Simulation Proposal for 2 Cyanoethyl Ether

The goal of any computer-generated simulation is to visualize an experiment or product, and ultimately generate a set of results corresponding to a desired value or variable while maintaining accuracy within reality. To identify the density of 2 cyanoethyl ether, I will run a LAMMPS simulation with an NPT ensemble to collect data for fluctuations in volume at different constant temperatures. Because of the relationship between volume, temperature, and pressure established by the equation pV=NkT, as well as Gay-Lussac’s Law, the volume can be calculated by using the data collected from the simulation. Per the equation, V=NkT/P, I can calculate the volume of 1000 molecules with a linear regression calculated (either on Microsoft Excell, Python’s Matplotlib/Numpy/Pandas libraries, or MatLab) when temperature is on the y-axis and pressure is on the x-axis. Then, I can find the density of a single molecule by dividing the molecular mass of the 2-CEE molecule by 1000 divided by the previously calculated volume.

To run my initial simulation, I will run the simulation from 300K to 230k in intervals of 10K, with 10,000 timesteps per each interval. In doing so, I hope to collect enough accurate data to capture the change in volume of the molecules as the temperature and pressure increase. To locate the best parameters of running an NPT simulation for this molecule, I will to increase the number of timesteps by 10,000 until I reach 100,000. By putting each of these simulations and output files in separate directories named based on the number of timesteps (e.g., 2CEE\_01, 2CEE\_02), I plan to keep both my files and directories organized enough to complete the analysis. This way, I can run the simulations on Abyss while storing the data well.