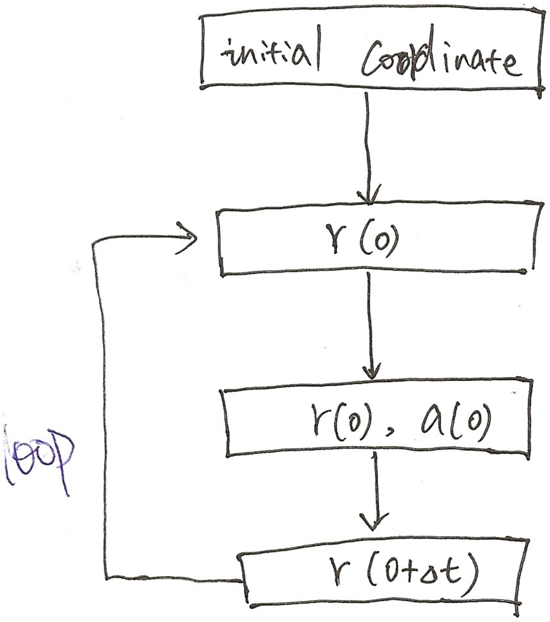
☆. Coordinate:



$\Leftarrow a_i = \frac{F_i}{m_i}$

$\Leftarrow r(t+\Delta t) = 2r(t) - r(t-\Delta t) + a(t)\Delta t^2$

※ when $t=0$, $r(t) = r(t-\Delta t)$

☆ minimum image convention:

If $dx > \frac{1}{2}L \Rightarrow dx = dx - L$

$dy > \frac{1}{2}L \Rightarrow dy = dy - L$

$dz > \frac{1}{2}L \Rightarrow dz = dz - L$

☆ velocity,

$$V_i(t+\Delta t) = V_i(t) + \frac{1}{2}\left[\frac{F_i(t)}{m_i} + \frac{F_i(t+\Delta t)}{m_i}\right]\Delta t$$

~~or:~~ $\cancel{v(t) = \frac{\quad}{2\Delta t}}$

System:

- 512 molecules
- $\varepsilon = 1$ kJ/mol, $\sigma = 0.3$ nm
- $V = 4 \times 4 \times 4$ nm (cube)
- $\Delta t = 2$ fs $\rightarrow$ (0.002 ps)
- $N_{steps} = 50{,}000$
- $T_{total} = 100$ ps
- $R_{cut\,off} = 1.5$ nm
- $m = 10.0$ amu (1 amu $= 1.66053892 \times 10^{-27}$ kg)

Calculate: ① potential, ② kinetic, ③ total energy.

④ total temperature.

☆: write these out every 50 steps

Solution:

Initial potential energy $= 290.4$ kJ/mol

Average total energy (should remain constant during the simulation) $= 292$ kJ/mol

Average temperature $= 170$ K

☆ Potential energy:

$$U = \sum_{i=1}^{N-1} \sum_{j>i}^{N} U_{ij}$$

$$U_{ij} = 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6} \right]$$

$$r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$$

☆ Kinetic energy:

$$E_k = \frac{1}{2} \sum m_i V_i^2$$

(m_i is constant for everyone ← 10.0 amu)

$$V(t) = \frac{r(t+\Delta t) - r(t-\Delta t)}{2\Delta t}$$

☆ Temperature:

$$T = \frac{\sum_i m_i V_i^2}{(3N-3)\, k_B}$$

$k_B = 1.3806488 \times 10^{-23}$ J/K

$N = 6.02214129 \times 10^{23}$ mol^{-1}

☆ Force Calculation

direction

X-Component: $F_{ij(x)} = \frac{24\varepsilon}{r^2} \cdot \left[2 \cdot \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \cdot x_{ij}$

Y-Component: $F_{ij(y)} =$ - - - - - - - $\cdot\, y_{ij}$

Z-Component: $F_{ij(z)} =$ - - - - - - - $\cdot\, z_{ij}$

$$F_{ij} = \sqrt{F_{ij(x)}^2 + F_{ij(y)}^2 + F_{ij(z)}^2}$$

$$\vec{F}_i = \sum_{j \neq i}^{N} \vec{F}_{ij}$$

energy

$\sum_i \frac{1}{2} m_i V_i^2$ kinetic energy

V_i

potential energy $\sum_i \sum_{j>i} V_{ij}$

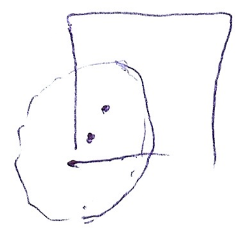
neighbor lists

$$\vec{F}_i \Leftarrow \sum_{j \neq 1} \left(- \frac{\partial V(r)}{\partial r} \Big|_{r=r_{ij}} \right) \cdot \frac{r_{ij}}{r}$$

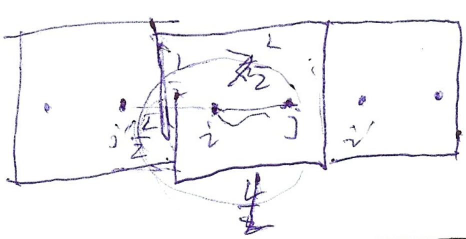
$$x\text{-component}_i \vec{F}_i = \sum_{j \neq i} \left(- \frac{\partial V(r)}{\partial r} \right) \cdot \frac{x_{ij}}{r_{ij}}$$

$$y \quad \vec{F}_{iy} = \sum_{j \neq i} \left(- \frac{\partial V(r)}{\partial r} \right) \cdot \frac{y_{ij}}{r_{ij}}$$

eg.



$$z \quad F_{iz} = \sum_{j \neq i} \left(- \frac{\partial V(r)}{\partial r} \right) \cdot \frac{z_{ij}}{r_{ij}}.$$



Set the initial conditions $r_i(t_0)$, $V_i(t_0)$, ……