भारतीय सांकेतिक विज्ञान संस्थ हैदराबाद
भारतीय प्रौद्योगिकी संस्थान हैदराबाद
Indian Institute of Technology Hyderabad

# Biomolecular Simulation BT2123

## Lecture 3 : Phase space and simple harmonic oscillator

Himanshu Joshi 09 January 2024

# Methodology : MD simulations

- Pick particles, masses and potential.

- Initialize positions and momentum.

$$-\frac{dU}{dr_i} = m_i \frac{d^2 r_i}{dt^2}$$

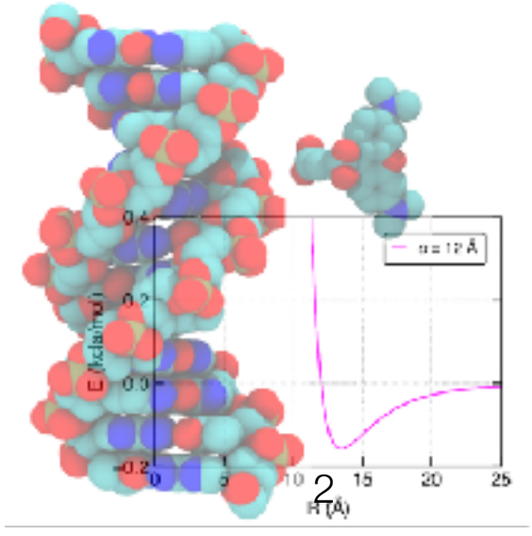
- Solve F = m a to determine r(t), v(t).

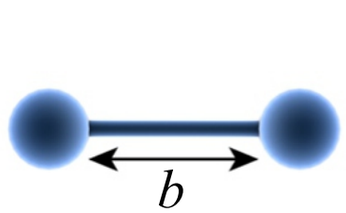
- Compute properties along the trajectory

- Try to use the simulation to answer physical questions.

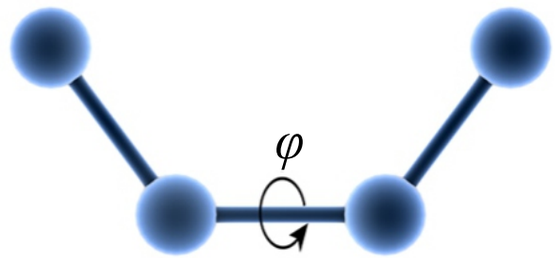
**Canonical ensemble**

N = 10, 000 to 1, 000,000
P= 1 atm
T= 300 K

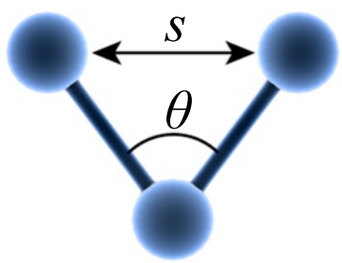




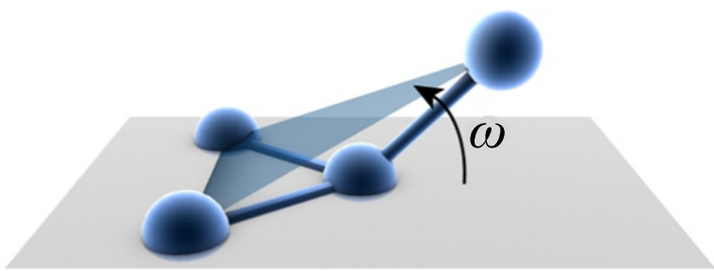
Bond Stretching



Proper dihedral torsion



Angle bending



Improper dihedral torsion

*Source: Behzad Mehrafrooz*

$$U = \sum_{\text{bonded}} \Big\{ \; k(r_{ij} - r_0)^2 + k_\theta(\theta - \theta_0)^2 + k(1 + \cos(n\psi + \phi)) \Big\}$$

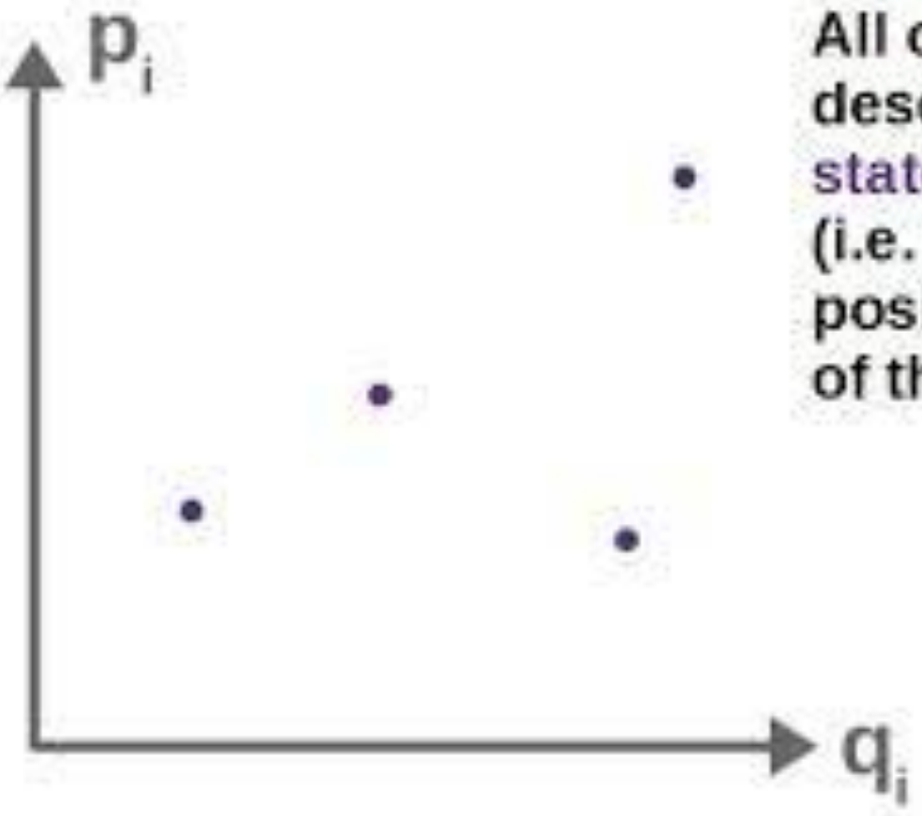
$$\sum_{i>j} \Big\{ \; -U_{\min}\left[\left(\frac{R_{\min}}{r_{ij}}\right)^{12} - 2\left(\frac{R_{\min}}{r_{ij}}\right)^{6}\right] + \frac{C q_i q_j}{\epsilon_0 r_{ij}} \Big\}$$

Hamiltonian mechanics

Newtonian mechanics

Lagrangian mechanics

# Phase space




- All of these points describe different states of the system (i.e. different values of position and momenta of the system)