Particle separation by biased Brownian motion

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Abstract

I have simulated movement of particles due to biased Brownian motion in a flashing ratchet potential. The result agree with prediction from experiment [J. S. Bader, *et al. Proc. Natl. Acad. Sci. USA*. 96(23):13165–13169, Nov. 9, 1999]. Particles of different size had different drift velocity and this can therefore be used as a method of separating different particles in a solution.

1. Introduction

Separation of particles of different size in a solution could be of interest in many applications. For example sorting cells by size in a biological sample. There are several ways to accomplish this. One of them is by applying a flashing ratchet potential. Here I take a look at separation of DNA molecules of different size by making a computer simulation based on the setup described in in [1] and in Fig. 2 in [2]. The aim is to be able to reproduce the results from [3] where the actual experiment took place.

2. The Langevin approach

2.1. Position of the problem

A ratchet potential is a flashing potential with an asymmetric 'sawtooth' shape. Initially the potential is 0, the collection of particles is located at 0, and the particles start to move randomly around due to their Brownian motion. When the potential is present at some later time, the particles will move to the corresponding well at their location. Because of the asymmetric shape of the potential, more particles will go to one side rather than another, and the group velocity of the ensemble is non-zero. The Langevin approach to solve this problem (in 1D) involves solving the equation of motion of the system. The system in this case contains two spherical particles with radius $\{r_1, r_2\}$ and mass $\{m_1, m_2\}$. The equation of motion for the particles in the medium can be found by Newton's 2$^{\text{nd}}$ law, and is given by:

$$m_i \frac{\mathrm{d}^2 \mathrm{x_i}}{\mathrm{dt}^2} = -\frac{\partial U}{\partial x}(x_i, t) - \gamma_i \frac{\mathrm{dx_i}}{\mathrm{dt}} + \xi(t) \qquad (1)$$

where i specify the particle, x is the position, t is time, U is the flashing ratchet-potential, $\gamma_i = 6\pi\eta r_i$ is the friction constant and $\xi(t)$ is stochastic variable that takes into account the collision with the solvent molecules. In the Langevin approach, the stochastic variable $\xi(t)$ can be assumed to have a Gaussian probability distribution with the properties

$$\langle \xi(t) \rangle = 0, \qquad \langle \xi(t)\xi(t') \rangle = 2\gamma_i k_{\mathrm{B}} T \delta(t - t')$$

where k_{B} is Boltzmann's constant and T is the temperature of the solvent.

Because the acceleration is small, and take place over a small time scale compared to the time scale of interest, the term $m_i \frac{\partial^2 x}{\partial t^2}$ can be neglected and we get an overdamped approximation. The equation of motion becomes

$$\frac{\partial U}{\partial x}(x_i, t) + \gamma_i \frac{\mathrm{dx_i}}{\mathrm{dt}} = \xi(t) \qquad (2)$$

The ratchet potential can be written in the form

$$U(x, t) = U_r(x)\, f(t),$$

where U_r is the 'sawtooth'-potential with period L and f is an asymmetric square signal with period τ to turn the potential on and off. U_r is defined as

$$U_r(x) = \begin{cases} \dfrac{x}{\alpha L}\Delta U, & 0 \le x < \alpha L \\ \dfrac{L - x}{L(1-\alpha)}\Delta U, & \alpha L \le x < L \end{cases}$$

and $f(t)$ is defined as

$$f(t) = \begin{cases} 0, & 0 \le t < \dfrac{3\tau}{4} \\ 1, & \dfrac{3\tau}{4} \le t < \tau \end{cases}$$

2.2. Numerical Implementation

By using the Euler scheme, equation (2) has the following approximate solution:

$$x_{n+1} = x_n - \frac{1}{\gamma_i}\frac{\partial U}{\partial x}(x_n, t_n)\, \delta t + \sqrt{\frac{2k_b T \delta t}{\gamma_i}}\hat{\xi}_n \qquad (3)$$

where δt is the time step, $t_n = n\delta t$ is the time and x_n is the position at iteration n. $\hat{\xi}_n$ is a random number drawn from a normal distribution.

If the time step is too large, the particle might jump through several variations of the potential within a single iteration, and the simulation would give a wrong result. To avoid this behaviour, the time step must be small enough such that the change in position is (to a high probability) within a region of constant force. Since $|\hat{\xi}| < 4$ more than 99.99 % of the time and αL id the shortest length with constant force (for $\alpha < 1/2$) the change in position form one time step to another should satisfy $|x_{n+1} - x_n| \ll \alpha L$. Given this constraint and equation (3) gives

$$\frac{1}{\gamma_i}\max\left|\frac{\partial \mathrm{U}}{\partial \mathrm{x}}\right|\delta \mathrm{t} + 4\sqrt{\frac{2\mathrm{k_B T}\delta \mathrm{t}}{\gamma_\mathrm{i}}} \ll \alpha \mathrm{L} \tag{4}$$

In reduced units, equation (3) becomes

$$\hat{x}_{n+1} = \hat{x}_n - \frac{\partial \hat{U}}{\partial \hat{x}}(\hat{x}_n, \hat{t}_n)\delta\hat{t} + \sqrt{2\hat{D}\delta\hat{t}}\,\hat{\xi}_n \tag{5}$$

where $\hat{x} = \frac{x}{L}$, $\hat{t} = \omega t$, $\omega = \frac{\Delta U}{\gamma_i L^2}$, $\hat{U}(\hat{x}, \hat{t}) = \frac{U(x,t)}{\Delta U}$ and $\hat{D} = \frac{k_B T}{\Delta U}$.

3. Result

3.1. Testing the code

For this simulation the physical parameters of the system is set to be:

$$\begin{aligned} r_1 &= 12\,\mathrm{nm}, \\ L &= 20\,\mu\mathrm{m}, \\ \alpha &= 0.2 \\ \eta &= 1\,\mathrm{mPa\,s} \\ k_\mathrm{B}T &= 26\,\mathrm{meV} \\ \Delta U &= 80\,\mathrm{eV} \end{aligned}$$

as given in [1] to resemble the experimental setup from [3].

When the potential difference ΔU between U_{min} and U_{max} is small compared to the thermal energy of the particles in the ensemble ($\Delta U < k_B T$) the particle is 'free' and moves around solely due to Brownian motion, unaffected by the sawtooth potential. On the other hand, if the potential different is large compared to the thermal energy of the particle, ($\Delta U > k_\mathrm{B}\mathrm{T}$), the particle is trapped in the potential well. Figure 1 and 2 shows the trajectory of a single particle with the potential present but no flashing.

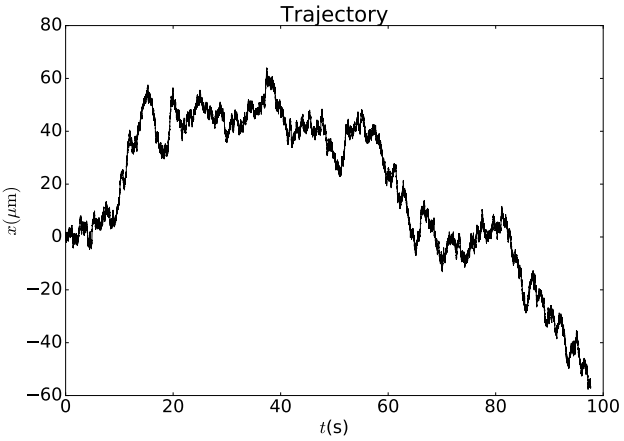

Figure 1: Single particle with $\Delta U = 0.1\,k_\mathrm{B}\mathrm{T}$. The particle is 'free'.

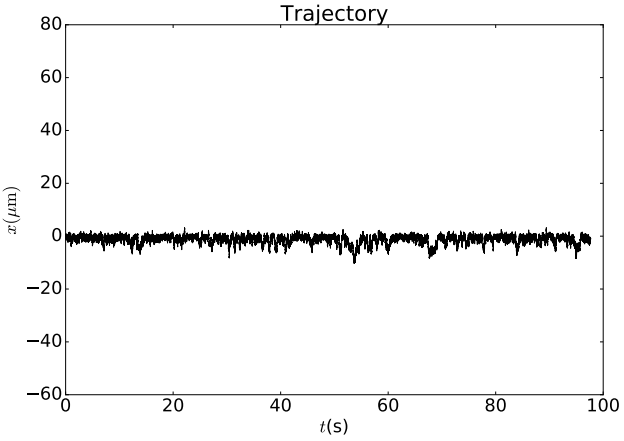

Figure 2: Single particle with $\Delta U = 10\,k_\mathrm{B}\mathrm{T}$. The particle is 'trapped'.

In thermal equilibrium, the distribution of occupied potential energies U is given by the Boltzmann distribution

$$p(U) = \frac{\exp\left(-\frac{U}{k_B T}\right)}{k_B T\left(1 - \exp\left(-\frac{U}{k_B T}\right)\right)} \tag{6}$$

where p is the probability density. Given eqn. (6), the probability density of visited potential for the two cases above is shown in figure 3 and 4.

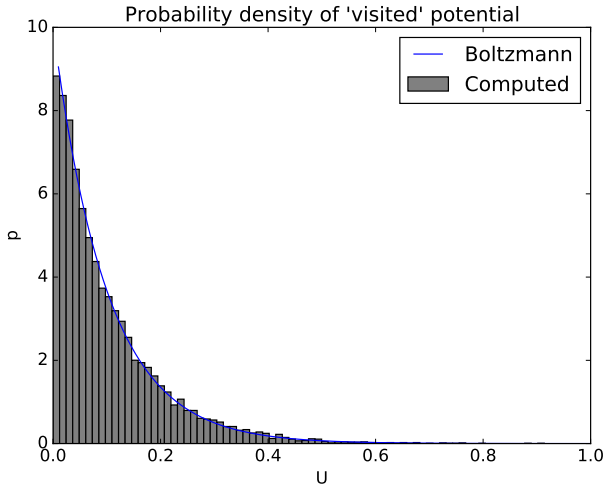

Figure 3: Probability density of visited potential with $\Delta U = 10\,k_{\mathrm{B}}\mathrm{T}$. Reduced units are used.

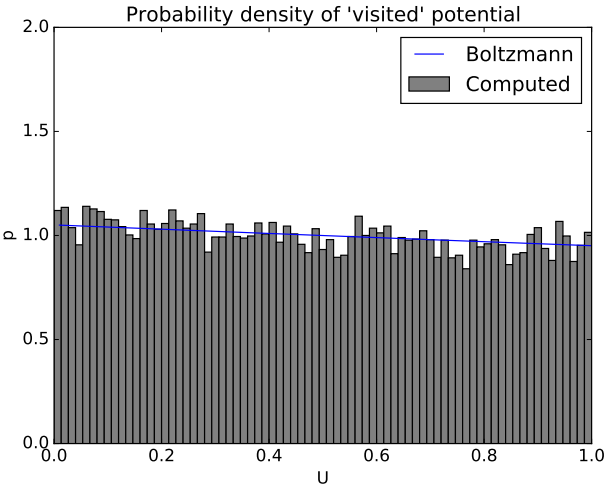

Figure 4: Probability density of visited potential with $\Delta U = 0.1\,k_{\mathrm{B}}\mathrm{T}$. Reduced units are used.

If the potential is turned off, the distribution of particles after some time t should follow the diffusion model. The solution to the diffusion equation in one dimension is

$$u(x,t) = \frac{1}{\sqrt{4\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right) \tag{7}$$

where u is the concentration of particles and D is the diffusivity defined as $D = \frac{k_{\mathrm{B}}T}{\gamma_i}$.

Figure 5 shows the actual distribution and the distribution calculated using eqn. (7).

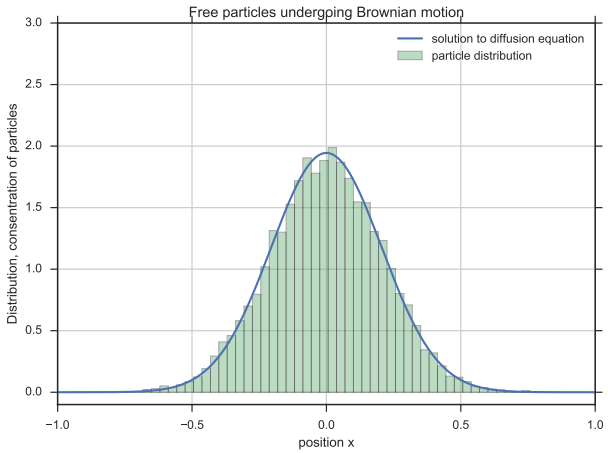

Figure 5: The distribution of particles after 0.45 s. 10000 particles. Reduced units are used.

3.2. Reproducing experimental result

By introducing a second particle with larger radius, $r_2 = 36\,\mathrm{nm}$, the average drift velocity as a function of the flashing period of the ratchet potential is calculated and is shown in 6.

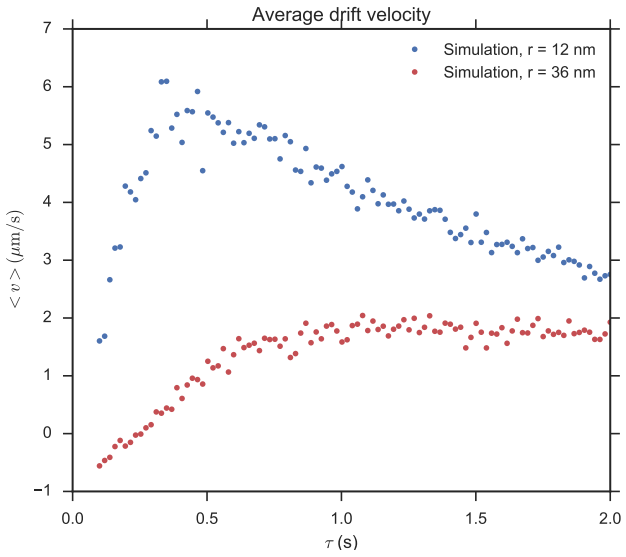

Figure 6: Average drift velocity as a function of flashing perod τ of the ratchet potential.

As seen in the figure above, different sized particles have different average drift velocities when exposed to the same ratchet potential. This would result in that different sized particles would become separated. The optimal flashing period τ_{op} (that results in highest average drift velocity) is $\tau_{op} \approx 0.5\,\mathrm{s}$ when $r = 12\,\mathrm{nm}$ and $\tau_{op} \approx 1.0\,\mathrm{s}$

when $r = 36\,\text{nm}$. The difference in average drift velocity is greatest when the flashing period of the ratchet potential is close to the optimal flashing period of the particles, and the separation would therefor be faster and easier around these optimal frequencies.

The flashing period of the potential is set to $\tau = 0.7$ as in [3]. The simulation was carried out with 1000 particles ($r = 12\,\text{nm}$) over a time period of 0, 10, and 20 cycles of the flashing potential. The distribution of particles is shown in figure 7, and the expected distribution from [3] is shown in figure 8

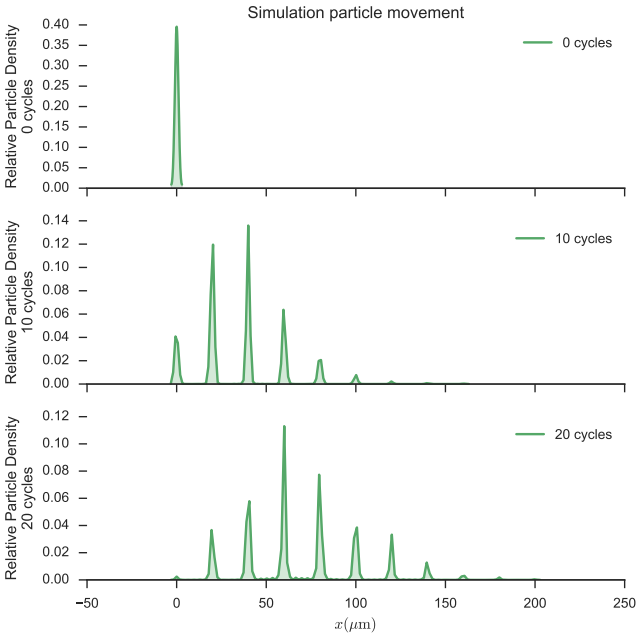

Figure 7: Particle distribution after 0, 10 and 20 cycles of the flashing potential. $\tau = 0.7\,\text{s}$. 1000 particles.

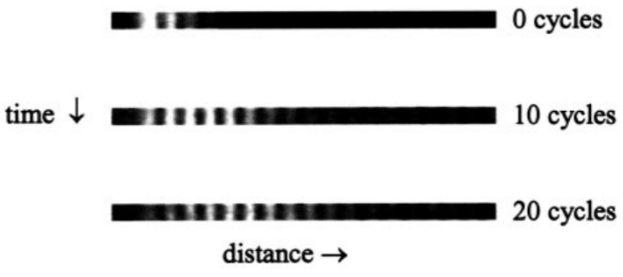

Figure 8: Expected distribution from experiment [3] after 0, 10 and 20 cycles.

The simulated distribution closely resembles the shape of the experimental results. When looking more closely at the 20 cycle simulation, figure 9 shows some of the particle trajectories.

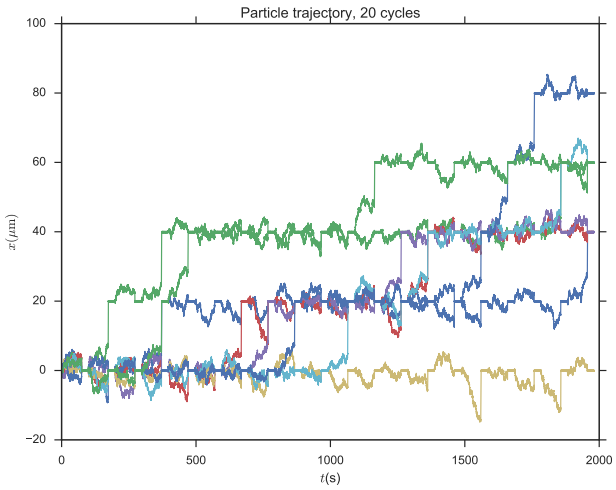

Figure 9: Particle trajectories. $\tau = 0.7\,\text{s}$. 8 out of 1000 particles are shown.

4. Conclusion

Dissolved particles of different size can be separated using a flashing ratchet potential. This exercise has numerically simulated the distribution of particles after being exposed to this kind of potential, as well as finding the optimal flashing period for maximum average drift velocity. The distribution of particles after they have been exposed to the ratchet potential seems to reproduce the results from the experiment done in [3].

References

[1] J-P. Banon, Biased Brownian Motion: An Application to Particle Separation, assignment in Computational Physics (TFY4235/FY8904), NTNU, Trondheim, Norway, 2016.

[2] R. Dean Astumian. Thermodynamics and Kinetics of Brownian Motor. *Science 9*, Vol. 256 no. 5314:917922, 1997.

[3] 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 of the United States of America*. 96(23):13165 – 13169, Nov. 9, 1999.