$$k \approx 8 \tag{0.1}$$
$$k = 3.9 \tag{0.2}$$
$$\gamma \tag{0.3}$$
$$\alpha \tag{0.4}$$
$$\alpha \tag{0.5}$$
$$\alpha \tag{0.6}$$
$$\gamma \tag{0.7}$$
$$\alpha \tag{0.8}$$
$$\gamma \tag{0.9}$$
$$\alpha \tag{0.10}$$
$$\alpha \tag{0.11}$$
$$\alpha \tag{0.12}$$
$$E_{\mathrm{A}} \tag{0.13}$$
$$p_{\mathrm{partial}} \tag{0.14}$$
$$\tau \tag{0.15}$$
$$A_S^D \tag{0.16}$$
$$t_{\mathrm{relax}} \tag{0.17}$$
$$t = 59 \tag{0.18}$$
$$t = 65 \tag{0.19}$$
$$t = 75 \tag{0.20}$$
$$t = 85 \tag{0.21}$$
$$t = 95 \tag{0.22}$$
$$t = 100 \tag{0.23}$$
$$n \tag{0.24}$$
$$1 \tag{0.25}$$
$$1 \tag{0.26}$$
$$1 \tag{0.27}$$
$$n \tag{0.28}$$
$$n \tag{0.29}$$
$$n \tag{0.30}$$

$$n \tag{0.31}$$

$$n \log n \tag{0.32}$$

$$n \tag{0.33}$$

$$n \tag{0.34}$$

$$n \tag{0.35}$$

$$n \tag{0.36}$$

$$1 \tag{0.37}$$

$$n \tag{0.38}$$

$$\frac{r_c^3}{s^3} n^2 \tag{0.39}$$

$$n \tag{0.40}$$

$$1 \tag{0.41}$$

$$1 \tag{0.42}$$

$$1 \tag{0.43}$$

$$r_s^3 \tag{0.44}$$

$$r_s^3 \tag{0.45}$$

$$c \tag{0.46}$$

$$n + c \tag{0.47}$$

$$n \log c \tag{0.48}$$

$$\log c \tag{0.49}$$

$$\log c \tag{0.50}$$

$$1 \tag{0.51}$$

$$r_s^3 \log c \tag{0.52}$$

$$r_s^3 \log c \tag{0.53}$$

$$\log c \tag{0.54}$$

$$n + c^{\frac{2}{3}} \tag{0.55}$$

$$n \log n \tag{0.56}$$

$$\log n \tag{0.57}$$

$$\log n \tag{0.58}$$

$$\log n \tag{0.59}$$

$$r_s^3 \log n \tag{0.60}$$

$$r_s^3 \log n \tag{0.61}$$

$$\log n \tag{0.62}$$

$$n \tag{0.63}$$

$$n \log n \tag{0.64}$$

$$k \log k \tag{0.65}$$

$$k \log k \tag{0.66}$$

$$k \log k \tag{0.67}$$

$$r_s^3 + n^{\frac{1}{3}} \tag{0.68}$$

$$r_s^3 \tag{0.69}$$

$$1 \tag{0.70}$$

$$nk \tag{0.71}$$

$$n \tag{0.72}$$

$$1 \tag{0.73}$$

$$1 \tag{0.74}$$

$$1 \tag{0.75}$$

$$n \tag{0.76}$$

$$n \tag{0.77}$$

$$n \tag{0.78}$$

$$n \tag{0.79}$$

$$n \tag{0.80}$$

$$k \tag{0.81}$$

$$b \tag{0.82}$$

$$k_r \tag{0.83}$$

$$d \leq r_c \tag{0.84}$$

$$r_c \tag{0.85}$$

$$r_s \tag{0.86}$$

$$s \tag{0.87}$$

$$k \tag{0.88}$$

$$k \tag{0.89}$$

$$k \tag{0.90}$$

$$k + 1 \tag{0.91}$$

$$atoms \tag{0.92}$$

$$size[3] \tag{0.93}$$

$$depth \tag{0.94}$$

$$atoms, spacesize, depth \tag{0.95}$$

$$cellsize[0] \leftarrow spacesize[0] \cdot 2^{-depth} \tag{0.96}$$

$$cellsize[1] \leftarrow spacesize[1] \cdot 2^{-depth} \tag{0.97}$$

$$cellsize[2] \leftarrow spacesize[2] \cdot 2^{-depth} \tag{0.98}$$

$$root \leftarrow \tag{0.99}$$

$$depth \tag{0.100}$$

$$atom \tag{0.101}$$

$$atoms \tag{0.102}$$

$$cellindex[0] \leftarrow \lfloor atom.pos[0]/cellsize[0] \rfloor \tag{0.103}$$

$$cellindex[1] \leftarrow \lfloor atom.pos[1]/cellsize[1] \rfloor \tag{0.104}$$

$$cellindex[2] \leftarrow \lfloor atom.pos[2]/cellsize[2] \rfloor \tag{0.105}$$

$$cell \leftarrow \tag{0.106}$$

$$root, cellindex \tag{0.107}$$

$$root \tag{0.108}$$

$$root \tag{0.109}$$

$$i[3] \tag{0.110}$$

$$allocate \tag{0.111}$$

$$cell, id, allocate \tag{0.112}$$

$$d \leftarrow \tag{0.113}$$

$$d = 0 \tag{0.114}$$

$$cell.children \tag{0.115}$$

$$cell.children \leftarrow \tag{0.116}$$

$$childid \leftarrow \tag{0.117}$$

$$2^{d-1} \tag{0.118}$$

$$2 \cdot \tag{0.119}$$

$$2^{d-1} \tag{0.120}$$

$$4\cdot \tag{0.121}$$

$$2^{d-1} \tag{0.122}$$

$$cell.children[childid], i, allocate \tag{0.123}$$

$$= \tag{0.124}$$

$$N \tag{0.125}$$

$$points \tag{0.126}$$

$$k \tag{0.127}$$

$$points, dim \leftarrow 0 \tag{0.128}$$

$$n \leftarrow \tag{0.129}$$

$$n = 0 \tag{0.130}$$

$$points, dim \tag{0.131}$$

$$points \tag{0.132}$$

$$dim \tag{0.133}$$

$$root \leftarrow points\left[\lfloor\frac{n}{2}\rfloor\right] \tag{0.134}$$

$$dim \leftarrow (dim + 1) \mod k \tag{0.135}$$

$$root.left \leftarrow \tag{0.136}$$

$$points\left[0 : \lfloor\frac{n}{2}\rfloor - 1\right], dim \tag{0.137}$$

$$root.right \leftarrow \tag{0.138}$$

$$points\left[\lfloor\frac{n}{2}\rfloor + 1 : n - 1\right], dim \tag{0.139}$$

$$root \tag{0.140}$$

$$\subset \tag{0.141}$$

$$\Leftrightarrow \tag{0.142}$$

$$\subset \tag{0.143}$$

$$\Rightarrow \tag{0.144}$$

$$k_d \tag{0.145}$$

$$_0 \tag{0.146}$$

$$_0 \in \tag{0.147}$$

$$\neq \emptyset \tag{0.148}$$

$$\in \tag{0.149}$$

$$\setminus \tag{0.150}$$

$$\in \tag{0.151}$$

$$\cap \tag{0.152}$$

$$\cap \tag{0.153}$$

$$\setminus \tag{0.154}$$

$$\alpha \tag{0.155}$$

$$r_d > \alpha^{-1} \tag{0.156}$$

$$r_d > \alpha^{-1} \tag{0.157}$$

$$\alpha \tag{0.158}$$

$$\alpha = 0 \tag{0.159}$$

$$\alpha < 0 \tag{0.160}$$

$$r_d > \alpha \tag{0.161}$$

$$r_d < \alpha \tag{0.162}$$

$$r_d < \alpha \tag{0.163}$$

$$\sim t \tag{0.164}$$

$$\sim t \tag{0.165}$$

$$\sim n_{\text{cyc.}} \tag{0.166}$$

$$\vec{F}(X) \tag{0.167}$$

$$V(X) \tag{0.168}$$

$$V(r_i j) \tag{0.169}$$

$$r_{\text{cut}} \tag{0.170}$$

$$\vec{F}_{ij}(r_{ij}) = \vec{\nabla} V(r_{ij}) \tag{0.171}$$

$$E = \sum_i \sum_{j \neq i} V(r_{ij}) \tag{0.172}$$

$$V_{\text{LJ}}(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right] \tag{0.173}$$

$$E = \sum_i \sum_{j \neq i} V_2\left(r_{ij}\right) + \sum_i \sum_{j \neq i} \sum_{i \neq k \neq j} V_3\left(r_{ij}, r_{ik}, \theta_{ijk}\right) + \ldots \tag{0.174}$$

$$V_{\alpha\beta}(r_{ij}) \tag{0.175}$$

$$i \tag{0.176}$$

$$F_\alpha \tag{0.177}$$

$$\rho_\beta(r_{ij}) \tag{0.178}$$

$$\alpha \tag{0.179}$$

$$\beta \tag{0.180}$$

$$E = \sum_i \left[F_\alpha \left(\sum_{j \neq i} \rho_\beta \left(r_{ij} \right) \right) + \frac{1}{2} \sum_{j \neq i} V_{\alpha\beta} \left(r_{ij} \right) \right] \tag{0.181}$$

$$E = \sum_i \left[F_\alpha \left(\bar{\rho}_i \right) + \frac{1}{2} \sum_{j \neq i} V_{ij} \left(r_{ij} \right) \right] \tag{0.182}$$

$$\sigma \tag{0.183}$$

$$\pi \tag{0.184}$$

$$\pi \tag{0.185}$$

$$\begin{aligned} E_{\text{system}} = \;& E_{\text{bond}} + E_{\text{lp}} + E_{\text{over}} + E_{\text{under}} + E_{\text{val}} + E_{\text{pen}} + E_{\text{coa}} + E_{\text{C2}} \\ & + E_{\text{tors}} + E_{\text{conj}} + E_{\text{H-bond}} + E_{\text{vdWaals}} + E_{\text{Coulomb}} \end{aligned} \tag{0.186}$$

$$E_{\text{bond}} \tag{0.187}$$

$$E_{\text{lp}} \tag{0.188}$$

$$E_{\text{over}} \tag{0.189}$$

$$E_{\text{under}} \tag{0.190}$$

$$\pi \tag{0.191}$$

$$E_{\text{val}} \tag{0.192}$$

$$E_{\text{pen}} \tag{0.193}$$

$$E_{\text{coa}} \tag{0.194}$$

$$_2 \tag{0.195}$$

$$E_{\text{C2}} \tag{0.196}$$

$$_2 \tag{0.197}$$

$$E_{\text{tors}} \tag{0.198}$$

$$E_{\text{conj}} \tag{0.199}$$

$$E_{\text{H-bond}} \tag{0.200}$$

$$E_{\text{vdWaals}} \tag{0.201}$$

$$E_{\text{Coulomb}} \tag{0.202}$$

$$t_{\text{relax}} \tag{0.203}$$

$$\tau \tag{0.204}$$

$$t_{\mathrm{relax}} \tag{0.205}$$

$$\tau \tag{0.206}$$

$$t_{\mathrm{relax}} = 50\,\mathrm{ps} \tag{0.207}$$

$$\tau = 0.02\,\mathrm{fs} \tag{0.208}$$

$$\Downarrow \tag{0.209}$$

$$\sigma_z = 1.2\,\text{Å} \tag{0.210}$$

$$\sigma_z = 6.4\,\text{Å} \tag{0.211}$$

$$\sigma_z = 8.0\,\text{Å} \tag{0.212}$$

$$\hat{=} \tag{0.213}$$

$$X_0 \tag{0.214}$$

$$\mathbb{X} \tag{0.215}$$

$$t_0 = 0 \tag{0.216}$$

$$X_n \in \mathbb{X} \tag{0.217}$$

$$E_i \tag{0.218}$$

$$X_{n-1} \tag{0.219}$$

$$X_n^i \tag{0.220}$$

$$E_i : X_{n-1} \to X_n^i \in \mathbb{X} \quad , \quad i \in [1, N] \tag{0.221}$$

$$E_i \tag{0.222}$$

$$r_i \tag{0.223}$$

$$R_i \tag{0.224}$$

$$R_N \tag{0.225}$$

$$r_i = r(E_i) \tag{0.226}$$

$$R_i = \sum_{j \leq i} r_j \tag{0.227}$$

$$u \tag{0.228}$$

$$X_n^i \tag{0.229}$$

$$X_n \tag{0.230}$$

$$N = 0 \tag{0.231}$$

$$R_N = 0 \tag{0.232}$$

$$X_n = X_n^i : R_{i-1} \leq u R_N < R_i \quad , \quad u \in [0, 1) \text{ gleichverteilt} \tag{0.233}$$

$$t_n = t_{n-1} + \frac{-\ln(u')}{R_N} \quad , \quad u' \in [0,1) \text{ gleichverteilt} \tag{0.234}$$

$$X_{n+1} \tag{0.235}$$

$$N = 0 \tag{0.236}$$

$$R_N = 0 \tag{0.237}$$

$$t_n > t_{\text{fin}} \tag{0.238}$$

$$E_i \tag{0.239}$$

$$X_n \tag{0.240}$$

$$X_n^i \tag{0.241}$$

$$\alpha \tag{0.242}$$

$$\tau_p \tag{0.243}$$

$$R \tag{0.244}$$

$$R \tag{0.245}$$

$$m \tag{0.246}$$

$$\vec{r} \tag{0.247}$$

$$\vec{p} \tag{0.248}$$

$$\vec{F}(R) \tag{0.249}$$

$$N \tag{0.250}$$

$$V \tag{0.251}$$

$$E \tag{0.252}$$

$$N = \text{const.} \qquad V = \text{const.} \qquad E = \text{const.} \tag{0.253}$$

$$i \tag{0.254}$$

$$\dot{\vec{r_i}} = \frac{\vec{p_i}}{m_i} \tag{0.255}$$

$$\dot{\vec{p_i}} = m\vec{a}_i = \vec{F}_i(R) \tag{0.256}$$

$$T \tag{0.257}$$

$$N = \text{const.} \qquad V = \text{const.} \qquad T = \text{const.} \tag{0.258}$$

$$T_{\text{Ziel}} \tag{0.259}$$

$$\overline{E_{kin}} = \frac{1}{2}\overline{mv^2} = \frac{d}{2}k_B T \tag{0.260}$$

$$T_{\text{Ziel}} \tag{0.261}$$

$$\tau \tag{0.262}$$

$$\vec{v}_i' = \vec{v}_i \cdot \sqrt{1 + \frac{\Delta t}{\tau}\left(\frac{T_{\text{Ziel}}}{T} - 1\right)} \tag{0.263}$$

$$s \tag{0.264}$$

$$\dot{\vec{p}_i} = \vec{F}_i - s\vec{p}_i \tag{0.265}$$

$$s \tag{0.266}$$

$$\tau \tag{0.267}$$

$$M \tag{0.268}$$

$$M \tag{0.269}$$

$$\tau \tag{0.270}$$

$$\dot{s} = \frac{1}{\tau M}\left(\sum_i \frac{p_i^2}{2m_i} - Ndk_B T\right) \tag{0.271}$$

$$N = \text{const.} \qquad p = \text{const.} \qquad T = \text{const.} \tag{0.272}$$

$$PV = Nk_B T + \frac{1}{d}\sum_{i=1}^{N} \vec{r}_i \cdot \vec{F}_i \tag{0.273}$$

$$\vec{X}_0 \tag{0.274}$$

$$\nabla E(X) \tag{0.275}$$

$$\alpha \tag{0.276}$$

$$\Rightarrow \tag{0.277}$$

$$\Rightarrow \tag{0.278}$$

$$\vec{X}_i = \vec{X}_{i-1} - \alpha \nabla E(\vec{X}_{i-1}) \tag{0.279}$$

$$\left|\vec{X}_i - \vec{X}_{i-1}\right| < X_{\text{tol}} \tag{0.280}$$

$$\max_k |X_{i,k} - X_{i-1,k}| < X_{\text{tol}} \tag{0.281}$$

$$\left|\nabla E(\vec{X}_{i-1})\right| < E_{\text{tol}} \tag{0.282}$$

$$i > i_{\text{tol}} \tag{0.283}$$

$$\min_\alpha f(X_i + \alpha \vec{s}_i) \to \alpha_i \tag{0.284}$$

$$\vec{X}_i = \vec{X}_{i-1} - \alpha_i \vec{s}_i \tag{0.285}$$

$$\tag{0.286}$$

$$\vec{s}_i = \Delta \vec{X}_i + \beta_i \vec{s}_{i-1} \tag{0.287}$$

$$\beta_i = \max\left(0, \frac{\Delta\vec{X}_i \cdot \left(\Delta\vec{X}_i - \Delta\vec{X}_{i-1}\right)}{\Delta\vec{X}_{i-1} \cdot \Delta\vec{X}_{i-1}}\right) \text{ (Polak-Ribire)} \tag{0.288}$$

$$Id \tag{0.289}$$

$$_2 \tag{0.290}$$

$$\tag{0.291}$$