

Assignment 19: Abstracting information from log.lammps

- If you are given a data file with certain format, can you write a code to read in the data, process them and visualise the content according to your need?
- Try this out on the file [log.lammps](#), which is part of an output produced by a Molecular Dynamics simulation software package LAMMPS.
- log.lammps is a formatted file containing assorted information of the LAMMPS output, such as "Step" "Atoms" "Temp" "Press" "PotEng" "KinEng" "TotEng" "Volume" "Enthalpy"

- Write a Mathematica code to abstract the data of "Step" "Atoms" "Temp" "Press" "PotEng" "KinEng" "TotEng" "Volume" "Enthalpy" from log.lammps.

Then plot

- Temp vs. Step
- PotEng vs. Step
- PotEng vs. Temp