Errata

1. In the derivation of the tree algorithm scaling starting on p. 20, the inner shell radius r_1 is defined as the radius beyond which particles can be grouped together in clusters. This can begin as soon as the inter-cluster distance θr_1 exceeds the mean particle separation a, i.e.:

$$\theta r_1 > a = n^{-1/3}$$

2. On p. 27, the initial expression for the potential in Cartesian coordinates should read:

$$\Phi_i(\mathbf{R} - \mathbf{r}_i) \quad = \quad -\frac{m_i}{\sqrt{(x-x_i)^2 + (y-y_i)^2 + (z-z_i)^2}}.$$

3. Equation (2.11) for the quadrupole moment of the parent cell on p. 30 should read:

$$\begin{aligned} Q_{xy}^{parent} &= \sum_d \left(\sum_i m_i x_i y_i - x_{sd} \sum_i m_i y_i \right. \\ &\qquad \left. - y_{sd} \sum_i m_i x_i + x_{sd} y_{sd} \sum_i m_i \right) \\ &= \sum_d \left(Q_{xy}^d - x_{sd} D_y^d - y_{sd} D_x^d + x_{sd} y_{sd} M^d \right). \end{aligned}$$

4. The Ewald summation for the potential (5.2) on p. 93 is missing the 'self-energy' correction $\Phi_s = -2\alpha q_i/\pi^{1/2}$. This is needed to cancel an identical, unphysical term contained in the k-space sum Φ_{II}. The latter is also missing a normalisation factor $|\mathbf{h}|^{-\mathbf{2}}$, so that the net potential should actually read:

$$\begin{aligned} \Phi_p &= \Phi_I + \Phi_{II} + \Phi_s \\ &= \sum_{\mathbf{n}} \sum_i q_i \frac{\mathrm{erfc}(\alpha r_{\mathbf{n}i})}{r_{\mathbf{n}i}} \\ &\quad + \frac{1}{\pi L} \sum_i \sum_{\mathbf{h} \neq 0} \frac{q_i}{|\mathbf{h}|^{\mathbf{2}}} \exp\left(\frac{-\pi^2 |\mathbf{h}|^2}{\alpha^2 L^2} \right) \cos\left(\mathbf{k} \cdot \mathbf{r}_{oi} \right) - \frac{2\alpha}{\pi^{1/2}} q_i, \end{aligned}$$

where $\mathbf{k} = 2\pi \mathbf{h}/L$.

5. As for the potential above, a factor $|\mathbf{h}|^{-\mathbf{2}}$ is missing from the k-space force term F_x^{II} on p. 94, which should read:

$$F_x^{II} \;=\; \frac{2}{L^2}\sum_i \sum_{\mathbf{h}\neq 0} \frac{q_i h_x}{|\mathbf{h}|^2} \exp\left(\frac{-\pi^2|\mathbf{h}|^2}{\alpha^2 L^2}\right) \sin\left(\mathbf{k}\cdot\mathbf{r}_{os}\right).$$

6. In the multipole expansion of the Ewald sum (5.5) the term $A(h)$ on p. 98 is also missing this factor, and should read:

$$A(h) = \frac{1}{|\mathbf{h}|^{\mathbf{2}}} \exp\left(\frac{-\pi^2|\mathbf{h}|^2}{\alpha^2 L^2}\right).$$

7. The shifting formulae on p. 99 should correspond to those on p. 30 and p. 31, namely:

$$\sum_i q_i x_i \quad\rightarrow\quad \sum_i q_i x_i - x_{sd}\sum_i q_i$$

$$\sum_i q_i x_i^2 \quad\rightarrow\quad \sum_i q_i x_i^2 - 2x_{sd}\sum_i q_i x_i + x_{sd}^2\sum_i q_i$$

$$\sum_i q_i x_i y_i \quad\rightarrow\quad \sum_i q_i x_i y_i - x_{sd}\sum_i q_i y_i - y_{sd}\sum_i q_i x_i + x_{sd}y_{sd}\sum_i q_i$$

8. The plasma frequency in (6.2) is normally referred to by the angular frequency ω_p, rather than the inverse period $\nu_p \equiv \tau_p^{-1}$, and is defined (in c.g.s. units) by:

$$\omega_p = \left(\frac{4\pi n_e e^2}{m_e}\right)^{1/2}.$$