Project 1. Brownian Dynamics, Fluctuations and Response.

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October 19, 2022

1

We know both η and ξ are a Gaussian white noise. ξ is a $\mathcal{N}(0,1)$ and η verifies:

$$\begin{aligned} \langle \eta_i^\alpha(t) \rangle &= 0,\ \forall\, i, t \\ \langle \eta_i^\alpha(t)\eta_j^\beta(t')\rangle &= 2\Gamma\delta(t-t')\delta^{\alpha\beta}\delta_{ij} \end{aligned} \tag{1}$$

So we can assume η and ξ are related by $\boldsymbol{\eta_i}(t) = A\boldsymbol{\xi}(t)$ then:

$$\langle \eta_i^x(t)\eta_i^x(t)\rangle = A^2\langle \xi_i^x(t)\xi_i^x(t)\rangle = 2\Gamma$$

It will be the same behaviour for y component so $A = \sqrt{2\Gamma}$. Eventually we obtain:

$$\gamma\dot{\mathbf{r}}_i(t) = \boldsymbol{\eta}_i(t) = \sqrt{2\Gamma}\boldsymbol{\xi_i}(t) \tag{2}$$

2

It is generated a sample of $N = 10^4$ random numbers uniformly distributed in the interval $[0,1]$. Using the Box-Müller method we generated the normal distribution shown in Figure 1 with the parameters $\mathcal{N}(0,1)$. After the data checking it is obtained the average $\mu = 1.47456 \cdot 10^{-3}$ and the variance $Var(N) = 0.99978$.

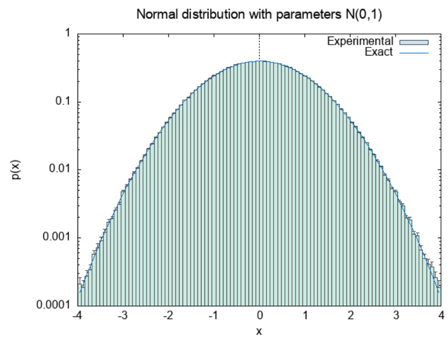

Figure 1: Normal distribution for a sample size $N = 10^4$ in a lin-log representation. The boxes width show the interval width. The "Exact" behaviour is given by $f(x) = \frac{1}{\sqrt{2\pi}} e^{\frac{-x^2}{2}}$ expression.

3

The following figure (Figure 2) shows how an origin located particles randomly moves due to the Brownian Dynamics. The equations which describe this motion are:

$$x_i(t + \delta t) = x_i(t) + \sqrt{2\Gamma \delta t} g_i^x \tag{3}$$

$$y_i(t + \delta t) = y_i(t) + \sqrt{2\Gamma \delta t} g_i^y \tag{4}$$

Both measured in μm. The constant values used are the following ones: $\Gamma = 3\mu N^2/s$, $\delta t = 0.1s$ and g_i^α where $\alpha = x, y$ is a random normal number.

4

In Figure 3 is shown the initial random configuration for $N = 1000$ particles confined in a box $L \times L$, where $L = 100\mu m$ so the Cartesian coordinates will be also given in μm. We obtain a final random configuration too after 100 steps for (3) and (4) equations, we used the same parameter values as in section 3. It is chosen $\delta t = 0.1s$ because the bigger the Euler Method error the bigger the width step, but δt has to be big enough to reach the $t \longrightarrow \infty$.

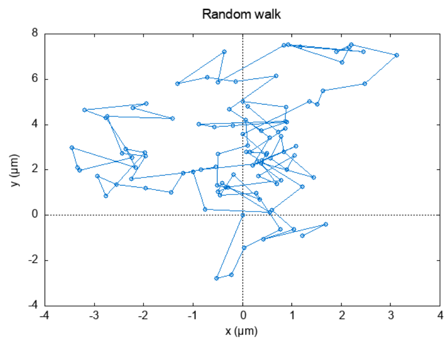

Figure 2: A single particle trajector due to the Brownian Dynamics for a 100 times δt steps, where $\delta t = 0.1s$.

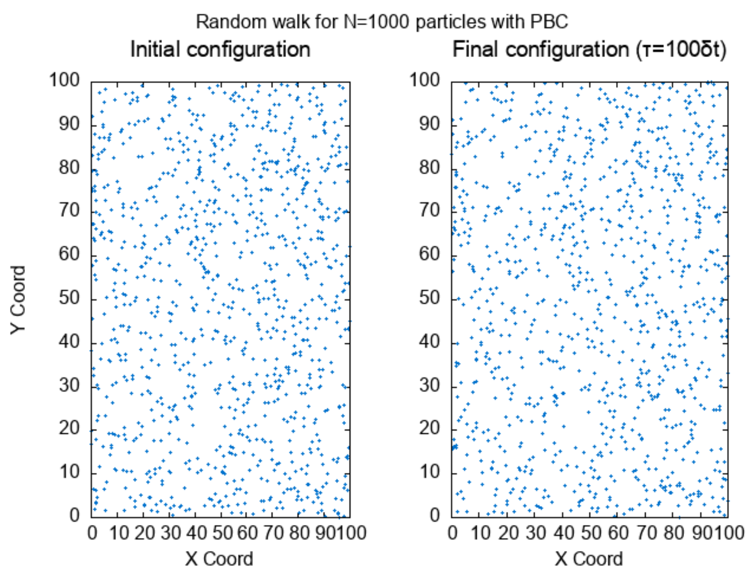

Figure 3: Initial and final configuration for $N = 1000$ particles after a time $\tau = 100\delta t$.

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Since they have a linear relation in a log-log representation, as we can see in Figure 4. We can asume $D = \Gamma^a$ where a is a number compressed in the interval $[0, 1]$.

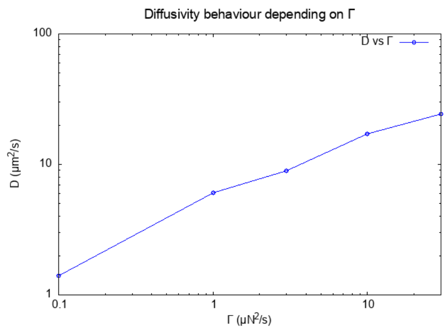

Figure 4: It is shown the diffusivity versus the Γ parameter in a log-log scale.

6

It is shown the distribution of the horizontal displacements of the particles in the absence of interactions. For different times measured in seconds. It is reproduced the exact solution of the diffusion equation.

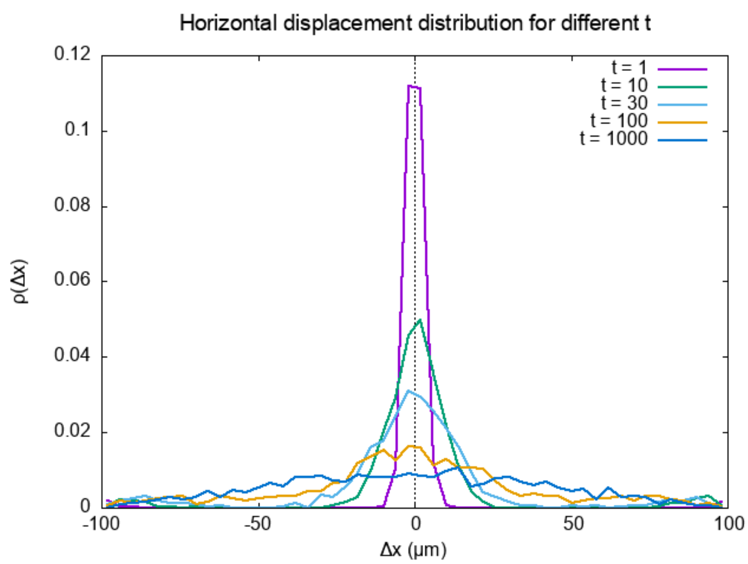

Figure 5: Horixontal displacement distribution for the N=1000 particles inside the box.