Computer Simulation of Liquids
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Second edition, Oxford University Press, 2017
List of errata up to August 11, 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

F Perez 2017-10-07

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

MPA 2017-04-04

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

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

MPA 2019-08-09

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

MPA 2019-08-09

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).

MPA 2019-07-30

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

MPA 2019-07-30

p36 ℓ 8 'Chapter 5' → 'Chapter 6'.

MPA 2019-07-30

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

Chapter 2

MPA 2019-08-11

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

MPA & Y Yang 2019-07-22

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

MPA 2019-07-18

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

Chapter 3

A Fleury 2018-08-02

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: MPA 2017-04-30

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

p142 The expression for $\mathrm{i}L_2'$ should have a factor of d: MPA 2017-04-30

$$\mathrm{i}L_2' = d(\mathcal{P}' - P)V\frac{\partial}{\partial p_\varepsilon}.$$

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 J Mikhail 2018-05-30

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

Chapter 6

p229 ℓ 8 'charges densities' → 'charge densities'. MPA 2017-04-19

Also, in eqn (6.43) there is a superfluous right parenthesis in the denominator, should be snafumeander 2019-01-24

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

p251 In eqn (6.106) the factor V should be $1/V$: J Dürholt 2018-04-13

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

Chapter 10

p344 In eqn (10.2b) $\displaystyle\int_{\mathbf{r}\in\mathrm{A}} \to \int_{\mathbf{r}\in\mathrm{B}}$. MPA 2017-03-07

Chapter 11

p362 ℓ 6 'Fig. 9.4' → 'Fig. 1.15(b)'. MPA 2019-07-30

p379 ℓ −16 'Chapter 9' → 'Chapter 3'. MPA 2019-07-30

Chapter 13

p420 ℓ −5 ‘described by eqn (1.36)’ → ‘described by eqn (1.20)’. MPA 2019-08-10

p443 ℓ −12 ‘described in Section 13.4’ → ‘described in Section 13.2’. MPA 2019-08-01

p444 ℓ 9 ‘described in Section 13.4’ → ‘described in Section 13.2’. MPA 2019-08-01