# ERRATA

## Erratum: "Constant pressure hybrid Molecular Dynamics–Monte Carlo simulations" [J. Chem. Phys 116, 55 (2002)]

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In the original paper the description of the reversible weak coupling algorithm had two deficiencies which lead to a slight violation of detailed balance if the algorithm is implemented as described. A correct description is given below.

In order to preserve time-reversal symmetry only $n-1$ scaling moves should be performed between $n$ molecular dynamics steps. The constant pressure MD can be disassembled into a rescaling move and a $NVT$ MD time step. A hybrid move now starts with a $NVT$ MD step, followed by $n-1$ rescaling and $NVT$ MD pairs. This point was omitted in the original paper.

There was a misprint in the actual rescaling formula [Eq. (9)] which should read

$$V_n = V_o\left(1+\tau_p^{-1}\Delta t\frac{p-p^*}{p^*}\right), \tag{9}$$

where $p^*$ is the target pressure, $p$ is the measured pressure, and $V_n$ and $V_o$ are the new and old volumes, respectively. The additional 1 was missing in the original paper.

In order to ensure reversibility the range from which target pressures $p^*$ are drawn must be sufficiently large. This stems from the fact that if the forward and backward scaling moves are performed according to Eq. (9), the resulting pressure (at $V_n$) cannot in general be predicted from the pressure at $V_o$; the range on $p^*$ ensures that the corresponding scaling factor for the reverse move can be obtained.

In certain cases where the relationship between the pressure of the system in volume $V_o$ and volume $V_n$ can be calculated analytically, e.g., if the compressibility is constant or analytically known, an analytical correction for the backward pressure can be implemented and selection from a range is not required. Note, however, that in this case the target pressures for forward and backward moves would be different.

The simulations in the original contribution used a sufficiently large pressure range, and the discussion and consequences of the paper remain unchanged.

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