Computer Simulation of Liquids
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List of errata up to January 24, 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 $\ell\,-16$ 'It quite possible' $\longrightarrow$ '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

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

Chapter 3

p116 All the masses in eqns (3.49ab) should be raised to the power -1: A Fleury 2018-08-02

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

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

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

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 $\ell 8$ 'charges densities' $\to$ '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) $\int_{\mathbf{r}\in\mathrm{A}} \to \int_{\mathbf{r}\in\mathrm{B}}$. MPA 2017-03-07