Proton Dynamics in Cavities

Dominik Wille

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2 Brownian Dynamics

The motion of a particle such as a proton in a fluid is primarily caused by collisions with other particles. This motion firstly was described by ROBERT BROWN who observed the motion of minute particles of pollen in water and is widely known as **brownian motion**.

2.1 Langevin Symulation

2.1.1 Priciple

The principle of a Langevin simulation generally is to consider collisions with other particles as a random force. And propergate the position of a particle over small time steps δt.

2.1.2 Physical background

An approach to describe situations with brownian motion was suggested by PAUL LANGEVIN who added the random force $\mathbf{Z}(t)$ in newtons equation of motion. This stochastic term represents the collision driven force. His equation, the Langevin equation reads:

$$m\ddot{\mathbf{r}} = -\lambda\dot{\mathbf{r}} + \mathbf{Z}(t) \tag{1}$$

where m is the mass of the particle, $\mathbf{r}$ the position of the particle and λ The friction constant.

Brownian dynamics can be represented with the so called **overdamped langevin equation** where the $m\ddot{\mathbf{r}}$ term is neglected. The equation for the prevailing situation therefore is:

$$\lambda\dot{\mathbf{r}} = \mathbf{Z}(t) \tag{2}$$

In order to get an iterable expression this expression is discretesated in time intervals Δt:

$$\int_t^{t+\delta t} \dot{\mathbf{r}}(t')\,dt' = \int_t^{t+\Delta t} \frac{\mathbf{Z}(t')}{\lambda}\,dt' \tag{3}$$

$$\mathbf{r}(t+\delta t) - \mathbf{r}(t) = \frac{1}{\lambda}\int_t^{t+\Delta t} \mathbf{Z}(t)\,dt' \tag{4}$$

$$\mathbf{r}(t+\delta t) - \mathbf{r}(t) \cong \boldsymbol{\zeta}(t,\varepsilon) \tag{5}$$

In the discussed 1–dimensional case ε is the step size and $\boldsymbol{\zeta}(t,\varepsilon)$ will be ε or $-\varepsilon$ with a chance of 50% each.

The position of a particle at time $t+\Delta t$ can easily derived from its position at time t.

$$\mathbf{r}(t+\delta t) = \mathbf{r}(t) + \boldsymbol{\zeta}(t,\varepsilon) \tag{6}$$

2.2 Connection to diffusion

The motion which is performed in the langevin simulation is widely known as a **random walk**. The probability $p(x,n)$ that a random walk comes to a position x after n steps. Is given by:

$$p(x,n) = \frac{\text{Number of ways to position } x}{\text{Total number of ways}} = \frac{N_x}{N} \tag{7}$$

Since there are 2 possible successors for every position the total number of ways doubles every step.

$$N = 2^n \tag{8}$$

The number of ways to the position x after n steps can be obtained by **Pascal's triangle**.

$$N_x = \binom{n}{k} \tag{9}$$

$$\text{with}\quad k = \frac{1}{2}\left(\frac{x}{\varepsilon} + n\right) \tag{10}$$

Therefore $p(x,n)$ follows as:

Step/Position	-3ε	-2ε	-1ε	0	ε	2ε	3ε
0				1			
1			1		1		
2		1		2		1	
3	1		3		3		1

Figure 1: Number of ways to different distances

$$p(x,n) = \binom{n}{k} \cdot 2^{-n} \tag{11}$$

A consequence of the **de Moivre–Laplace theorem** is that for large numbers of steps ($n \to \infty$) this expression can be approximated with the following gaussian curve:

$$p(x,n) \cong \sqrt{\frac{2}{n\pi}} \exp\left(\frac{-x^2}{2\varepsilon^2 n}\right) \tag{12}$$

The probability function $p(x,n)$ has valid values only for values

$$x \in \{x \mid x = z \cdot 2\varepsilon + \varepsilon\,(n \bmod 2),\ z \in \mathbb{Z} \land |x| \leq n\varepsilon\} \tag{13}$$

For other values x the probability is 0. This means that there is only one value per 2ϵ interval, therefore the probability density function $\rho(x,n)$ is:

$$\rho(x,n) = \frac{1}{2\varepsilon}\, p(x,n) = \frac{1}{\varepsilon\sqrt{2\pi n}} \exp\left(\frac{-x^2}{2\varepsilon^2 n}\right) \tag{14}$$

The probability density function of a **random walk** fulfills the diffusion equation (*Note:* $n = {}^{t}/_{\delta t}$):

$$\frac{\partial}{\partial t}\rho(x,t) = D\frac{\partial^2}{\partial x^2}\rho(x,t) \tag{15}$$

$$\text{with} \quad D = \frac{\varepsilon^2}{2\delta t} \tag{16}$$

What means that a random walk can also be seen as a diffusion process.

2.3 Mean square distance

Obviously the expectation value after n steps $\langle x_n \rangle = 0$. What can be derived from:

$$\langle x_n \rangle = \int_{-\infty}^{\infty} x \cdot \rho(x,t) \; dx = 0 \tag{17}$$

But the **mean square distance** (MSD) is:

$$\langle x_n^2 \rangle = \int_{-\infty}^{\infty} x^2 \cdot \rho(x,t) \; dx = 2Dt \tag{18}$$