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

Second edition, Oxford University Press, 2017
List of errata up to August 10, 2019

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), $T_{\alpha\beta} \rightarrow T^{ab}_{\alpha\beta}$. In eqn (1.21), $A_{\alpha\beta} \rightarrow A^{ab}_{\alpha\beta}$.

p17 In eqn (1.22), $B_{\alpha\beta} \rightarrow B^{ab}_{\alpha\beta}$, $T_{\alpha\beta} \rightarrow T^{ab}_{\alpha\beta}$, $(\alpha^a)^{-1} \rightarrow (\alpha^a)^{-1}_{\alpha\beta}$.
In eqn (1.23) and ℓ 15, $\tilde{T}_{\alpha\beta} \rightarrow \tilde{T}^{ab}_{\alpha\beta}$. 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 8 'Chapter 5' → 'Chapter 6'.

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

Chapter 2

p66 ℓ 19, $k_\mathrm{B}T/V\beta_T \rightarrow k_\mathrm{B}T/V\beta_S$.

p67 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:

$$\mathbf{r}_{12}(t+\delta t) = \mathbf{r}'_{12}(t+\delta t) + \left(m_1^{-1} + m_2^{-1}\right)\lambda^{(\mathrm{r})}_{12}\mathbf{r}_{12}(t) - m_2^{-1}\lambda^{(\mathrm{r})}_{23}\mathbf{r}_{23}(t)$$
$$\mathbf{r}_{23}(t+\delta t) = \mathbf{r}'_{23}(t+\delta t) - m_2^{-1}\lambda^{(\mathrm{r})}_{12}\mathbf{r}_{12}(t) + \left(m_2^{-1} + m_3^{-1}\right)\lambda^{(\mathrm{r})}_{23}\mathbf{r}_{23}(t).$$

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

$$\mathbf{v}_{12}(t+\delta t) = \mathbf{v}'_{12}(t+\delta t) + \left(m_1^{-1} + m_2^{-1}\right)\lambda^{(\mathrm{v})}_{12}\mathbf{r}_{12}(t+\delta t) - m_2^{-1}\lambda^{(\mathrm{v})}_{23}\mathbf{r}_{23}(t+\delta t)$$
$$\mathbf{v}_{23}(t+\delta t) = \mathbf{v}'_{23}(t+\delta t) - m_2^{-1}\lambda^{(\mathrm{v})}_{12}\mathbf{r}_{12}(t+\delta t) + \left(m_2^{-1} + m_3^{-1}\right)\lambda^{(\mathrm{v})}_{23}\mathbf{r}_{23}(t+\delta t)$$

p141 In the equation at the top of the page the sign of $\mathbf{r} \cdot \mathbf{f}$ is wrong:

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

p142 The expression for iL_2' should have a factor of d:

$$iL_2' = d(\mathcal{P}' - P)V\frac{\partial}{\partial p_\varepsilon}.$$

Chapter 4

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: $-\mathcal{V}_m^{(6)} \to +\mathcal{V}_m^{(6)}$, 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

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

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

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

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 10

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

Chapter 11

p362 ℓ 6 'Fig. 9.4' $\to$ 'Fig. 1.15(b)'.

p379 ℓ −16 'Chapter 9' $\to$ 'Chapter 3'.

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'.