### MOLECULAR DYNAMICS SIMULATION

why simulation?

- replace expt.
- provoke expt.
- explain expt.
- and in establishing intellectual property.

Moreaure Modeling?

deserip of the atomic & molecular inter that govern microscopic 2 macroscopic behaviors of physical systems.

relation/connection b/w the macroscopic world provided by the theory of statistical mechanics.

#### Computational Took

Quantint Mechanics

(QM) Electronic

Structure (Schrödinger)

- · accurate · expensive)
- 10400 atoms small 10-100 Ps SYSTEM

classical Molecular Mechanits

(MM)

Emperical Forces (New ton)

- · less accurate
- · fast

104 - 105 atoms 10 - 100 ns

Mixed Quantum/ Classica (QM/MM)

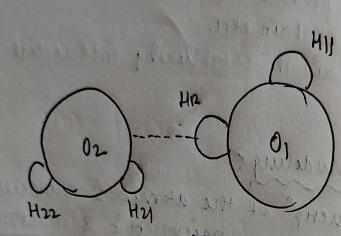
point mass, no electrons

104\_105 atoms

10-100 PS

# Proveins - performs functions in the order of milisee.

### 23/8/23



(2011 Yo11 Zo1) (2021 YO2 ZO2) (2411 YHIII ZHIV) (2421 YH221 ZH22)

(WM)

adole and the

3N raniables

of siderales

Monte Carlo 3N-6 Vaniables 20/6/33 solvation - water Periodic stochastic Boundary boundary conditions conde region of interest fully solvated is solvated in a central cell is water sphere at lasm simulated, in the environment produced by the repitition of the Explicit cell in all him. Solvew Model 00000000 > 0000000 --(00007-peniodic Repeats of each box has System of uniform no of INTEREST atoms, the algorithm takes care of otherwise terat applic? oplaws of physics becomes i MPOSETHLE a1b1c=[0, n] Electrostatic Energy of Crystal

 $V = \underbrace{\begin{cases} 3329i9j} \\ 3329i9j \end{cases}$  a=0, b=0, c=0  $\downarrow \text{ original box in } x \text{ dim}$ 

Periodic repeats of words. (Xi+La, yi, ti), (xi+dLa, yi, ti)+++(xi+NLa, yi (Xithal yithaiti), Xit hurier Transforme of Gaussian Charge Distible  $g(n) = \int g(x)e^{-2\pi ixh}dx$ each atmic- a charge:  $g'(h) = \int \exp(-kx^2) \exp(-i2nxh) dx$ = exp (-ah2) adding together for all atoms = g!(h)
& fourier transform again to
get the total every # Coarse Grain Models; centre of mass All-atom model (A1-A4) 16 (CH2 or CH3 atoms) contra at man (B1-B4)1

## VMD - Visualization.

Gromacs

Minimal input for MM

middle Minimis (released and

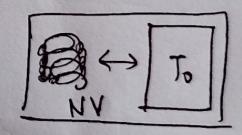
Structural Energetical (Thermod)
properties properties Topologicai properties force field NIVIT starting conform discript of the describing of the molecule NIPIT the force matdin

invalent connectivity of the molecules to be modeled

X-ray struc, NMR data/ Meoretical moder

aching on each atom of the molecules

fredoction dynastics MARINE ME



MD flowchart (M) Initial coord. (X-ray, NMR) Structure minimiz (release strain) (solvation (if explicit solvent) initial vélocities assignment. Hearing dynamics (T to 300K) Egbration, dymanuice (control of 12 struc es molecules TOKA of modeled Rescale structok? velocities Production dynamics (NVE/NVT, NPT) Analysis of trajectory Calcula of macroscopic values