Introduction

Polymer folding is an important process in biology and chemistry. This is particularly true in biology for proteins, whose function is strongly dependent on how their 3D structure is folded togeather. In chemistry, polymer folding has significant application in understanding the material properties of materials, including assessing the strength and flexibility, giving us the ability to design better materials and tailor them for various applications including advanced composites and space technology.

In this project, I simulated a polymer chain through the bead-chain model in order to understand how temperature affects the changes in a polymer folding. I aimed to assess the stability of the polymer chain through analysis of radius of gyration, end-to-end distance, and potential energy in order to find ways to prevent polymer folding under low temperatures for material design with regard to space applications.

Methods

In this simulation, I used the bead-spring model, where the polymer chain is reperasented by a line of beads connected togeather via springs. In this model beads represent the repeating units of the polymer and the springs match up to the bonds connecting those repeating units.

I used Harmonic Potentials to model the interactions between adjacent beads. This was further enhanced via Lennard-Jones Potentials, which use excluded volume repulsive potentials between beads seperated by just one spacer and attractive potentials between beads with more than one spacer. I then use the velocity verlet algorithm on the computed forces to integate the equations of motion and simulate movement.

In order to simulate positions, I used the periodic boundary conditions, which are able to take out the edge effects that would limit a finite system. These conditions work by making particles that leave one side of the simulation re-enter through the opposite side, effectively creating an infinite system.

Lastly, after simulating positions, computing forces, and integrating, I applied a velocity rescaling themostat in order to maintain constant temperature by constantly rescaling particle velocities throughout the system to match the desired temperature.

I primarily tested the effects of changing temperature range from 0.1 to 1 in order to understand how the polymer performed under different temperature configurations. Then values of k and repulsive epsilon were varied in order to find values that prevent low temperature folding ranging from 0 to 5. Lastly, I varied the chain length from 5 to 25 in order to understand how the length of the polymer chain affects folding behavior.
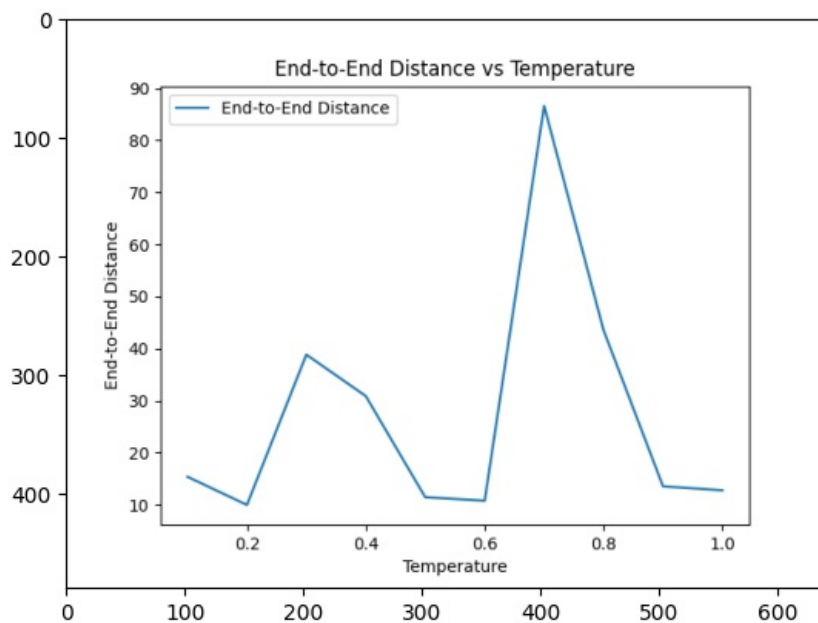
Results

Temperature

We first kept the polymer length at 20 with epsilon repulsive and k at 1, varying temperature from 0.1 to 1. The corresponding plot is show below.
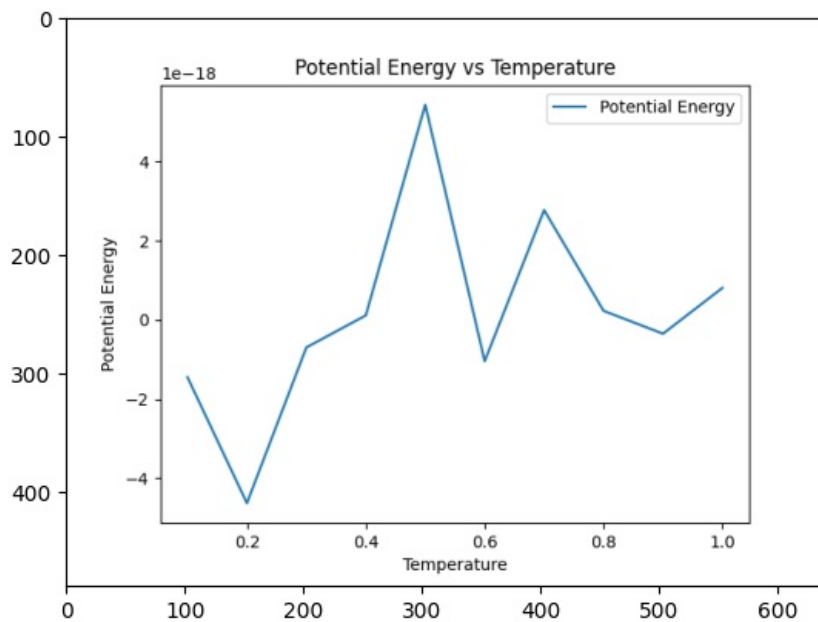
```
In [1]:   import matplotlib.pyplot as plt
          import matplotlib.image as mpimg
          img = mpimg.imread('pics/radius.png')
          imgplot = plt.imshow(img)
          plt.show()
```
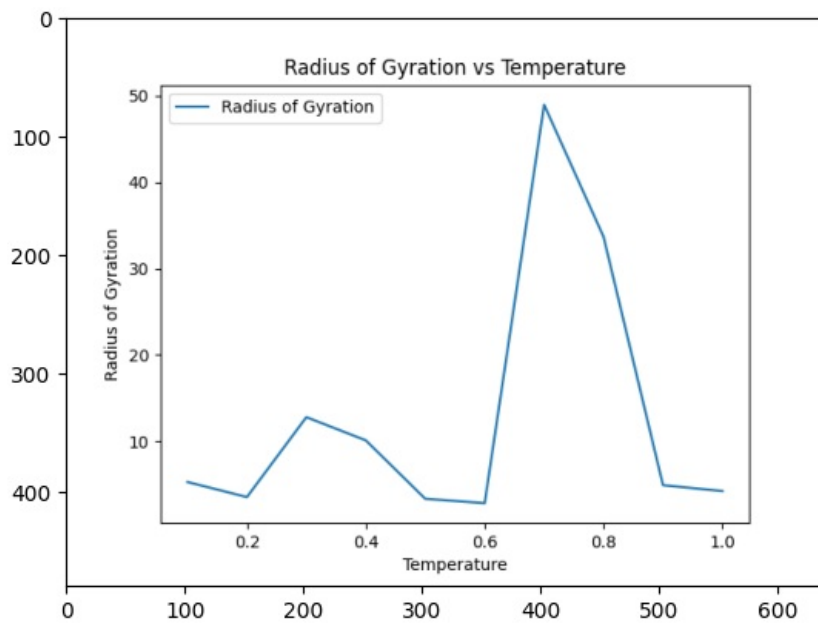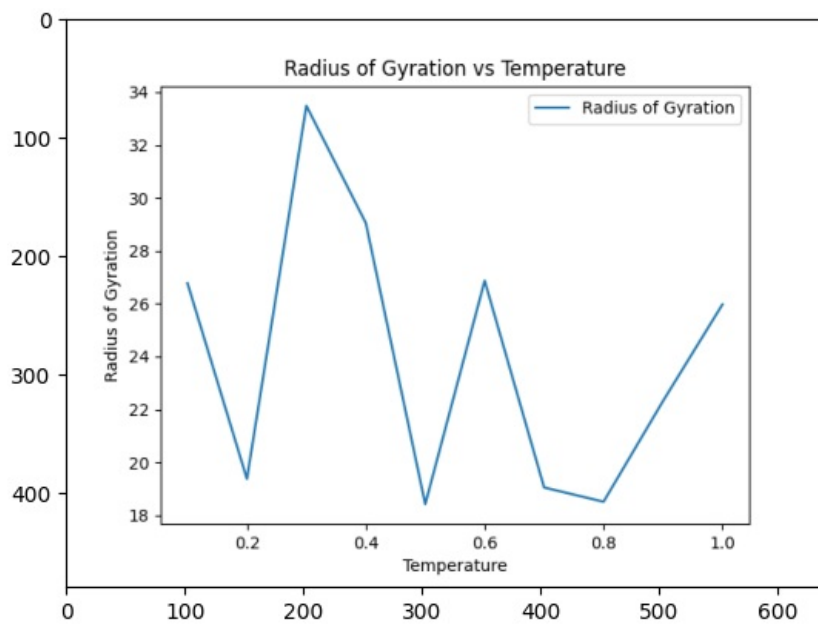
```python
In [4]: import matplotlib.pyplot as plt
        import matplotlib.image as mpimg
        img = mpimg.imread('pics/U.png')
        imgplot = plt.imshow(img)
        plt.show()
```

Potential Energy vs Temperature

1e−18

Potential Energy

Potential Energy

0.2   0.4   0.6   0.8   1.0
Temperature

In this simulation, we observed a phase transition from folded to unfolded around 0.6 temperature which can be seen from the radius of gyration plot which shows how the radius of gyration goes from being relatively small and constant to spiking upward which indicates that the dimensions of the polymer chain have increased substantially. This is further backed by the change in the end-to-end distance spiking around the same value and in the potential energy chart, where you see a build-up in potential energy just before 0.6, before the system reconfigures at 0.6 in order to find a more optimal energy configuration.

In [5]:
```python
# k = 0
import matplotlib.pyplot as plt
import matplotlib.image as mpimg
img = mpimg.imread('pics/k0.png')
imgplot = plt.imshow(img)
plt.show()
```

Radius of Gyration vs Temperature

Radius of Gyration

Radius of Gyration

0.2   0.4   0.6   0.8   1.0
Temperature

In [7]:
```python
# k = 2
import matplotlib.pyplot as plt
import matplotlib.image as mpimg
img = mpimg.imread('pics/k2.png')
imgplot = plt.imshow(img)
plt.show()
```
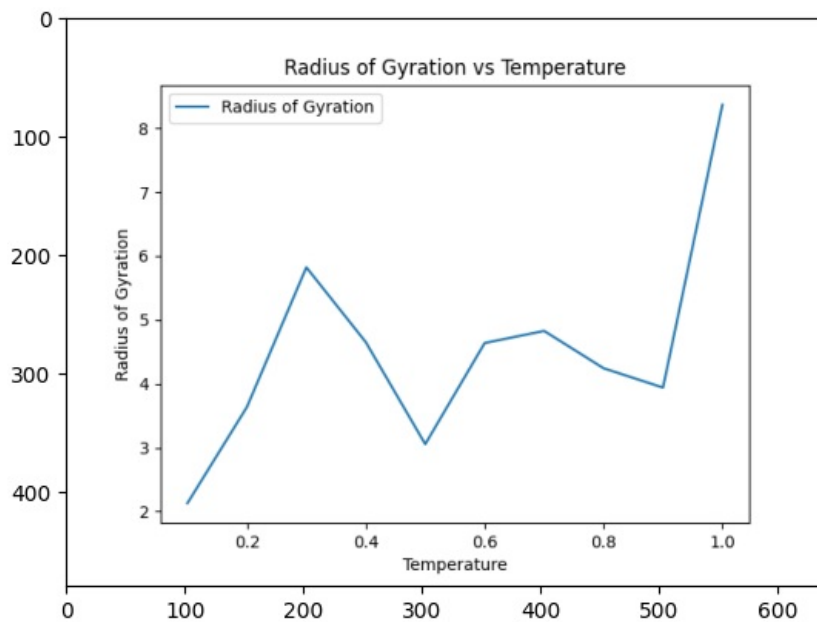
Spring Constant

As I increased the spring constant, generally the temperature at which we saw a large spike in a radius of gyration increased. This is indicative of the polymer unfolding and shows that as we increase the strength of adjacent bonds, it becomes harder and harder for the polymer to get out of the initial configuration. You can see in the above plot that for the maximum tried k value, its not until about 0.9 temperature that you get the spike in radius of gyration. Generally, lower values of k appear to make the polymer more nimble and allow it to make changes quicker in order to adapt to changes in the system.

In [10]:
```python
# epsilon repulsive = 0
import matplotlib.pyplot as plt
import matplotlib.image as mpimg
img = mpimg.imread('pics/e0.png')
imgplot = plt.imshow(img)
plt.show()
```
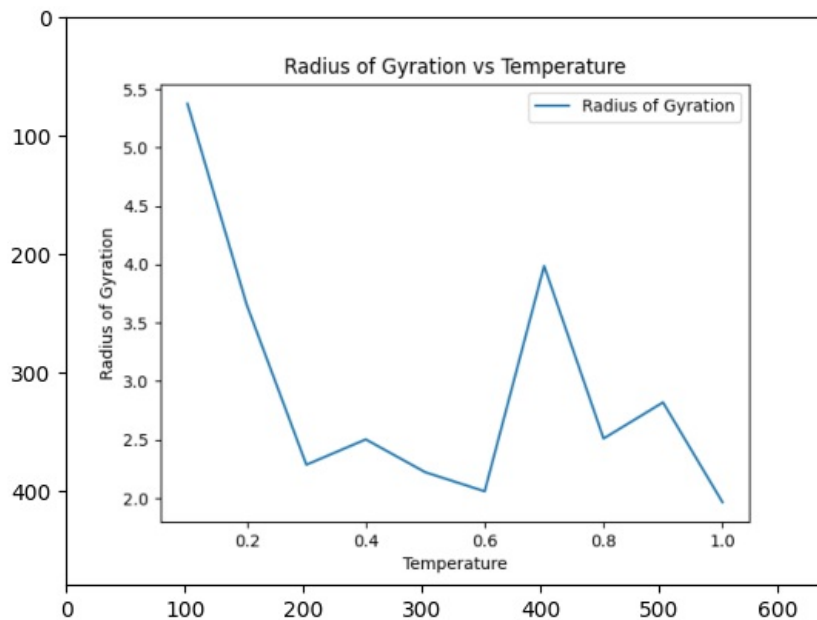

In [11]:
```python
# epsilon repulsive = 2
import matplotlib.pyplot as plt
import matplotlib.image as mpimg
img = mpimg.imread('pics/e2.png')
imgplot = plt.imshow(img)
plt.show()
```
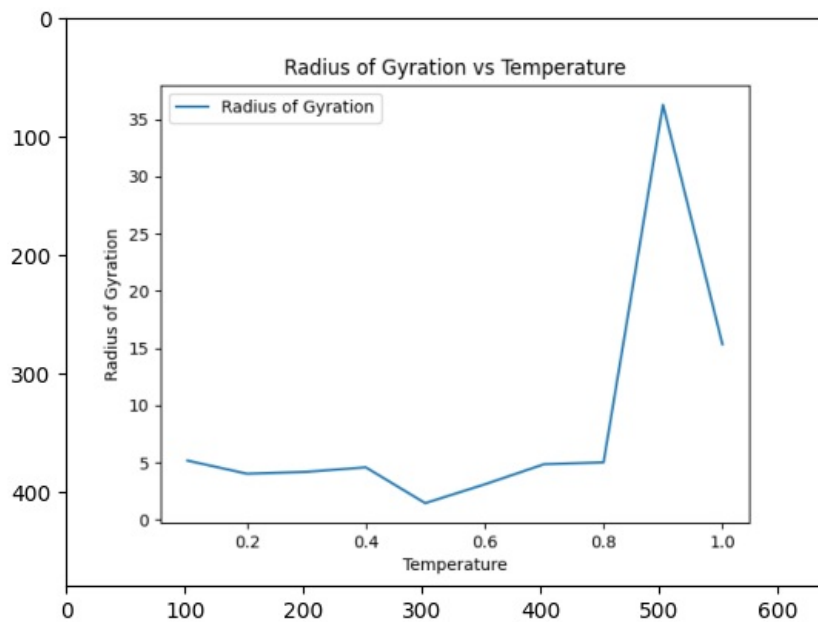
Epsilon Repulsive

For lower levels of epsilon repulsive, the spikes in radius of gyration happened earlier, leaving me to conclude that with lower epsilon repulsive the polymer was more willing to take on a unfolded state at lower temperatures. This is a somewhat suprising result given that I would have expected it to be harder to remain folded if there were stronger excluded volume effects. I would guess that with higher levels of epsilon repulsive, the polymer is more resistant to moving so is attempting to stay folded for longer but I am a little unsure.

```
In [12]: # chain length = 5
         import matplotlib.pyplot as plt
         import matplotlib.image as mpimg
         img = mpimg.imread('pics/n5.png')
         imgplot = plt.imshow(img)
         plt.show()
```
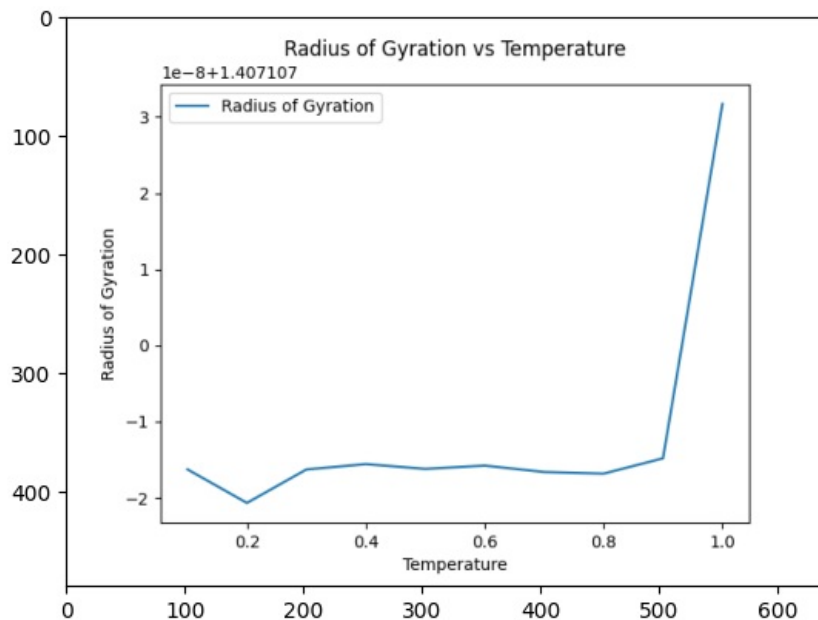


```
In [13]: # chain length = 25
         import matplotlib.pyplot as plt
         import matplotlib.image as mpimg
         img = mpimg.imread('pics/n25.png')
         imgplot = plt.imshow(img)
         plt.show()
```

Radius of Gyration vs Temperature
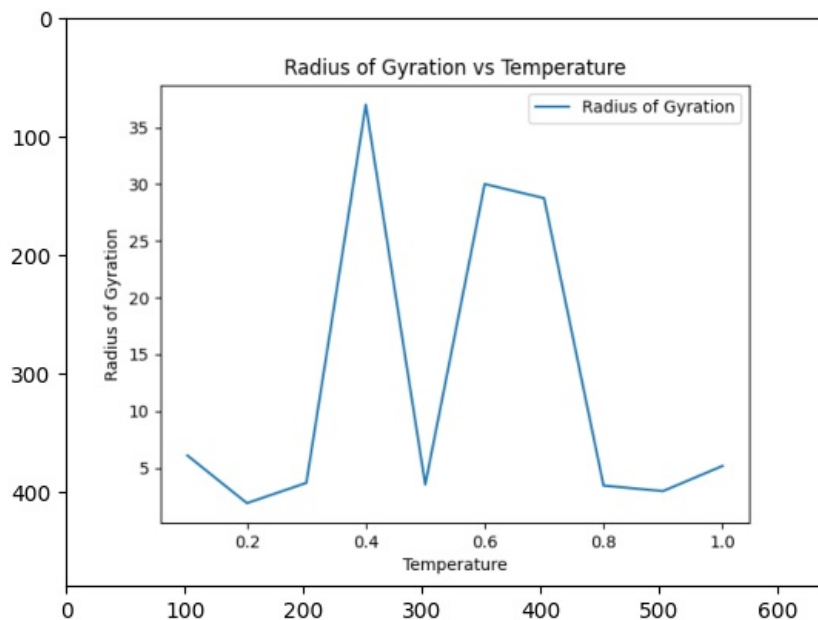
Chain Length

For higher chain lengths, it became more likely that the polymer would obtain an unfolded configuration. This can be seen in the charts as the higher 25 length chain has a much earlier initial spike, showing how it was at a lower temperature that it transitioned from a folded to an unfolded configuration. This is in line with what I would expect given that for higher chain lengths it's harder to manage a folded configuration with everything being so close and stronger volume effects.

Discussion

As temperature increased and the polymers started to gain sufficient potential energy in order to override the interactions, they began to obtain a higher radius of gyration and end-to-end distance. This is probably due to attractive interactions dominating under low temperature conditions and gradually as temperature increased, the repulsive potentials began to take over, leading to the shown unfolding.

The spring constant k represents the strength of the bonds between adjacent repeating units in the bead-spring model. Thus we would expect that with a larger k, the unfolded configuration would be harder to achieve as there are more bonds to overcome. This was the result seen in the simulation, where the failure point where the polymer undergoes a phase transition, gradually moves farther and farther out as I increased k.

Epsilon Repulsive represents the repulsive potentials used in the Lennard Jones model for beads seperated by one spacer in order to simulate excluded volume effects. In the simulation, lower repulsive potential tended to create earlier failure points which does not align with what I intially would expect: that it would be harder to take a folded configuration if there is greater resistance to putting repeating units in close proximity. It appears as though for higher values of epsilon repulsive the beads were more resistant to movement and were more likely to take on folded configurations in order to maintain outward movement.

Polymer chain length represent the size of the polymer and in the simulation, as the length of the chains increased, it became more likely that the polymer would adopt an unfolded configuration which makes sense given that it would be harder for a much longer chain to maintain its integrity and would like to stretch itself out to the greatest extent.

If we want to pick the best polymer for a space application that will remain unfolded you would want to maximize values of k, minimize epsilon repulsive, and maximize chain length.

Conclusion

In this project, I have investigated the folding unfolding transition in the bead-spring model using Lennard-Jones and Harmonic Potentials. These results show that unfolding is dependent on temperature, spring constants, epsilon repulsive, and chain length and offer insights into how we should design space materials.

For future projects, I would perform energy minimization before starting the MD simulation to ensure greater robustness of simulation results.