Basics of Molecular Dynamics Simulation

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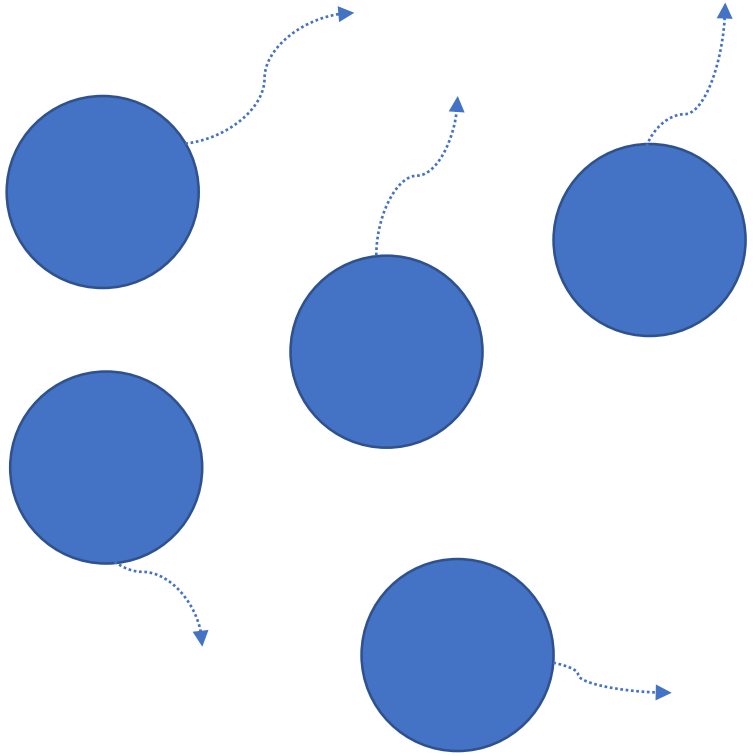
Objective (Molecular Dynamics)

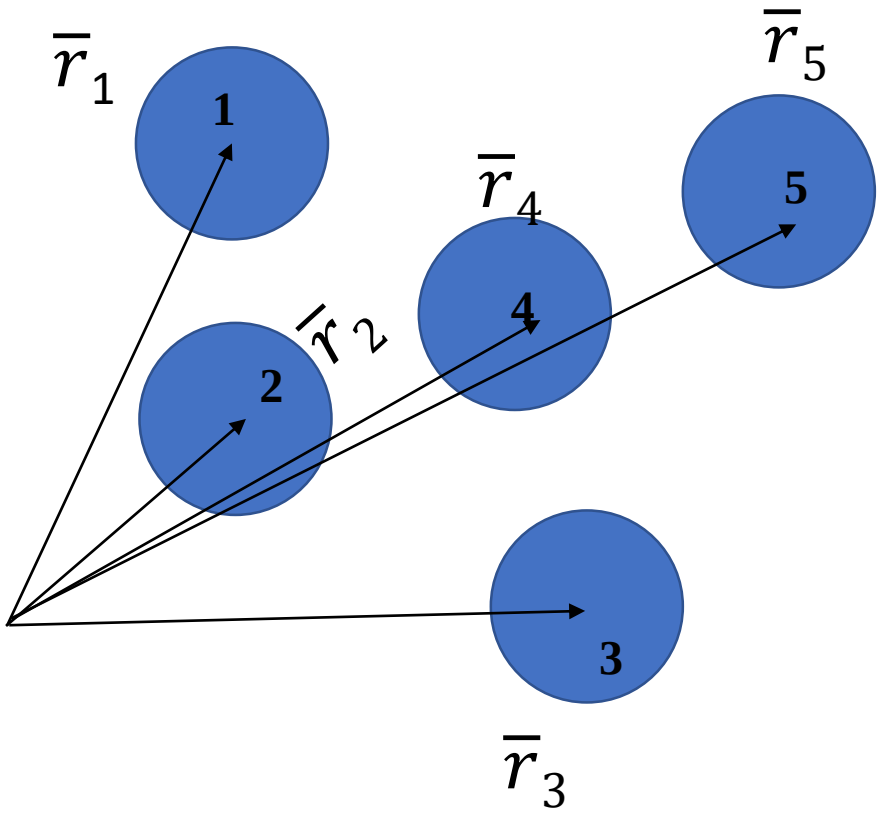


Given a collection of “N” particles

How the particle will move with Time

Trajectory

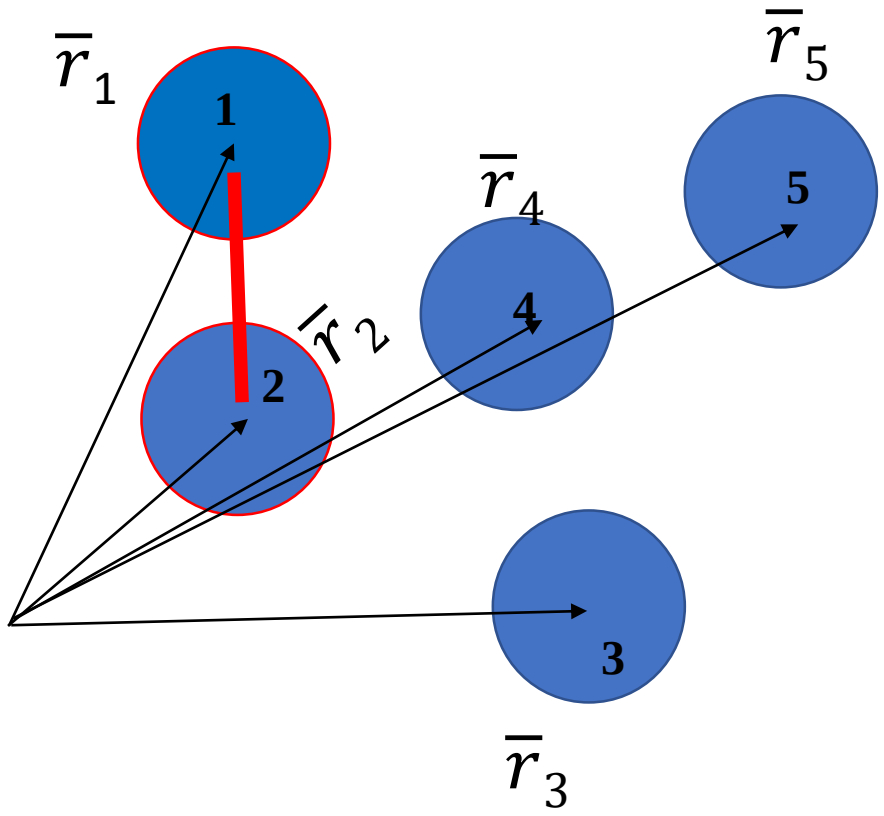
Objective (Molecular Dynamics)



What I need ?

1. Where the “N” particles are (initial position)
   Velocities of “N” particles (initial velocities)

Objective (Molecular Dynamics)



What I need ?

1. Where the "N" particles are (initial position)
   Velocities of "N" particles (initial velocities)

2. What is the interatomic energy (U) ?

Given 'N' position corresponds to a Energy (U)

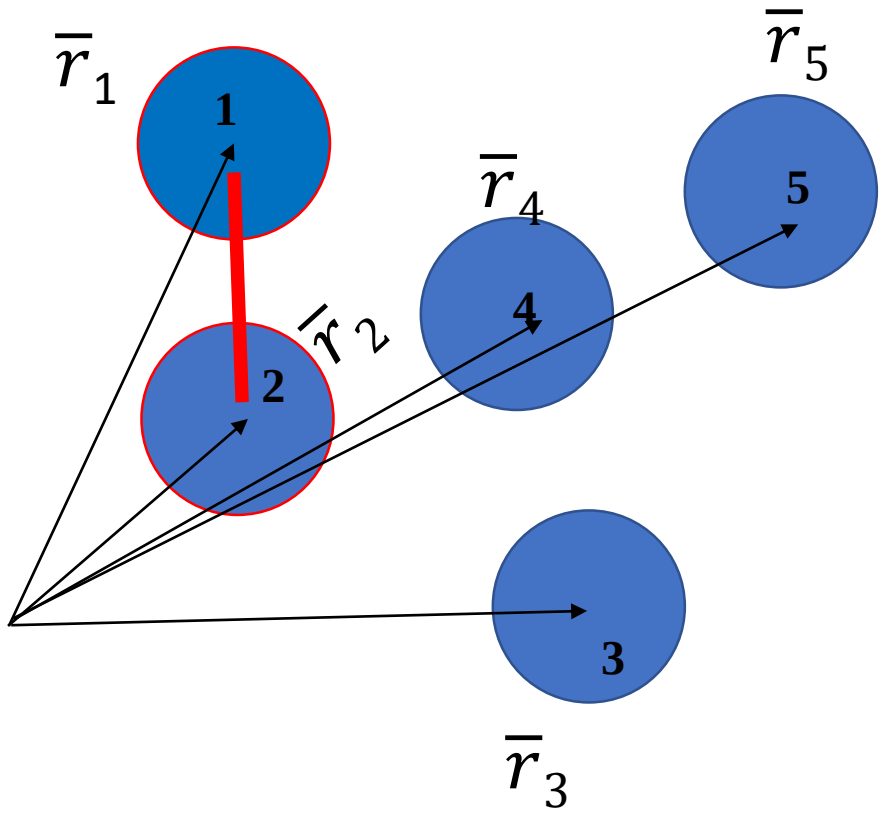
Every pair of particles apply forces to each other (e.g, 1 &2)

$$\overline{F}_{2 \rightarrow 1} = - \overline{F}_{1 \rightarrow 2}$$

$$\overline{F}_{3 \rightarrow 1} = - \overline{F}_{1 \rightarrow 3}$$

$$\overline{F}_{4 \rightarrow 1} = - \overline{F}_{1 \rightarrow 4}$$

Objective (Molecular Dynamics)



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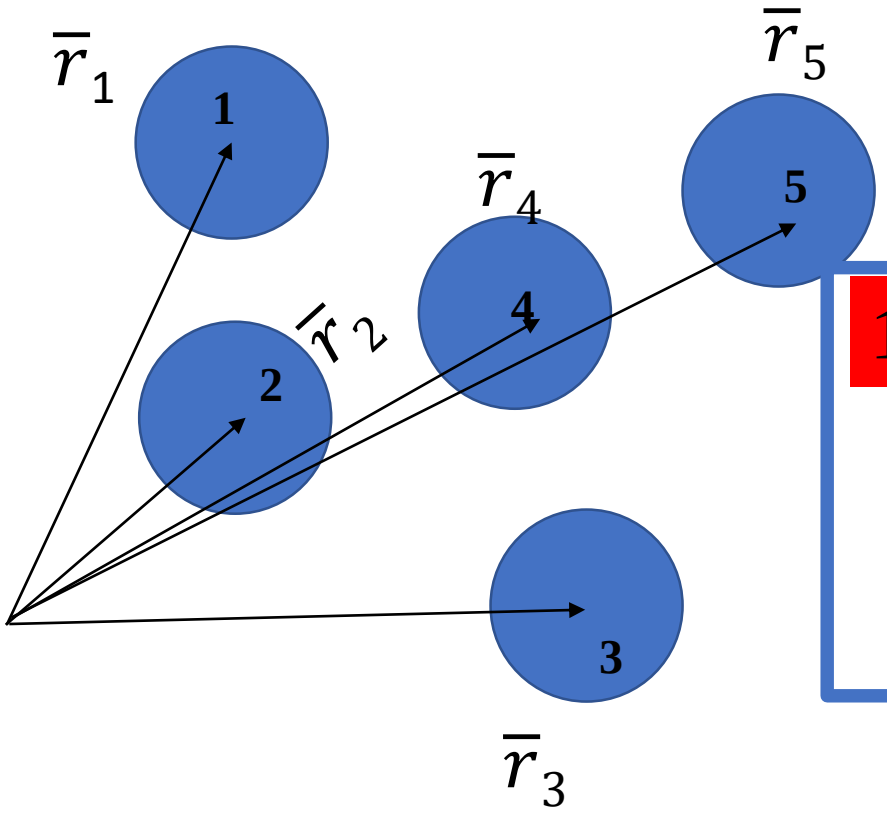
$\overline{F}_{2 \rightarrow 1}$?

If you want to know the forces you need to know Energy U_{12} (Depends on distance, $\overline{r}_{12}$)

MD cycle (Four Steps)



1

$\{\bar{r}_i\}(0)$ $\{\bar{r}_i\}(dt)$

$\{\bar{v}_i\}(0)$ $\{\bar{v}_i\}(dt)$

$i \in [1, N]$

2

$U_{ij}(r_{ij})$

$U_{total} = \sum U_{ij}(r_{ij})$

$i > j$

3

$\bar{F}_{j \to i} = -\frac{\partial U_{ij}}{\partial r_{ij}}\vec{r}$

$\bar{F}_i = \sum \bar{F}_{j \to i}$

$i \neq j$

4

Newtons Law

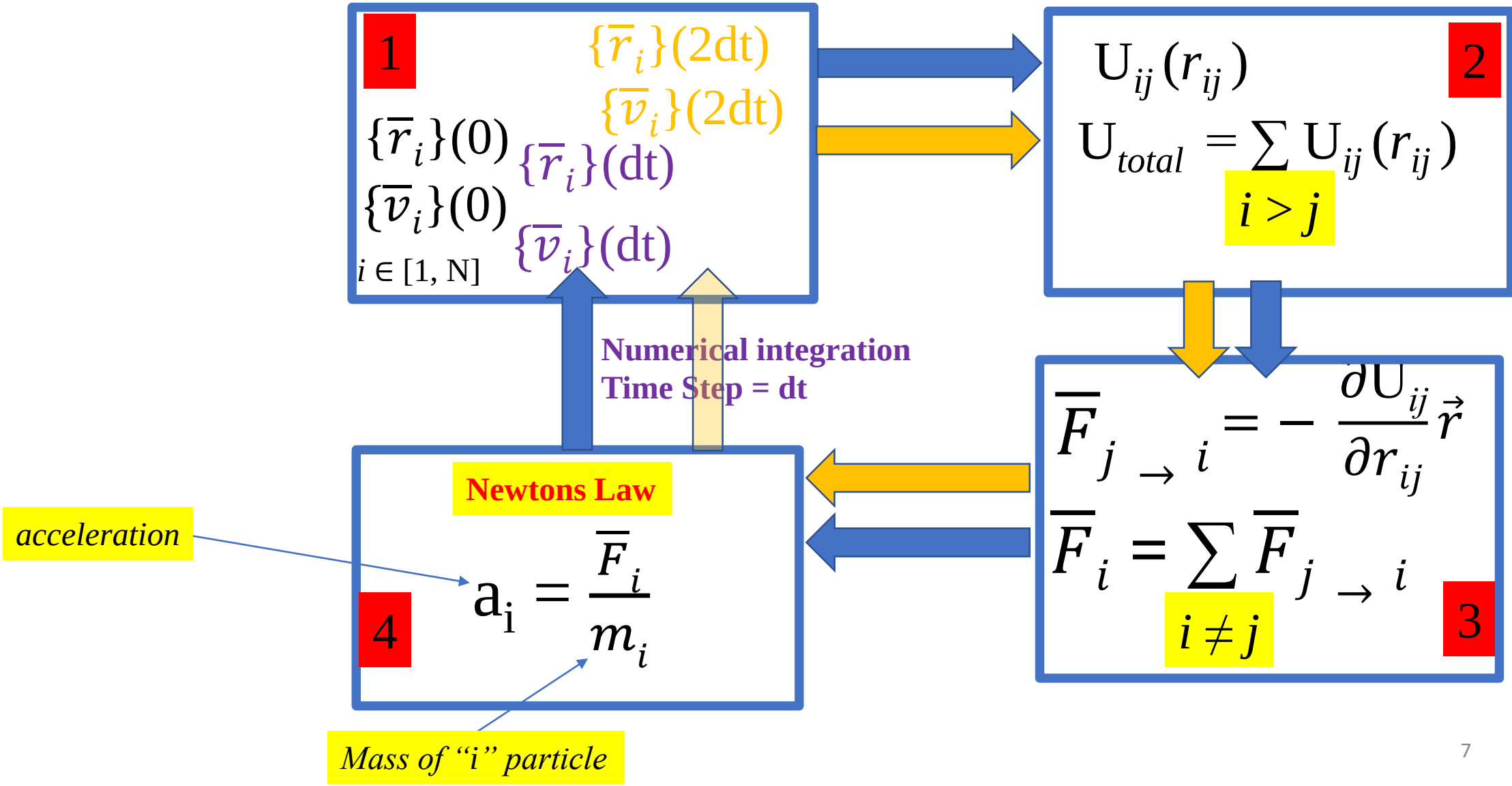
$a_i = \frac{\bar{F}_i}{m_i}$

acceleration

Mass of "i" particle

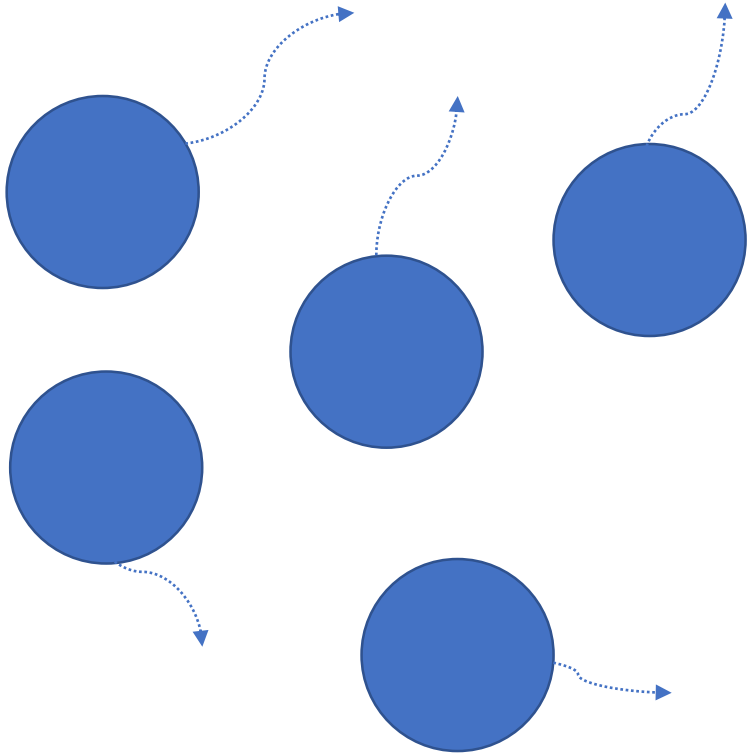
Numerical integration
Time Step = dt

MD cycle (Four Steps)



MD cycle (Four Steps)

0 → dt →2 dt → 3dt ….



Outcome = Trajectory

MD cycle (Four Steps)

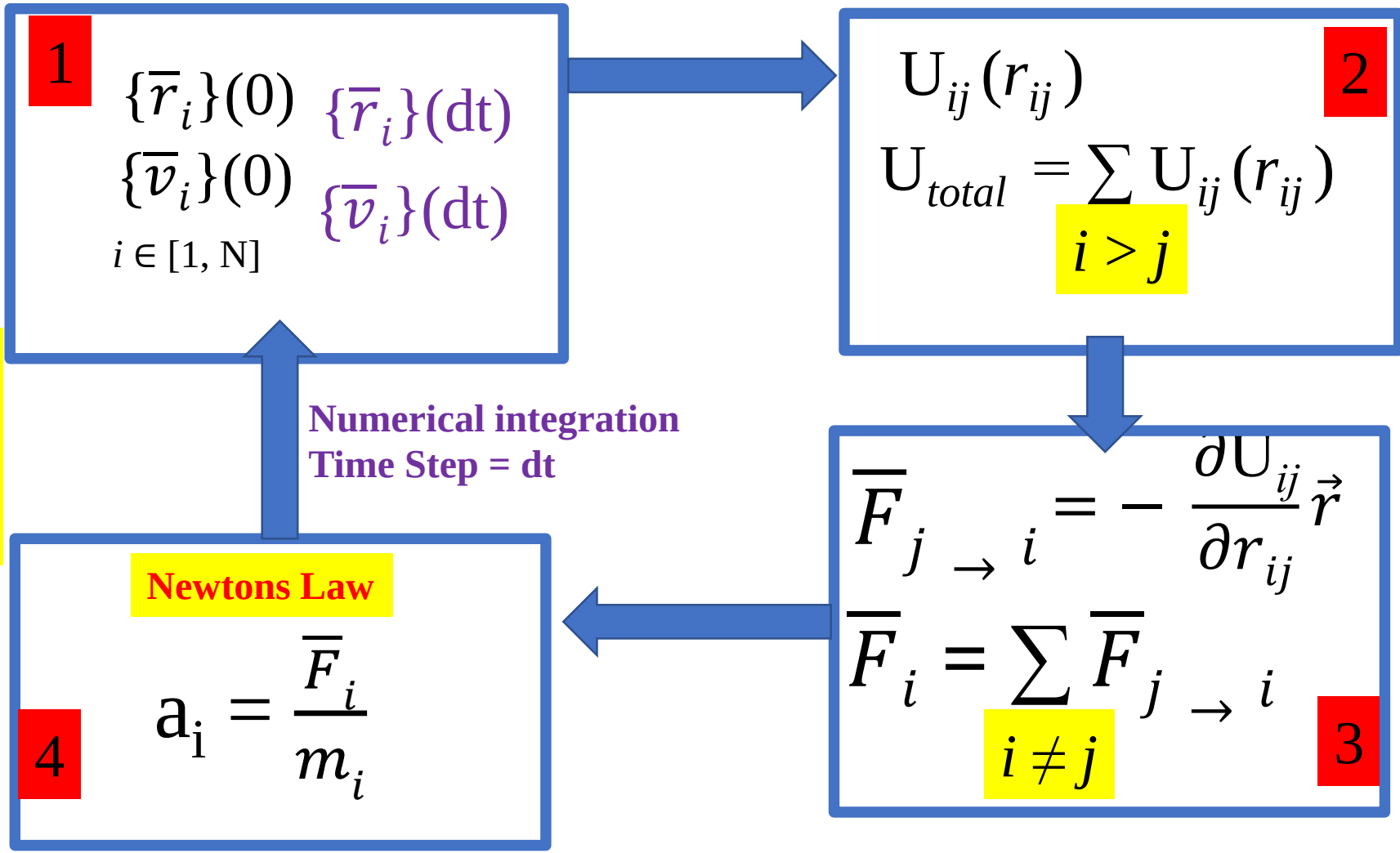
Needs to Know ?

r(0), v(0), U(r)

Key for accuracy ?

- ***Force filed U***
- ***Numerical integration (Choice of "dt")***

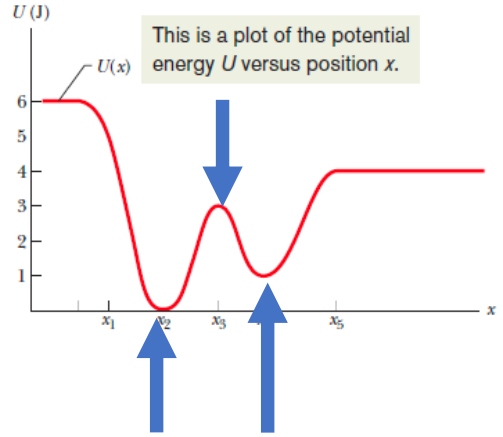
Usually
t = 1- 2 fs



Why it is called Classical Molecular Dynamics ?

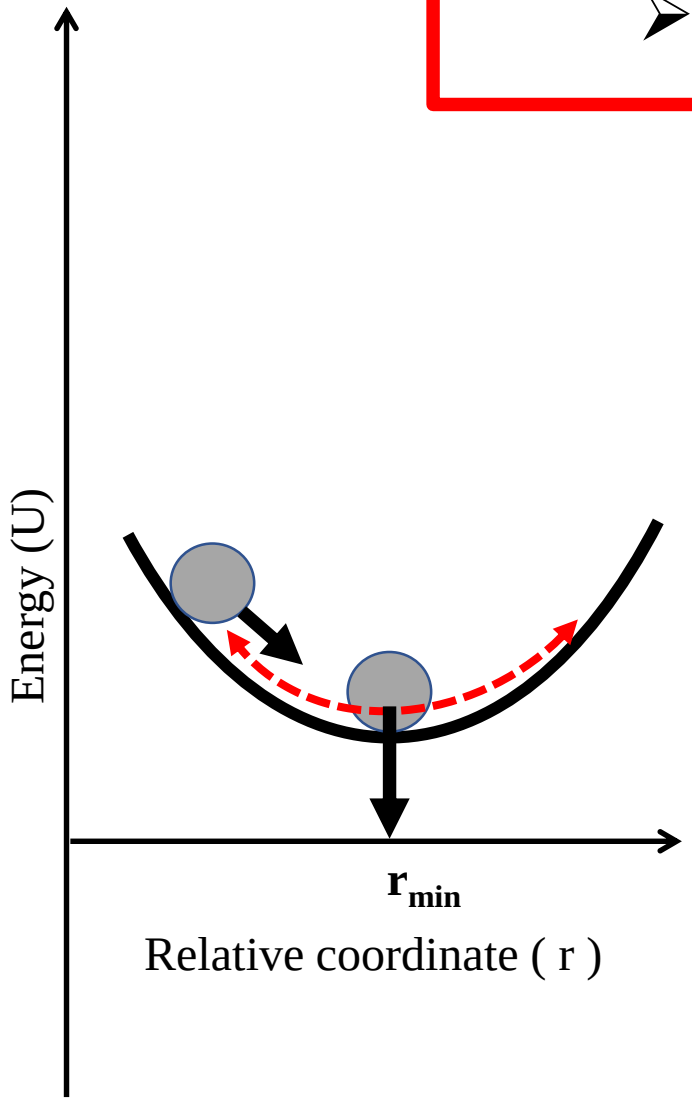
Use of Classical equation of motion (F = m a, Time evolution)

Energy Minimization do not have Time (NOT DYNAMICS)



Molecular Dynamics ≠ Energy Minimization

➢ **F = m a** **(Classical Mechanics)**



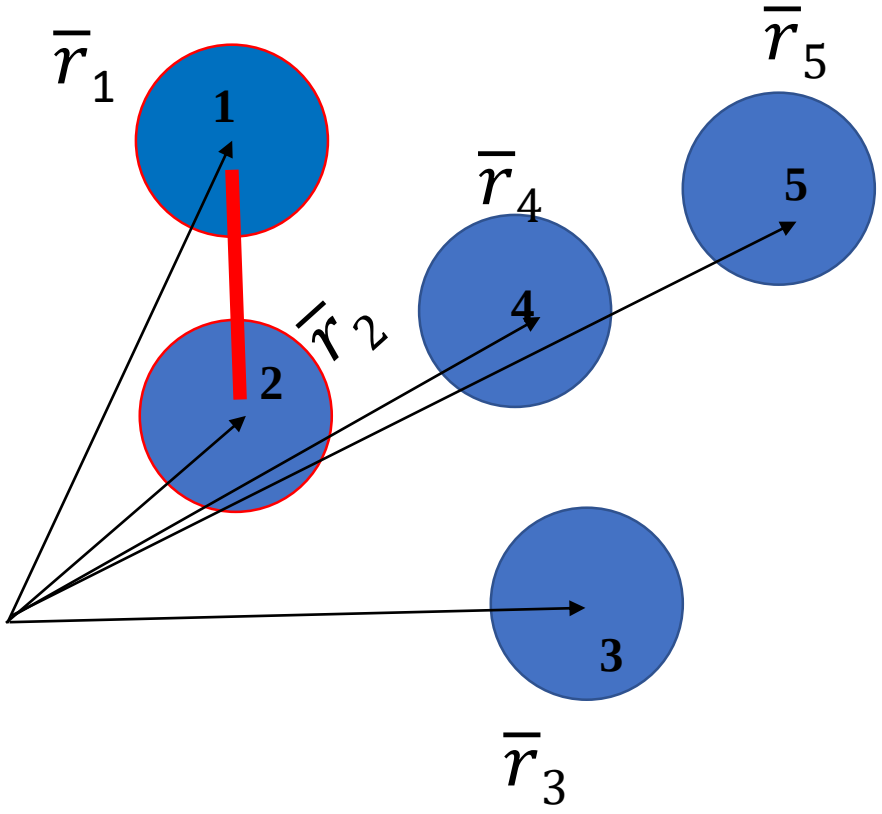
$$F_{r=rmin} = -(dU/dr)_{r=rmin} = 0$$

NO MORE MOVEMENT

Thank GOD:
Nothing is at zero kelvin

KEEP MOVING AROUND THE MINIMA

We already know U_{12} (Force-Field)



CHARMM Potential Function

$$U(\vec{R}) = \underbrace{\sum_{bonds} k_i^{bond}(r_i - r_0)^2}_{U_{bond}} + \underbrace{\sum_{angles} k_i^{angle}(\theta_i - \theta_0)^2}_{U_{angle}} + \underbrace{\sum_{dihedrals} k_i^{dihe}[1 + \cos(n_i\phi_i + \delta_i)]}_{U_{dihedral}} + \underbrace{\sum_i \sum_{j \neq i} 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] + \sum_i \sum_{j \neq i} \frac{q_i q_j}{\epsilon r_{ij}}}_{U_{nonbond}}$$

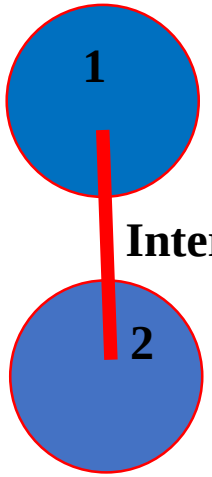
PDB file → geometry

Topology → PSF file

parameters → Parameter file

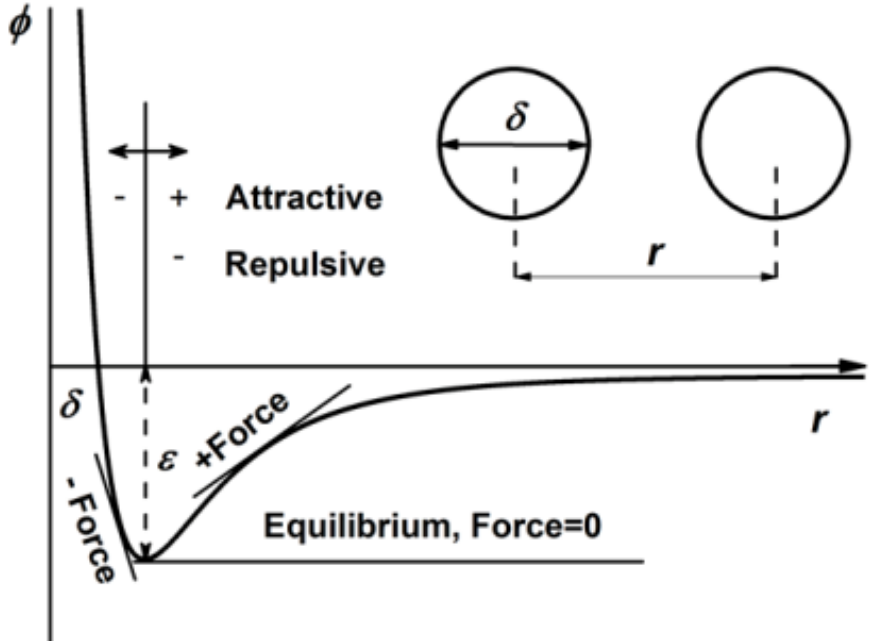
If my particles do not have internal structure

U_{12} (Force-Field) → $\overline{F}_{2 \rightarrow 1}$?



Interatomic distance= r

$$\overline{F}_{2 \rightarrow 1} = -\frac{\partial U}{\partial r}\vec{r}$$



https://lammpstube.com/2020/02/10/lennard-jones-potential/

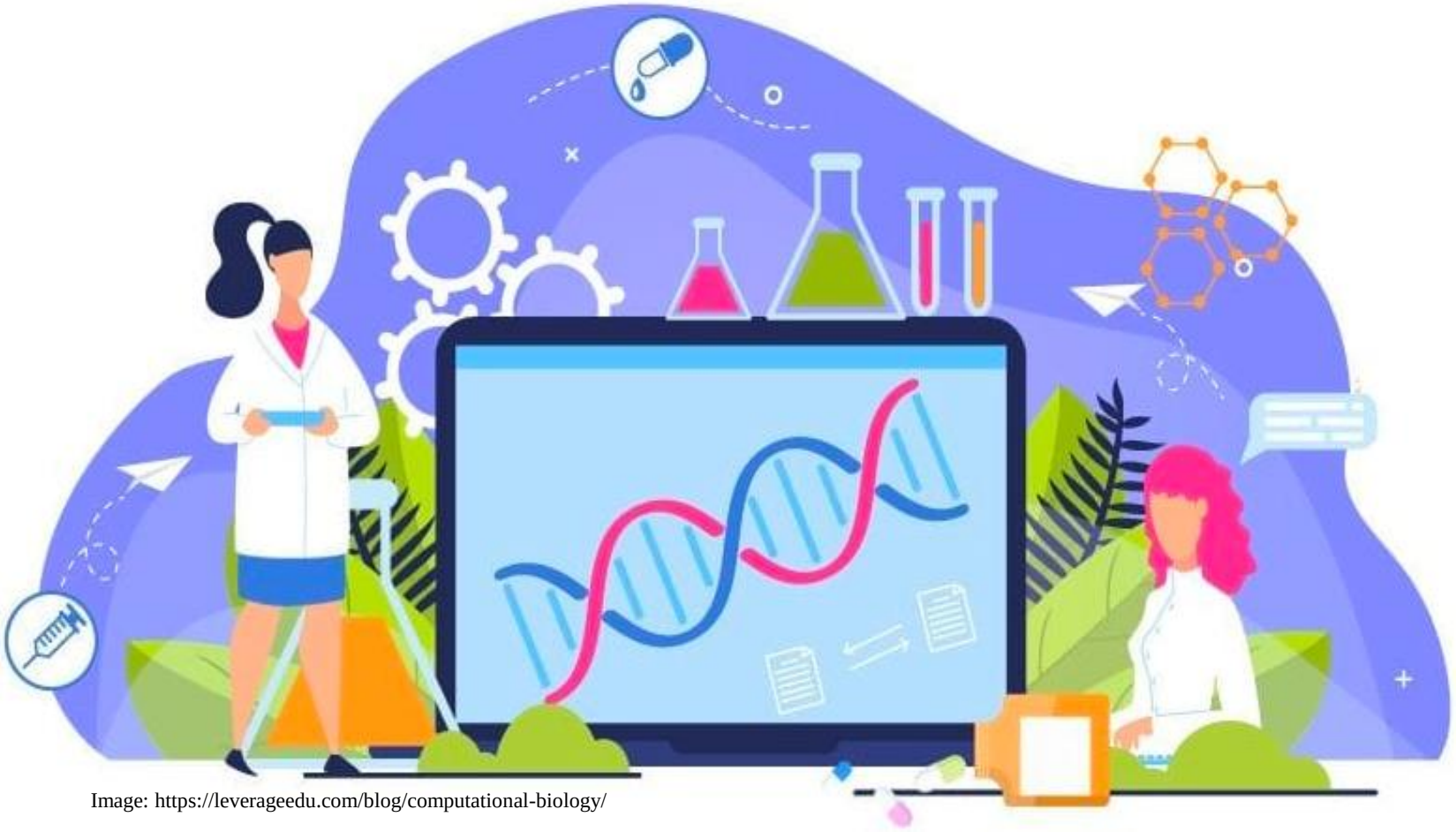


Image: https://leverageedu.com/blog/computational-biology/

Next : Numerical Integration and Position/Velocity update