The most important resource you will need is the LAMMPS manual.

<https://docs.lammps.org/Manual.html>

**Run a simple energy minimization and temperature ramp of UO2**

Input script to run - EAM\_equil.lammps

**What’s in script:**

This outlines that the simulation will use periodic boundaries

boundary p p p

This is the the type of structure file … check the structure file to make sure this is consistent

atom\_style full

This is what units your results will be in

units metal

These are two variables created that will be used later. They are damping variables to be used with the thermostat and barostat

variable THERMO\_DAMP equal 0.1

variable BARO\_DAMP equal 0.5

Reads in the structure file and assigns the variables “O” and “U” to the oxygen and uranium atoms, respectively.

read\_data UO2-single\_cell.lmpstruct

variable O equal 1

variable U equal 2

Assigns the charges to the relevant species

set type $O charge -1.1104

set type $U charge 2.2208

This defines the interatomic potential used. Coulombic interactions and a many-bodied EAM

• In LAMMPS, forcefields are called "pairstyles"

• Need to specify:

• style

• cutoff distance

• interaction coefficients

• maybe more depending on the pairstyle

Use Kspace style to add long-range electrostatics

kspace\_style pppm 1.0e-5

variable SR\_CUTOFF equal 11.0

pair\_style hybrid/overlay coul/long ${SR\_CUTOFF} eam/alloy

pair\_coeff \* \* coul/long

pair\_coeff \* \* eam/alloy CeThUNpPuAmCmO.eam.alloy O U

Extends the cell 4 times in the x , y and z directions

replicate 4 4 4

Creates an initial velocity for 300 K on all the atoms

velocity all create 300 160278

Sets the timestep for each step – work out the time for each step for units metal

timestep 0.002

Sets up an NPT fix from 300 K to 300 K using the damping parameters defined earlier

fix thermostat\_fix all npt temp 300 300 ${THERMO\_DAMP} aniso 0.0 0.0 ${BARO\_DAMP}

Defines the style of thermos output and how many steps the output will be printed

thermo\_style one

thermo 10

Parameters to adjust neighbour list – don’t worry about this for now

neigh\_modify delay 0 every 1 check yes

This runs the previous fix

run 25000

To create a new fix, first unfix the previous fix. For example,

unfix thermostat\_fix

Then can make a new fix. For example, doing a temperature ramp from 300 K to 500 K

fix thermostat\_fix\_ramp all npt temp 300 500 ${THERMO\_DAMP} aniso 0.0 0.0 ${BARO\_DAMP}

To dump out files for visualization in Ovito use the command. Important to use this before the run command. This will dump out structures every 100 timesteps. Check in Ovito.

dump cfg\_dump all cfg 100 addatom\_\*.cfg.gz mass type xs ys zs vx vy vz

dump\_modify cfg\_dump sort id element O U

To do:

* Minimize a UO2 structure
* Equilibrate at 300 K
  + Plot out relevant information to make sure system has equilibrated
  + Might need to adjust thermos output to a custom one e.g

thermo\_style custom step temp press vol lx ly lz enthalpy etotal pe

* Heat structure to 1000 K and equilibrate
  + Plot out relevant information to make sure system has equilibrated
* Calculate lattice parameter at 1000 K and compare to value in potential paper
* Heat up structure until melting
  + Check dumps in Ovito to see if system has melted
  + Has system melted at temperature you expected? – get melting temperature of UO2 for this potential in melting paper.