Homework 3

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Problem 1

* Three simulations at 250K 300K and 350K were done on NPT ensemble
* The average value of the enthalpy in each case was evaluated discarding the initial spikes.
* Central difference scheme was used to evaluate the Cp
* Cp300 = (av.Enth)250 – (av.Enth)350 / (2\*50)
* **the value of Cp300 was found to be 1.0765 eV/K**
* Similarly the the average volumes were evaluated.
* The CTE was also calculated using the central difference scheme.
* **CTE300 = 4.47e-5 K-1**
* The isothermal compressibility was taken to be 0.01385 Gpa-1
* Using the relation between between Cp and Cv
* **Cv300 = 1.0583 eV/K**

Problem 2

* Similar procedure as the first problem was used to calculate the Cv.
* NVT was done on the optimized structure of the NPT simulation at 300K
* **Cv300 was found to be 1.0199 eV/K**

Problem 3

