Modelling Polymer Dynamics

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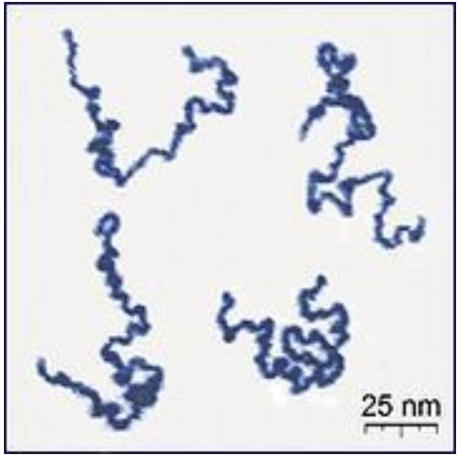
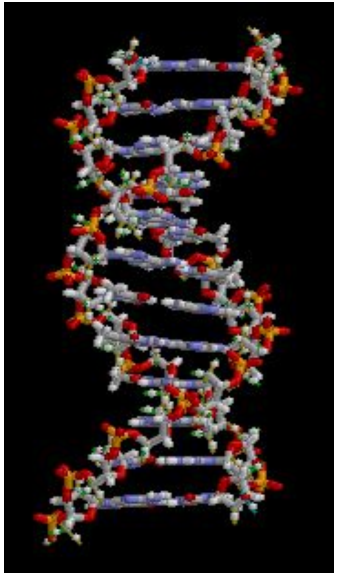
PS10 Final Project

Polymers

- “Substance or material consisting of large macromolecules with repeating subunits” (Wikipedia)





Movement

- Based on Boltzmann Distribution
- Due to thermal fluctuations

$$P(X) = Ae^{\frac{-\epsilon_i}{k_B T}}$$

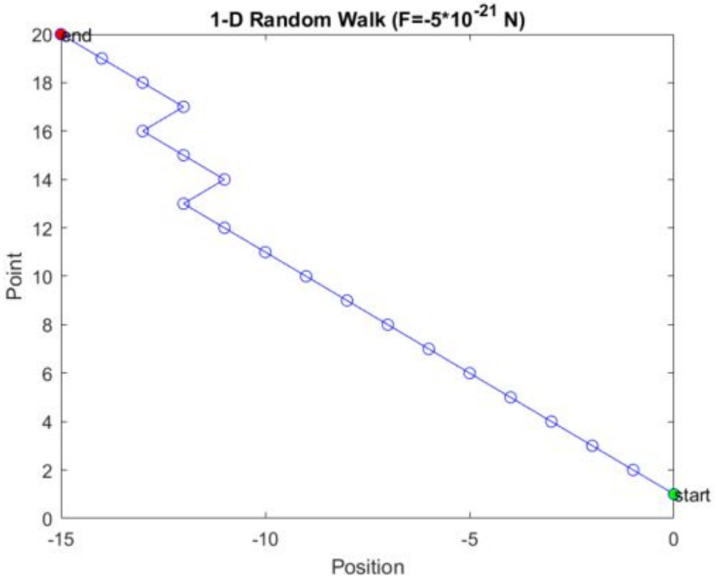
1D Polymer Dynamics

Probability Distribution (1D)

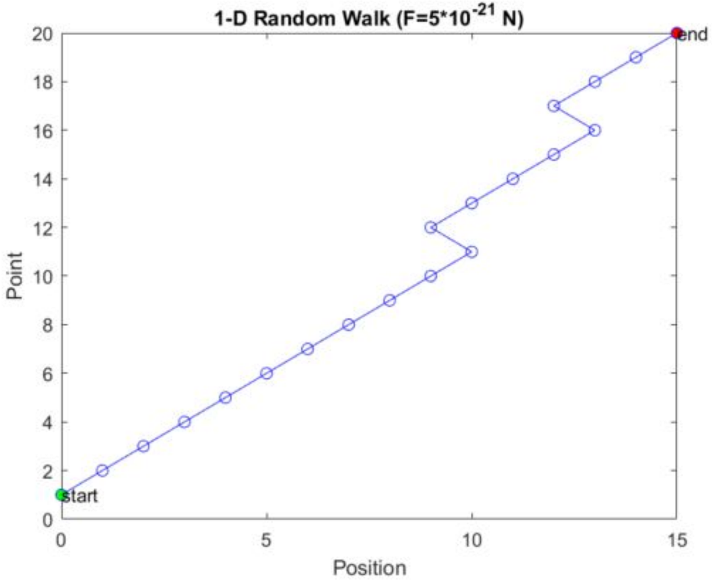
$$P(L|R) = \frac{e^{\frac{-\epsilon_i}{k_B T}}}{2\cosh(\frac{FL}{k_B T})}$$

$$\epsilon_i = \pm FL$$

Polymer 1D Simulation Results



Leftward Force



Rightward Force

2D Polymer Dynamics

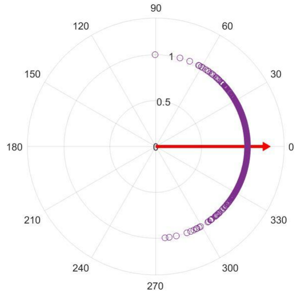
Probability Distribution (2D)

$$P(\theta) = Ae^{\frac{-\epsilon_i}{k_B T}}$$

$$A = \frac{1}{\int_0^{2\pi} e^{\frac{-\epsilon_i}{k_B T}} d\theta}$$

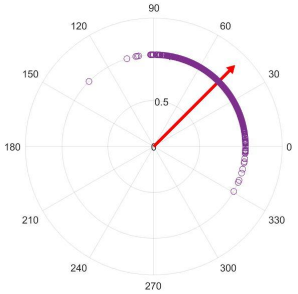
$$\epsilon_i = -\vec{L} \cdot \vec{F} = -L \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix} \cdot \begin{bmatrix} F_x \\ F_y \end{bmatrix}$$

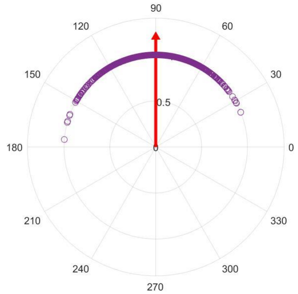
Probability Distribution (2D)



Rightward Force
θ=0 rad.

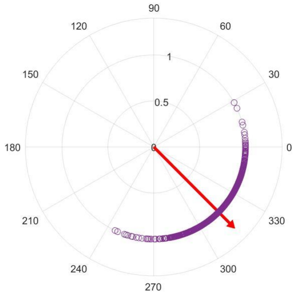
Up-Right Force
θ=π/4 rad.





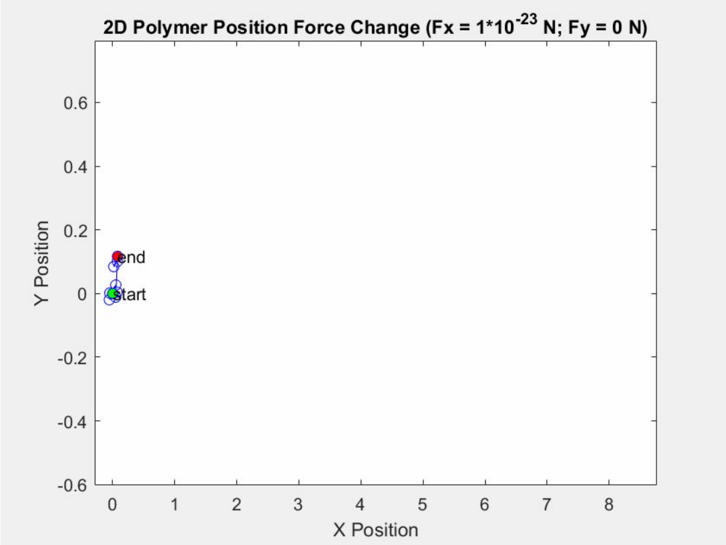
Upward Force
θ=π/2 rad.

Down-Right Force
θ=-π/4 rad.

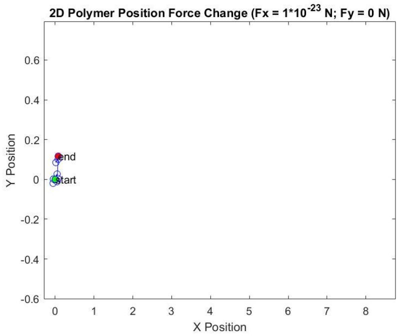


Increasing Force (2D)

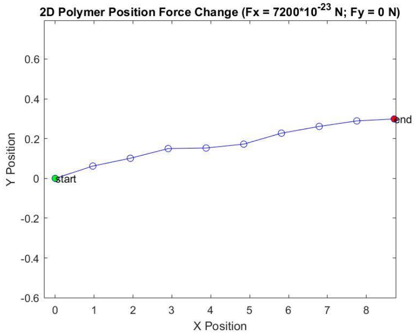
$$P(\theta) = Ae^{\frac{-\vec{L}\cdot\vec{F}}{k_B T}}$$



Start position

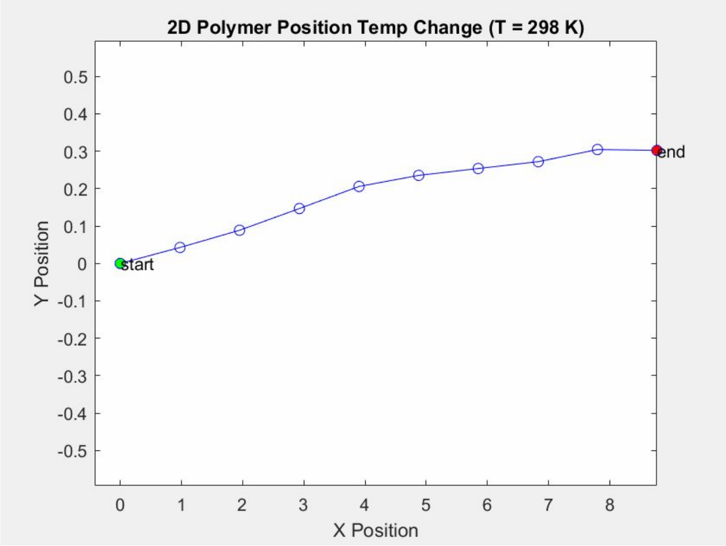


End position

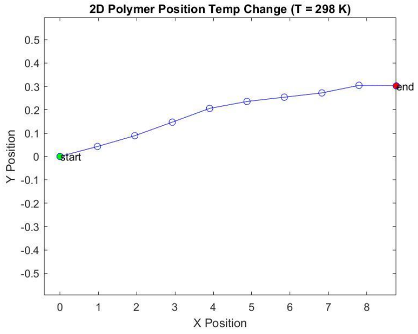


Increasing Temperature (2D)

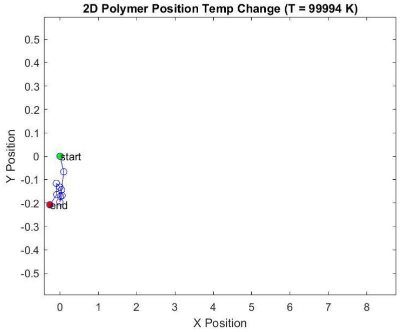
$$P(\theta) = Ae^{\frac{-\vec{L}\cdot\vec{F}}{k_B T}}$$



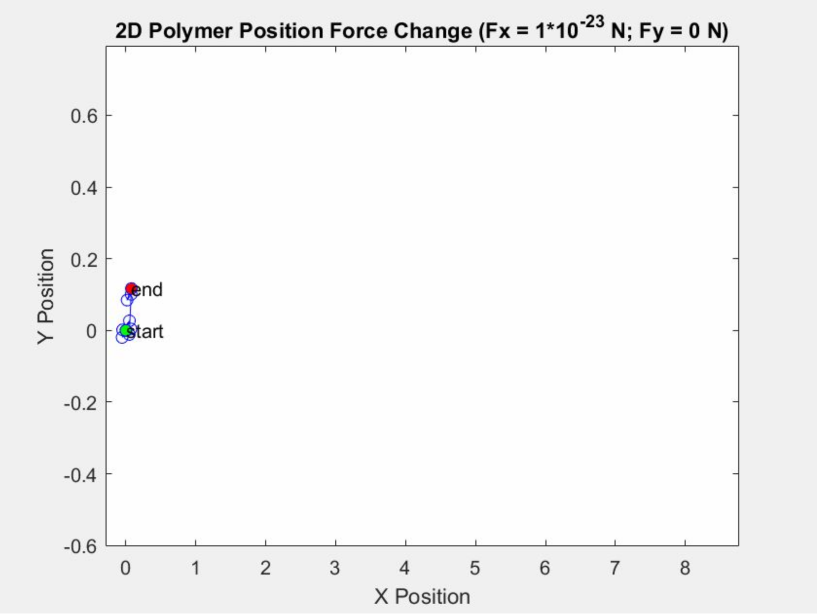
Start position

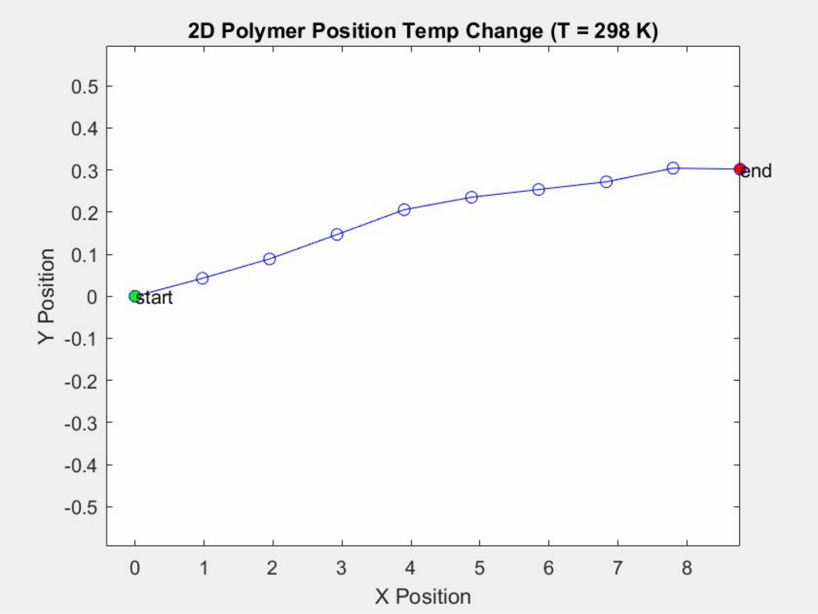


End position



Polymer 2D Simulation Results





3D Polymer Dynamics

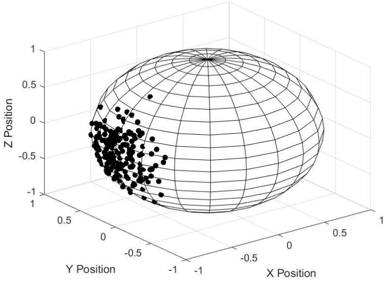
Probability Distribution (3D)

$$P(\theta) = Ae^{\frac{-\epsilon_i}{k_B T}}$$

$$A = \frac{1}{\int_0^{\pi} \int_0^{2\pi} e^{\frac{-\epsilon_i}{k_B T}} d\theta d\phi}$$

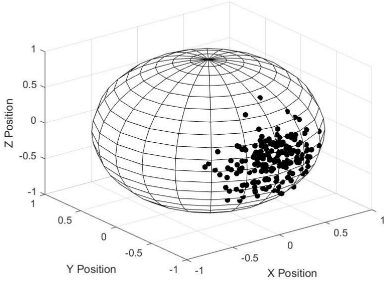
$$\epsilon_i = -\vec{L} \cdot \vec{F} = -L \begin{bmatrix} \sin\phi\cos\theta \\ \sin\phi\sin\theta \\ \cos\phi \end{bmatrix} \cdot \begin{bmatrix} F_x \\ F_y \\ F_z \end{bmatrix}$$

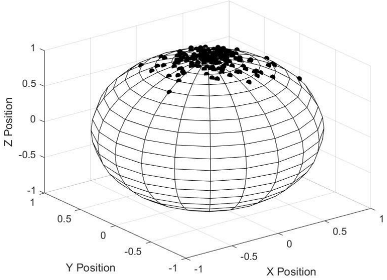
Probability Distribution (3D)



X Force
$[F\ 0\ 0]^T$

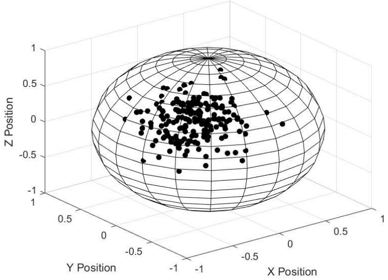
Y Force
$[0\ F\ 0]^T$





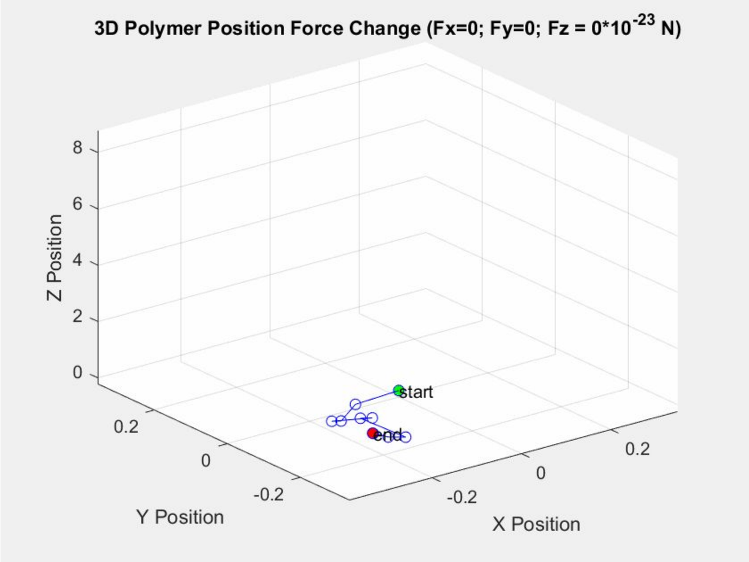
Z Force
$[0\ 0\ F]^T$

XYZ Force
$[-F\ -F\ F]^T$

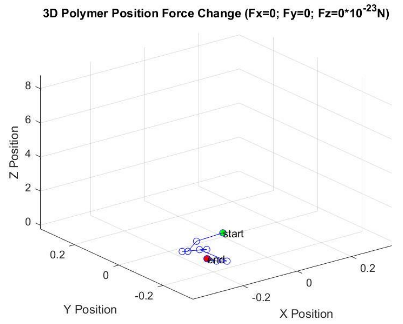


Increasing Force (3D)

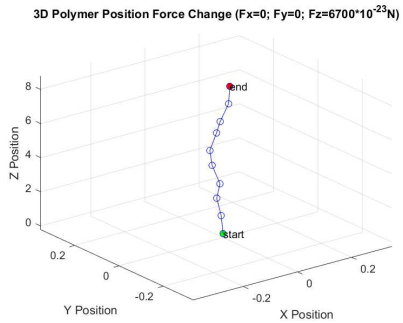
$$P(\theta, \phi) = A e^{\frac{-\vec{L} \cdot \vec{F}}{k_B T}}$$



Start position

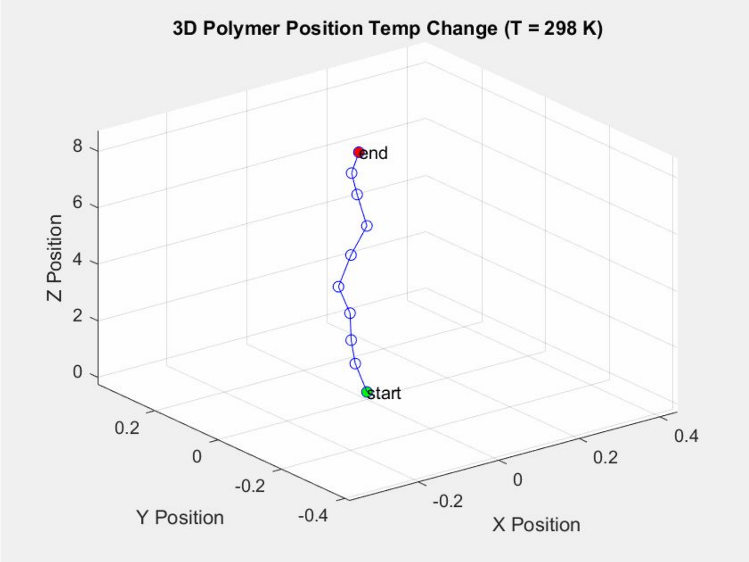


End position

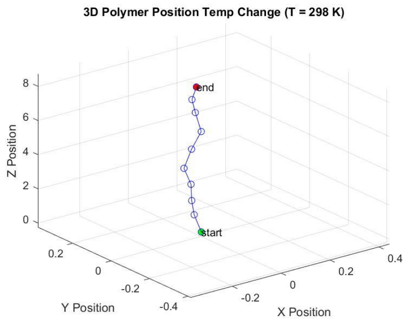


Increasing Temperature (3D)

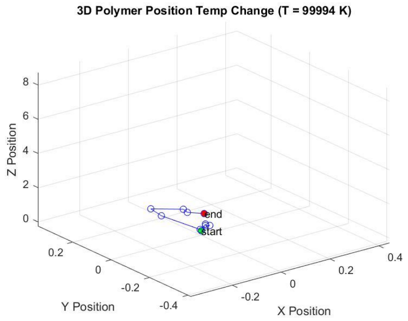
$$P(\theta, \phi) = Ae^{\frac{-\vec{L}\cdot\vec{F}}{k_B T}}$$



Start position



End position



Polymer 3D Simulation Results