Brownian Dynamics, Fluctuations and Response

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1. From the overdamped Langevin equation

$$\gamma\dot{\mathbf{r}}_i = \eta_i(t)$$

where η is a stochastic process we can write $\xi = \frac{\eta}{\sqrt{2\Gamma}}$ where ξ will be gaussian noise with zero mean and unit variance. Indeed,

$$\langle \xi_i^\alpha(t) \rangle = 0 \;\; \forall i, t \qquad \langle \xi_i^\alpha(t)\xi_j^\beta(t') \rangle = \delta(t-t')\delta^{\alpha\beta}\delta_{ij}$$

2. We now generate a set of $N = 10^4$ random numbers following a normal distribution $\mathcal{N}(0,1)$ with the Box-Muller algorithm and represented their distribution in a histogram. We can see the results in Figure 1, along with their mean and variance for X and Y values and the gaussian curve those values yield.

3. It is not straightforward to differentiate the Langevin equation since ξ is not differentiable, but considering a Wiener process $w = \int \xi \, dt$ we arrive to the form

$$\begin{aligned} x_i(t+\delta t) &= x_i(t) + \frac{g_i^x}{\gamma}\sqrt{2\Gamma\delta t} \\ y_i(t+\delta t) &= y_i(t) + \frac{g_i^y}{\gamma}\sqrt{2\Gamma\delta t} \end{aligned} \tag{1}$$

Using this procedure, we can now simulate a single particle in an open box located initially at the origin $(0,0)$ and with $\gamma = 1$. An example of the possible trajectories these particles can follow is represented in Figure 2, where each color represents a different particle that, starting from the origin, updates its position according to the above equations.

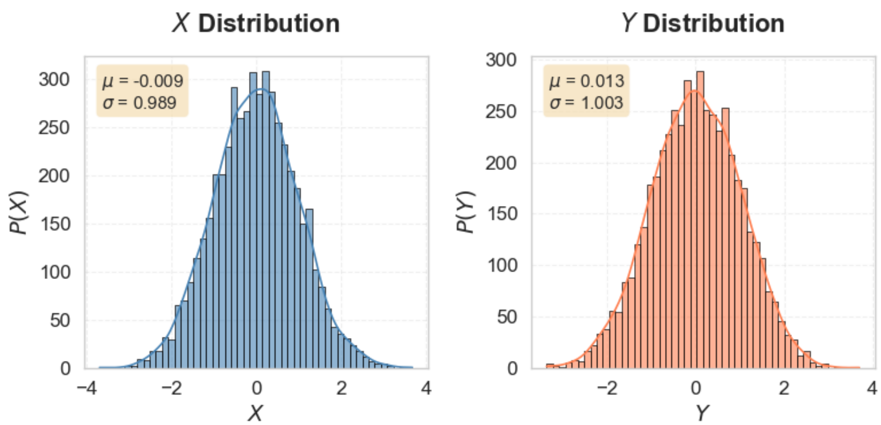

Figure 1: X and Y distribution when generating 1000 random numbers drawn from $\mathcal{N}(0, 1)$.

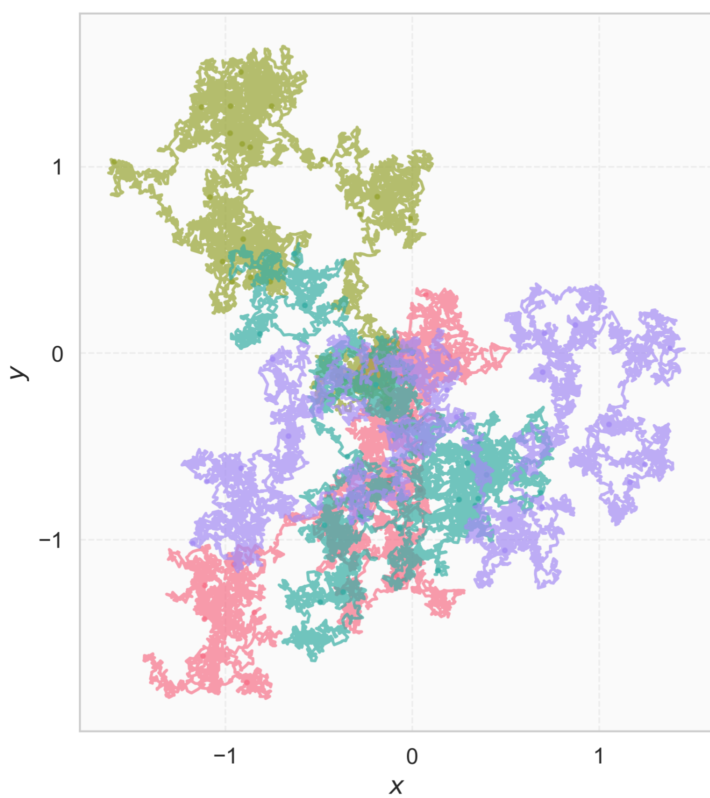

Figure 2: Different trajectories for the stochastic movement of four particle.

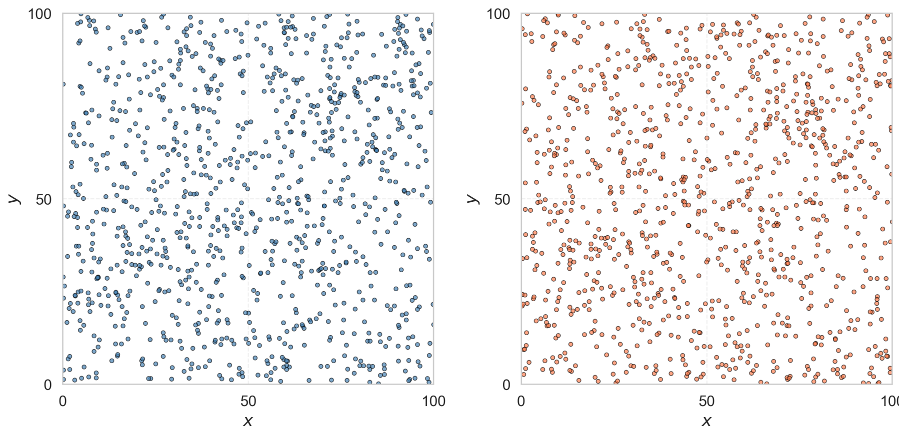

Figure 3: First and last time step for a system of $N = 1000$ particles which evolve according to brownian dynamics for a time $\tau = 100\delta t$. Now, the positions of particles are initialized randomly from a uniform distribution in the LxL box with periodic boundary conditions.

4. We now intend to implement periodic boundary conditions (PBC), restricting the particles to move inside a LxL box and keeping track of boundary crossings in both directions.

Also, the time step δt will determine the accuracy of our numerical solution. We would normally want a small time step to avoid multiple-box crossings per step, although the runtime of the algorithm increases by a factor $1/\delta t$. For our computations, we have chosen $\delta t = 0.001$, which is a reasonable value that preserves the balance between accuracy and runtime.

5. We are now interested in computing the Mean-square displacement (MSD) of $N = 1000$ particles as:

$$\Delta^2(t) = N^{-1} \sum_{i=1}^{N} \langle (\mathbf{r}_i(t) - \mathbf{r}_i(0))^2 \rangle$$

for different values of Γ and compute the value of the diffusivity, defined as

$$D = lim_{t\to\infty} \frac{\Delta^2(t)}{4t}$$

We see the results of this computation in Figure 4. We clearly observe a linear relationship between Γ and the diffusivity D. The fact that Γ and D take the same value should not come as a surprise since, from Eqs. 1:

$$\langle (\Delta x)^2 \rangle = \frac{2\Gamma}{\gamma^2} \delta t$$

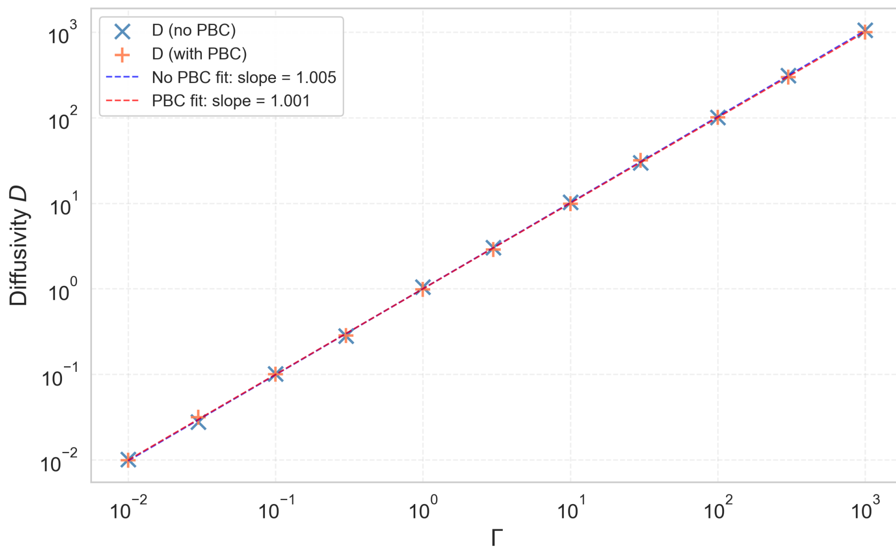

Figure 4: Relation between Γ and diffusivity D calculated with and without PBC.

Taking $\gamma = 1$ and computing x and y contributions for all particles after a time t we have:

$$\Delta^2(t) = \langle \Delta x(t) \rangle^2 + \langle \Delta y(t) \rangle^2 = 4\Gamma t$$

which does not depend on the particle i located at $\mathbf{r}_i$. Therefore we can see that in the limit $t \to \infty$, $D = \Gamma$.