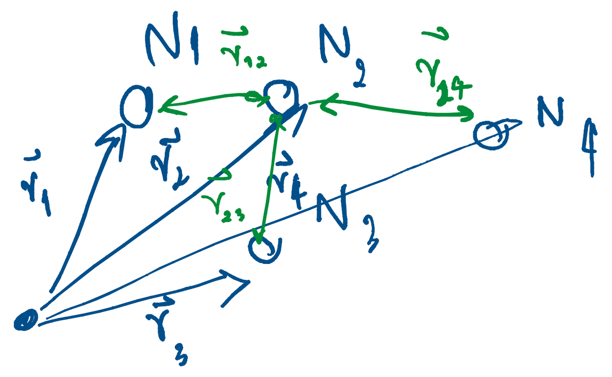
MD

Tuesday, November 3, 2020 11:07 AM



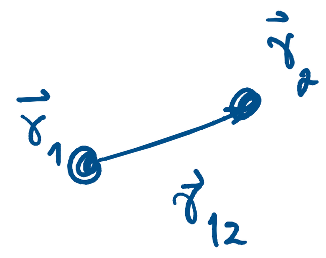
update → dt

$\{\vec{r}(t)_i\}$ $i \in [1, N]$
$\{\vec{v}(t)_i\}$ $i \in [1, N]$

→

$$U_{ij} = \frac{1}{4\pi\varepsilon} \frac{q_i q_j}{\vec{r}_{ij}}$$

$$U_{tot} = \sum_{i>j} U_{ij}$$



↓

$$\vec{F}_{j\to i} = -\Delta U_{ij}$$

$$\vec{F}_i = \sum_{i \neq j} \vec{F}_{j \to i}$$

←

$$\vec{a}(t)_i = \frac{\vec{F}_i}{m_i}$$

↑ Numerical integration

$\boxed{\text{Energy}}$

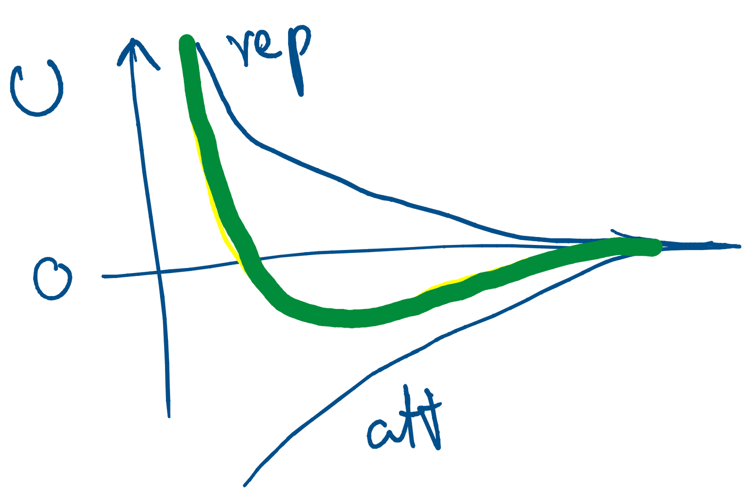
1) Coulomb $\quad U_{ij} = \frac{1}{4\pi\varepsilon_0} \frac{q_i q_j}{\vec{r}_{12}}$ ↗ Attraction ↘ Repulsive

2) vdW $\quad U_{vdw} = \frac{-A}{r^6}$ $\quad$ Attraction - Cohesive

dipole-dipole interaction

$\vec{r} \to \infty$ $\quad$ 3) Electronic

$$U = \frac{-A}{r^{12}}$$



velocity-verlet scheme → No velocity in calculation

$$\vec{r}(t+dt) = \vec{r}(t) + \frac{d\vec{r}(t)}{dt} \cdot dt + \frac{1}{2}\frac{d^2\vec{r}(t)}{dt^2} dt^2 + \ldots \quad -①$$

Taylor expansion

$$\vec{r}(t-dt) = \vec{r}(t) - \frac{d\vec{r}(t)}{dt} \cdot dt + \frac{1}{2}\frac{d^2\vec{r}}{dt^2} dt^2 - \ldots \quad -②$$

① - ② $\quad \vec{r}(t+dt) - \vec{r}(t-dt) = 2 \underbrace{\frac{d\vec{r}(t)}{dt}}_{v(t)} \cdot dt$

$$v(t) = \frac{\vec{r}(t+dt) - \vec{r}(t-dt)}{2 \cdot dt}$$