Assignment 2 - TFY4235
Biased brownian motion

Thorvald M. Ballestad

March 20, 2020

Task 1
Euler scheme

$$x_{n+1} = x_n - \frac{1}{\gamma_i}\frac{\partial U}{\partial x}\delta t + \sqrt{\frac{2k_BT\delta t}{\gamma_i}}\hat{\xi}_n. \tag{1}$$

Introducing

$$\hat{x} = \frac{x}{L}, \quad \hat{t} = \omega t, \quad \omega = \frac{\Delta U}{\gamma_i L^2}, \quad \hat{U}(\hat{x}, \hat{t}) = \frac{U(x,t)}{\Delta U}, \quad \hat{D} = \frac{k_BT}{\Delta U}, \tag{2}$$

(1) can be rewritten as

$$\hat{x}_{n+1} = \hat{x}_n - \frac{\partial \hat{U}}{\partial \hat{x}}(\hat{x}, \hat{t})\delta\hat{t} + \sqrt{2\hat{D}\delta\hat{t}}\hat{\xi}_n. \tag{3}$$

Here $\hat{U} = \hat{U}_r(\hat{x})f(\hat{t})$ where

$$\hat{U}_r(\hat{x}) = \begin{cases} \frac{\hat{x}}{\alpha}, & \text{if } 0 \leq \hat{x} < \alpha \\ \frac{1-\hat{x}}{1-\alpha}, & \text{if } \alpha \leq \hat{x} < 1 \end{cases}, \quad f(\hat{t}) = \begin{cases} 0 & \text{if } 0 \leq \hat{t} < \frac{3\omega\tau}{4} \\ 1 & \text{if } \frac{3\omega\tau}{4} \leq \hat{t} < \omega\tau \end{cases}. \tag{4}$$

The criterion for δt in dimensionless quantities become

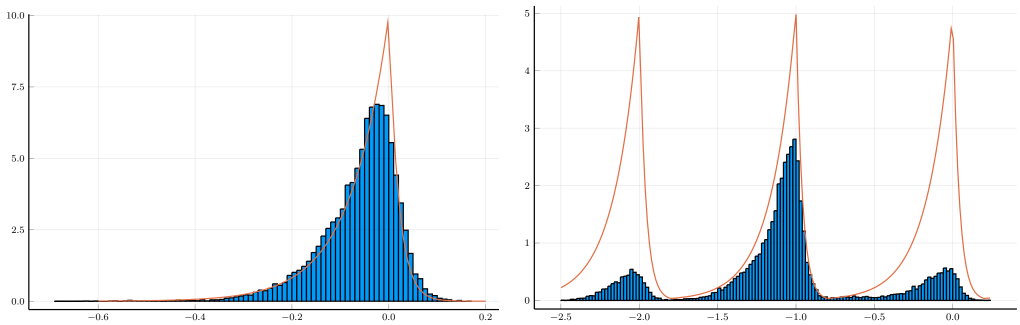
$$\max\left|\frac{\partial \hat{U}}{\partial \hat{x}}\right|\delta\hat{t} + 4\sqrt{2\hat{D}\delta\hat{t}} \ll \alpha \tag{5}$$

Task 7
The Boltzmann distribution

$$p(U) = \frac{e^{-\frac{U}{k_BT}}}{k_BT\left(1 - e^{-\frac{\Delta U}{k_BT}}\right)}. \tag{6}$$

Which, in dimensionless quantities is

$$p(\hat{U}) = \frac{e^{-\hat{U}/\hat{D}}}{\hat{D}\left(1 - e^{-1/\hat{D}}\right)}. \tag{7}$$



(a) $D = \frac{1}{10}$

(b) $D = \frac{1}{5}$

Figure 1: Simulated distribution, histogram, and the theoretical Boltzmann distribution, solid line, for $D = \frac{1}{10}$ and $D = \frac{1}{5}$.

Task 8

One should choose ΔU such that diffusion is maximized, without particles reaching over to neighbouring wells when the potential is on. There will be three regimes of drift velocity, (1) too high frequency on the flashing will not allow the particles to diffuse enough, and we will see very little drift. (2) correct frequency will allow particles to diffuse beyond α and thus be trapped in the next well when the potential is turned on again. (3) the final regime will be a too large period, where particles will move both left and right, ie. they diffuse more than $1 - \alpha$, and are trapped in wells in both directions.

We will now set $\Delta U = 80\,\text{eV}$ and let $r = r_1$.

Task 9 With $D = 2 \times 10^{-4}$ simulating to $t = 7000$ for different τ, with 500 relizations for each τ, the drift velocities shown in figure 2 was found. The drift velocity is here defined as the position in the final step. From the figure one sees that the τ that optimizes drift velocity, τ_{opt} is 110.

Drift velocitites for $\tau = 100, 110, 120, 130, 140$ are 7.160835818693163, 7.174037267938745, 7.2548174835795 74, 7.297040033152324, 7.198623178831086.

Another simulation, with $\tau = 10, 30, 60, 80100, 120$ gives 0.02214625656038857, 2.730464062719224, 6.0891858241978 61, 7.046632812276713, 7.463267755732644, 7.468415404324993.

Task 11

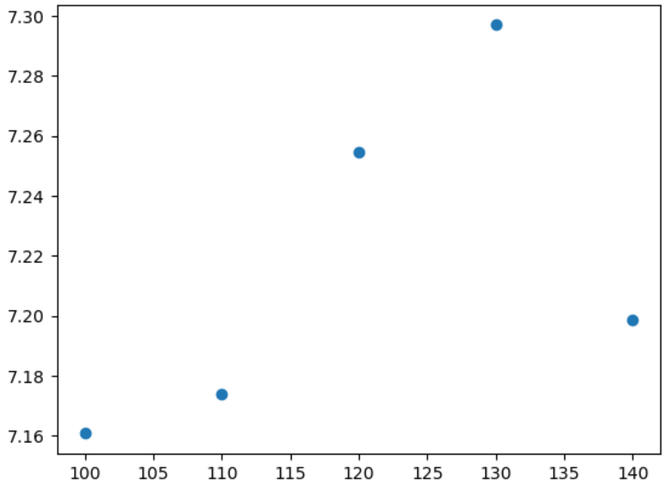


Figure 2: Drift velocity for different flashing periods τ. Calculated for $D = 2 \times 10^{-4}$ with $t_{\text{end}} = 7000$ and 500 relizations for each τ.

We now consider a particle with radius $r_2 = 3r_1$. Thus $\gamma_2 = 3\gamma_1$ and $\omega_2 = \frac{1}{3}\omega_1$. Thus, this corresponds to scaling the time with a factor 3.

Task 12

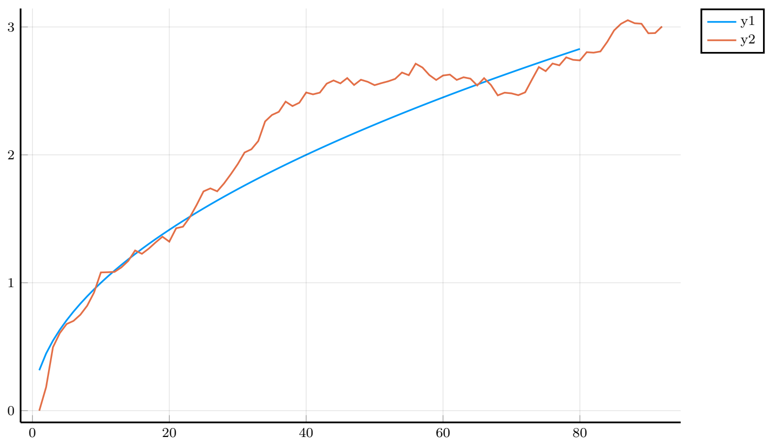


Figure 3: Standard deviation of an ensable as a function of time. The solid line is a fit curve, which scales like $\sqrt{t}$, showing that the standard deviation behaves as expected. Calculated with $D = 2 \times 10^{-4}, t_{end} = 7000, \tau = 110$.