Molecular Dynamics Simulations

Simulations of the motion of atoms and molecules. Trajectories of molecules (position versus time) are calculated by numerically solving equations of motion originating from the Newton laws:

Force=mass* acceleration, F=m*a

Forces between interacting particles and potential energy are defined by molecular mechanics force fields.

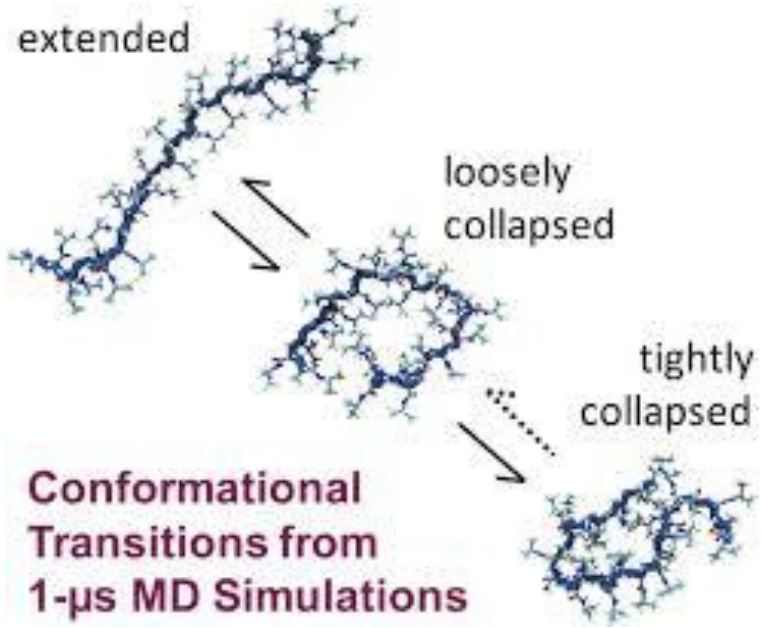
Main area of applications: materials science and modeling of biomolecules.

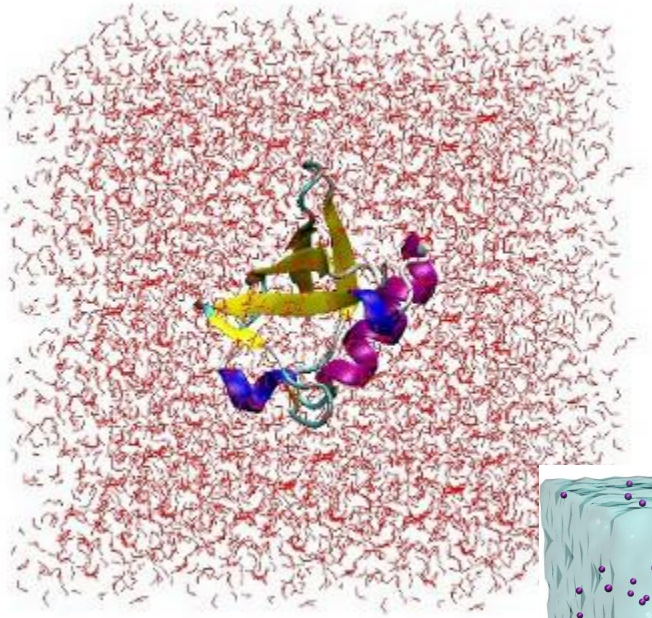
Examples of potential: gravitation field, electrostatic field

Potential energy – characterises forces that depend only on the position of the particle in space. Consequently, the potential energy also depends only on the position

Force field – the set of forces

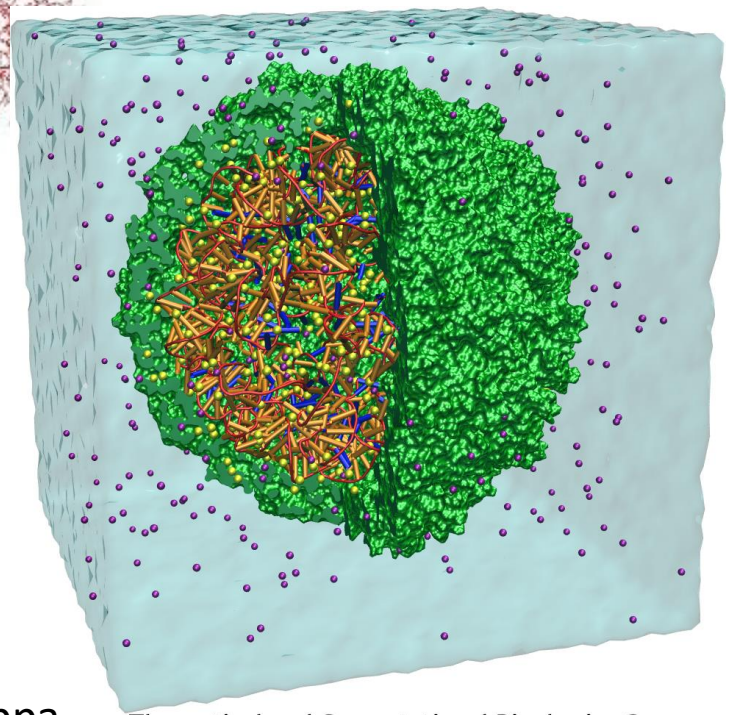
Molecular Dynamics Simulations





http://ringo.ams.stonybrook.edu/index.php/MD_Simulation:_Protein_in_Water

https://pubs.acs.org/doi/pdf/10.1021/acs.jpcb.6b09165?rand=fu7wimf5



https://www.ks.uiuc.edu/Research/STMV/images/virus_webpage.full.png

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Molecular Dynamics Simulations

- Each atom is treated as a single particle
- Each particle has an radius and polarizability
- Interactions are treated as “springs” with an equilibrium distance (harmonic oscillators)
- Atoms are treated as a hard spheres (balls)
- Collisions are perfectly elastic (the total kinetic energy and momentum is conserved, no changes in the particle shape)
- Atomic charges remain unchanged during the motion
- Bonds cannot be created (or destroyed)

Limitations

bigger systems for longer timescales – longer computation time

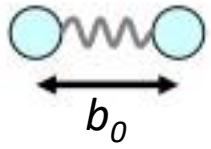
- protein aggregation on atomistic level, adsorption and diffusion mechanisms
- enzymes activity and insight into detailed catalytic activity mechanisms

Molecular Dynamics Simulations

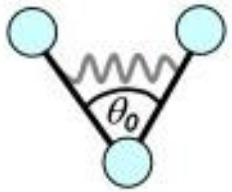
- Build the molecule – find the (*x,y,z*) position of all atoms
- Create (or apply existing) the force field
- Find the optimal structure (energy minimization)
- Solve the Newton's equations of motions of all atoms in the force field for each time point

Molecular Dynamics Simulations

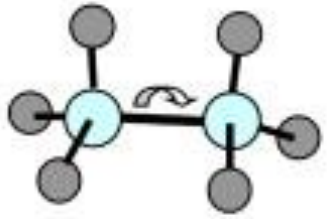
$$U(\vec{R}) = \frac{1}{2}\sum_{bonds} K_b (b - b_0)^2 +$$



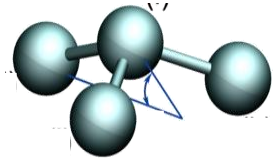
$$\frac{1}{2}\sum_{angles} K_\theta (\theta - \theta_0)^2 +$$



$$\sum_{dihedrals} K_\phi \left[1 + \cos(n\phi - \delta)\right] +$$



$$\sum_{impropers} K_\omega (\omega - \omega_0)^2 +$$

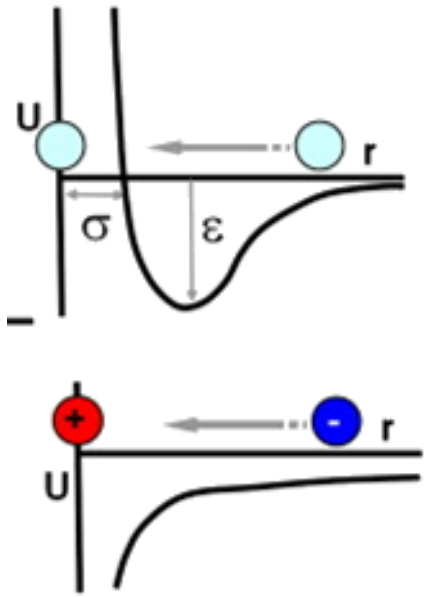


[Basic Principles of Molecular Dynamics (MD) - ARCHIE-WeSt](www.archie-west.ac.uk › 2012/06)
www.archie-west.ac.uk › 2012/06

Molecular Dynamics Simulations

$$\sum_{i>j}\left(\frac{A_{ij}}{r_{ij}^{12}}-\frac{B_{ij}}{r_{ij}^{6}}\right)+$$

$$\sum_{i>j}\frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}$$



Energy minimization methods -
to compute the equilibrium configuration of molecules

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Molecular Dynamics Simulations

The Verlet algorithm

Taylor expansion

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \frac{d\vec{r}_i(t)}{dt}\Delta t + \frac{1}{2}\frac{d^2\vec{r}_i(t)}{dt^2}\Delta t^2 + \frac{1}{6}\frac{d^3\vec{r}_i(t)}{dt^3}\Delta t^3 + O(\Delta t^4)$$

$$\vec{r}_i(t-\Delta t) = \vec{r}_i(t) - \frac{d\vec{r}_i(t)}{dt}\Delta t + \frac{1}{2}\frac{d^2\vec{r}(t)}{dt^2}\Delta t^2 - \frac{1}{6}\frac{d^3\vec{r}_i(t)}{dt^3}\Delta t^3 + O(\Delta t^4)$$

$$\vec{r}_i(t+\Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t-\Delta t) + \frac{d^2\vec{r}_i(t)}{dt^2}\Delta t^2 + O(\Delta t^4)$$

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Molecular Dynamics Simulations

The Verlet algorithm

Velocity:

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

Kinetic Energy:

$$E(t) = \sum_{i=1}^{N} \frac{m\vec{v}_i(t)^2}{2}$$

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Molecular Dynamics Simulations

The Verlet algorithm

The position of the atom is updated with Δt step

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \vec{v}_i(t)\Delta t + \frac{1}{2}\vec{a}_i(t)\Delta t^2$$

The velocity is updated with $\left(\Delta t + \Delta t/2\right)$ step:

$$\vec{v}_i\left(t+\frac{\Delta t}{2}\right) = \vec{v}_i(t) + \frac{1}{2}\vec{a}_i(t)\Delta t$$

Acceleration at $(t+\Delta t)$:

$$\vec{a}_i(t+\Delta t) = -\left(\frac{1}{m_i}\right)\nabla U\left(\vec{r}_i(t+\Delta t)\right)$$

Velocity at: $(t+\Delta t)$ $\vec{v}_i(t+\Delta t) = \vec{v}_i\left(t+\frac{\Delta t}{2}\right) + \frac{1}{2}\vec{a}_i(t+\Delta t)\Delta t$

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