

A temperature calculator for replica exchange molecular dynamics simulations - Corrections

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Corrections to the equations in this paper are explained in bold font.

The average probability of exchange over the entire simulation $\langle P \rangle$ can be related to the energy distributions, U_1 and U_2 :

$$\begin{aligned}\langle P(T_1 \leftrightarrow T_2) \rangle &= \int_{-\infty}^{\infty} P(T_1 \leftrightarrow T_2) \rho_{U_2-U_1}(u) du \\ &= \int_{-\infty}^0 \rho_{U_2-U_1}(u) du + \int_0^{\infty} e^{-Cu} \rho_{U_2-U_1}(u) du\end{aligned}\quad (6)$$

where $\rho_{U_2-U_1}(u)$ is the probability of having a certain energy difference $U_2 - U_1$. **Note that a minus sign was missing in e^{-Cu} .**

The integral of $\rho_{U_2-U_1}(u)$ can then be written

$$\int_{-\infty}^u \rho_{U_2-U_1}(u') du' = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{u - \mu_{12}}{\sigma_{12}\sqrt{2}} \right) \right] \quad (7)$$

(**note that a prime ' was inserted in the integration variable**) which after insertion into Eqn. 6 yields:

$$\begin{aligned}\langle P(T_1 \leftrightarrow T_2) \rangle &= \frac{1}{2} \left[1 + \operatorname{erf} \left(-\frac{\mu_{12}}{\sigma_{12}\sqrt{2}} \right) \right] + \\ &\quad \frac{1}{2} e^{\left(C\mu_{12} + \frac{C^2\sigma_{12}^2}{2} \right)} \left[1 + \operatorname{erf} \left(\frac{\mu_{12} + C\sigma_{12}^2}{\sigma_{12}\sqrt{2}} \right) \right]\end{aligned}\quad (8)$$

The second half of the equation involves a product of a very large number and a very small number. Due to the lack of an in-built error function in the PHP programming language the integral is evaluated numerically.