TFY4235 - Biased Brownian Motion

Karl Kristian Ladegård Lockert[a]

[a] *Institutt for fysikk, Norges Teknisk-Naturvitenskapelige Universitet, N-7491 Trondheim, Norway.*

Abstract

By implementing an Euler-scheme for numerical computation of the Langevin equation with a flashing potential, drifting of particles in a Ratchet potential is achieved. Moreover, filtering of two different kinds of particles is realized. The optimal flashing time τ is found to be $\tau_{\text{op}} = 0.52$ for a particle similar to that of Bader et al. The particle densities reach a maximum average drift speed of approximately 4.5μm/s, deviant from the results in [1]. A re scaling of the time-axis predicts the optimal flashing time for a particle with a larger mass. The distributions follow a prescribed analytical particle densities for an absent potential to great precision.

Introduction

This assignment on biased Brownian motion is about solutions of stochastic differential equations. The Euler scheme of the equation is, as presented in ref. [2],

$$x_{n+1} = x_n - \frac{1}{\gamma_i}\frac{\partial U}{\partial x}\left(x_n, t_n\right)\delta t + \sqrt{\frac{2k_B T \delta t}{\gamma_i}}\hat{\xi}_n. \quad (1)$$

We could use a higher order numerical scheme to calculate the solutions, but there is a trade off in the stochastic processes taking place at each time step, and must be dealt with carefully if a numerical scheme with multiple function evaluations as each step is chosen.

In this report, an investigation how a stochastic process is affected by a flashing potential is to be done. The implementation is made by first rewriting the problem to dimensionless constants. After ensuring the use of a good pseudo-random generator, the physical differences of the problem for a non-flashing potential with different heights will be discussed, and a comparison with the analytical Boltzmann distribution of particles will be presented. After this, flashing of the potential given in (3) will be turned on, and an investigation of the average drifting velocity will be carried out, and optimal flashing times will be deduced. The particle density will be shown to evolve as an analytic model for an absent potential, and will also work as a filtering mechanism when comparing multiple particle types.

All the implementation is written in Python 3.7, with heavy usage of packages such as NumPy, SciPy and Numba to vastly improve the performance of the programming language. None of the calculations has been very time consuming individually, and the variety of parameters that are checked is part reason for that. Even thought 10000 particles is far below Avogadros number (macroscopic), the array containing all data points for 10 seconds for these particles is above 4GB of data, and has proved as a well functioning way for filling a hard-drive with data in record time.

Reduced units and numerical randomness

By rewriting Equation (1) in terms of the reduced units, also presented in ref. [2], we get the equation on the desired form, which is

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

By inserting the presented definitions in the Euler-scheme In reduced units, the ratchet potential may be written as

$$\hat{U}(x,t) = \hat{U}_r(x)\hat{f}(t), \quad (3)$$

with

$$\hat{U}_r(x) = \begin{cases} \frac{x}{\alpha} & ,0 < x < \alpha \\ \frac{1-x}{1-\alpha} & ,\alpha \leq x < 1 \end{cases} \quad (4)$$

$$\hat{f}(t) = \begin{cases} 0 & ,0 < t < \frac{3}{4}\tau \\ 1 & ,\frac{3}{4}\tau \leq t < 1 \end{cases}, \quad (5)$$

where both position and time are in reduced units as well. Inserting the reduced units in the criterion formulae for the time step, we obtain the reduced unit criterion

$$\max\left|\frac{\partial \hat{U}}{\partial \hat{x}}\right|\delta t + 4\sqrt{2D\delta t} \ll \alpha \quad (6)$$

As the Euler scheme Equation (2) is strongly dependent on a stochastic variable, ξ, one ought to check that the pseudo-random number generator is good enough. In contrast to nature, which is probabilistic, a machine interpreting binary numbers can never be 100% random. Luckily,

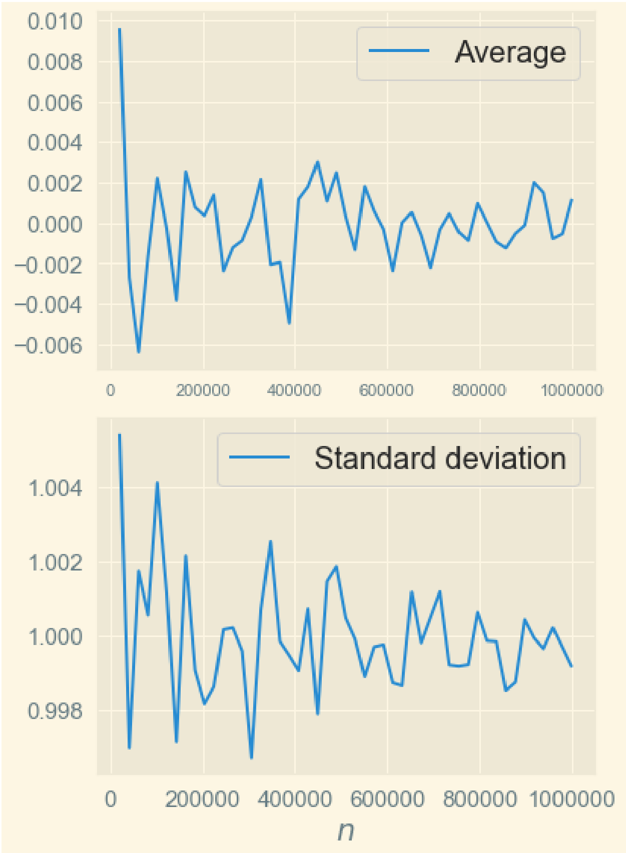

Figure 1: The average and standard deviation of NumPy's normal distribution as a funtion of n, the number of draws from the distribution.

r_1	12 nm
L	20μm
α	0.2
η	1mPa
k_BT	26meV
ΔU	80eV

Table 1: Experimental values for a given particle, as presented in refs. [2, 1]

there exist excellent numerical libraries with good pseudo-random distributions. The one used in this implementation is NumPy's [3] normal distribution. In Figure 1, we see the mildly fluctuating standard deviations and average, around 1 and 0 correspondingly.

Simulation without flashing

For comparison with experiments, the implementation will, as suggested, be that of the experimental parameters in ref. [1]. These values are presented in Table 1. The task is now to normalize these values and implement 2.

To check that our implementation works, we first simulate the particle in a non-flashing potential, $\hat{f}(t) = 1$, for two different values of ΔU. Comparing the distributions with the Boltzmann distribution requires that our system is in thermal equilibrium. By letting the simulation run for a long time, say 10s, this is fulfilled. Simulations of 10000 individual particles for $\Delta U = 0.1k_BT$ and $\Delta U = 10k_BT$ has been computed. The tolerance for the time step has been set so that the left hand side of Equation (6) is less than 0.08α, i.e. smaller than 10% of α. Let us first address some of the physics of the problem. The stationary potential is shown in Figure 2, and for the parameter $\alpha = 0.2$, which we will stick to for the rest of the assignment, the potential is steeper to the right than to the left, given the starting point at the origin. Thus, we can immediately suspect that the average position of a particle with thermal energy much lower than the potential will be slightly negative. If the energy is almost equal to the potential height, we suspect that thermal fluctuations will play a greater role in in the distribution of particles, as the probability of "jumping" across the top will increase. With these considerations in mind, we can prescribe the distribution for the $\Delta U = 10k_BT$ - case to be comparable to a uniform distribution. For the $\Delta U = 0.1k_BT$-case, we expect the distribution of particles to be much higher for lower values of the potential, for the same reason as previously discussed.

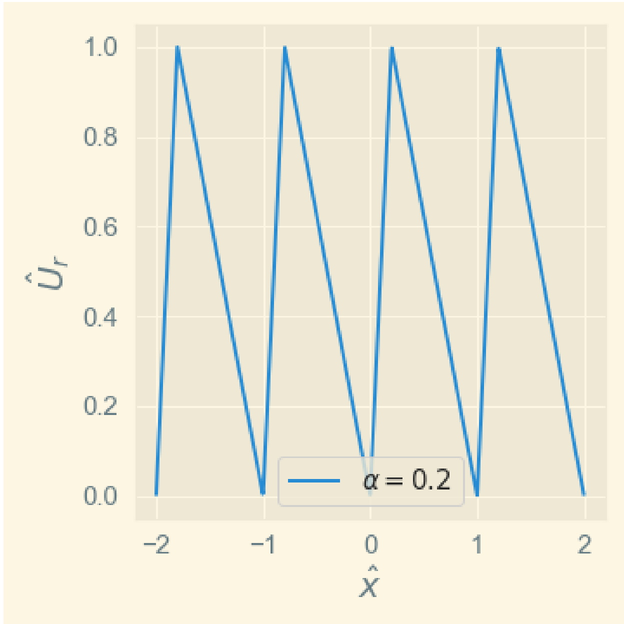

Figure 2: The normalized Ratchet potential.

In Figure 3, we see the trajectories of five particles during their 100 first steps in the iteration. These particles have a thermal energy ten times higher than the maximum value of the potential, and are somewhat unconstrained. Although this is only five particles, and not a large ensemble of particles, the amount of information one can deduce from these graphs are very limited. We can, however, notice that the trajectories shown in Figures 3 and 4 are in

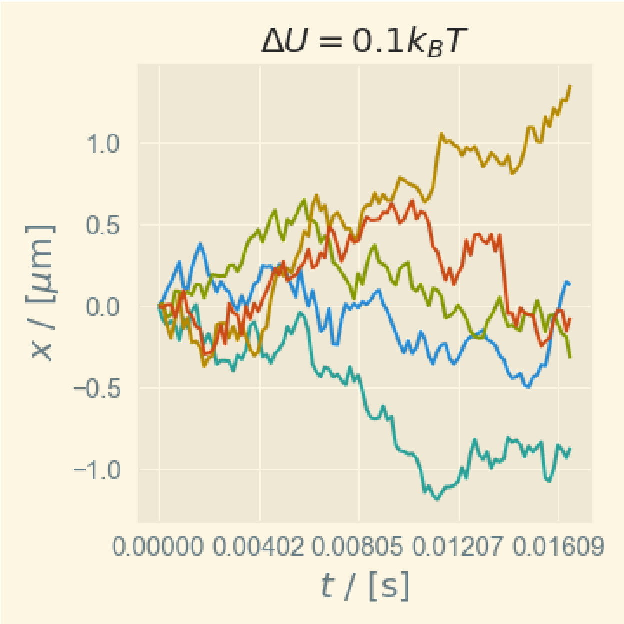

Figure 3: The 100 first steps of 5 particles with $\Delta U = 0.1k_BT$.

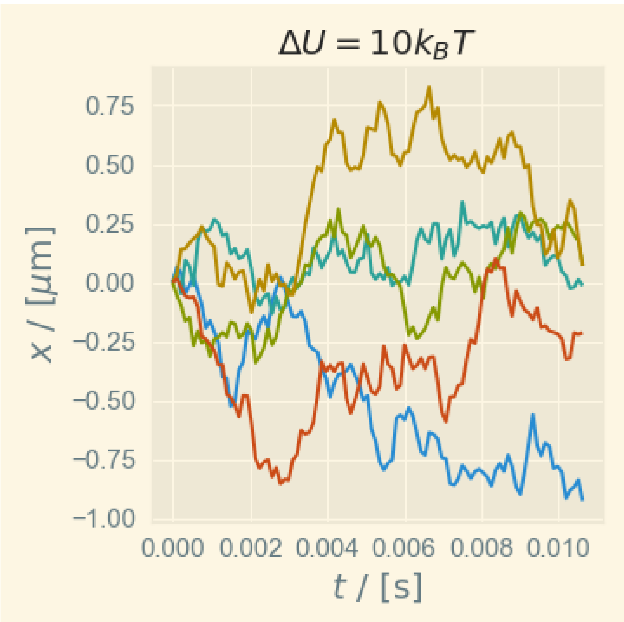

Figure 4: The 100 first steps of 5 particles with $\Delta U = 10k_BT$.

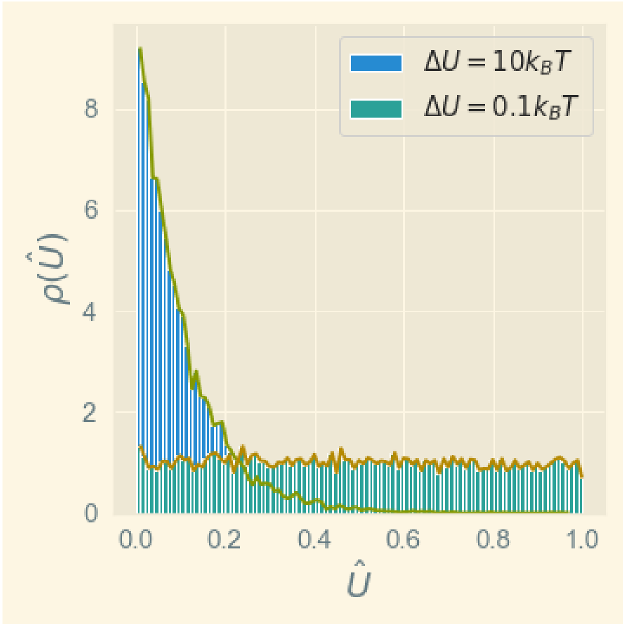

Figure 5: Histogram of the energy occupation after 10 seconds in the constant ratchet potential.

agreement to our physical prescription; the $\Delta U = 10k_BT$-case seems to drift (on average) to a slightly negative value, and the $\Delta U = 0.1k_BT$-case is more reminiscent of a one dimensional random walk. These heuristic arguments will be justified with more results from the computations.

In Figure 5, the occupied energies of the particles for the two different cases are shown. These results were calculated for an ensemble of 10000 particles of the type in Table 1, with the potential changed. As predicted, the thermal fluctuations play a massive role in letting the diffuse. For the $\Delta U = 0.1k_BT$-case, the distribution appears as if it is uniform. Comparing the distributions with the (normalized) Boltzmann-probability density at thermal equilibrium, given by [2]

$$\rho(U) = \beta \frac{\mathrm{e}^{-\beta U}}{1 - \mathrm{e}^{-\beta \Delta U}}, \tag{7}$$

we find that the distributions fit quite well, as shown in Figures 6 and 7.

Using flashing to propagate the particles

As we now have seen, and also can see from Equation (2), the steepness of the potential (force) plays a crucial role in the drifting of the particles. Now, as is the idea in ref. [1], we can utilise this property to transport particles by turning this potential on and off. The idea is to have the particles localized, which we now have seen requires a potential much greater than the thermal energy, for some time (potential on). We then turn the potential off, letting the ensemble diffuse (Brownian motion). Now, because $\alpha = 0.2$, there is a shorter path across the top of the

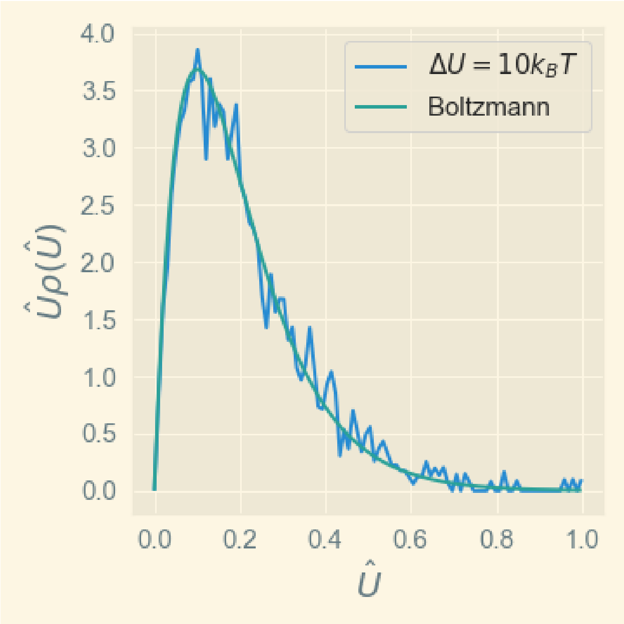

Figure 6: The energy occupation probability density and the corresponding analytic normalized Boltzmann-distribution for $\Delta U = 10k_BT$. Simulation of 10000 equal non-interacting particles

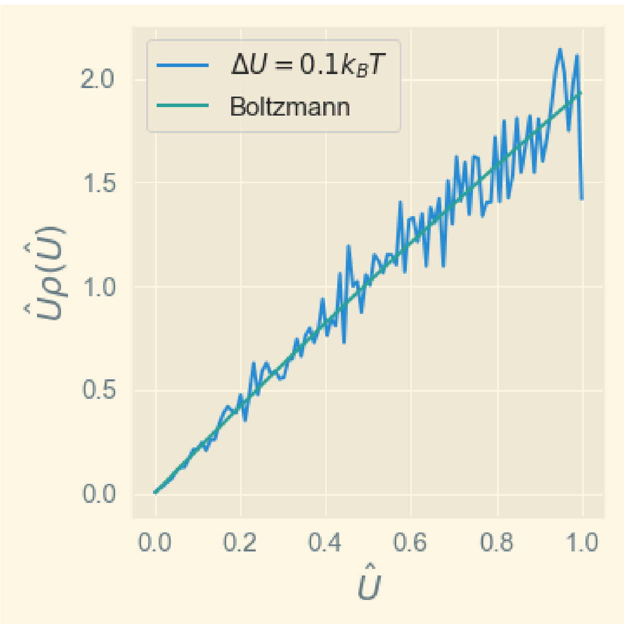

Figure 7: Same as in Figure 6, with $\Delta U = 0.1k_BT$.

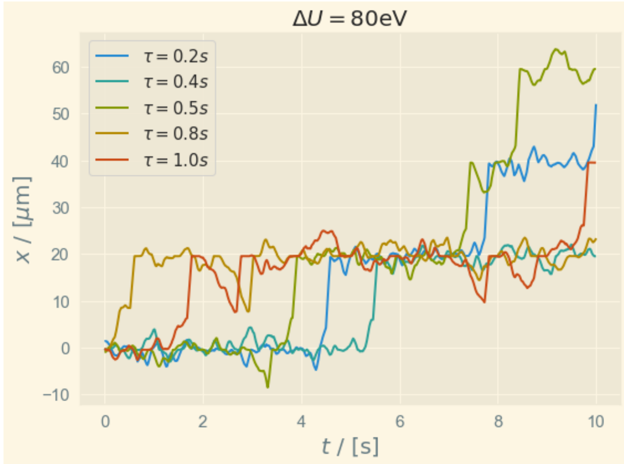

Figure 8: Moving average over 1000 time steps for trajectories of single particles at varying τ. A moving average is used to give a simpler plot.

potential moving to the right, than to the left (assuming we start near the bottom of the potential). This means that, for a proper frequency, we can transport particles of a type towards the right. For frequencies that are too low (too long times between turning on and off), the particles will have diffused in both directions, making the average transport velocity very low. On the other hand, if the frequency is too high, the particles will not have time to diffuse in any direction at all, making the ensemble as a whole stationary. Thus we have the three regions of drift efficiency, and an optimal period τ_{op} corresponding to the highest average velocity.

In Figure 8, some single particle trajectories are plotted for different values of τ. Note that a moving average of 1000 points is used, but this should not impair the data too much, as 1000 points is less than 1% of the total points in each trajectory. Figure 8 does not tell us much, as the trajectories of single particles are not necessarily representative of the mean trajectory of the ensemble as a total. To see how the collective behaviour is affected by the potential turning on and off, we must compute average drifts for different τ.

Comparing the results for the drift velocity in Figure 9 with figure 2.b. in ref [4], we see that the trend for the average velocities does match. While the shape of the velocities does match, the velocity it self is deviant from the results in ref. [1], where frequency was 0.7Hz, and the DNA-molecules have moved approximately $4-6\mu$m after 10 cycles. This means that the drift velocity is approximately $0.6-0.8\mu$m/s, which is an entire order of magnitude off. We find our optimal τ to be $\tau_{\text{op}} \simeq 0.52$s.

Filtering particles

We are now considering a particle similar to that of Table 1, but with a different radius $r_2 = 3r_1$. In the reduced

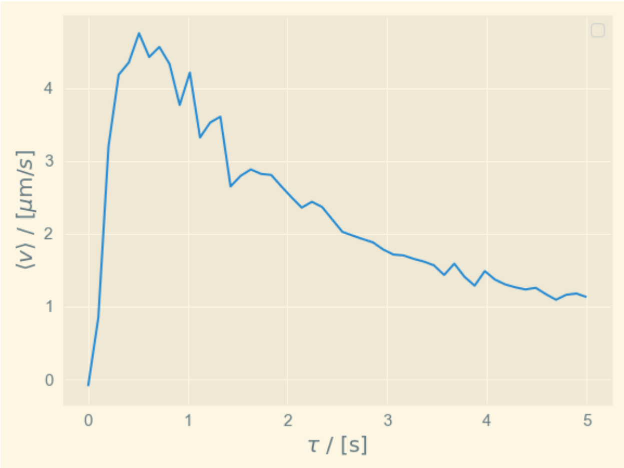

Figure 9: Average drift velocities for an ensemble of 1000 particles of the type in Table 1.

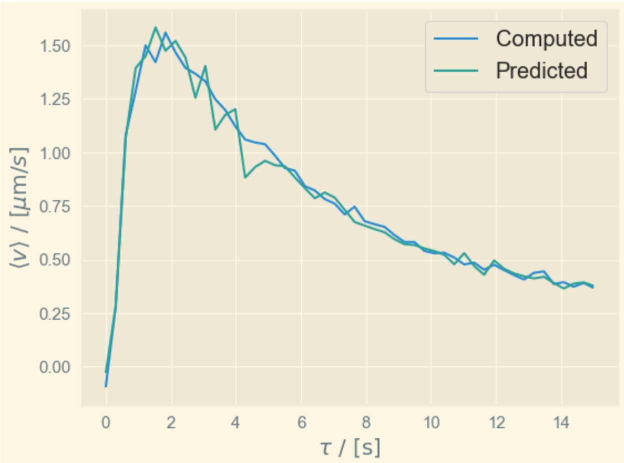

Figure 10: Both the predicted and computed results for the second particle. The prediction is a re-scaling of Figure 9.

units presented in [2], we have $\gamma_i = 6\pi\eta r_i$ with $\omega = \frac{\Delta U}{\gamma_i L^2}$ and $\hat{t} = \omega t$. This implies that $t_2 = 3t_1$, i.e the change in radius corresponds to a change in the time scale of a factor 3. Thus, we expect that $\tau_{\mathrm{op},2} = 3\tau_{\mathrm{op},1}$. This prediction can be made by scaling the time in Figure 9, and by comparing these results with the numerical calculations of the second parameters, we obtain a very similar graph, as we should. This is presented in Figure 10, where both the predicted (time scaling) and computed drift velocities are shown. From a physical perspective, it is intuitive to think that lighter particles are itinerant, not as settled as heavier particles, and therefore have both larger drift velocity and shorter optimal flashing times.

If we now turn off the potential completely, we can in Figure 11 see that the time evolution of our particle follows (up to statistical noise) the distribution given in ref. [2]

$$n(x,t) = \frac{N}{\sqrt{4\pi D t}} \mathrm{e}^{-\frac{x^2}{4Dt}}. \qquad (8)$$

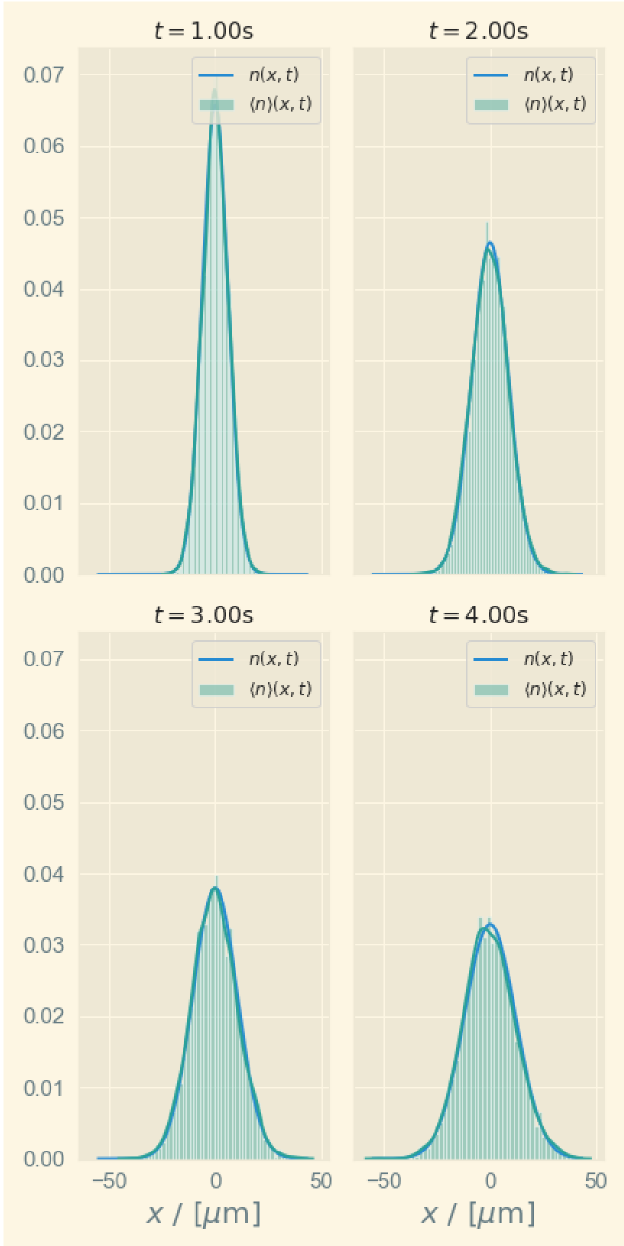

Figure 11: The time evolution of the ensemble at $U(x,t) = 0$. The blue line is the analytical expression from Equation (8) normalised to a probability density per particle. The green line is a Gaussian kernel density estimation of the probability density. The ensemble consists of 5000 particles.

Using the previously found optimal time $\tau_{\mathrm{op}} = 0.52$s for the first type of particle, we can to some extent filter the particles. This is because the average drift velocity of particle 2 is lower at $\tau = \tau_{\mathrm{op}}$ than for particle 1, c.f. Figures 9 and 10. These trajectories are presented in Figure 12, with a Gaussian kernel density estimate of the distributions for visual aid. The distributions diffuse, but with an average velocity towards the right. The shape of the estimate of the drifting distribution from Figure 12 is reminiscent of a itinerant Gaussian packet modulated by a periodic func-

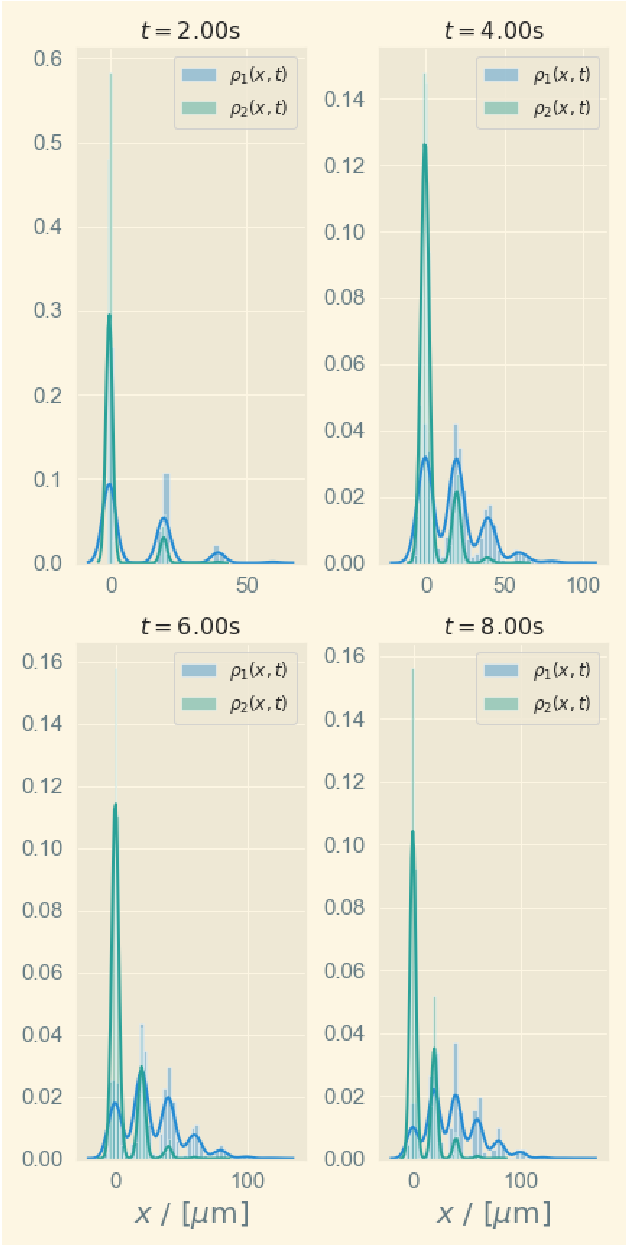

Figure 12: The particle densities for some time intervals. ρ_1 represents the density of particles as in Table 1, while ρ_2 has radius $r_2 = 3r_1$. The thick lines are estimates of the underlying distributions, using a Gaussian kernel.

tion, and can perhaps be modelled by

$$f(x,t) = \frac{A}{\sqrt{t}} \exp\left\{-B\frac{(x-vt)^2}{t}\right\}\left(1-\frac{1}{2}\sin(Cx)\right). \quad (9)$$

Now this equation seems to mach the travelling distribution, but finding the differential equation that it satisfies is hard. A somewhat qualified guess would be to guess for equations on a somewhat similar form as the "Convection-diffusion equation", with a modified oscillating term

$$\frac{\partial f}{\partial t} - D\frac{\partial f}{\partial x} + v\frac{\partial^2 f}{\partial x^2} = \alpha(\cos(Cx)). \quad (10)$$

This is at best a guess that might have some similar properties, but is not tested at all. The term would correspond to an extra sources / sinks in the diffusion, and is thus not guaranteed to exhibit conservation of number of particles.

Concluding remarks

This assignment has given insight in how simple numerical schemes together with a relatively low number of particles (≤ 10000), give results with defined trends that have a simple, yet intuitive, physical interpretation. Moreover, the assignment has given insight in how one can filter particles of different sizes by tuning a flashing potential. Most of the task-relevant coding has been developed in notebooks, but the core functionality in standard programming environments.

References

[1] J S Bader, R W Hammond, S A Henck, M W Deem, G A Mcdermott, J M Bustillo, J W Simpson, G T Mulhern, and J M Rothberg. DNA transport by a micromachined Brownian ratchet device. *Proceedings of the National Academy of Sciences*, 96(23):13165–13169, 1999.

[2] J. Banon and I. Simonsen. Assignment 2: Biased brownian motion: An application to particle separation. `http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/Assignments/TFY4235_Assignment_02.pdf`, 2020.

[3] Travis Oliphant. NumPy: A guide to NumPy. USA: Trelgol Publishing, 2006–. [Online; accessed 23.02.2020].

[4] R Dean and Astumian. Thermodynamics and Kinetics of a Brownian Motor. *Science*, 276(5314):917–922, 1997.