Tutorial Day 2: Materials

Introduction:

The Molecular Dynamics (MD) simulations will be performed using the LAMMPS package, widely used within the material science community. You can download it from:

http://lammps.sandia.gov/

or use the version installed in the VMware for you.

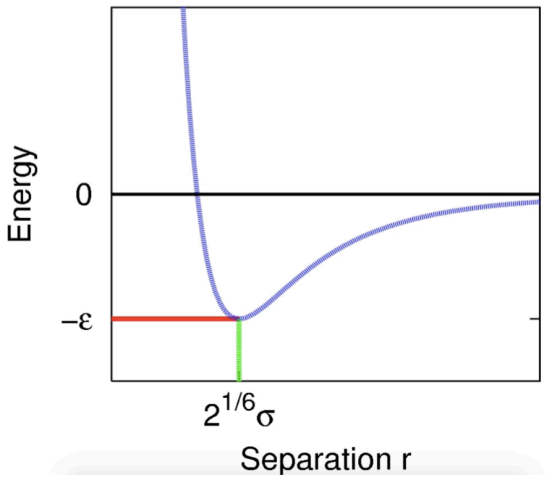
In this exercise we will calculate the melting point of a material. We will consider Ar, which in solid form packs in the fcc structure. The experimental melting point for Argon is 84 K, so our temperatures will be mostly well below room temperature.

The Lennard-Jones parameters for Argon are:

ε=0.010832 eV

σ=3.345 Å

and the mass of Ar is 40.0 amu where 1 amu=1.66×10^{-27} kg. You won't need to enter this information into any files. All that information is taken into account in the file `forcefield.lmp`



As well as the file `forcefield.lmp`, you will need the following files:

- `fcc_0.pdb` and `fcc.lmp` : These contain the coordinates of a supercell of solid fcc Ar in pdb format and LAMMPS format respectively. You can visualize the structure by using VMD by typing: `vmd fcc_0.pdb`
- `liq_0.pdb` and `liq.lmp` : These contain the coordinates of a supercell of liquid Ar in pdb format and LAMMPS format respectively. You can visualize the structure by using VMD by typing: `vmd liq_0.pdb`
- `int_0.pdb` and `int.lmp` : These contain the coordinates of a supercell which contains both liquid Ar and solid Ar in pdb format and LAMMPS format respectively. Note that the supercell is double the size as the previous ones. You can visualize the structure by using VMD by typing: `vmd int_0.pdb`
- `lammps.inp` : is the input file for lammps. It contains all the information

about the conditions to run the MD simulation (temperature, ensemble, thermostats, etc). You can read the file by typing: `vi lammps.inp`

Exercise 1: Melt a solid Ar

Using `fcc.lmp`, `forcefield.lmp` and `lammps.inp`, you will explore the temperature at which the structure melts.

The file `lammps.inp` calls for `forcefield.lmp` and `coord.lmp`. First copy the initial coordinates into `coord.lmp` :

```
copy fcc.lmp coord.lmp
```

Edit the line "`variable temp equal ...`" in `lammps.inp`, and chose a temperature for the MD simulation to run. Save and close the file.

Run the MD simulation by typing:

```
mpirun -np 6 lammps -in lammps.inp
```

you can redirect the output from the screen into a file if you desired by typing:

```
mpirun -np 6 lammps -in lammps.inp > lammps.out
```

Your output file will contain the thermodynamical quantities you need. You can modify lammps.inp and include more if you wanted. For this exercises you need the potential energy (PE) and the temperature.

LAMMPS will also produce a file `trajectory.dcd` which can be visualize with VMD. It contains frames of your MD simulations. You can change the frequency of the frames in the line in `lammps.inp`: "`variable ntraj equal ...`"

You can visualize the simulation by typing: `vmd fcc_0.pdb trajectory.dcd`

If you have chosen a temperature above the melting point, the structure would have

Your aim is to plot PE. vs. Temperature and find at which temperature the structure melts.

Exercise 2: Freeze liquid Ar

Copy the coordinates on liquid Ar into coord.lmp and repeat the same exercise as Exercise 1. Your aim is to plot PE. vs. Temperature and find at which temperature the structure freezes.

```
copy liq.lmp coord.lmp
```

Exercise 3: Two phases of Ar

Copy the coordinates of the structure with liquid and solid into coord.lmp and repeat the same exercise again.

```
copy int.lmp coord.lmp
```

In this case, you should change the conditions around pressure, so that pressure in z can vary. Edit the line in lammps.in:

```
variable npttype  string  iso
```

into

```
variable npttype  string      z
```

Once again, your aim is to plot PE. vs. Temperature and find at which temperature the structure is stable. If you visualize the MD run, at the melting temperature the interface should not move.

Are the answers from all three exercises the same?
Which method would you use for an unknown material?