A temperature calculator for replica exchange molecular dynamics simulations - Corrections

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Corrections to the equations in ref. [1] 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:

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

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

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

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

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

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.

The code underlying the webserver is now available at `https://github.com/dspoel/remd`.

References

[1] A. Patriksson, D. van der Spoel, A temperature predictor for parallel tempering simulations, Phys. Chem. Chem. Phys. 10 (2008) 2073–2077.