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Computational Problem Solving

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Project 2: Polymer Simulations in Python

Introduction:

Polymers hold relevance across many scientific disciplines and their behaviors can be modeled effectively when appropriately simplified for basic molecular dynamic simulations. This project will utilize python to model a polymer made up of like-monomers that will exert and experience the same forces as one another. The system will rely on both bonding and nonbonding interactions that the monomers experience and the effect on varying bond rigidity and temperature will be investigated to inform us what set of parameters would be ideal for a polymer that is meant to maintain its integrity and remain unfolded at low temperatures. By understanding how certain parameters of the polymer permit for this behavior, there can be better selection of materials based on how they are expected to match these simulated parameters.

Methods:

To model the system in python a basic polymer was constructed with the most essential forces included only. The polymer was modeled to be 20 beads long, with bonds made up of harmonic oscillators that included k-values that would be manipulated during trials. The Lennard-Jones attractive interaction when r is greater than sigma was included, along with a volume exclusion interaction that prevents the polymer from existing in one point in space. The code in the function named “initialize chain” in the script will allow for the polymer to be

initialized without fear of overlap. The system is dynamically relaxed via molecular dynamics and velocity rescaling. By rescaling the velocities of the system to hold a given temperature, the system will lose its rapid movements and gets it to a relatively low energy configuration. Then, equilibrium sampling of the system begins to characterize how the polymer behaves under the chosen temperature, bond strength and repulsive effects.

Results:

The following plots all display how different characteristics of the polymer change under temperature of the system. The Radius of gyration, is a measure of how far the beads are from their center of mass, where the center of mass is calculated, then the difference between this position and the beads position is squared and then the squared distance is average and the square root is taken. The second parameter is simply the end to end distance where the linear-distance between the first and last particle is calculated. The final metric of interest is the potential energy of the system under the given parameters. The phase transition will be marked by finding the gradient of these parameters and where this change is most rapid because this should be around where a phase transition is expected. A folded polymer would be expected to be dominated by attractive interactions and the radius of gyration would be relatively small, but if there is a massive change towards a higher radius of gyration the beads are moving apart. The highest radius of gyration would be when a given polymer is least folded so going in a direction of higher radius of gyration should be a sign of a folded to unfolded transition. The first 6 figures are modeled with a k-value of 1.0 and a repulsive interaction value of 1.0. The 7th figure has a repulsive interaction value of 8.0 and a k-value of 5.0. The repulsive interaction variable will

contribute to the magnitude of the repulsive non-bonding interactions and the k-value is simply for the stiffness of the spring that is described by the harmonic oscillator model of bonds.

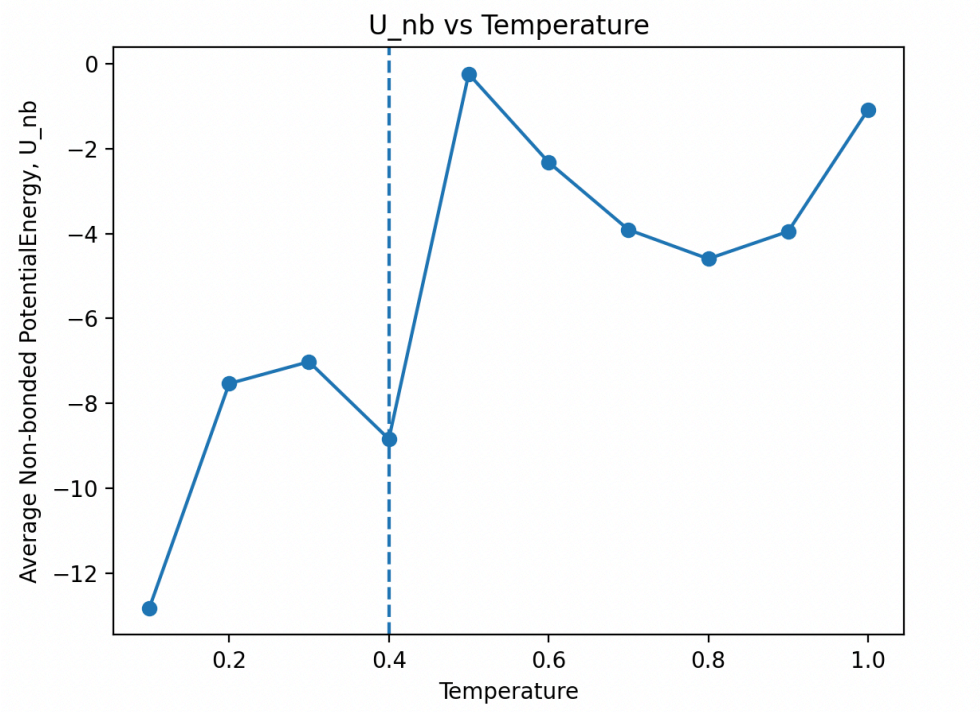

Figure 1: Temperature and Potential energy of the polymer when modeled with a k-value of 1.0 and a repulsive interaction value of 1.0.

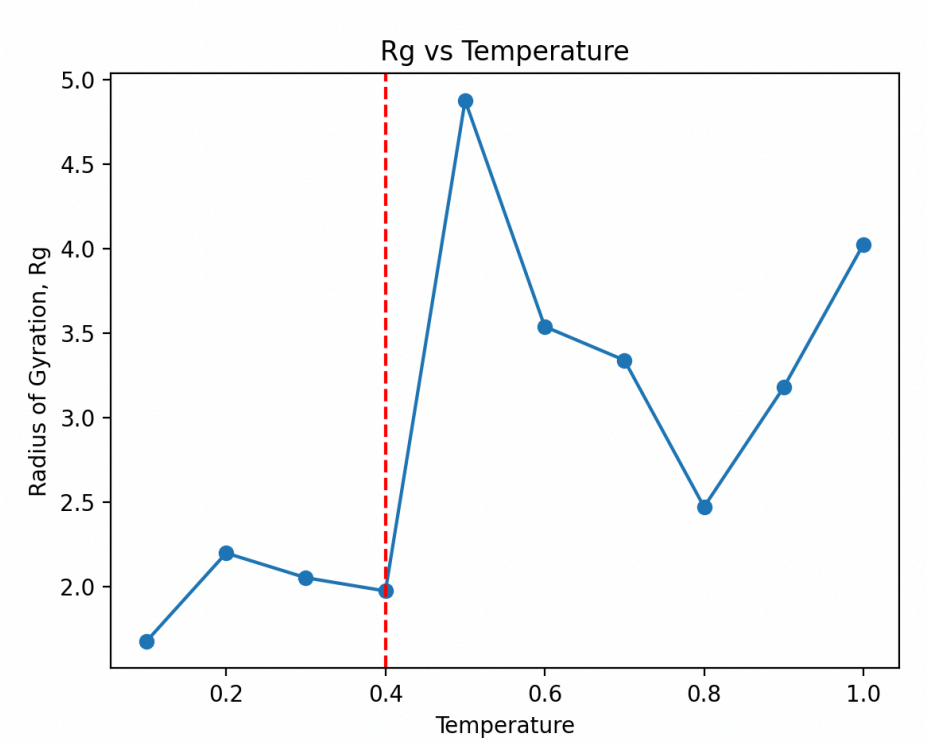

Figure 2: Temperature and Radius of Gyration of the polymer when modeled with a k-value of 1.0 and a repulsive interaction value of 1.0.

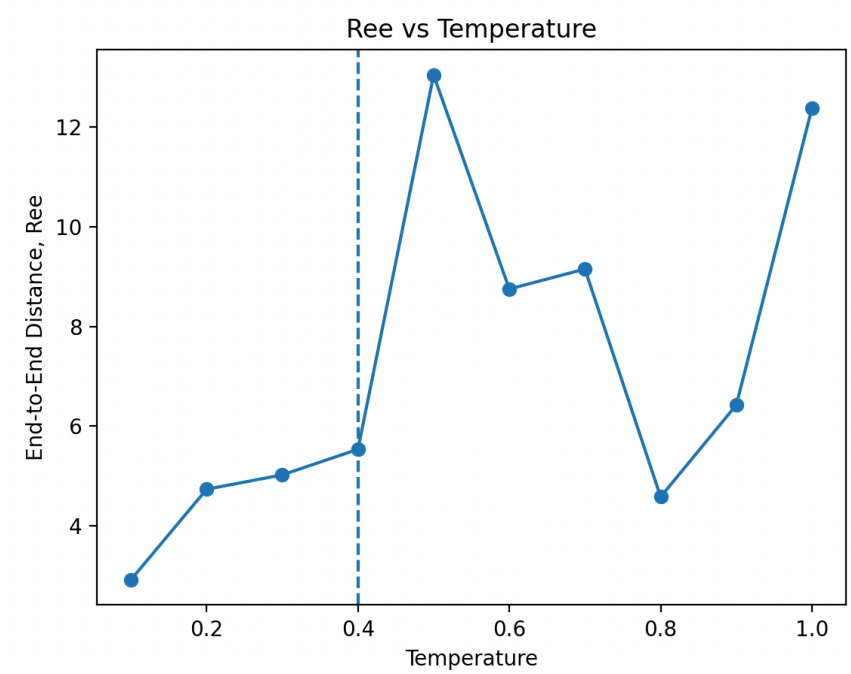

Figure 3: Temperature and end-to-end distance of the polymer when modeled with a k-value of 1.0 and a repulsive interaction value of 1.0.

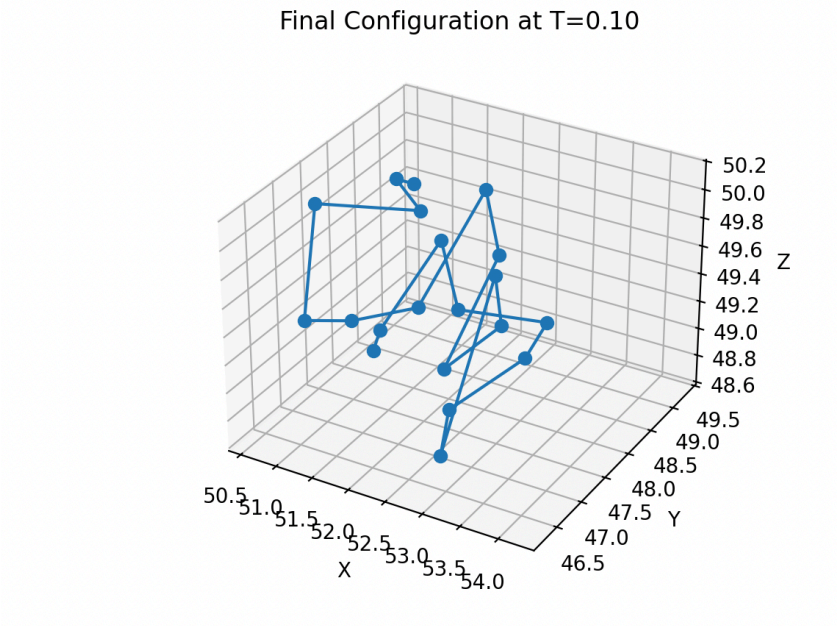

Figure 4: A snapshot of the polymer at the lowest sampled temperature (.1) with a k-value of 1.0 and a repulsive interaction value of 1.0.

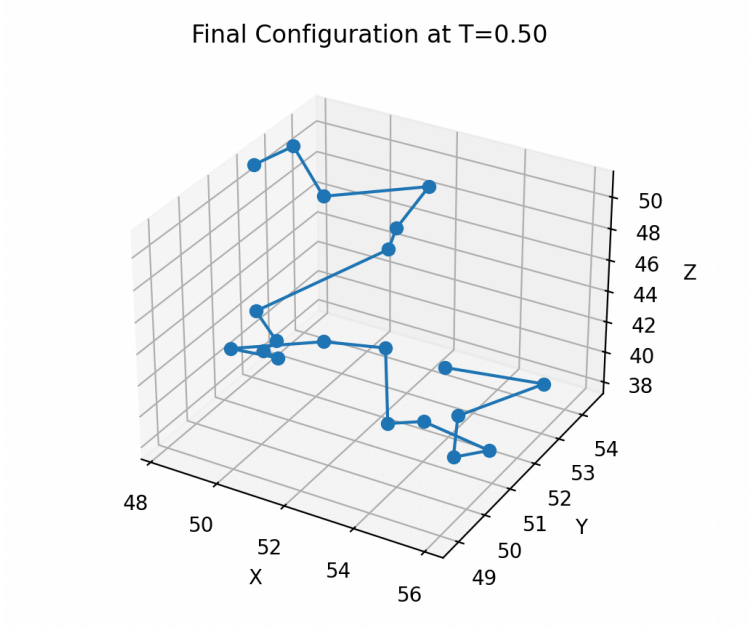

Figure 5: A snapshot of the polymer close to the estimated phase change temperature with a k-value of 1.0 and a repulsive interaction value of 1.0.

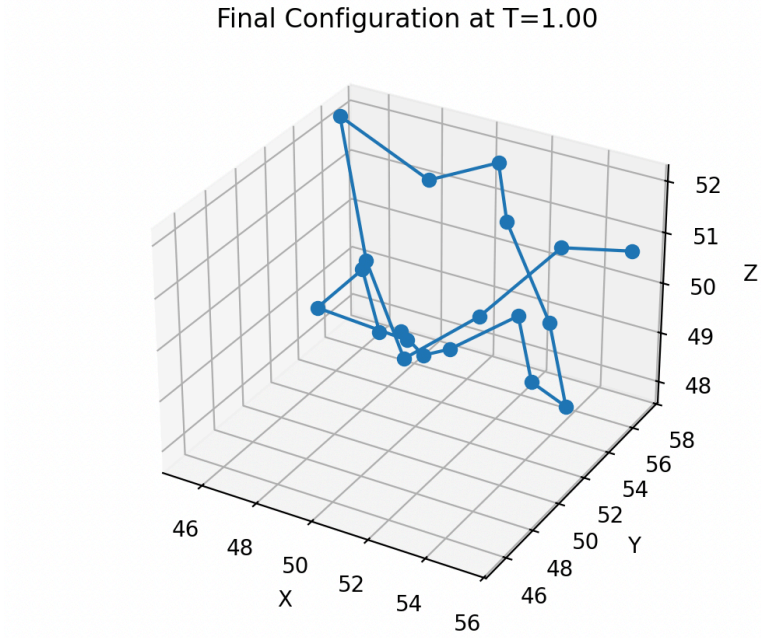

Figure 6: A snapshot of the polymer at the highest sampled temperature with a k-value of 1.0 and a repulsive interaction value of 1.0.

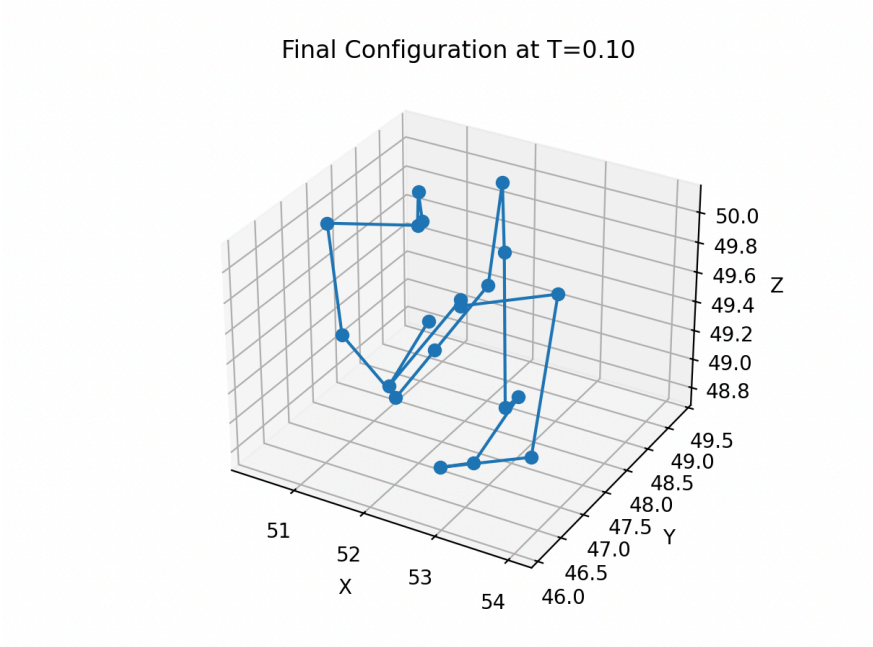

Figure 7: A snapshot of the polymer modeled at the lowest sampled temperature but modified parameters, with a k-value of 5.0 and a repulsive interaction value of 8.0.

Discussion:

To determine a phase change temperature for the starting parameters where the k-value is 1.0 and the repulsive interaction is 1.0, the gradient of each of the variables of interest is taken and all experience a sudden change in gradient at T= .4. This marks a period where the polymer is expanding which can be seen in its Radius of Gyration that peaks around .5. It is logical that it was experiencing some moderate folding below this temperature, especially at the minimum temperature of .1. However, when analyzing the polymer snapshot at a temperature of .1, some areas appear relatively folded and compact but there is certainly some expansion that shows that the temperature minimum isn't strong enough to lead to an aggressive downshift in energy. However, when contrasted to the snapshots at a temperature of .5 and the temperature 1.0

snapshots, it's clear that there is some level of folding that could jeopardize a polymer with these characteristics in space. In order to adopt a conformation at low temperatures that is similar to the moderate temperatures, the repulsive interaction and the bond stiffness were both increased, which made it far more energetically unfavorable for the particles to pack tightly. This can be seen in figure 7 as its level of packing and folding is closer to that of Figures 5 and 6 than Figure 4.

A better understanding through a simple way of modeling is essential for real-world applications of polymers. The inherent characteristics that lead to differences in our simplified parameters of repulsion and bond strength are of great interest for real-world polymers. NASA has studied different polymers at temperatures below the phase change of gas and looked at how properties like molecular weight affect overall brittleness and stability under these intense conditions.

Conclusion:

This study has demonstrated how a simple modelling of a generic polymer in python can allow for further study of what parameters can be optimized in order to design an ideal polymer for low temperature scenarios. By comparing plots of radius of gyration, end to end distance and potential energies across different temperatures, we could compare the effects of repulsive nonbonding interactions and bonding strength by varying them. The maximum slope was found to determine what temperature most likely corresponded to a phase change between a coil-globule-like transition. We were able to prevent collapse at low temperatures with significant increases to the k-value and repulsive parameters. While the model is a good tool to understand rough magnitudes of forces in comparison to one another, it doesn’t directly consider a bending effect and how the rigidity of the backbone directly affects its ability to fold.

Furthermore, we only explored a homogenous chain which simplified the study but doesn't capture all real world polymers. Further space polymer simulations should be mindful of these enhancements to the polymer and should find more physically relevant parameters than the end to end distance and radius of gyration because these give a good idea of packing but not if the polymer of interest has maintained its structural integrity or form.

Sources:

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https://wexlergroup.github.io/comp-prob-solv/lecture-25-project-2/