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

\[ F = \frac{dP}{dt} = \frac{d(m \cdot v)}{dt} = \frac{dm}{dt} \cdot v + m \cdot \frac{dv}{dt} = \frac{dm}{dt} \cdot v + m \cdot a \]

\[ \vec{F} \propto \vec{\nabla} P \]

• Newton's Third Law:
  – For every action there is an equal and opposite reaction
Laws of Thermodynamics

- Laws of thermodynamics describe 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

$F_{Bnd}$

$F_{\text{Angle}}$

$V_0$
Assignment of Initial Velocities in MDS

- **Xplor-NIH** provides the following three methods of assigning initial velocities:
  - **Blotzman-Maxwell distribution**
    - IASVel = MAXWell
      
      \[
      \vec{v}_i = \left( \frac{m_i}{2\pi k_B T_l} \right)^{\frac{3}{2}} e^{-\frac{3m_i \delta^2}{2k_B T_l}}
      \]
  
  - **Uniform distribution**
    - IASVel=UNIFORM
      
      \[
      \vec{v}_i = U\left[0, \frac{T_l k_B}{m_i}\right]
      \]
  
  - **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

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

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