

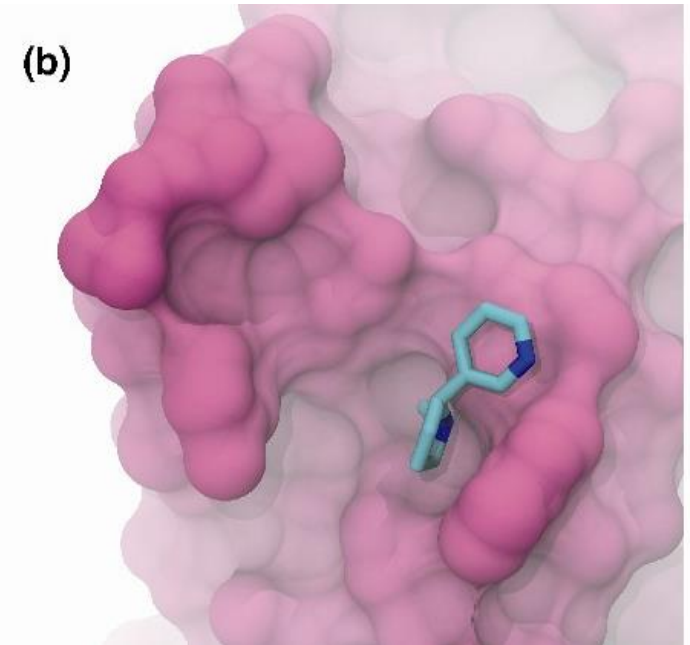
Molecular Dynamics Simulations

Ahmet Sacan

Some figures/examples are from: ...

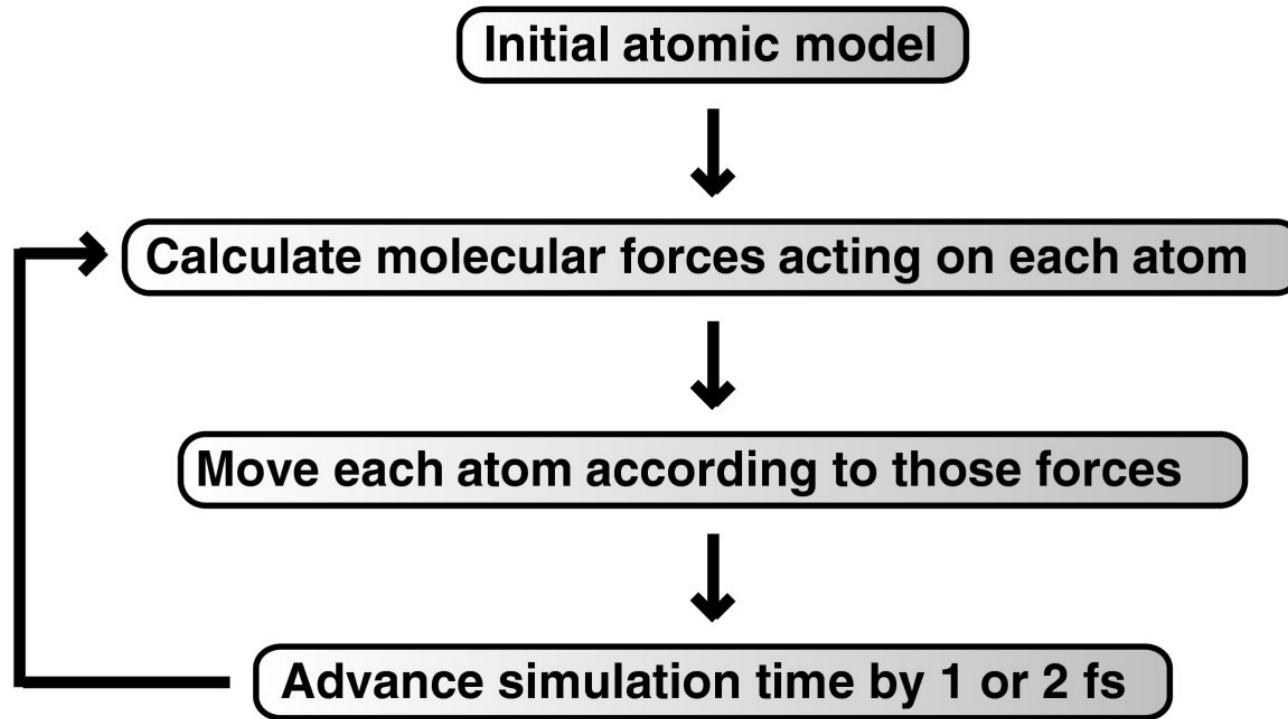
Molecular Dynamics (MD) Simulations

- Simulate a chemical system at an atomic scale
 - Real-world experiments may be too costly not possible
- Applications:
 - Identify 3D structure of molecules
 - Identify interactions among molecules
 - Drug design
 - Study material properties

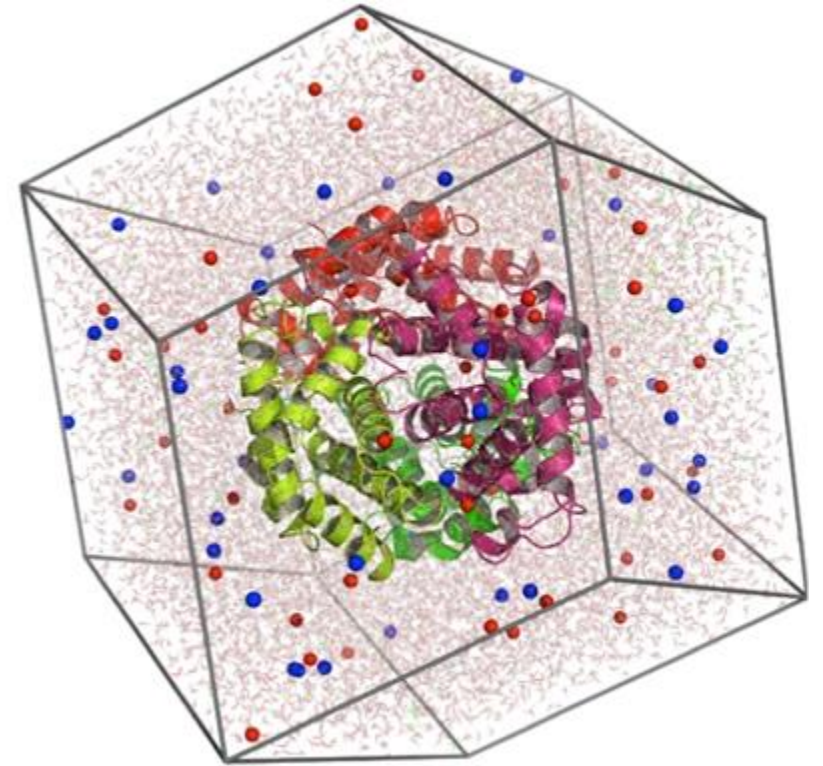


Durrant & McCammon, 2011

Steps in MD



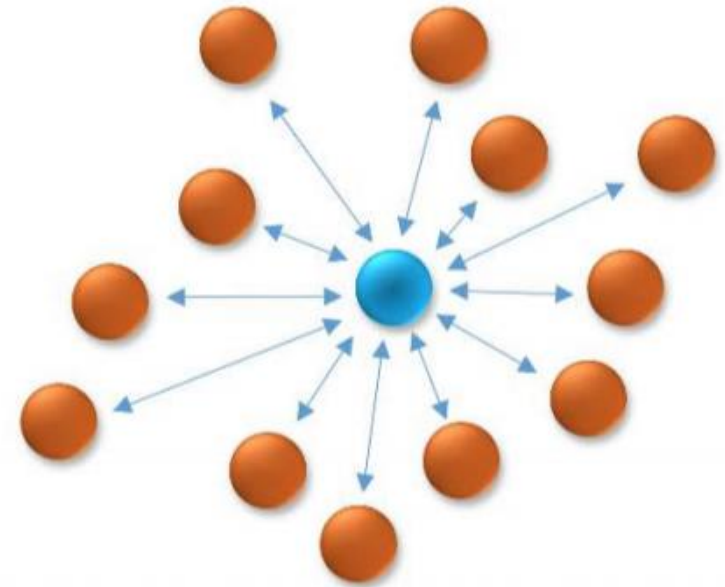
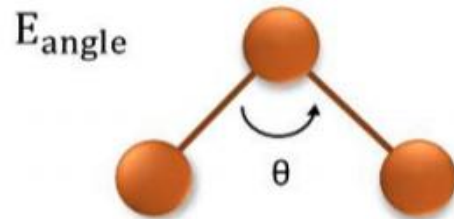
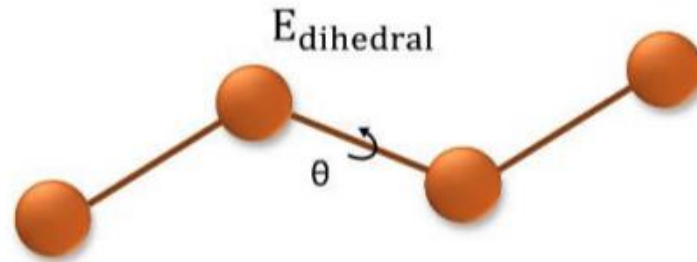
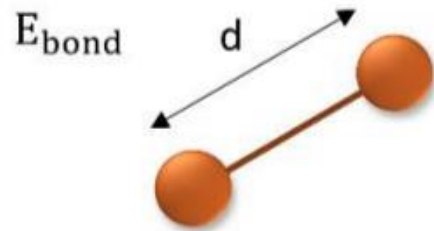
Durrant & McCammon, 2011



<https://www.creative-proteomics.com/services/molecular-dynamics-simulation-service.htm>

Energy Functions used in Force-fields

- Bonded (bond, angle, dihedral) and non-bonded energies (Vander-Waals, electrostatic)



$$E_{\text{non-bonded}} = E_{\text{elec}} + E_{\text{vdW}}$$