

Analysis of a polymer in Outerspace temperatures:

Introduction:

The goal of this experiment was to simulate a polymer in extremely cold conditions of outer space. This was done because many polymers fold and become brittle or break under such conditions.

Methods:

A program was constructed that would create a linear chain of n particles. Since the mass of a monomer in the polymer chain was left vague the mass of tyrosine (181.19 amu), was used to calculate the forces and energies, since it seemed to be a viable polymer stand in. The force exerted by the bond between these particles was calculated using simple harmonics with a spring constant that was altered between experiments. Particles that weren't neighbors interacted with each other using a Lenord-Jones potential, with a sigma of 1, an epsilon attractive of 0.5, and a variable epsilon repulsive from 0.5 to 3.5. Temperatures varied from 0.1 to 5.0 Kelvin, since the average temperature in space is 2.5 kelvin. The particles were moved around using Verlet velocity, where every 0.01 nanoseconds the particles were moved, their acceleration based on the surrounding forces were calculated, and then the particles were moved again with this in mind. Every 100 steps velocities were rescaled to match the outside temperature using an Anderson thermostat function. The polymer was simulated in a cubic box with a 100nm side length and periodic boundary condition. Once each chain was created, but prior to simulation a metropolis algorithm of 1000 steps was used to place each particle in their minimum energy state, and each particle was then given a random velocity. The simulation was run for 10,000 steps, or a total of 100 nanoseconds.

Results:

K values and epsilon repulsive were iterated until values were found where the potential energy increased steadily with temperature, but the end-to-end distance and radius of gyration were approximately the same. A graph of the final polymer at the highest simulated temperature was graphed. The values graphed were average potential energy, end-to-end distance, and radius of gyration, all with respect to temperature.

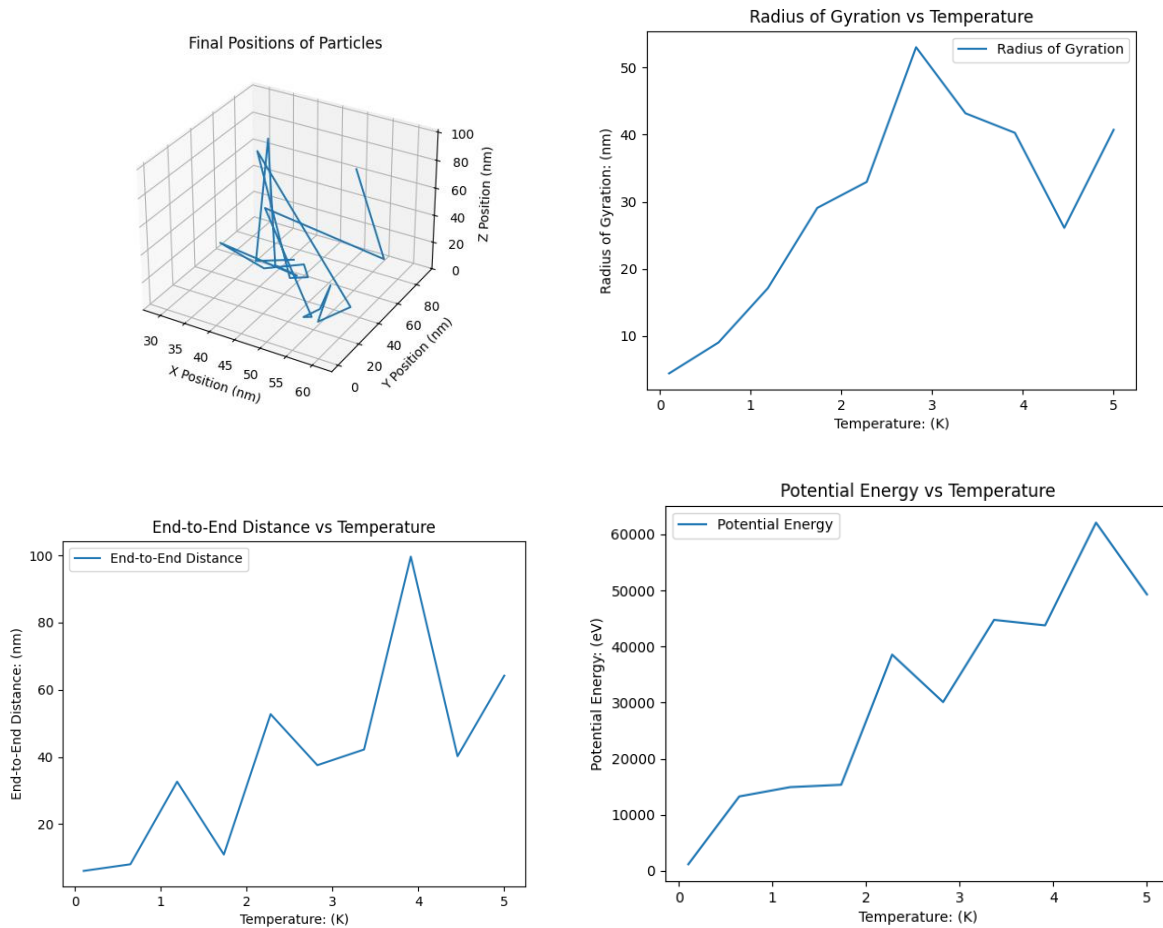


Figure 1: A chain of 20 monomers simulated with a spring constant of 300, a repulsive Lennard-Jones epsilon of 2.5, and simulated temperatures from 0.1 to 5.0 kelvin. The upper left-hand graph is the final position of the particles after being simulated at their highest temperature. The upper right-hand graph is radius of gyration in nanometers versus temperature. The lower left-hand graph is end-to-end distance versus temperature, and the lower right-hand graph is potential energy versus temperature.

Figure 1 is an example of a polymer that folds in cold temperatures. This is not the desired result. Not only is this apparent from the graph of the polymer, but also from the steady increase in radius of gyration and end-to-end distance. Both of these measure how spread out the polymer is, either from its center of mass, or from one of its ends to the other respectively. For a polymer not to fold in on itself the radius of gyration and end-to-end distance must not decrease with temperature. Although potential energy will still steadily climb, since when the particles are placed into an environment with more energy, they will

turn that heat energy into potential energy and move into a conformation that is not as favored by their internal forces.

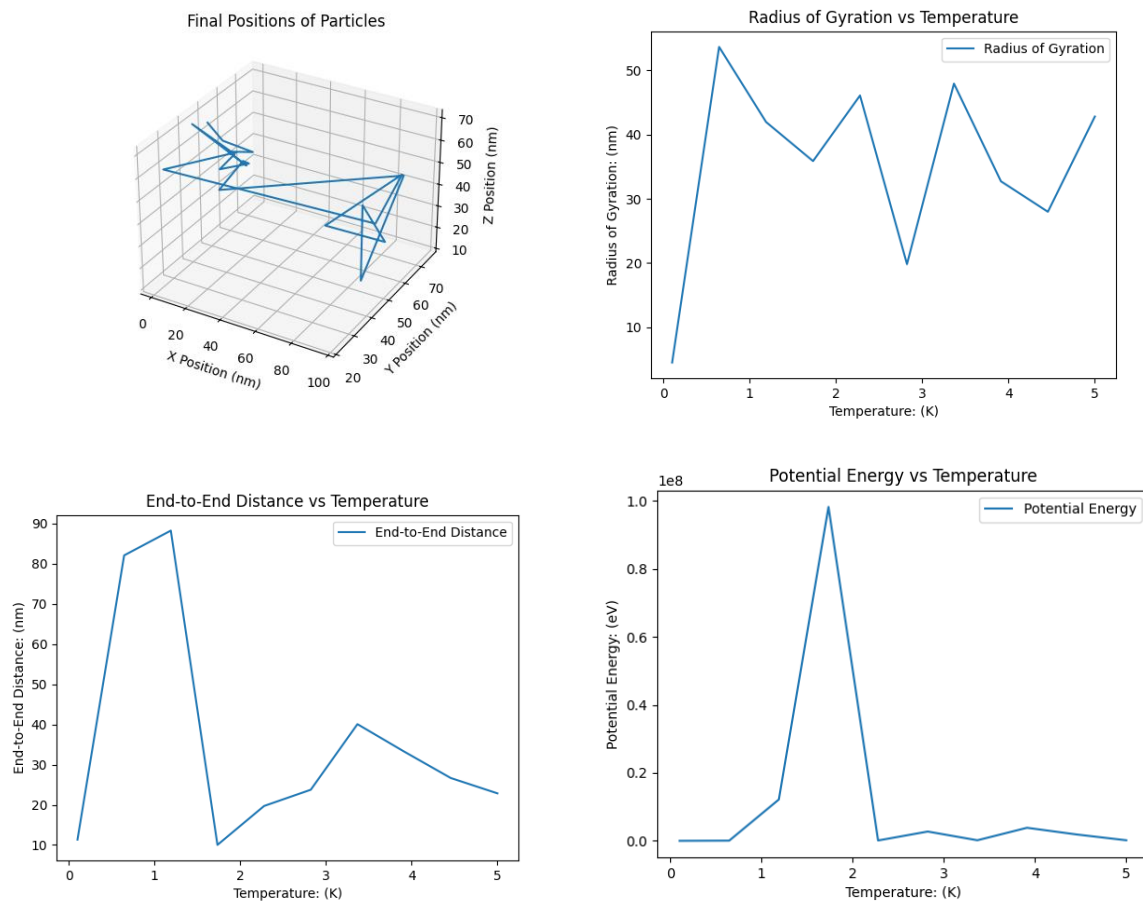


Figure 2: A chain of 20 monomers simulated with a spring constant of 400, a repulsive Lennard-Jones epsilon of 3.5, and simulated temperatures from 0.1 to 5.0 kelvin. The upper left-hand graph is the final position of the particles after being simulated at their highest temperature. The upper right-hand graph is radius of gyration in nanometers versus temperature. The lower left-hand graph is end-to-end distance versus temperature, and the lower right-hand graph is potential energy versus temperature.

The polymer in figure 2 suffers from a different problem. The radius of gyration seems relatively level as temperature increases, but there is an unexplained spike in both potential energy and end-to-end distance. This was likely due to a fault in the simulation, especially since the peak in potential energy is several orders of magnitude larger than any other potential energy on the graph. This fault makes this entire set of results questionable

at best, even though the final positions of the polymer show a relatively unfolded polymer. Unfortunately, this was the result of several otherwise promising simulations.

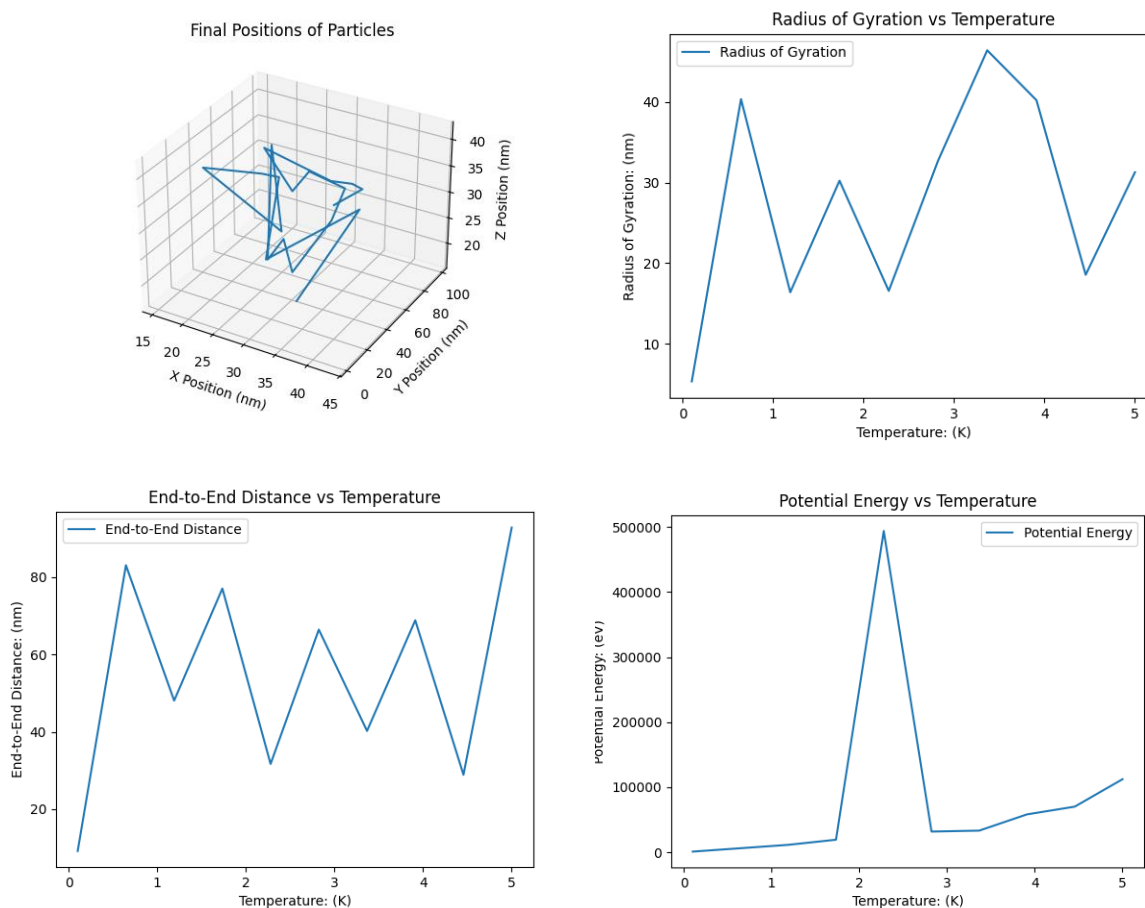


Figure 3: A chain of 20 monomers simulated with a spring constant of 300, a repulsive Lennard-Jones epsilon of 1.5, and simulated temperatures from 0.1 to 5.0 kelvin. The upper left-hand graph is the final position of the particles after being simulated at their highest temperature. The upper right-hand graph is radius of gyration in nanometers versus temperature. The lower left-hand graph is end-to-end distance versus temperature, and the lower right-hand graph is potential energy versus temperature.

Figure 3 shows the best polymer simulated. Although there is a potential energy spike at Kelvin, which likely means the data there is dubious, the spike is not so massive that it obfuscates the rest of the potential energy slope. Here a sight of a end-to-end distance and radius of gyration, which does not depend on temperature can clearly be seen. Only at 0.1 kelvin does the polymer seem to bunch up. However, except at this temperature, and 2 Kelvin, which must be ignored because of the potential spike, the radius of gyration and

end-to-end distance are significantly larger. The graph of the polymer itself also appears to be more open, unfortunately despite what the end-to-end distance and radius of gyration imply, it still seems to be folded somewhat into a doughnut shape, though it is significantly more spread out than the other polymer analyzed at this temperature (Figure 1).

Size Matters:

To ensure this was in fact the best distance for the polymer more sizes were tested a 10-monomer chain and a 30-monomer chain.

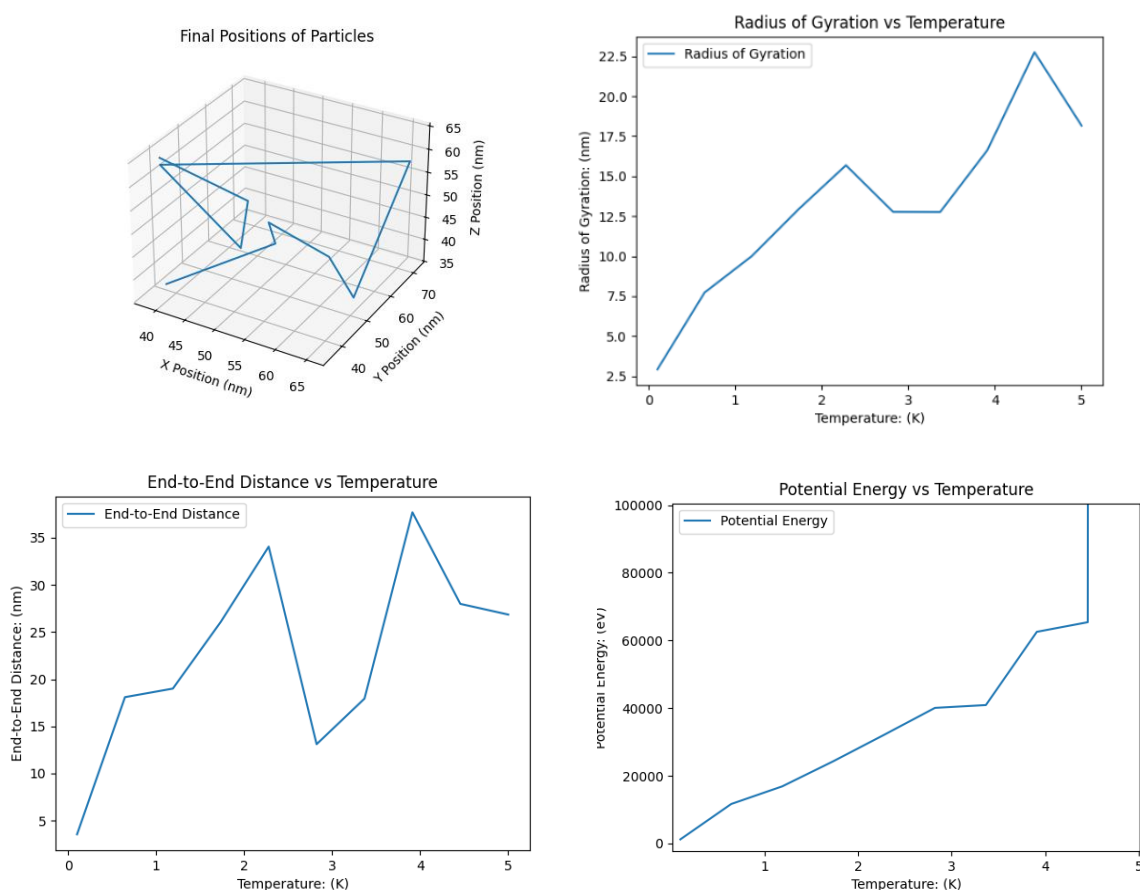


Figure 4: A chain of 10 monomers simulated with a spring constant of 300, a repulsive Lennard-Jones epsilon of 1.5, and simulated temperatures from 0.1 to 5.0 kelvin. The upper left-hand graph is the final position of the particles after being simulated at their highest temperature. The upper right-hand graph is radius of gyration in nanometers versus temperature. The lower left-hand graph is end-to-end distance versus temperature, and the lower right-hand graph is potential energy versus temperature.

The first thing to notice is how this polymer seems to fold at low temperatures when the same properties are applied to it that were applied to the other polymer (Figure 4). This is

rather surprising and seems to imply that every chain length will have its own ideal chain properties to prevent folding. The second thing to notice is that, ignoring the potential spikes, this chain has about the same potential energy as the previous chain, and the 30-monomer chain (Figure 5). This means that the potential energy must not be impacted much by chain length for some reason.

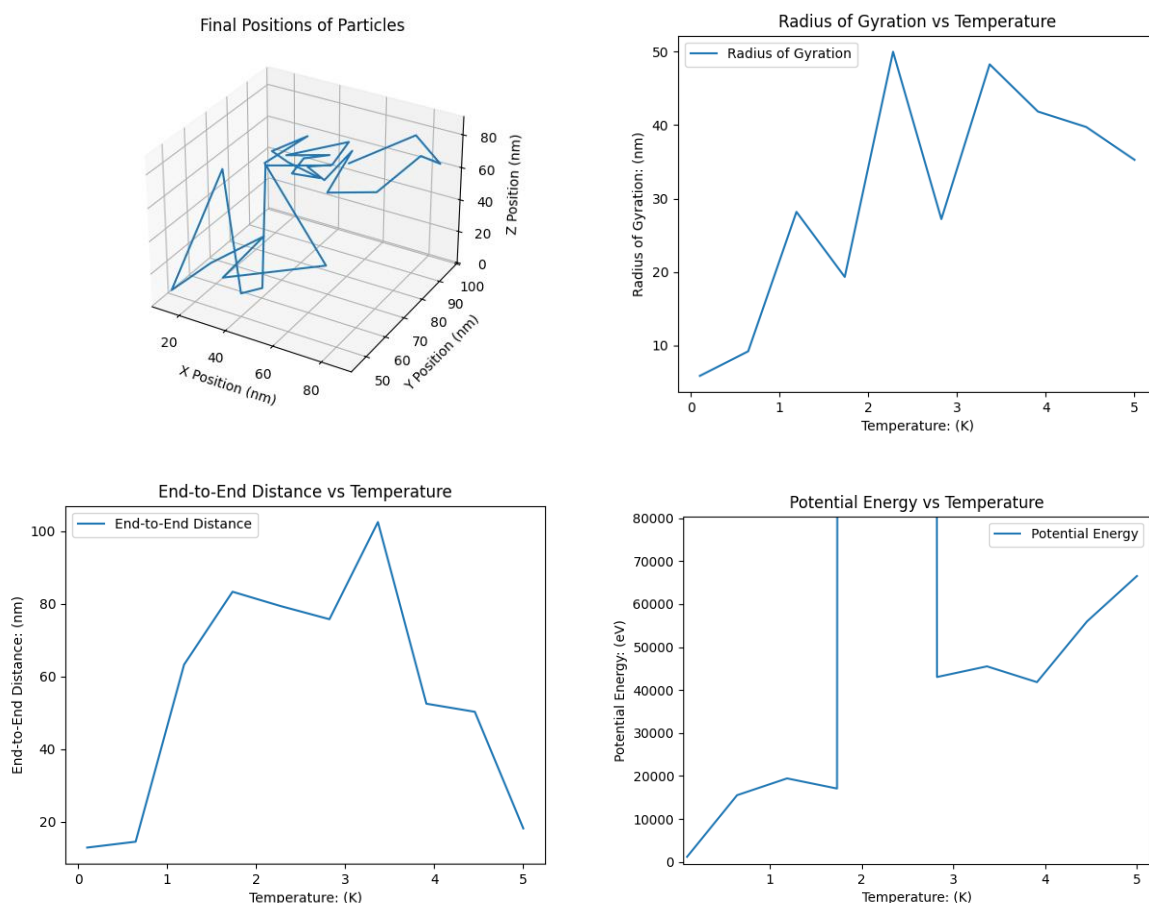


Figure 5: A chain of 30 monomers simulated with a spring constant of 300, a repulsive Lennard-Jones epsilon of 1.5, and simulated temperatures from 0.1 to 5.0 kelvin. The upper left-hand graph is the final position of the particles after being simulated at their highest temperature. The upper right-hand graph is radius of gyration in nanometers versus temperature. The lower left-hand graph is end-to-end distance versus temperature, and the lower right-hand graph is potential energy versus temperature.

The 30-monomer chain reveals two interesting truths about the simulated chain. Firstly, as expected it appears that the ideal repulsive epsilon, and spring constant vary with chain length. The second thing of note is that despite being relatively unfolded, the ends of the final polymer are close together (Figure 5). This is reflected in the end-to-end distance, which goes up and then back down again. This seems to suggest that end-to-end distance may not be the best measure of folding, since it only depends on the two terminal monomers, no matter how large the chain is. If this was done on massive polymers radius of gyration would be a much better measure of folding.

Discussion:

The best properties I found for the polymer were a 300 spring constant and an epsilon repulsive of 2.5, however the graph is still far from ideal as the illustration still shows a good deal of folding. There are likely better values out there that I failed to find in my extensive testing. Despite this the large and consistent radius of gyration and end-to-end distance suggest that these are the values that show the least impact from temperature. The values found would also only work for a polymer of 20 length, as they don't appear to work for chains that are shorter or longer. This shows the difficulty of designing a space polymer since despite iterating through over a dozen values, I only found one that sort of works at a very specific chain length. The glitch with the spikes in potential energy were also problematic although now, in retrospect unfortunately their cause has occurred to me. Although I optimized the initial positions of the monomers, I never optimized the initial velocities, so it is very likely the start of the simulation resulted in large amounts of particle collision. Still this project shows the power of computer simulation since it would be incredibly difficult to construct the near absolute zero environment necessary for the tests. In addition, it is very likely that more information on real world polymers would allow simulations to take less shots in the dark like this one did. Overall computer simulation allows experimentation under conditions that would be challenging or otherwise impossible to recreate in the real world.