NTNU
Norwegian University of
Science and Technology

Molecular Dynamics Simulation

theories and principles

Senbo Xiao

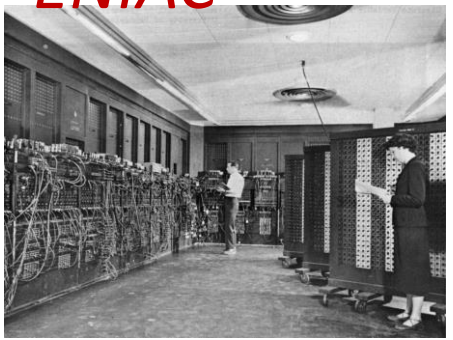
Outline

- Briefs on computer simulations
- Introductory Molecular Dynamics (MD) simulations
- Practice of MD simulations

Computer simulations

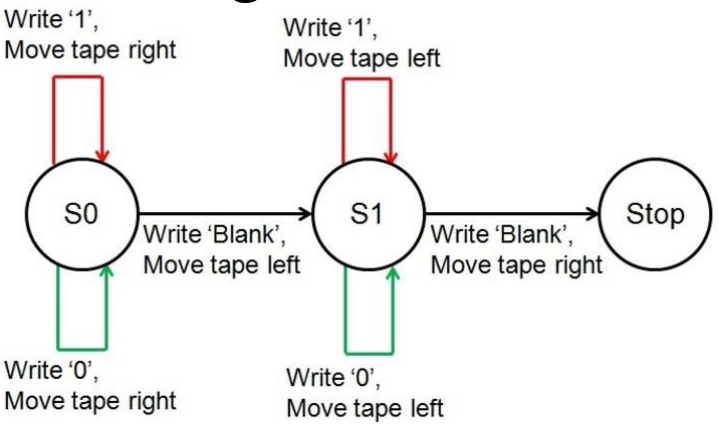
Alan Turing

ENIAC



The Norwegian e-infrastructure

The Turing machine



Nicholas Metropolis

Martin Karplus

Chemistry 2013

Computer simulations

Computer simulations in research:

- Verification of theories
- Explanation and prediction of experimental results
- Independent exploratory tools

Computer simulations

Applications of computer simulations

Formation of galaxy

Weather forecast

Massive explosion study

Flight simulation

"The day after tomorrow"

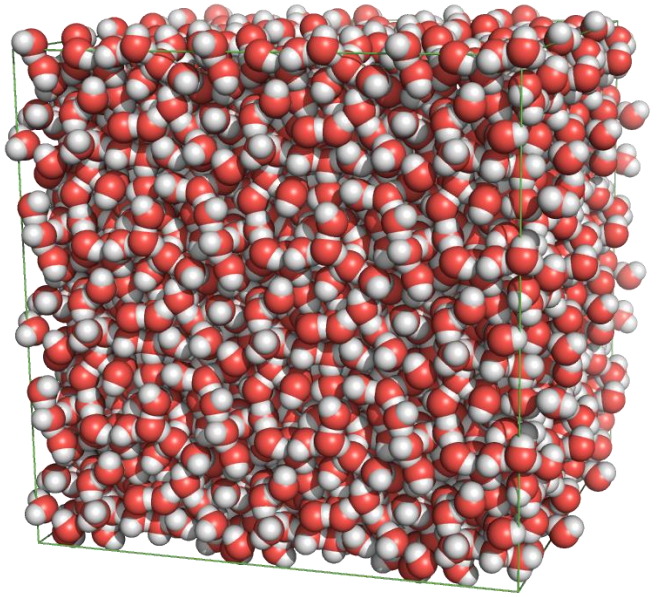
High pressure phenomenon

Chemical diffusion in the primitive universe

Ultrafast dynamics of Super-small system

Molecular Dynamics (MD) simulations

- Atomistic resolution
- Classic physics (Newton's laws of motion)
- Small system (nanometers)
- Small time scale (nanoseconds)



A water box

Molecular Dynamics (MD) simulations

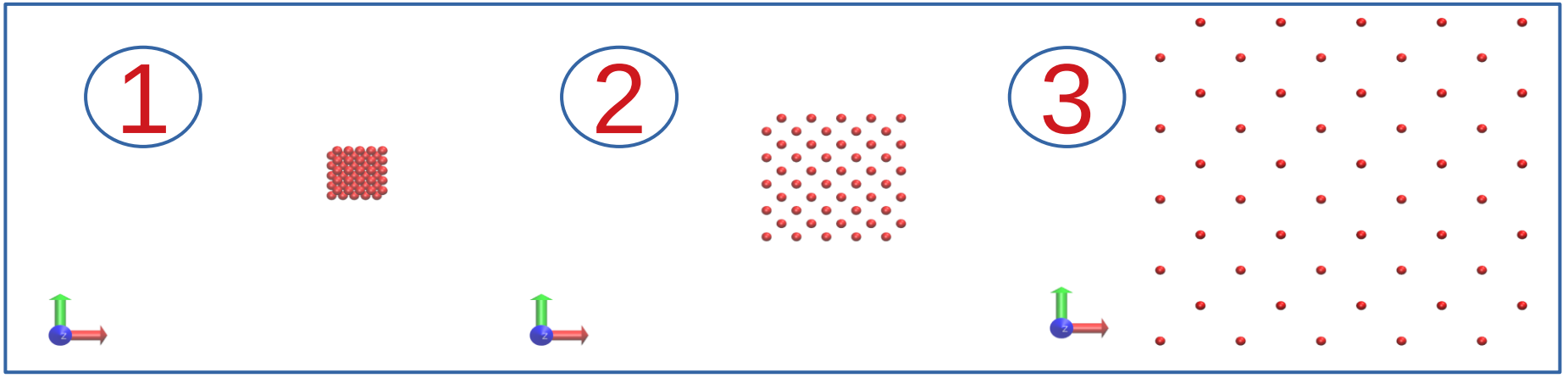
- Simulate interactions of particles (*atoms, molecules, granules, ...*)
- Predict time evolution of N-body systems
- Require parameters of initial atom coordinates, velocities, interaction potentials, ...
- Use finite time step to integrate Newton's laws of motion:

$$m_i \vec{a_i} = \vec{F_i} \quad / \quad m_i \frac{d\vec{v_i}}{dt} = \vec{F_i} \quad / \quad m_i \frac{d^2\vec{r_i}}{dt} = \vec{F_i}$$

Molecular Dynamics (MD) simulations

Examples:

1. Calculation cohesive energy: **Not** MD



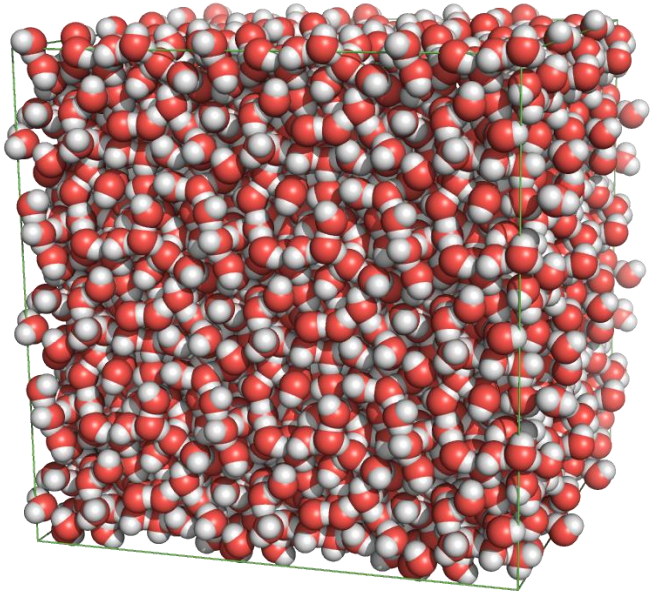
Molecular Dynamics (MD) simulations

Examples:

2. Equilibrating water molecules: MD

Water molecules diffusion at

a temperature of 300K

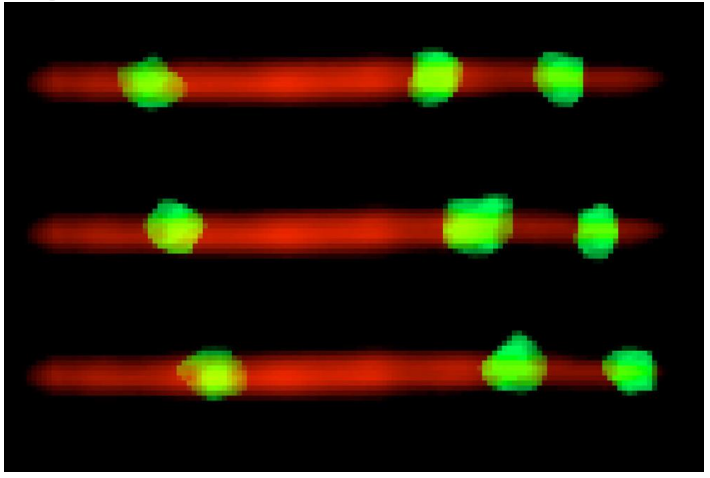


A water box

MD simulation as a powerful tool

Comparison of tools for studying a single protein:

1) Single molecule microscopy



2) X-ray crystallography

3) MD simulation

MD simulation as a powerful tool

Comparison of tools for studying a single protein:

1) Single molecule microscopy

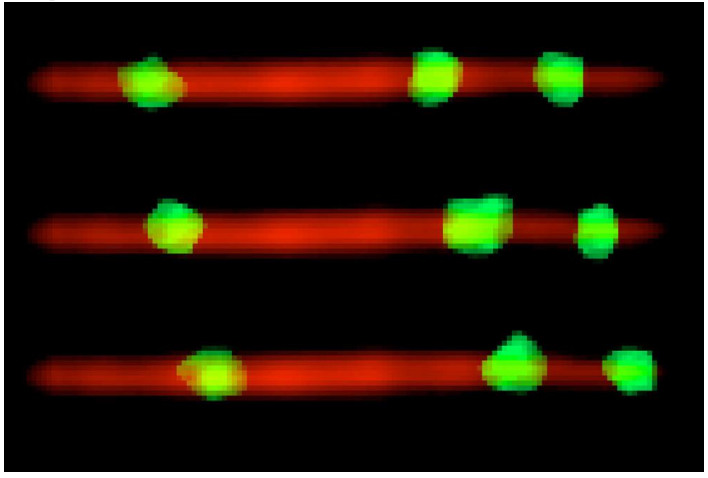
2) X-ray crystallography

3) MD simulation

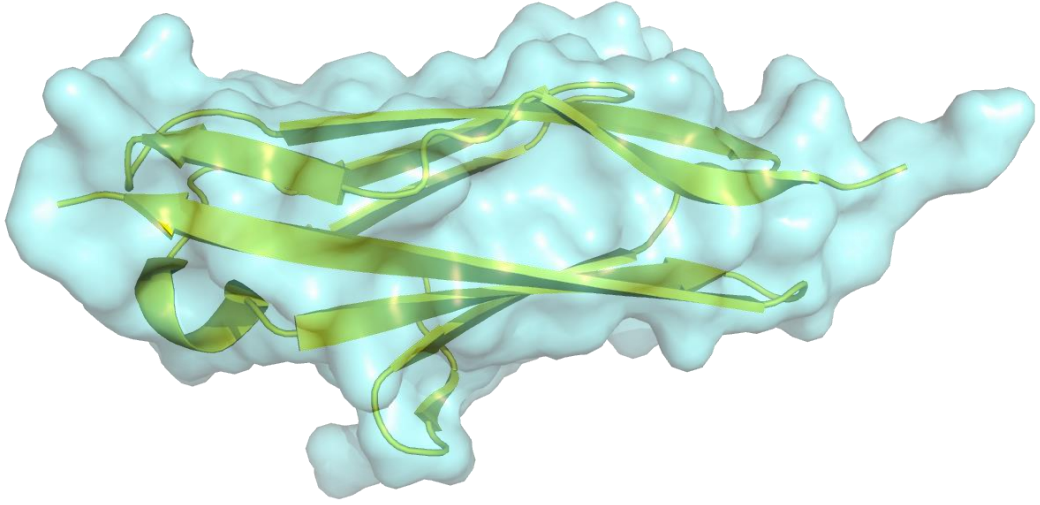
MD simulation as a powerful tool

A comparison of tools for studying a single protein:

1) Single molecule microscopy



2) X-ray crystallography

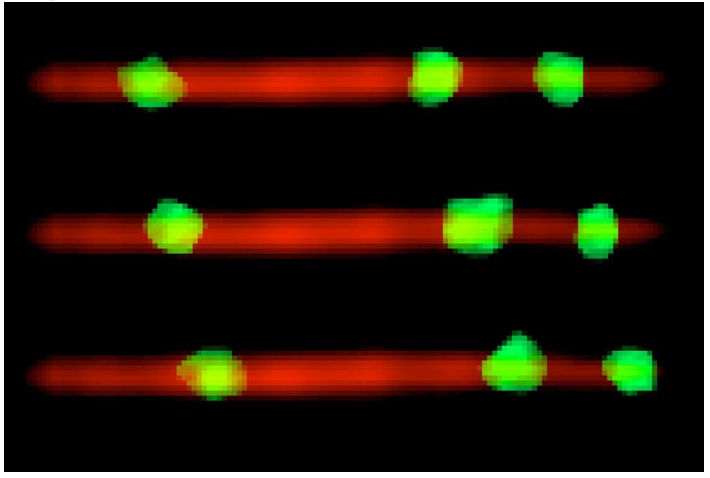


3) MD simulation

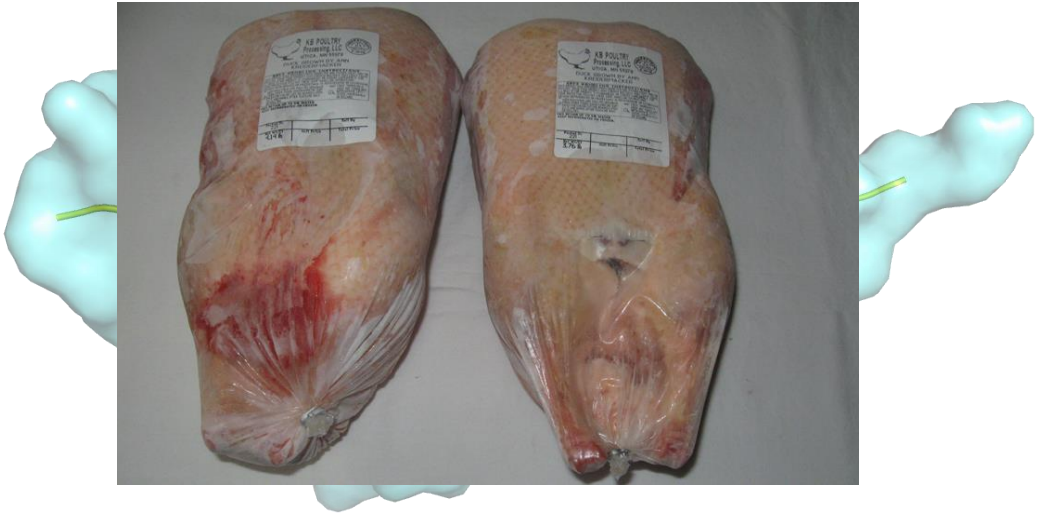
MD simulation as a powerful tool

A comparison of tools for studying a single protein:

1) Single molecule microscopy



2) X-ray crystallography



3) MD simulation

MD simulation as a powerful tool

A comparison of tools for studying a single protein:

3) MD simulation

Practice of MD simulations

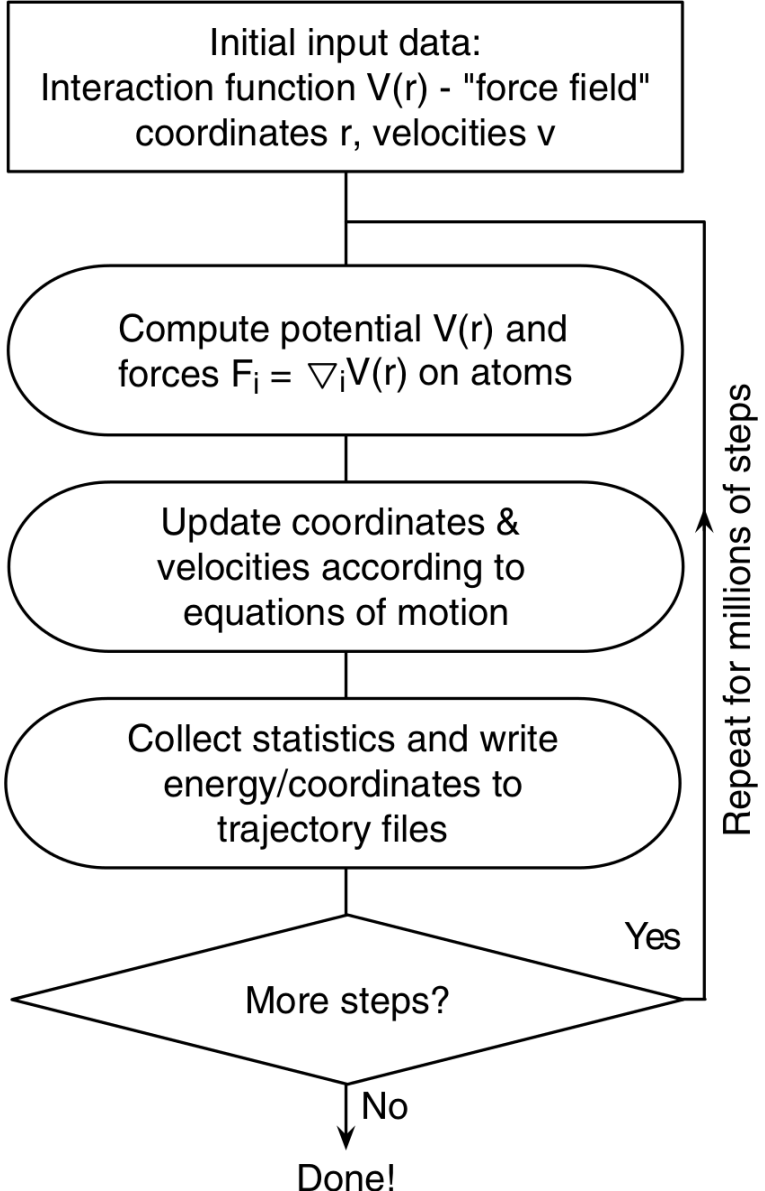
Common procedure of MD simulations

(Analysis not included)

Implementation of classical mechanics

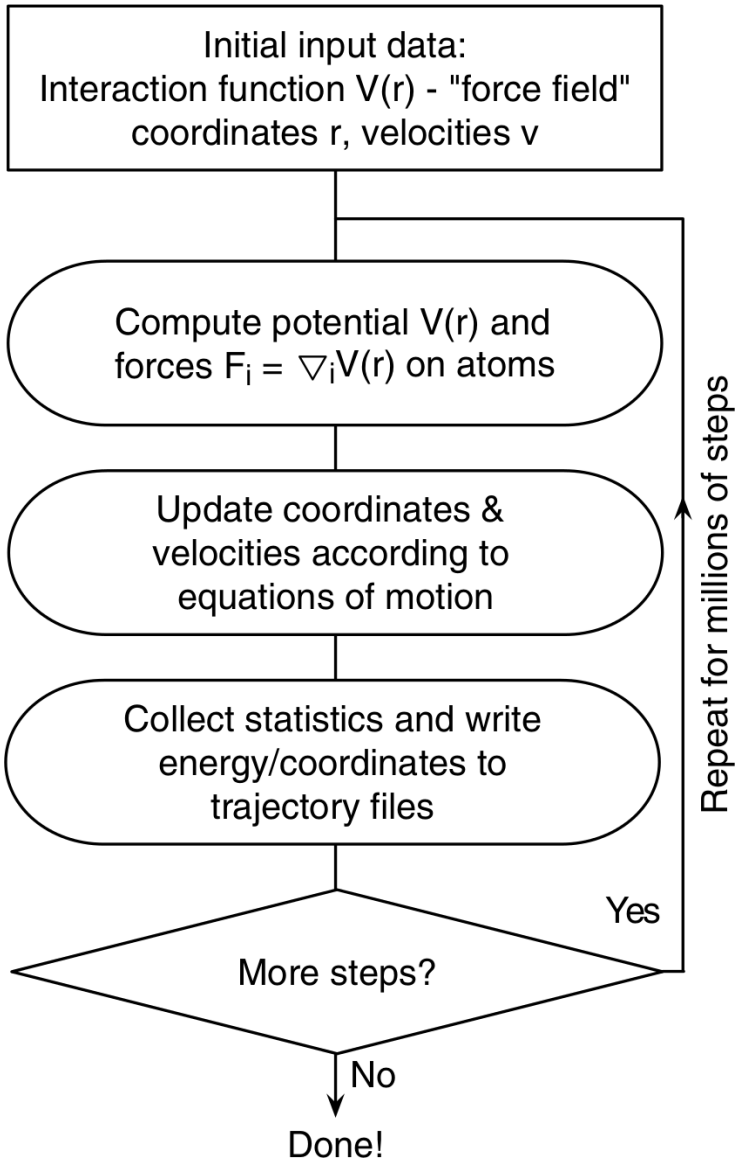
Newton's equation of motion:

$$m_i\overrightarrow{a_i} = \overrightarrow{F_i} \qquad m_i\frac{d\overrightarrow{v_i}}{dt} = \overrightarrow{F_i} \qquad m_i\frac{d^2\overrightarrow{r_i}}{dt} = \overrightarrow{F_i}$$



This part is the atomistic modeling section, and deviates depends on individual project.

This part is the real MD running section. Generally, one simple command.



Practice of MD simulations

Common procedure of MD simulations

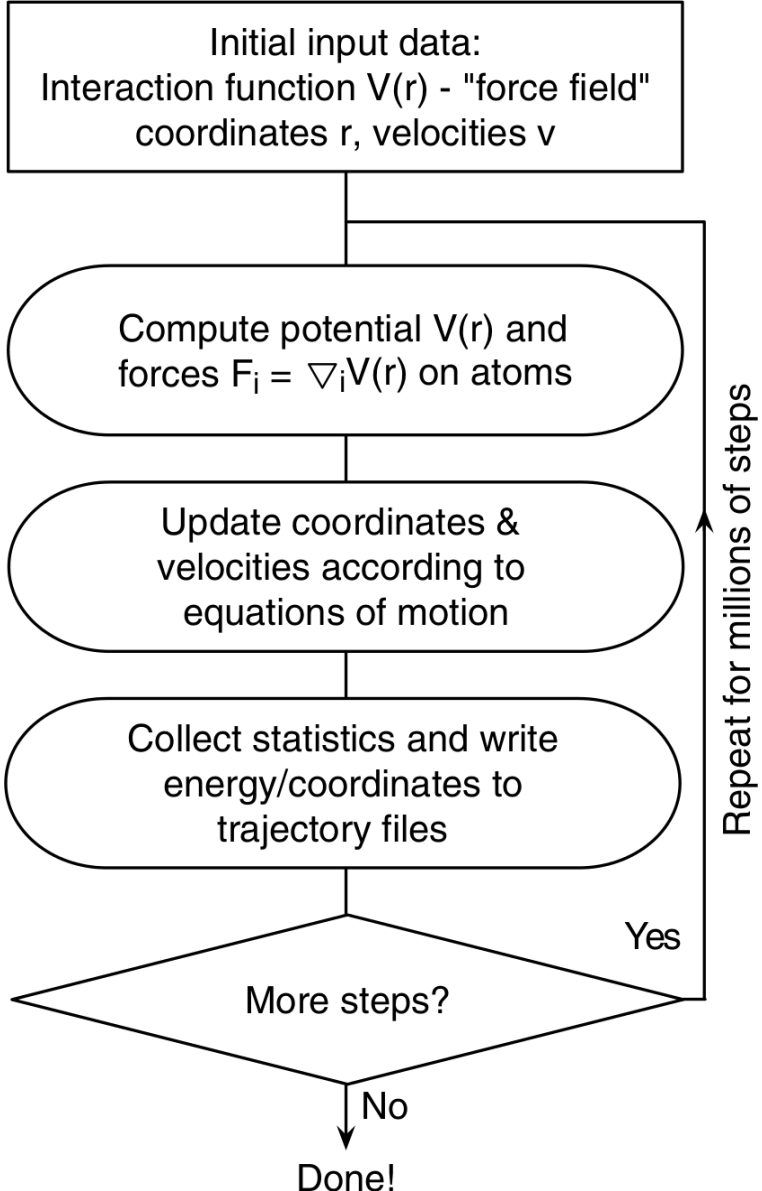
(Analysis not included)

There are multiple ways to calculate force in simulations:

ab initio MD

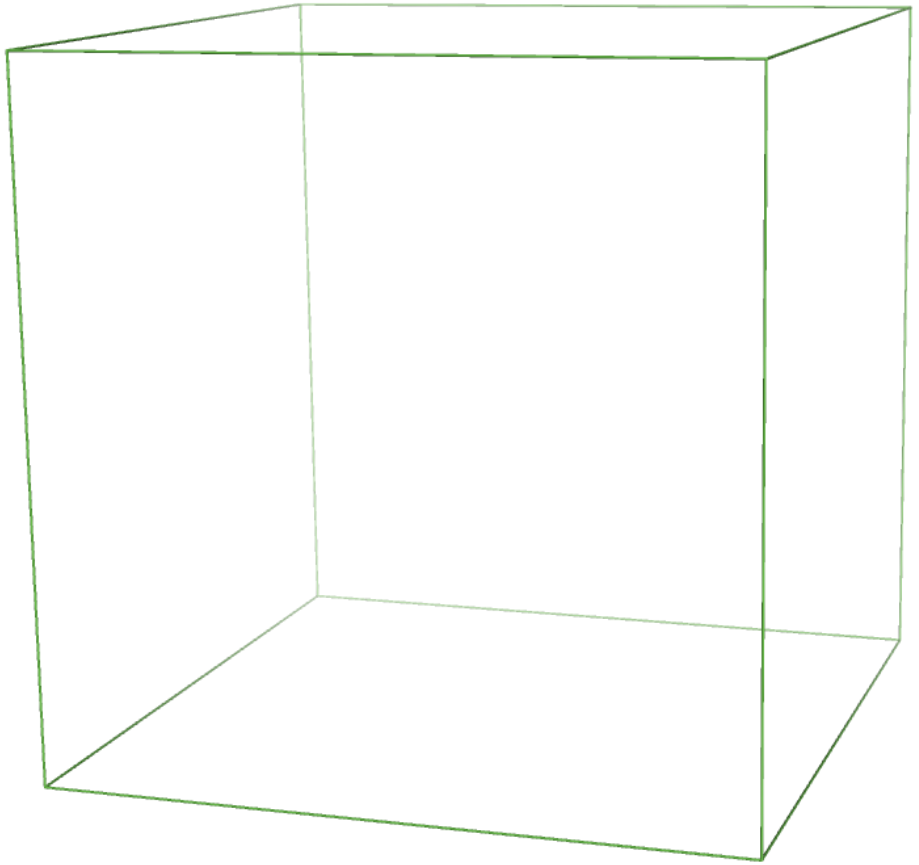
first-principles MD

...



Practice of MD simulations

Building a MD simulation system from scratch

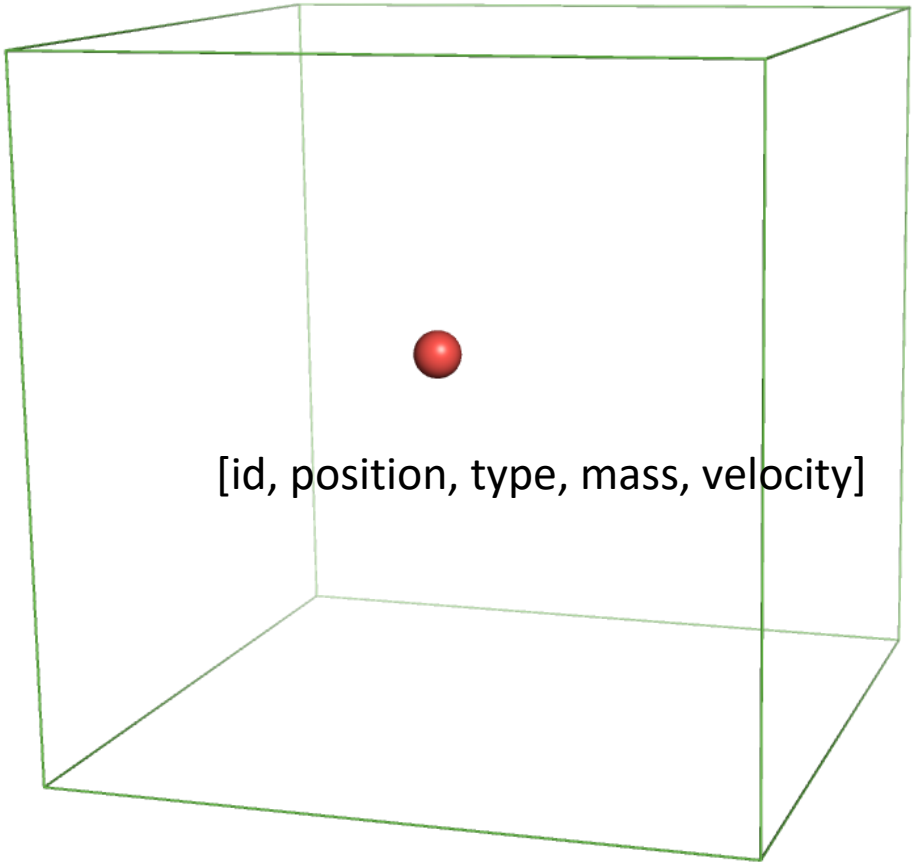


Setting simulation box

Setting up boundary

Practice of MD simulations

Building a MD simulation system from scratch

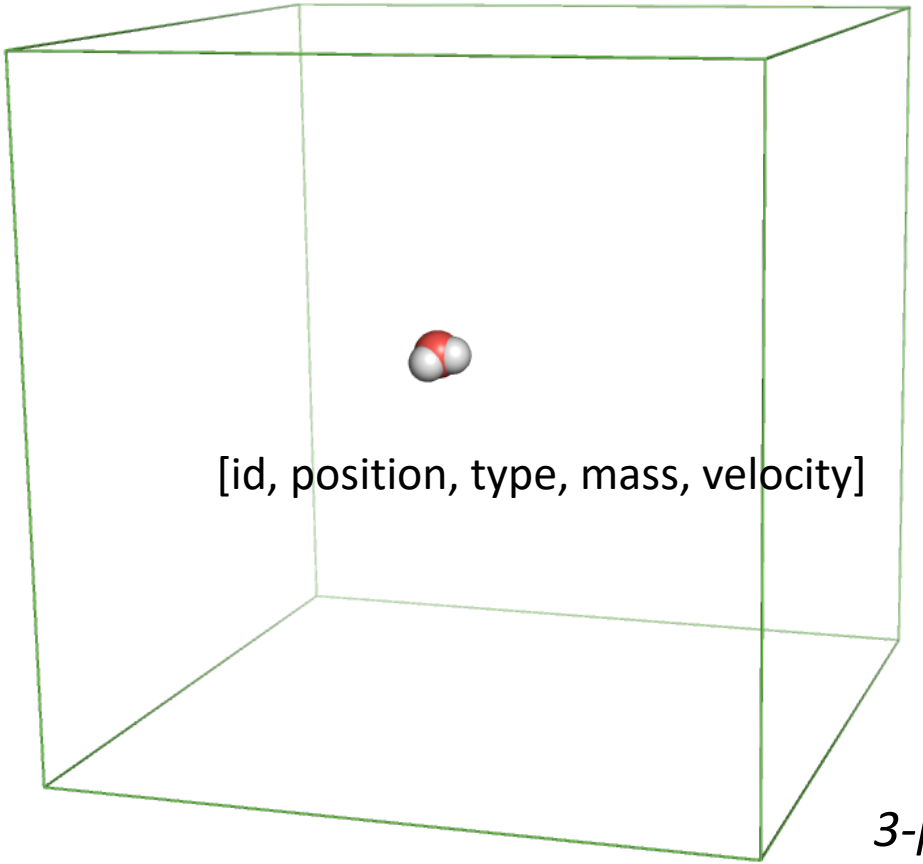


Putting points in the box

Defining properties

Practice of MD simulations

Building a MD simulation system from scratch



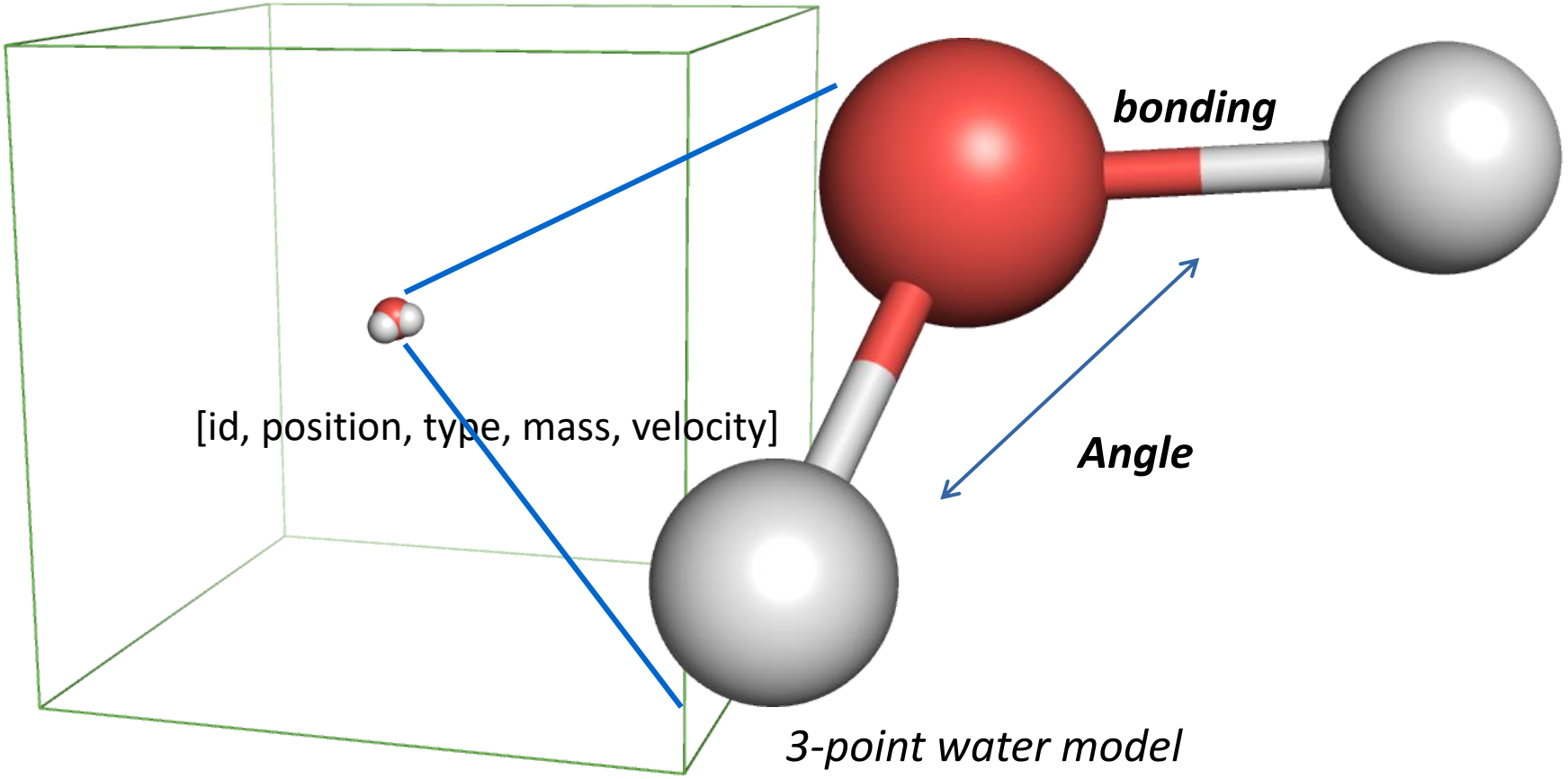
Putting more points

Defining more properties

3-point water model

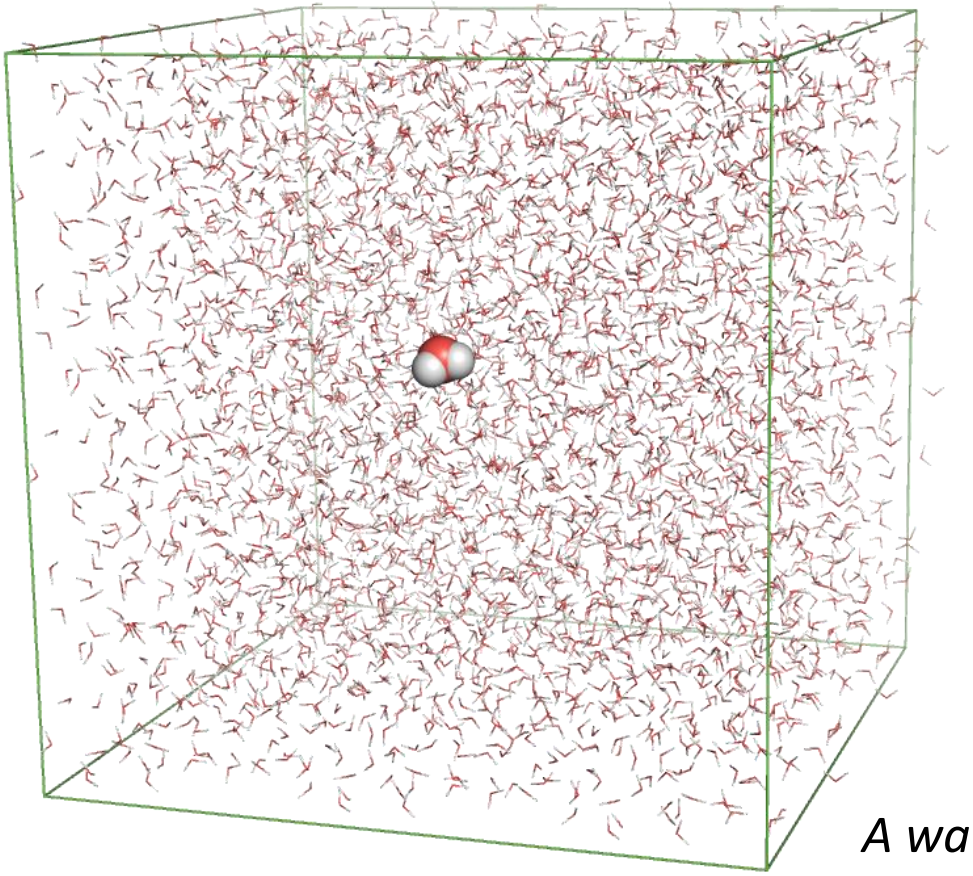
Practice of MD simulations

Building a MD simulation system from scratch



Practice of MD simulations

Building a MD simulation system from scratch



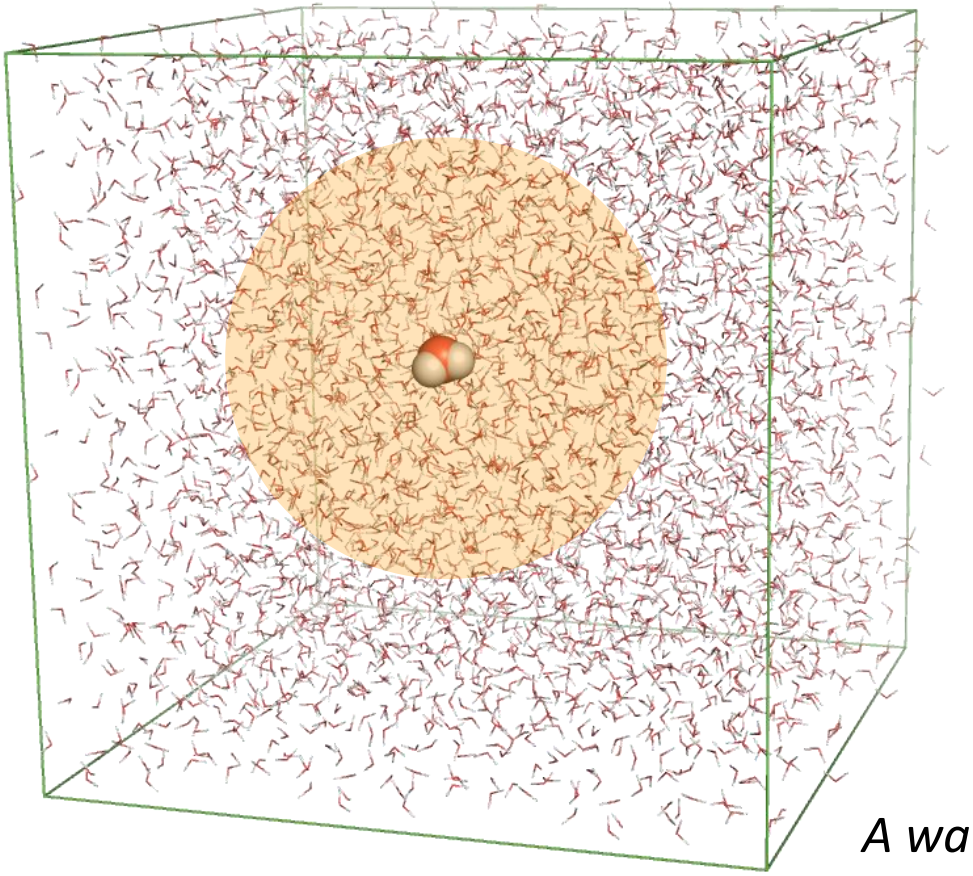
A water box

Making many

Copy & paste

Practice of MD simulations

Building a MD simulation system from scratch



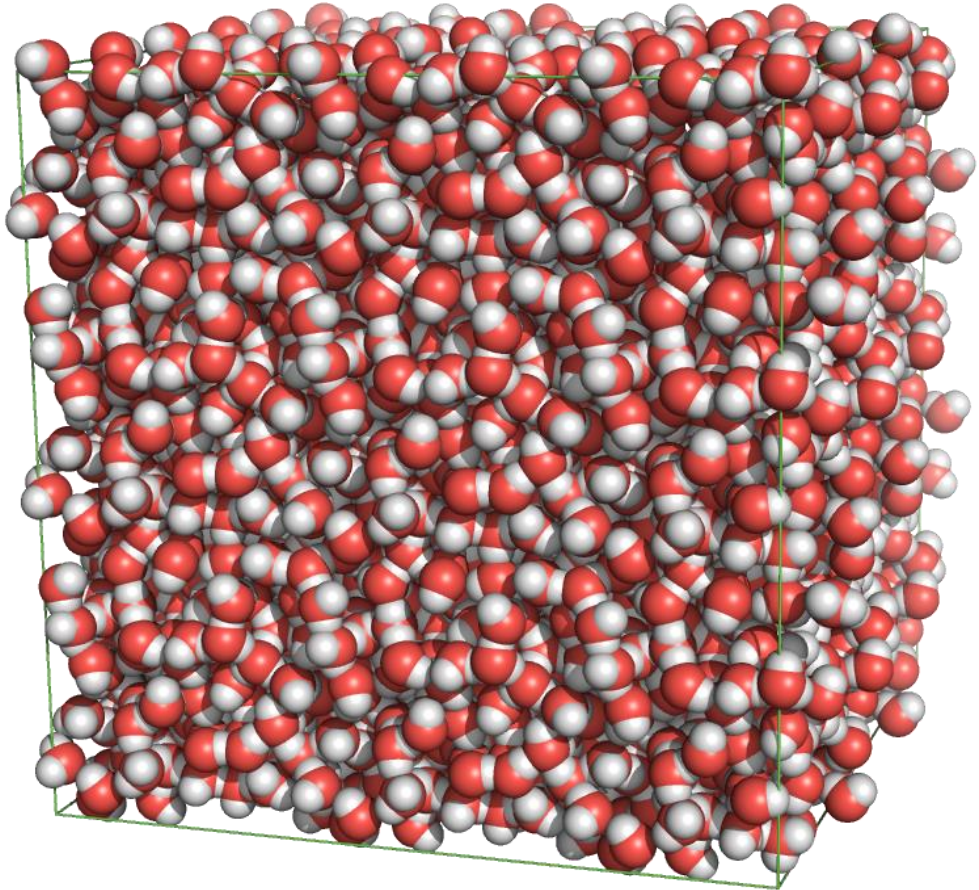
A water box

Computational efficiency

Defining cut-off

Practice of MD simulations

Building a MD simulation system from scratch



Done structural modeling

Practice of MD simulations

Building a MD simulation system from scratch

Modeling process

1. simulation box

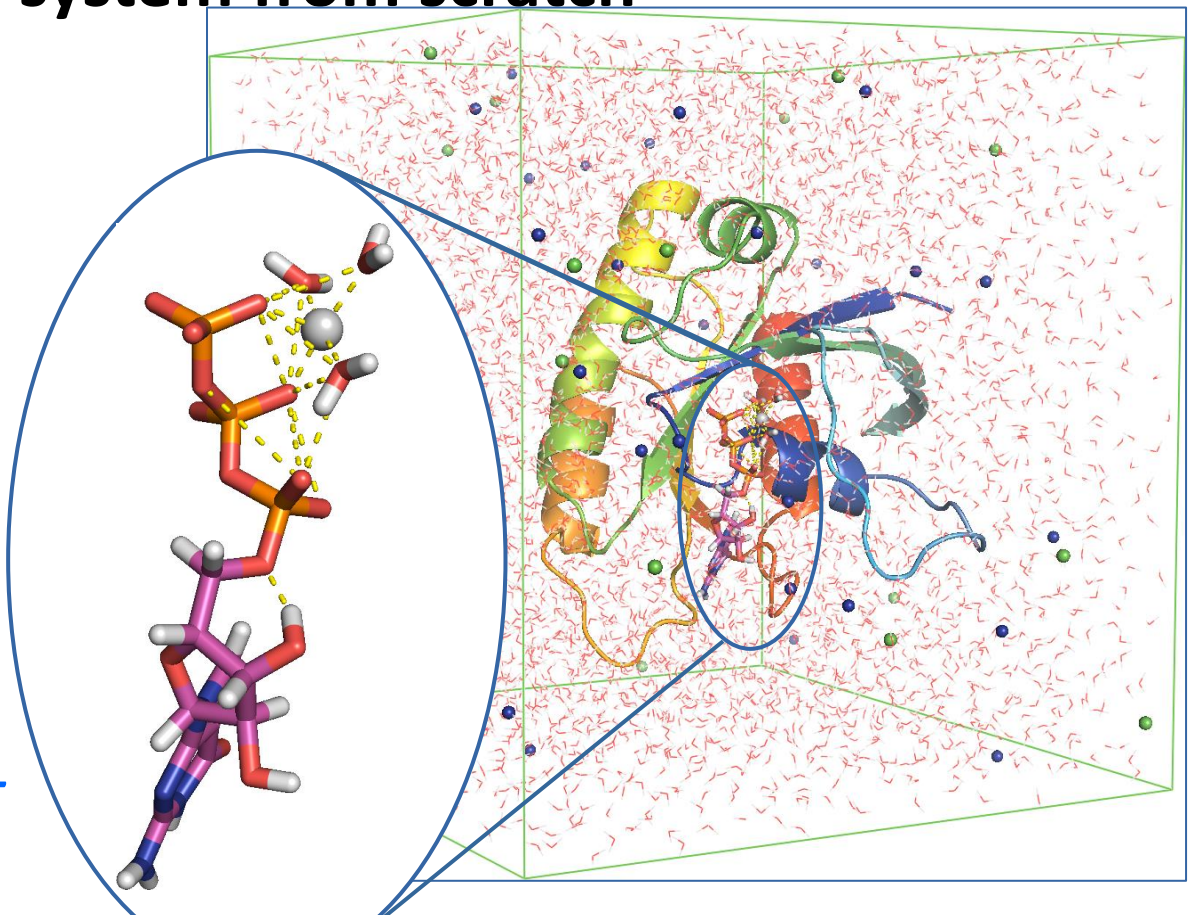
2.boundary

3. biomolecules

4. ligands

5. solvation

6. cytosol environment



Practice of MD simulations

Building a MD simulation system from scratch

Modeling process

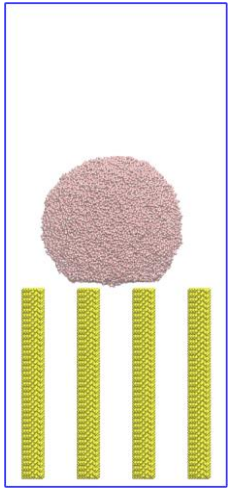
1. simulation box

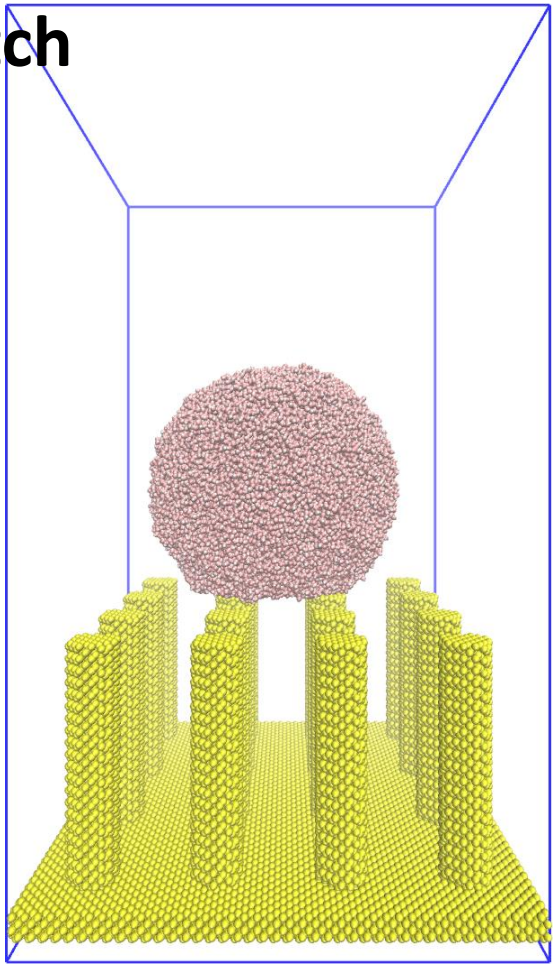
2.boundary

3. periodicity?

4. water droplet size?

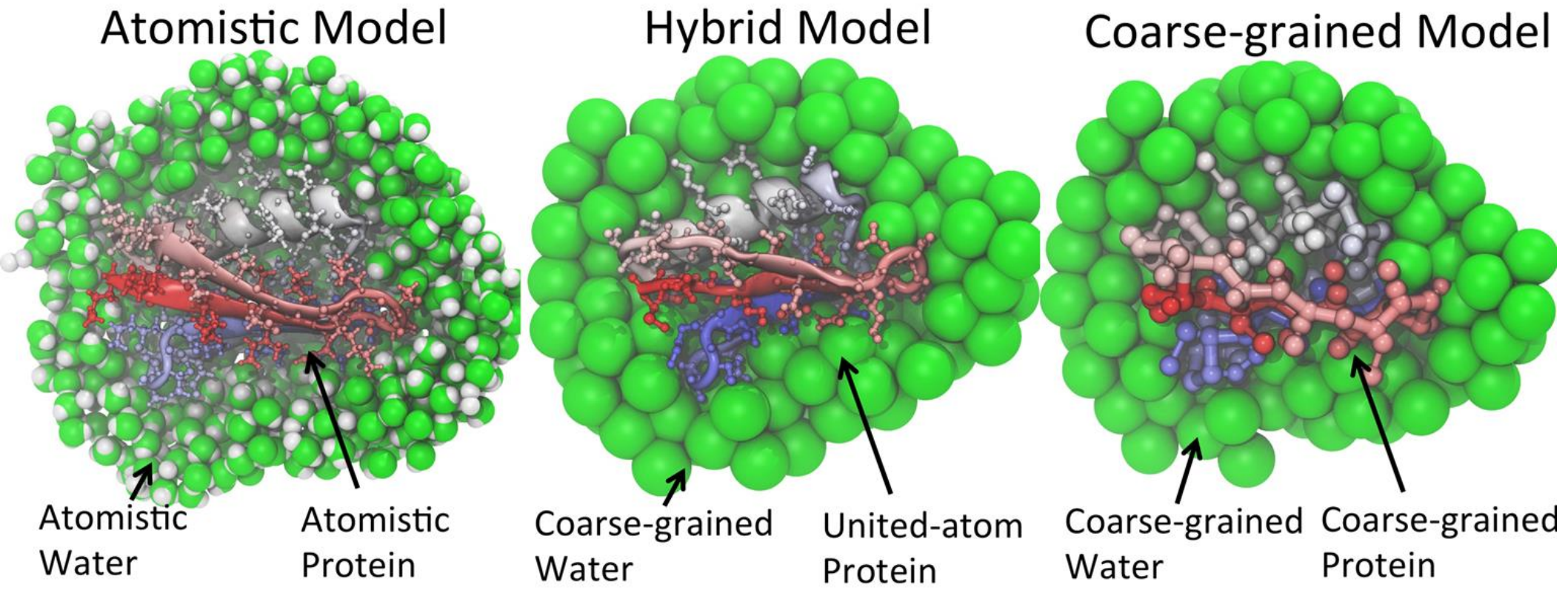
5. pillar hight?





Practice of MD simulations

Complexities and resolutions



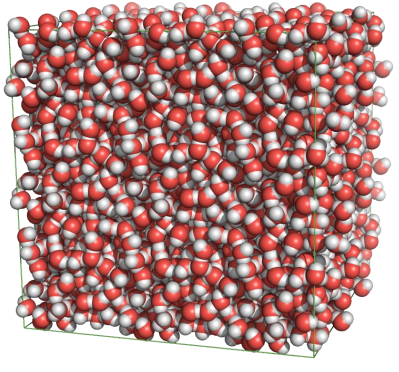
Practice of MD simulations

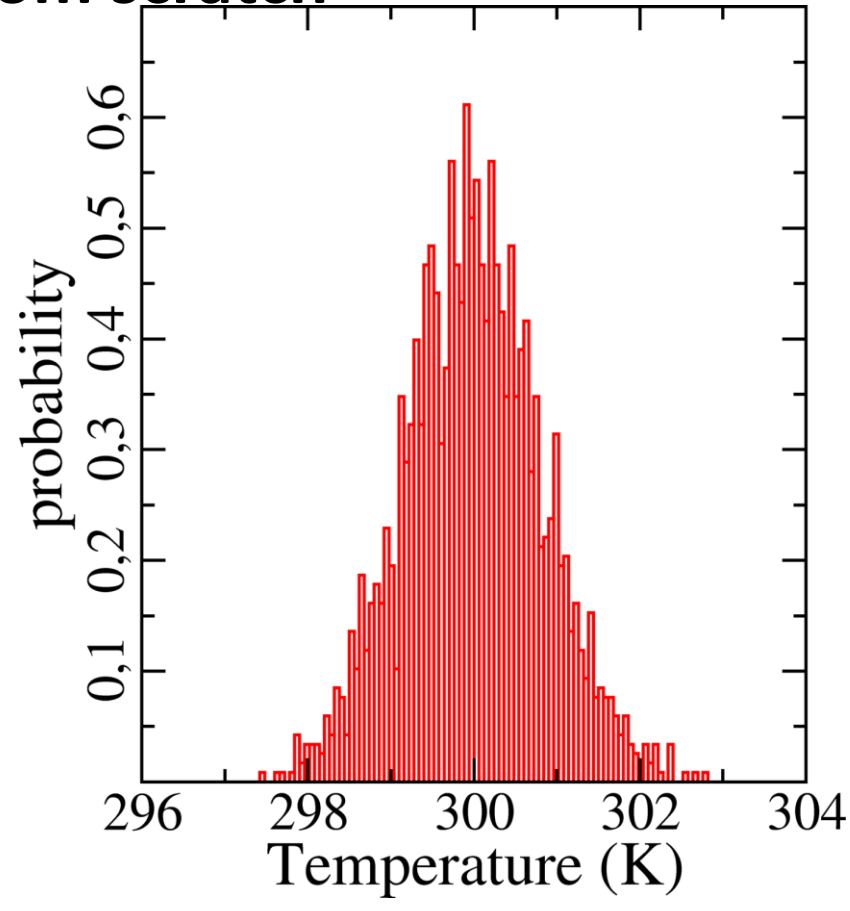
Building a MD simulation system from scratch

Define temperature

by assign velocities on particles

$$\left\langle \frac{1}{2} m_i v_i^2 \right\rangle = \frac{3}{2} k_b T$$



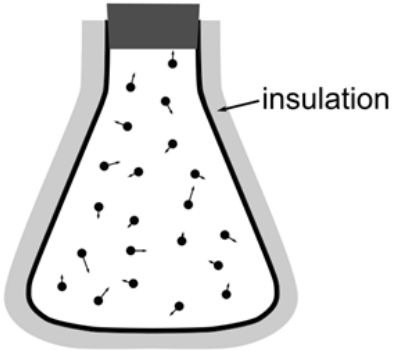


Practice of MD simulations

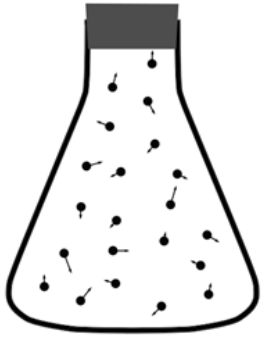
Building a MD simulation system from scratch

Choose ensemble (simulation conditions):

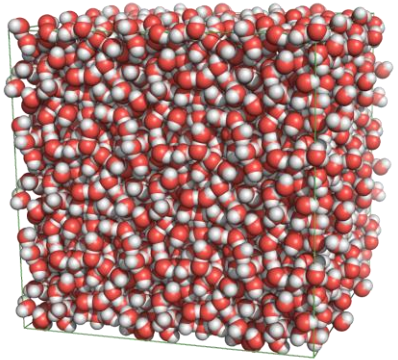
Npt, **NVT**, **NVE**, …

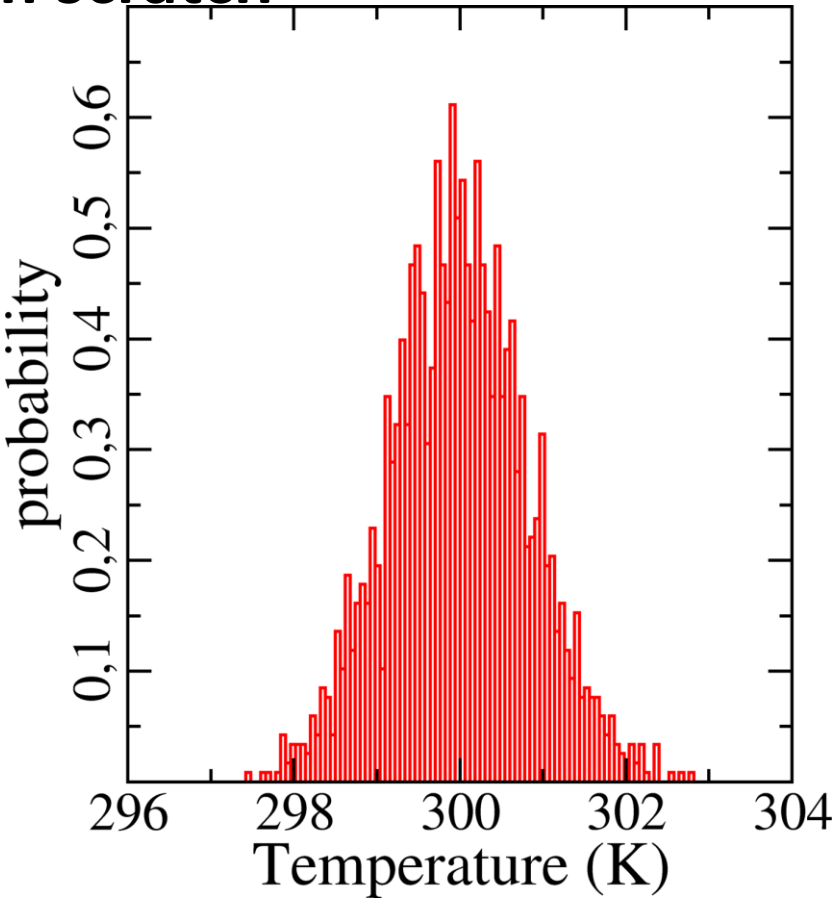


Microcanonical



Canonical



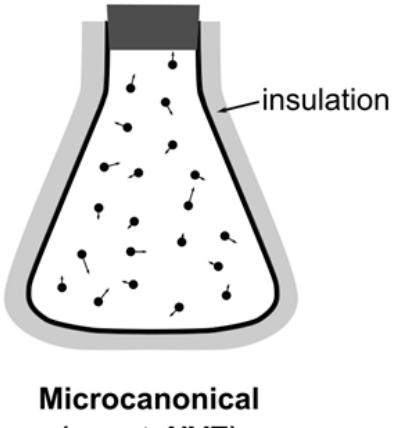


Practice of MD simulations

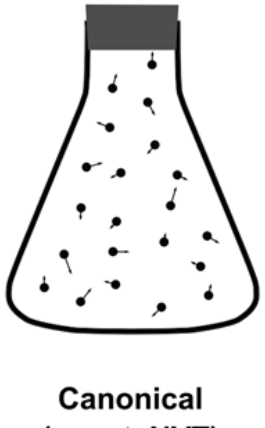
Building a MD simulation system from scratch

Pressure tensor:

$$P = \frac{1}{V}\left\{\sum_i mv_i^2 - \sum_{i<j} r_{ij}F_{ij}\right\}$$



Microcanonical



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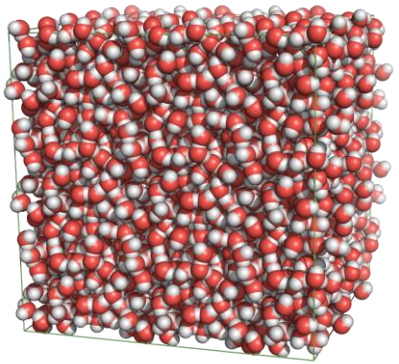
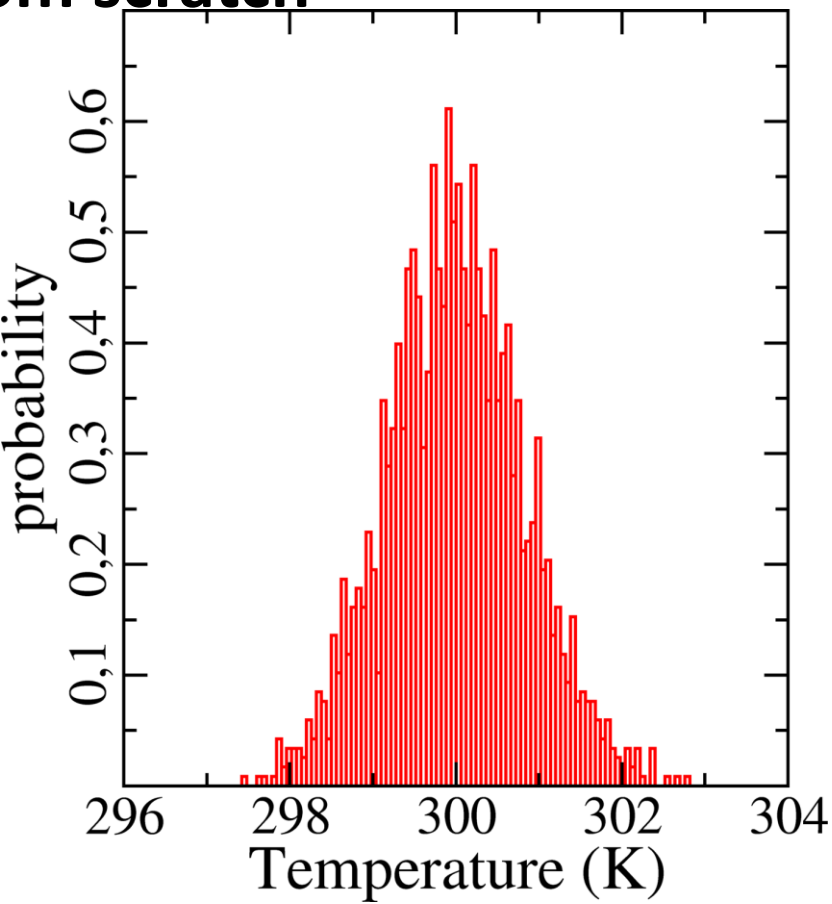




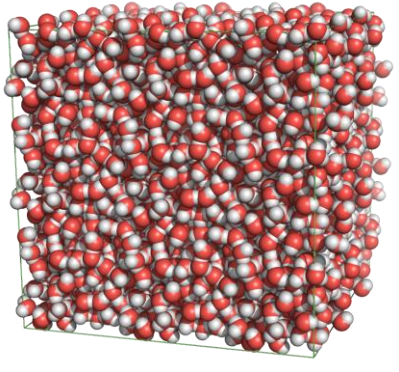
Practice of MD simulations

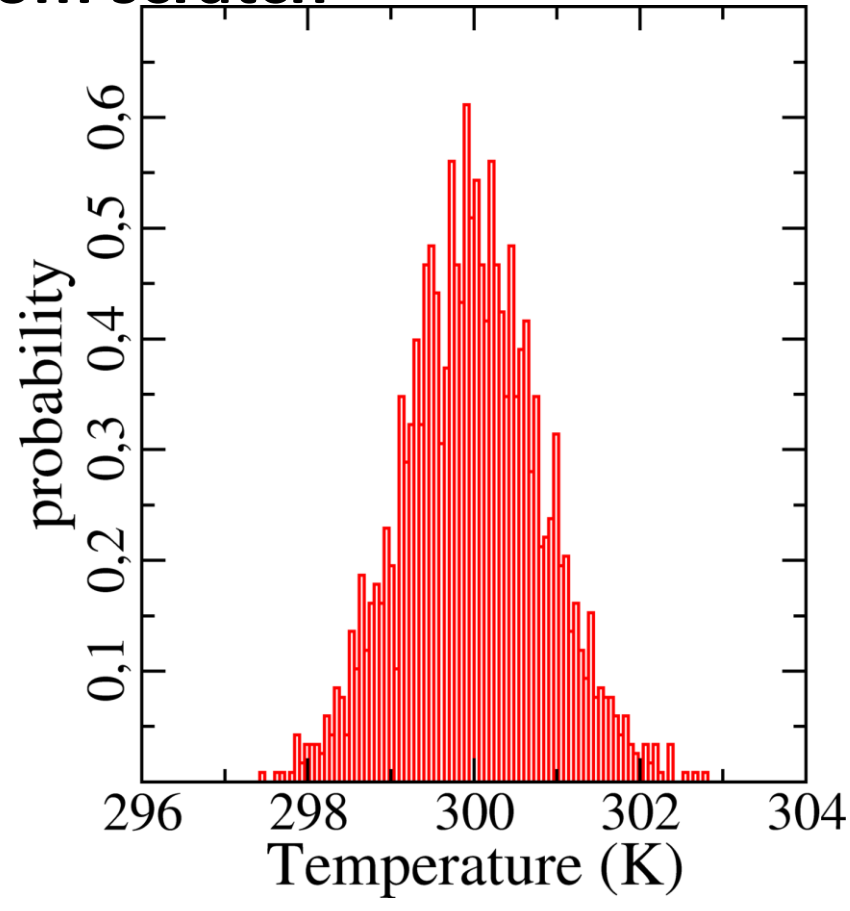
Building a MD simulation system from scratch

Setting constraint, adding extra field, applying force, …

Setting output frequency and variables.

Run and collect data ….

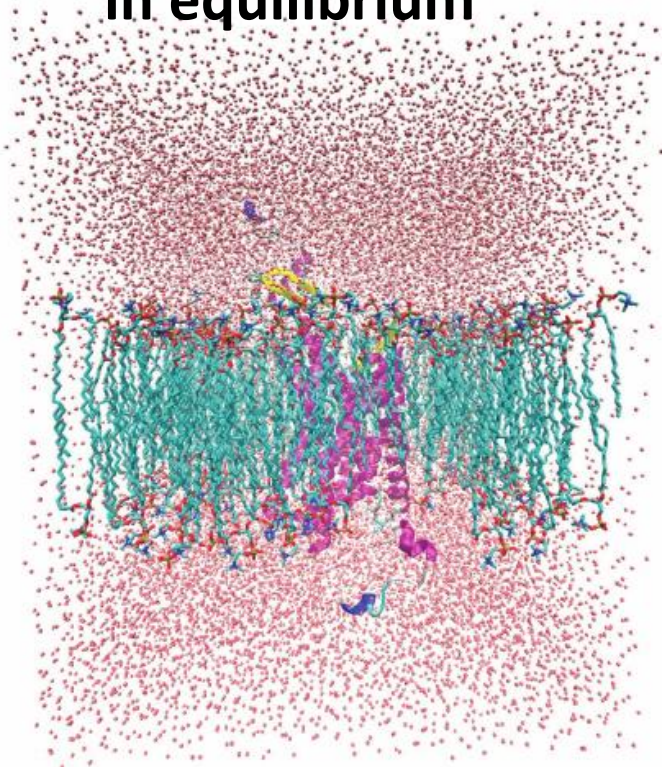




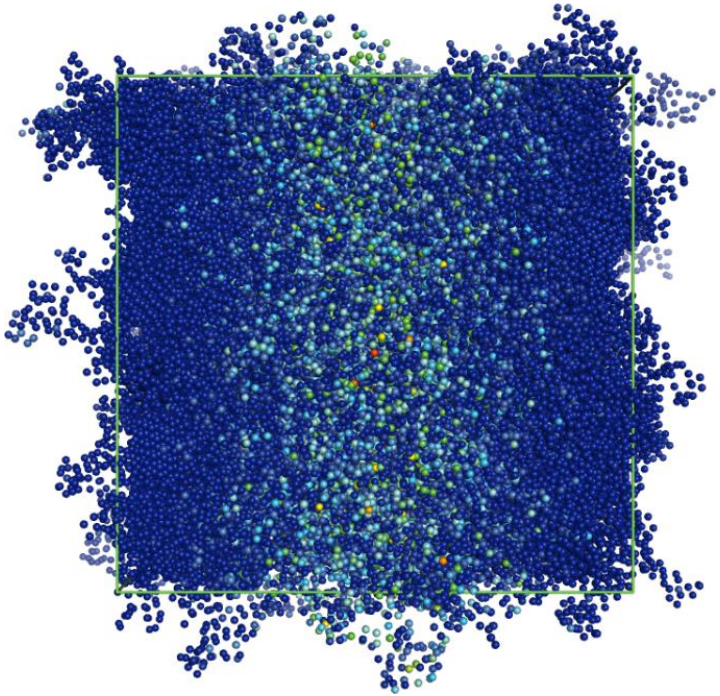
Practice of MD simulations

Equilibrium vs. Non-equilibrium

Membrane protein in equilibrium



Thermal transport in polymer nanocomposites



Practice of MD simulations

General guidelines:

- Think about the question before doing anything
- Choose or borrow potential/force-field parameters if possible
- (try not to make new potential/force-field parameter)
- Statistics, repetition and repetition
- Control simulations, significance tests
- ...

Molecular Dynamics (MD) simulations

Chemistry and biology

Structural prediction, drug design, energy calculation, dynamics of large biomolecules, ...

Computational physics and statistics

theory verification, many-body motion, ensemble properties, phase transition, ...

Materials science

crystal defects, material performance, microscopic fracture, interface design, melting, nanostructuring, ...

Molecular Dynamics (MD) simulations

Pros:

1. Only need description of inter-atomic interactions
2. No assumption is made
3. Provide atomistic coordinate and velocity trajectories

...

Cons:

1. Classical inter-atomic interactions
2. Poor description of light elements' motion
3. Small time and size scales

...

Further reading

1. D. Frenkel, B. Smit

   Understanding Molecular Simulation

   -From Algorithms to Applications

   Academic Press

2. D. C. Rapaport

   The Art of Molecular Dynamics Simulation

   Cambridge University Press