

Errata to “Molecular dynamics and the accuracy of numerically computed averages”

Stephen D. Bond
Department of Computer Science,
University of Illinois,
Urbana, IL 61801-2302, USA

Benedict J. Leimkuhler
School of Mathematics,
University of Edinburgh,
Edinburgh EH9 3JZ, UK

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This errata applies to the printed version of “Molecular dynamics and the accuracy of numerically computed averages”, appearing in *Acta Numerica* (2007), volume 16, pages 1–65.

- On page 37, line 22 should read

$$\frac{\bar{D}\bar{\rho}_h}{\bar{D}t} + \bar{\rho}_h \nabla_z \cdot \bar{f} = 0,$$

where $\bar{D}/\bar{D}t$ denotes the total derivative with respect to the modified vector field, \bar{f} .

- On page 37, line 24 should read

$$\omega \left(\frac{D\rho}{Dt} + \rho \nabla_z \cdot f \right) + \rho \left(\frac{\bar{D}\omega}{\bar{D}t} + h^s \omega \nabla_z \cdot g \right) + h^s \omega g \cdot \nabla_z \rho = 0.$$

- On page 37, line 27 should read

$$\frac{\bar{D}\omega}{\bar{D}t} + h^s \omega (\nabla_z \cdot g + g \cdot \nabla_z \ln \rho) = 0.$$

- On page 37, equation 3.1 on line 29 should read

$$\bar{\rho}_h = \frac{1}{C} \rho \omega = \frac{1}{C} \rho \exp \left[-h^s \int (\nabla_z \cdot g + g \cdot \nabla_z \ln \rho) dt \right],$$

where the time integral is along the flow of the modified vector field.

- On page 39, equation 3.8 on line 12 should read

$$\bar{\rho}_{2,h}^{\text{NHE}} \propto \rho_{\text{NH}} \exp \left[-h^2 \int (\nabla \cdot f_{[2]} + f_{[2]} \cdot \nabla \ln \rho_{\text{NH}}) dt \right],$$

where the time integral is along the flow of the modified vector field.

- On page 40, the fourth line from the bottom should read

$$\bar{\rho} = \frac{1}{C} \int \int_{p_s \eta} e^{(N_f+1)\eta} \delta \left[e^\eta \left(H(q, p) + \frac{p_s^2}{2\mu} + g k_B T \eta + h^2 G(q, e^\eta, p, p_s) - H_N^0 \right) \right] dp_s d\eta,$$

- On page 46, line 18 should read

$$\lim_{S \rightarrow \infty} \frac{1}{S} \int_0^S f_N(w_N(t)) dt = \frac{1}{C_N} \int f_N(w) e^{-\frac{1}{kT} H(w; N)} dw,$$

where C_N is a normalizing constant.