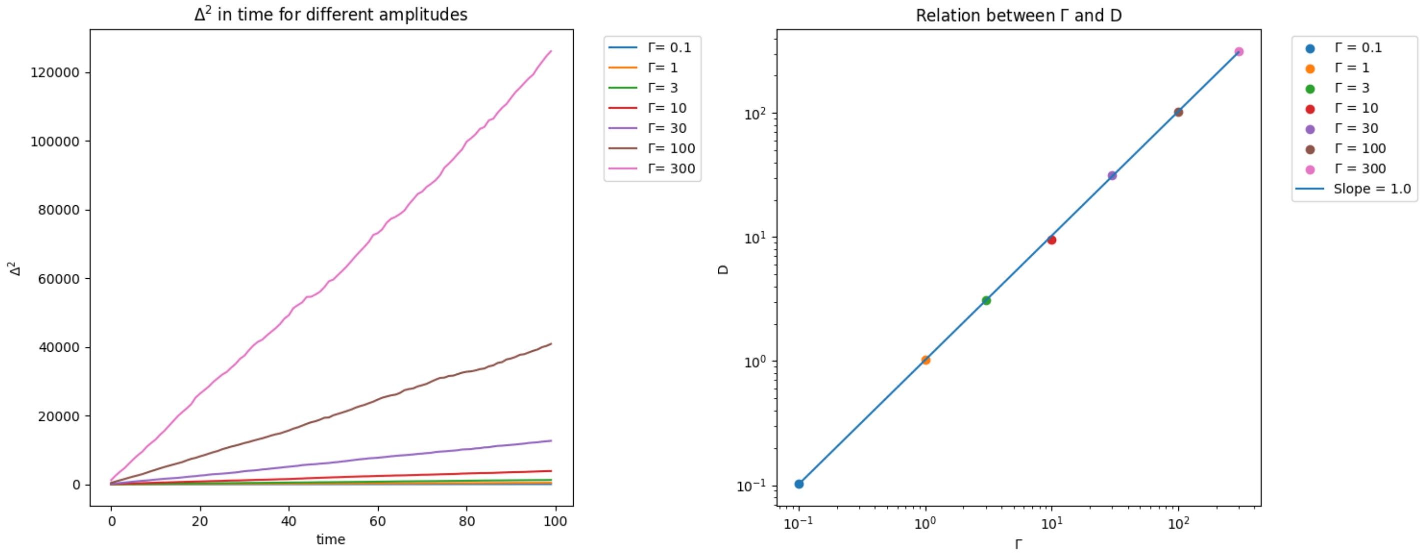


Figure 4: 4.a) Mean square displacement, Δ^2, averaged for N=1000 particles for different amplitudes of the noise term Γ. 4.b) Relation between diffusivity, D, and the amplitude of the noise term.

6 Exercise 6: Diffusion equation

The solution for the diffusion equation is: $P(\Delta x, t) = \frac{1}{\sqrt{4\pi Dt}} \cdot e^{-x^2/4Dt}$. The following picture shows time snapshots of 1000 particle's random walks and the fitting to this solution.

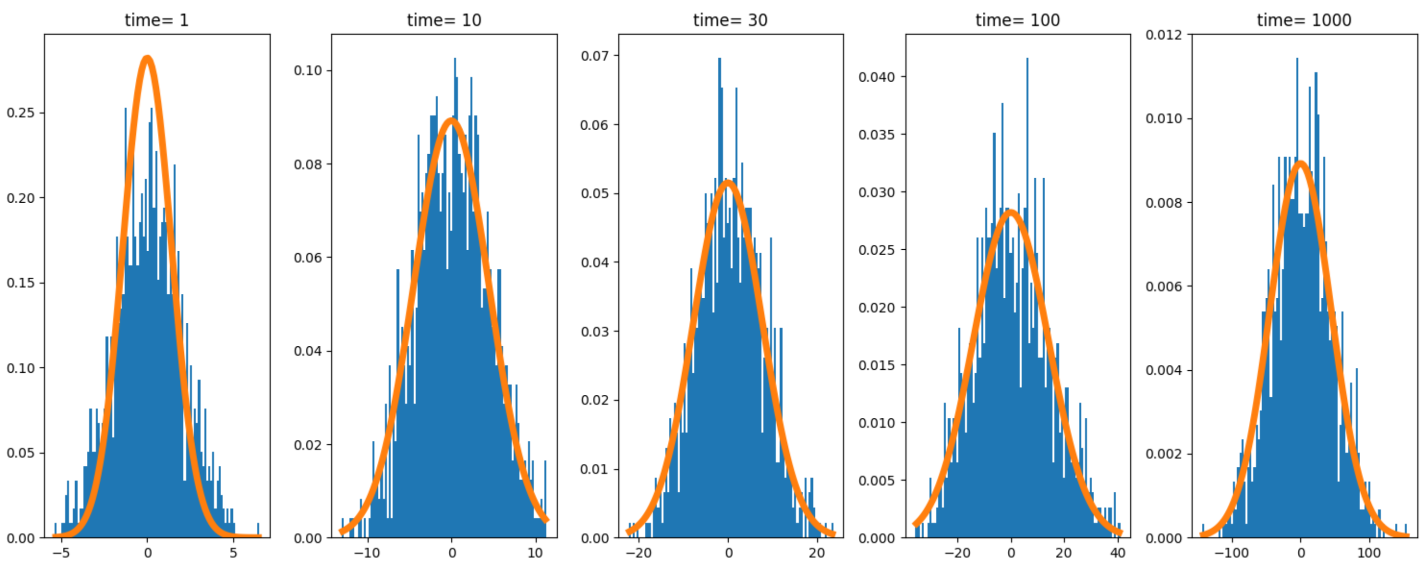


Figure 5: Histogram made of positions of each particle at selected times. The theoretical result is plotted in orange

7 Exercise 7: Diffusion equation and Boltzmann distribution

The Boltzann distribution is $\Psi_0(\{r_i(t)\}) = Z^{-1} e^{-U/k_B T}$ and the Fokker-Planck equation is:

$$\frac{\partial \Psi(\{\mathbf{r}_i(t)\})}{\partial t} = \sum_i \left[D\nabla_i^2 \Psi(\{\mathbf{r}_i(t)\}) - \gamma^{-1} \nabla_i \cdot (F_i \Psi(\{\mathbf{r}_i(t)\}) \right] \tag{7.6}$$

In order to prove that the Boltzmann distribution is a solution of this equation we must substitute it in the equation and prove that $\frac{\partial \Psi(\{\mathbf{r}_i(t)\})}{\partial t} = 0$.

$$\frac{\partial \Psi_0(\{r_i(t)\})}{\partial t} = \sum_i \left[D\left(-\frac{U''(x)}{k_B T} e^{-U/k_B T} + \frac{U''(x)^2}{k_B^2 T^2} e^{-U/k_B T} \right) - \gamma^{-1} \left[U''(x) e^{-U/k_B T} - \frac{U'(x)^2}{k_B T} e^{-U/k_B T} \right] \right] Z^{-1}$$

Knowing that $\frac{k_B T}{D} = \gamma$ the first term is equal to the last one:

$$\frac{\partial \Psi_0(\{r_i(t)\})}{\partial t} = 0$$

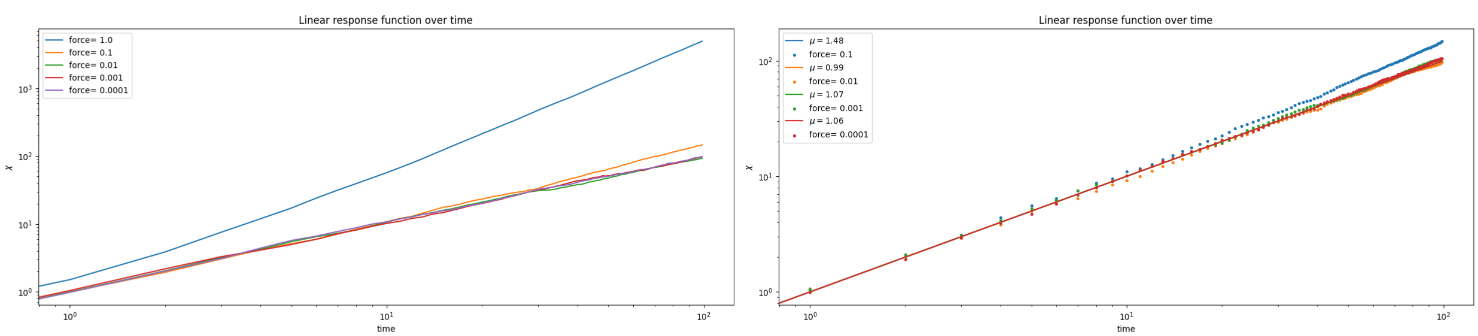
So, we have acchieved an stationary solution of the Fokker-Planck equation.

8 Exercise 8: Linear response function

We added a small force in the x axes and plotted the response function based on the mean square displacement on the x axes:

$$\chi(t, 0) = \frac{1}{2k_B T} \Delta_x^2(t, 0) \tag{8.7}$$

Setting $k_B T = 1$ we can see the linear response regime is acchieved when the perturbation is really small, f<0.1. We can see the computationally found μ, Figure 6.b), are equal to the diffusion constant D=1. This means a diffusive regimen is still conserved even if a small perturbation is applied on the system. For strong forces the system displays a ballistic behaviour, as it can be seen in Figure 6.a) for force=1, so there displacement of the particle will not be that of a random walk.



(a) (b)

Figure 6: 6.a) linear response, χ, over time for different forces. 6.b) Close-up showing the response to the smaller forces and their results, obtained computationally by linear regression, for μ.

References

[1] Livi R, Politi P., *Nonequilibrium Statistical Physics: A Modern Perspective.*, Cambridge: Cambridge University Press, 2017.

[2] M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids*, Oxford university press. https://global.oup.com/booksites/content/9780198803195/