

Computer Simulation of Liquids

Michael P. Allen and Dominic J. Tildesley

Second edition, Oxford University Press, 2017

List of errata up to August 17, 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’ \rightarrow ‘It is quite possible’.

F Perez
2017-10-07
MPA
2017-04-04

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

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

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

MPA
2019-08-09
MPA
2019-08-09

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).

MPA
2019-07-30
MPA
2019-07-30
MPA
2019-07-30

p35 ℓ 11 ‘see Chapter 13’ \rightarrow ‘see Chapter 14’.

p36 ℓ 8 ‘Chapter 5’ \rightarrow ‘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, $\mu_n \rightarrow \mu_c$.

MPA
2019-08-11
MPA & Y Yang
2019-07-22

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

p67 ℓ 2, ‘(eqn (2.82))’ \rightarrow ‘(eqn (2.62))’.

ℓ 8, between eqns (2.85) and (2.86), ‘viral’ \rightarrow ‘virial’.

MPA
2019-08-13
MPA
2019-07-18

Chapter 3

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

A Fleury
2018-08-02

$$\begin{aligned}\mathbf{r}_{12}(t + \delta t) &= \mathbf{r}'_{12}(t + \delta t) + (m_1^{-1} + m_2^{-1})\lambda_{12}^{(r)}\mathbf{r}_{12}(t) - m_2^{-1}\lambda_{23}^{(r)}\mathbf{r}_{23}(t) \\ \mathbf{r}_{23}(t + \delta t) &= \mathbf{r}'_{23}(t + \delta t) - m_2^{-1}\lambda_{12}^{(r)}\mathbf{r}_{12}(t) + (m_2^{-1} + m_3^{-1})\lambda_{23}^{(r)}\mathbf{r}_{23}(t).\end{aligned}$$

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

$$\begin{aligned}\mathbf{v}_{12}(t + \delta t) &= \mathbf{v}'_{12}(t + \delta t) + (m_1^{-1} + m_2^{-1})\lambda_{12}^{(v)}\mathbf{r}_{12}(t + \delta t) - m_2^{-1}\lambda_{23}^{(v)}\mathbf{r}_{23}(t + \delta t) \\ \mathbf{v}_{23}(t + \delta t) &= \mathbf{v}'_{23}(t + \delta t) - m_2^{-1}\lambda_{12}^{(v)}\mathbf{r}_{12}(t + \delta t) + (m_2^{-1} + m_3^{-1})\lambda_{23}^{(v)}\mathbf{r}_{23}(t + \delta t)\end{aligned}$$

p120 ℓ 14 ‘eqn (2.161)’ \rightarrow ‘eqn (2.167)’.

MPA
2019-08-13

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

MPA
2017-04-30

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

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

MPA
2017-04-30

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

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

MPA
2019-08-14

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

p218 $\ell - 4$ ‘(see Fig. 5.6(b))’ \rightarrow ‘(see Fig. 6.2(b))’.

p222 Equation (6.16) has the wrong sign:

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

p229 $\ell 8$ ‘charges densities’ \rightarrow ‘charge densities’.

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

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

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 9

p333 $\ell 14$ ‘(see Section 4.5)’ \rightarrow ‘(see Section 4.4)’,
 $\ell - 2$ ‘(eqn (4.41))’ \rightarrow ‘(eqn (4.42))’.

p337 $\ell 21$ ‘liquid-vapour’ \rightarrow ‘liquid–vapour’.

Chapter 10

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

Chapter 11

p360 $\ell - 7$ ‘eqn (2.153)’ \rightarrow ‘eqn (2.159)’.

p362 $\ell 6$ ‘Fig. 9.4’ \rightarrow ‘Fig. 1.15(b)’.

p379 $\ell - 16$ ‘Chapter 9’ \rightarrow ‘Chapter 3’.

Chapter 13

p420 $\ell - 5$ ‘described by eqn (1.36)’ \rightarrow ‘described by eqn (1.20)’.

p443 $\ell - 12$ ‘described in Section 13.4’ \rightarrow ‘described in Section 13.2’.

p444 $\ell 9$ ‘described in Section 13.4’ \rightarrow ‘described in Section 13.2’.

MPA
2019-08-15
MPA
2019-08-16

MPA
2017-04-19
snafumeander
2019-01-24

J Dürholt
2018-04-13

MPA
2019-08-15
MPA
2019-08-17

MPA
2017-03-07

MPA
2019-08-13
MPA
2019-07-30
MPA
2019-07-30

MPA
2019-08-10
MPA
2019-08-01
MPA
2019-08-01