TFY4235 NTNU

Computational Physics Assignment I

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Todo list

Abstract

1 Introduction

If one wants to separate particles in a solution, there are several techniques one can use to obtain this. Here, considering a constituents of different mass and size, the particles will be separated by the use of a perodic asymmetric potential serving as a set of potential wells. By switching the potential on and off with a certain time period, one can bias the particles´brownian motion such that lighter and smaller particles are more likely to cross the potential barriers and jump to the neighboring wells than the larger and heavier ones. This is called to use a rachet potential

2 Modeling of The Problem

2.1 Theory

A small particle placed in a solution will be subject to random collisions with the solvent and constituent molecules. The force on the particle due to the collisions varies in both force and direction and causes the particle to move in an unregular and unpredictable pattern or *Brownian Motion*. In addition to the fluctuating force the particles are also subject to viscous drag, such that the extent of the particles erratic movement is decided by their mass and size/surface.

Now, consider two constituents of spherical particles with radius r_1, r_2 and masses m_1, m_2, respectively. The 1D equation of motion for particle i is given by Newton's 2$^{\text{nd}}$ law

$$m_i \frac{d^2x}{dt^2} = \underbrace{-\frac{\partial}{\partial x} U(x_i, t)}_{\text{potential force}} \underbrace{- \gamma_i \frac{dx_i}{dt}}_{\text{friction force}} + \xi(t), \tag{1}$$

where $\gamma_i = 6\pi\eta r_i$ is the friction constant, U is the potential energy and ξ is a stochastic variable modeling the particle's brownian motion. Furthermore, the potential is assumed to have the form of

$$U(x,t) = U_r(x) f(t), \tag{2}$$

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

whith $U_r(x)$ being the spatial part, having an asymmetric saw-tooth shape with periodicity L. The time dependency is described $f(t)$ which is a square wave signal, turning the potential on and off, with a period of τ. $\alpha \in [1, 0]$ is the asymmetry factor, giving how much the potential is skewed (with $\alpha = 0.5$ being the symmetric case).

The resulting iterative numerical scheme, based on the equations above, is a forward Euler given by

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

Choosing

$$\hat{x} = \frac{x}{L}, \qquad \hat{t} = \omega t, \qquad \hat{U}(\hat{x}, \hat{t}) = \frac{U(x,t)}{\Delta U}, \qquad \omega = \frac{\Delta U}{\gamma_i L^2}, \qquad \hat{D} = \frac{k_B T}{\Delta U} \tag{5}$$

such that

$$\begin{aligned} \frac{\partial}{\partial x} U(x,t) &= \frac{\partial}{\partial x}\big(\Delta U \cdot \hat{U}(\hat{x}, \hat{t})\big) \\ &= \Delta U \cdot \frac{\partial}{\partial x}\big(\hat{U}_r(\hat{x})\big)\hat{f}(\hat{t}) \\ &= \Delta U \cdot \frac{\partial \hat{U}_r(\hat{x})}{\partial \hat{x}}\frac{\partial \hat{x}}{\partial x}\hat{f}(\hat{t}) \\ &= \frac{\Delta U}{L} \cdot \frac{\partial}{\partial \hat{x}}\hat{U}_r(\hat{x}, \hat{t}) \end{aligned}$$

$\big($note that $f(t) = \hat{f}(\hat{t})\,\big)$, equation (4) can be rewritten in reduced units

$$\hat{x}_{n+1} = \hat{x}_n - \frac{\partial}{\partial \hat{x}} \hat{U}(\hat{x}_n, \hat{t}_n)\delta\hat{t} + \sqrt{2\hat{D}\delta\hat{t}}\,\hat{\xi}. \tag{6}$$

Box-Müller Algorithm

A gaussian probability distribution is used to model the particles brownian motion. The stochastic variable is obtained using the Box-Müller algorithm. Assuming mean $\mu = 0$ and unit standard deviation the 2D gaussian distribution can be expressed as

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$$p(x) = \frac{1}{2\pi} e^{-\frac{x^2+y^2}{2}} = \frac{1}{2\pi} e^{-\frac{r^2}{2}}$$

using cartesian coordinates. Since the distribution is radially symmetric, it is a good choice to use polar coordinates (r,ϕ), with $x = r\cos\theta$, $y = r\sin\theta$ and $\theta \in [0, 2\pi]$. Due to the radial symmetry θ is uniformly distributed on its interval and may be sampled using

$$\theta = 2\pi\xi_2.$$

The resulting distribution function as a function of r

$$\begin{aligned} P(r' \leq r) = P(r) &= \int_0^{2\pi} \int_0^r \frac{1}{2\pi} e^{-\frac{r'^2}{2}} r' dr' d\theta \\ &= \int_0^r e^{-\frac{r'^2}{2}} dr' \\ &= 1 - e^{-\frac{r^2}{2}}, \end{aligned}$$

which we can rewrite to

$$r = \sqrt{-2ln(1 - P(r))} = \sqrt{-2ln(1 - \xi')} = \sqrt{-2ln\xi_1}.$$

By choosing two independent uniformly distributed numbers, ξ_1,$\xi_2 \in U(0, 1)$, setting $P(r) = \xi_1$ and $\theta = 2\pi\xi_2$,

$$x = r\cos\theta = \sqrt{-2ln\xi_1}\cos(2\pi\xi_2) \tag{7a}$$

$$y = r\sin\theta = \sqrt{-2ln\xi_1}\sin(2\pi\xi_2). \tag{7b}$$

are two uncorrelated gaussian distributed numbers.

Time Step Size

99.99% of the time, the random number drawn from the gaussian distribution follows that $|\hat{\xi}| < 4$. Assuming $0 < \alpha < 1/2$, the shortest length of a constant force region is given by αL. To get a reasonable answer the iterations must satisfy

$$|x_{n+1} - x_n| \ll \alpha L. \tag{8}$$

By inserting the iteration scheme, Eq.(6), the expression can be rewritten

$$L|\hat{x}_{n+1} - \hat{x}_n| \ll \alpha L$$
$$\left| -\frac{\partial}{\partial \hat{x}} \hat{U}(\hat{x}_n, \hat{t}_n)\delta\hat{t} + \sqrt{2\hat{D}\delta\hat{t}}\,\hat{\xi}\,\right| \ll \alpha.$$

In the shortest region the particle experiences the largest force. Assuming that $|\hat{\xi}| < 4$ together with that the force and the kick act in the same direction, the criterion becomes

$$\max\left|\frac{\partial}{\partial \hat{x}} \hat{U}(\hat{x}_n, \hat{t}_n)\right|\delta\hat{t} + 4\sqrt{2\hat{D}\delta\hat{t}} \ll \alpha. \tag{9}$$

2.2 Implementation

3 Results

4 Discussion

5 References