MD Simulation
Part II

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Newton's Laws of Motion

- Newton's laws are the corner stones of the classical physics
- Newton's First Law (law of inertia):
  - If the vector sum of all forces on an object sum up to zero, then the velocity and trajectory of that object will remain unchanged
- Newton's Second Law:
  - Acceleration of an object is proportional to the sum of forces applied to that object

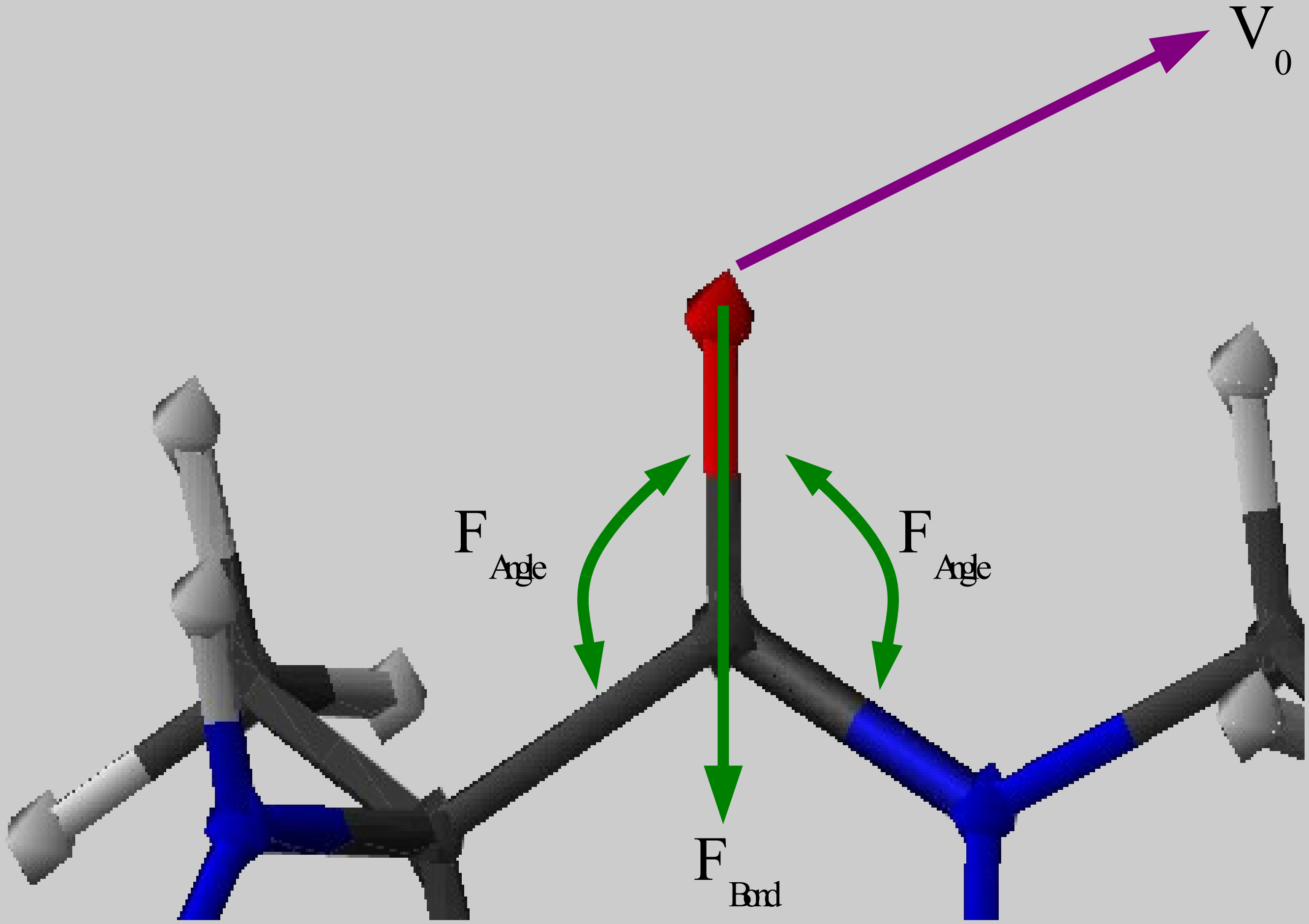
$$F = \frac{dP}{dt} = \frac{d\left(m \cdot v\right)}{dt} = \frac{dm}{dt} \cdot v + m \cdot \frac{dv}{dt} = \frac{dm}{dt} \cdot v + m \cdot a \qquad \vec{F} \propto \vec{\nabla} P$$

- Newton's Third Law:
  - For every action there is an equal and opposite reaction

Laws of Thermodynamics

- Laws of thermodynamics describe describe the transport of heat and work in thermodynamic processes
- They are mostly concerned with closed systems
- First Law (conservation of energy):
  - Energy can neither be created nor destroyed. It can only change forms.
- Second Law:
  - Energy systems have a tendency to increase their entropy rather than decrease it.
- Third Law:
  - As temperature approaches absolute zero, the entropy of a system approaches a constant minimum.

Basics of MD Simulation



Assignment of Initial Velocities in MDS

- Xplor-NIH provides the following three methods of assigning initial velocities:
  - Blotzman-Maxwell distribution
    - IASVel = MAXWell

$$\vec{v}_i = \left(\frac{m_i}{2\pi k_B T_I} \right)^{\frac{3}{2}} e^{\left(-3m_i \delta^2 \big/ 2k_B T_I \right)}$$

  - Uniform distribution
    - IASVel=UNIForm

$$\vec{v}_i = U\left[0, \frac{T_I k_B}{m_i} \right]$$

  - Current velocities stored in vectors Vx, Vy and Vz
    - IASVel= CURRent

set seed=432324368 end
vector do (vx=maxwell(4000.)) (all)
vector do (vy=maxwell(4000.)) (all)
vector do (vz=maxwell(4000.)) (all)

Role of Temperature in MD Simulations

- Temperature has an impact on the initial and therefore the intermediate velocities
- Xplor-NIH allows three methods of controlling temperature
- We will only use velocity rescaling
  - IEQFrq= frequency of the velocity rescaling

$$v_i^{new} = \begin{cases} v_i^{old}\sqrt{3\,n\,k_B T_0 / \left\langle \sum_i m v_i^{old}(t)^2 \right\rangle} & \text{If ISCVel} = 0 \\ v_i^{old}\sqrt{3\,n\,k_B T_0 / \left\langle m v_i^{old}(t)^2 \right\rangle} & \text{If ISCVel} = 1 \end{cases}$$

Demonstration

- Examine and understand
  - MDS.BM.inp
  - MDS.FixedV.inp