Aalto University

Errata

Hanne Antila
Simulations of Polyelectrolyte Interactions in Salt
School of Chemical Technology
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Chapter 3.3, page 45, equation 3.22

A factor of ½ is missing from the last row of the algorithm. It correctly reads:

$$\begin{aligned} \boldsymbol{v}_n(t+\frac{1}{2}\Delta t) &= \boldsymbol{v}_n(t-\frac{1}{2}\Delta t) + \frac{\Delta t}{m}\boldsymbol{F}_n(t) \\ \boldsymbol{r}_n(t+\Delta t) &= \boldsymbol{r}_n(t) + \Delta t \boldsymbol{v}_n(t+\frac{1}{2}\Delta t) \\ \boldsymbol{v}_n(t) &= \frac{1}{2}\left(\boldsymbol{v}_n(t+\frac{1}{2}\Delta t) + \boldsymbol{v}_n(t-\frac{1}{2}\Delta t)\right), \end{aligned} \tag{3.22}$$

Chapter 3.4., page 50

The Monte Carlo algorithm should read:

This is realized by setting the transition probability from state m to state n equal to 1 if the move is downhill in energy ($U_n - U_m = \Delta U_{nm} < 0$). If the move is uphill in energy ($\Delta U_{nm} > 0$), the move is accepted with a probability $W_{m\to n}$ defined by the ratio of probabilities of the initial and final states

$$W_{m\to n} = \frac{P(\boldsymbol{r}_n^N)}{P(\boldsymbol{r}_m^N)} = e^{-\beta(U_n - U_m)}. \tag{3.27}$$

A simple implementation of Metropolis Monte Carlo algorithm reads

1. Select a particle at random, and calculate energy of the initial configuration U_m
2. Give the particle a random displacement, $r' = r + \Delta$, and calculate the energy of the trial configuration U_n.
3. Accept or reject the move:
   (a) if $\Delta U_{nm} < 0$, accept configuration n.
   (b) if $\Delta U_{nm} > 0$, calculate $W_{n\to m} = e^{-\beta(U_n - U_m)}$ by drawing a random number $RAND$ from uniform distribution between 0 and 1 and accepting n if $W_{m\to n} > RAND$. Otherwise, reject the trial configuration and stay at m.
4. Repeat.