Computer Simulation of Liquids
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List of errata up to March 20, 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'. — F Perez 2017-10-07

p14 In eqn (1.15) the signs of the odd-order terms are wrong: — MPA 2017-04-04

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

p15 In eqn (1.20), $T_{\alpha\beta} \rightarrow T^{ab}_{\alpha\beta}$. In eqn (1.21), $A_{\alpha\beta} \rightarrow A^{ab}_{\alpha\beta}$. — MPA 2019-08-09

p17 In eqn (1.22), $B_{\alpha\beta} \rightarrow B^{ab}_{\alpha\beta}$, $T_{\alpha\beta} \rightarrow T^{ab}_{\alpha\beta}$, $(\alpha^a)^{-1} \rightarrow (\alpha^a)^{-1}_{\alpha\beta}$. — MPA 2019-08-09
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'. — MPA 2019-07-30

p36 ℓ 7, $v(r) \sim r^3 \rightarrow v(r) \sim r^{-3}$. — Bian Li 2022-04-02
ℓ 8, 'Chapter 5' → 'Chapter 6'. — MPA 2019-07-30

p42 ℓ 3 Remove sentence 'Some of these methods … Appendix A.' — MPA 2019-07-30

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

p66 ℓ 19, $k_\mathrm{B}T/V\beta_T \rightarrow k_\mathrm{B}T/V\beta_S$. — MPA & Y Yang 2019-07-22

p67 ℓ 2, '(eqn (2.82))' → '(eqn (2.62))'. — MPA 2019-08-13
ℓ 8, between eqns (2.85) and (2.86), 'viral' → 'virial'. — MPA 2019-07-18

Chapter 3

A Fleury 2018-08-02

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

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

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

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

MPA 2019-08-13

p120 ℓ 14 'eqn (2.161)' → 'eqn (2.167)'.

MPA 2023-02-11

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).'

MPA 2017-04-30 2019-08-21

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:

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

MPA 2017-04-30

p142 The expression for $\mathrm{i}L'_2$ should have a factor of d:

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

MPA 2019-08-14

p145 In the equations, $T_{\alpha\beta} \to T^{ab}_{\alpha\beta}$ 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: $-\mathcal{V}_m^{(6)} \to +\mathcal{V}_m^{(6)}$, giving

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

Chapter 6

p218 ℓ −4 '(see Fig. 5.6(b))' → '(see Fig. 6.2(b))'. MPA 2019-08-15

p222 Equation (6.16) has the wrong sign: MPA 2019-08-16

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

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

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

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

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

Chapter 9

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).' B Vorselaars 2023-02-11

p333 ℓ 14 '(see Section 4.5)' → '(see Section 4.4)', MPA 2019-08-15
ℓ −2 '(eqn (4.41))' → '(eqn (4.42))'.

p337 ℓ 21 'liquid-vapour' → 'liquid–vapour'. MPA 2019-08-17

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

p360 ℓ −7 'eqn (2.153)' → 'eqn (2.159)'. MPA 2019-08-13

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 12

B Vorselaars 2023-02-11

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

MPA 2019-08-10

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

MPA 2019-08-01

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'.

Appendix D

MPA 2019-08-19

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

MPA 2019-08-19

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

Appendix E

J Mikhail 2021-09-30

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)

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.

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