Computer Simulation of Liquids
Michael P. Allen and Dominic J. Tildesley

Second edition, Oxford University Press, 2017
List of errata up to March 21, 2023

Line numbers below do not include section headings, equations, figures etc.
Negative line numbers are counted up from the bottom of the page.

Chapter 1

p11 ℓ −16 'It quite possible' → 'It is quite possible'.

p14 In eqn (1.15) the signs of the odd-order terms are wrong:

$$+T_\alpha \rightarrow -T_\alpha \qquad \text{and} \qquad +\tfrac{1}{3}T_{\alpha\beta\gamma} \rightarrow -\tfrac{1}{3}T_{\alpha\beta\gamma}.$$

p15 In eqn (1.20), $T_{\alpha\beta} \rightarrow T_{\alpha\beta}^{ab}$. In eqn (1.21), $A_{\alpha\beta} \rightarrow A_{\alpha\beta}^{ab}$.

p17 In eqn (1.22), $B_{\alpha\beta} \rightarrow B_{\alpha\beta}^{ab}$, $T_{\alpha\beta} \rightarrow T_{\alpha\beta}^{ab}$, $(\alpha^a)^{-1} \rightarrow (\alpha^a)_{\alpha\beta}^{-1}$.
In eqn (1.23) and ℓ 15, $\tilde{T}_{\alpha\beta} \rightarrow \tilde{T}_{\alpha\beta}^{ab}$. Also in this equation the factor $4\pi\epsilon_0$ should be omitted for consistency with eqn (1.17).

p35 ℓ 11, 'see Chapter 13' → 'see Chapter 14'.

p36 ℓ 7, $v(r) \sim r^3 \rightarrow v(r) \sim r^{-3}$.
ℓ 8, 'Chapter 5' → 'Chapter 6'.

p42 ℓ 3 Remove sentence 'Some of these methods … Appendix A.'

Chapter 2

p55 In eqn (2.35), $N_n \rightarrow N_c$; in eqns (2.35), (2.36) and ℓ −4, $\mu_n \rightarrow \mu_c$.

p66 ℓ 19, $k_B T/V\beta_T \rightarrow k_B T/V\beta_S$.

p67 ℓ 2, '(eqn (2.82))' → '(eqn (2.62))'.
ℓ 8, between eqns (2.85) and (2.86), 'viral' → 'virial'.

Chapter 3

p116 All the masses in eqns (3.49ab) should be raised to the power -1:

$$\mathbf{r}_{12}(t + \delta t) = \mathbf{r}'_{12}(t + \delta t) + \left(m_1^{-1} + m_2^{-1}\right)\lambda_{12}^{(r)}\mathbf{r}_{12}(t) - m_2^{-1}\lambda_{23}^{(r)}\mathbf{r}_{23}(t)$$

$$\mathbf{r}_{23}(t + \delta t) = \mathbf{r}'_{23}(t + \delta t) - m_2^{-1}\lambda_{12}^{(r)}\mathbf{r}_{12}(t) + \left(m_2^{-1} + m_3^{-1}\right)\lambda_{23}^{(r)}\mathbf{r}_{23}(t).$$

The same correction should be applied to eqns (3.53ab); in addition, all the bond vectors in eqns (3.53ab) should be evaluated at $t + \delta t$:

$$\mathbf{v}_{12}(t + \delta t) = \mathbf{v}'_{12}(t + \delta t) + \left(m_1^{-1} + m_2^{-1}\right)\lambda_{12}^{(v)}\mathbf{r}_{12}(t + \delta t) - m_2^{-1}\lambda_{23}^{(v)}\mathbf{r}_{23}(t + \delta t)$$

$$\mathbf{v}_{23}(t + \delta t) = \mathbf{v}'_{23}(t + \delta t) - m_2^{-1}\lambda_{12}^{(v)}\mathbf{r}_{12}(t + \delta t) + \left(m_2^{-1} + m_3^{-1}\right)\lambda_{23}^{(v)}\mathbf{r}_{23}(t + \delta t)$$

p120 ℓ 14 'eqn (2.161)' $\to$ 'eqn (2.167)'.

p131 ℓ 19, the sentence should read: 'It is relatively straightforward to combine it with constraint algorithms (Ryckaert and Ciccotti, 1986); see, however, Peters et al. (2014).'

p139 ℓ -3, the last 3 sentences of section 3.8, beginning with 'Also...', should be replaced by: 'Also, the distribution is not canonical (it may tend to isokinetic as $\tau \to 0$ and microcanonical as $\tau \to \infty$ (Morishita, 2000)). Recently it has been shown that these equations of motion do not preserve *any* distribution (Petersen and Searles, 2022). The Berendsen thermostat is quite widely used, but in view of the risk of generating incorrect results (see e.g. Braun et al., 2018), alternatives are to be preferred.'

p141 In the equation at the top of the page the sign of $\mathbf{r} \cdot \mathbf{f}$ is wrong, and a factor $1/dV$ was omitted from the correction term:

$$\mathcal{P}' = \mathcal{P} + (1/gV)\mathbf{p} \cdot \mathbf{p}/m = \frac{1}{dV}\left(\alpha\mathbf{p} \cdot \mathbf{p}/m + \mathbf{r} \cdot \mathbf{f}\right) - \frac{\partial V}{\partial V}.$$

p142 The expression for iL'_2 should have a factor of d:

$$iL'_2 = d(\mathcal{P}' - P)V\frac{\partial}{\partial p_\varepsilon}.$$

p145 In the equations, $T_{\alpha\beta} \to T_{\alpha\beta}^{ab}$ and $\left|\mathbf{p}_{\mu a}\right|^2/m_{\mu a} \to \left|\mathbf{p}_{\mu a}\right|^2/2m_{\mu a}$.

Chapter 4

J Mikhail
2018-05-30

p162 In the second part of eqn (4.34), defining the terms $\mathcal{V}_m^{(12)}$ and $\mathcal{V}_m^{(6)}$, the negative sign is wrong: $-\mathcal{V}_m^{(6)} \rightarrow +\mathcal{V}_m^{(6)}$, giving

$$\mathcal{V}_m = 4\epsilon \sum_i \sum_{j>i} \left(\frac{\sigma}{L_m s_{ij}^m}\right)^{12} - 4\epsilon \sum_i \sum_{j>i} \left(\frac{\sigma}{L_m s_{ij}^m}\right)^6$$
$$= \mathcal{V}_m^{(12)} + \mathcal{V}_m^{(6)}.$$

Chapter 6

MPA
2019-08-15

p218 ℓ −4 '(see Fig. 5.6(b))' $\rightarrow$ '(see Fig. 6.2(b))'.

MPA
2019-08-16

p222 Equation (6.16) has the wrong sign:

$$(\mathbf{f}_{ij})_\alpha = q_i \widehat{T}_{\alpha\beta}\mu_{j\beta} - q_j \widehat{T}_{\alpha\beta}\mu_{i\beta}.$$

MPA
2017-04-19

p229 ℓ 8 'charges densities' $\rightarrow$ 'charge densities'.

snafumeander
2019-01-24

Also, in eqn (6.43) there is a superfluous right parenthesis in the denominator, should be

$$b(k_x) = \frac{\exp\big(i(P-1)k_x\ell\big)}{\sum_{q=0}^{P-2} \exp(ik_x\ell q)M_P(q+1)}.$$

J Dürholt
2018-04-13

p251 In eqn (6.106) the factor V should be $1/V$:

$$\mathcal{V}_{\text{correction}}^{qq} = \frac{2\pi}{V}\left(\sum_i q_i z_i\right)^2$$

Chapter 9

B Vorselaars
2023-02-11

p323 ℓ 5 The sentence beginning 'Smc' should read 'Asymptotically, the rejection rate of both smc, and fb with $\lambda = \frac{1}{2}$, approaches zero, proportional to the third power of the typical step size (see section 12.3 and e.g. Gupta et al., 1990; Vorselaars, 2023).'

MPA
2019-08-15

p333 ℓ 14 '(see Section 4.5)' $\rightarrow$ '(see Section 4.4)',
ℓ −2 '(eqn (4.41))' $\rightarrow$ '(eqn (4.42))'.

MPA
2019-08-17

p337 ℓ 21 'liquid-vapour' $\rightarrow$ 'liquid–vapour'.

Chapter 10

MPA
2017-03-07

p344 In eqn (10.2b) $\int_{r\in A} \rightarrow \int_{r\in B}$.

Chapter 11

p360 ℓ −7 'eqn (2.153)' → 'eqn (2.159)'.

p362 ℓ 6 'Fig. 9.4' → 'Fig. 1.15(b)'.

p379 ℓ −16 'Chapter 9' → 'Chapter 3'.

Chapter 12

p388 ℓ −5 Before the sentence starting 'A sample…', insert 'Typically, the rejection rate for a single-step HMC move is proportional to δt^3 at small δt (Gupta et al., 1990).'.

Chapter 13

p420 ℓ −5 'described by eqn (1.36)' → 'described by eqn (1.20)'.

p443 ℓ −12 'described in Section 13.4' → 'described in Section 13.2'.

p444 ℓ 9 'described in Section 13.4' → 'described in Section 13.2'.

Appendix D

p502 ℓ −5 'eqns (D.1a) and (D.2b)' → 'eqns (D.1a) and (D.1b)'.

p505 ℓ −5 'integral of eqn (D.14a)' → 'integral of eqn (D.14b)'.

Appendix E

p510 ℓ 12 '…generating $X_i = 1$, but allows the possibility of $X_i = 0$;' → '…generating $\xi_i = 1$, but allows the possibility of $\xi_i = 0$;'.

Bibliography (additional items)

Braun, E., Moosavi, S. M., and Smit, B. (2018). Anomalous effects of velocity rescaling algorithms: the flying ice cube effect revisited. *J. Chem. Theor. Comput.* **14**, 5262–5272.

Gupta, S., Irbäc, A., Karsch, F., and Petersson, B. (1990). The acceptance probability in the hybrid Monte Carlo method. *Phys. Lett. B* **242**, 437–443.

Peters, E. A. J. F., Goga, N., and Berendsen, H. J. C. (2014). Stochastic dynamics with correct sampling for constrained systems. *J. Chem. Theor. Comput.* **10**, 4208–4220.

Petersen, C. F. and Searles, D. J. (2022). Equilibrium distribution functions: connection with microscopic dynamics. *Phys. Chem. Chem. Phys.* **24**, 6383–6392.

Vorselaars, B. (2023). Efficient Langevin and Monte Carlo sampling algorithms: the case of field-theoretic simulations. *J. Chem. Phys.* **158**, 114117.