Errata

Hanne Antila
Simulations of Polyelectrolyte Interactions in Salt
School of Chemical Technology
Aalto University publication series DOCTORAL DISSERTATIONS 21/2016
Date of Errata: 23.03.2016

Chapter 3.3, page 45, equation 3.22

A factor of $\frac{1}{2}$ is missing from the last row of the algorithm. It correctly reads:

$$v_n(t + \frac{1}{2} \Delta t) = v_n(t - \frac{1}{2} \Delta t) + \frac{\Delta t}{m} F_n(t)$$

$$r_n(t + \Delta t) = r_n(t) + \Delta t v_n(t + \frac{1}{2} \Delta t)$$

$$v_n(t) = \frac{1}{2} \left( v_n(t + \frac{1}{2} \Delta t) + v_n(t - \frac{1}{2} \Delta t) \right)$$

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

\[
W_{m\to n} = \frac{P(r^N_m)}{P(r^N_n)} = e^{-\beta(U_n - U_m)}. \tag{3.27}
\]

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.