Proton Dynamics in Cavities

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1 Introduction

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 Simulation

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:

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

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

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

Where ε is the mean step distance and $\boldsymbol{\zeta}(t,\varepsilon)$ random vector with mean norm ε. Both will be discussed later on.

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

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

3 Conclusion

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