Biased brownian motion
Simulation of particles in flashing ratchet potential

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Abstract

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1 Introduction

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2 Theory

$$m_i \frac{\mathrm{d}^2 x_i}{\mathrm{d}t^2} = -\frac{\partial U}{\partial X}(x_i, t) - \gamma_i \frac{\mathrm{d}x_i}{\mathrm{d}t} + \xi(t), \tag{1}$$

$\gamma_i = 6\pi\eta r_i$ is a friction constant.

$$\gamma_i \frac{\mathrm{d}x_i}{\mathrm{d}t} = -\frac{\partial U}{\partial x}(x_i, t) + \xi(t) \tag{2}$$

Let

$$U(x,t) = U_r(x) f(t), \tag{3a}$$

$$U_r(x) = \begin{cases} \frac{x}{\alpha L}\Delta U & , 0 \le x < \alpha L \\ \frac{L-x}{L(1-\alpha)} & , \alpha L \le x < L \end{cases}, \quad f(t) = \begin{cases} 0 & , 0 \le t < \frac{3\tau}{4} \\ 1 & , \frac{3\tau}{4} \le t < \tau \end{cases}. \tag{3b}$$

We introduce the Euler scheme

$$x_{n+1} = x_n - \frac{1}{\gamma_i}\frac{\partial U}{\partial x}(x_n, t_n)\delta t + \sqrt{\frac{2k_B T \delta t}{\gamma_i}}\hat{\xi}_n. \tag{4}$$

Must choose

$$|x_{n+1} - x_n| \ll \alpha L$$

which by insertion into (4) yields

$$\frac{1}{\gamma_i} \max \left| \frac{\partial U}{\partial x} \right| \delta t + 4\sqrt{\frac{2 k_B T \delta t}{\gamma_i}} \ll \alpha L, \tag{5}$$

where we used the fact that $|\hat{\xi}_n| < 4$ with 99.99% probability.

The Boltzmann distribution is given as

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

Diffusion equation gives density of particles for given x and t

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

3 Method

Convert the Euler scheme (4) into a dimensionless system by introducing

$$\hat{x} = \frac{x}{L}, \quad \hat{t} = \omega t, \quad \omega = \frac{\Delta U}{\gamma_i L^2}, \quad \hat{U}(\hat{x}, \hat{t}) = \frac{U(x,t)}{\Delta U}, \quad \hat{D} = \frac{k_B T}{\Delta U}. \tag{8}$$

This gives the scheme

$$\hat{x}_{n+1} = \hat{x}_n - \frac{\partial \hat{U}}{\partial \hat{x}}(\hat{x}, \hat{t}) \delta \hat{t} + \sqrt{2 \hat{D} \delta \hat{t}} \hat{\xi}_n. \tag{9}$$

Will perform two tests for numerical validity: correspondence with the Boltzmann distrbution when the potential is turned on, and correspondence with the diffusion equation when the potential is turned off.

4 Results and discussion

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5 Conclusion

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