Exercise 8 Molecular Dynamics

In this exercise we will use LAMMPS again. We will simulate the melting of naphthalene.

a) For this simulations you will need `md-bulk.in`. You might want to make a new directory put your new output. We will use the restart file from the minimization that you performed earlier min_restart. Do not forget to copy this to the new directory as well.

b) Run `lmp_serial < md-bulk.in`. This will take a while. You can continue with the next question.

c) Open the `md-bulk.in` file. Most of it is similar to `minimize.in`. The MD magic happens in the bottom lines. Look up on `https://lammps.sandia.gov/doc/fix_nh.html` what the numbers mean. What will be the temperature profile?

d) We would like to see melting of naphthalene. The experimental melting temperature is 80 °C. Do you expect to see melting in the MD simulation at lower, higher or exactly the correct temperature? Why? How do you expect to observe the melting?

e) Hopefully the simulation is now done. Let us check the answers, starting with the temperature profile. Plot this in a new Jupyter Notebook (Use python2 else it will not work). You will see temperature fluctuations on top of the temperature profile as given to LAMMPS by the `fix npt`. These fluctuations change with temperature. Why? What will happen if you change the system size?

f) Plot the different cell dimensions as function of the time. You will see a clear change. This is accompanied by a small change in energy of the non-bonded interactions. Estimate the temperature at which the changes occur. How does it compare to 80 °C? Did you expect this?

g) Download the trajectory file and view with VMD. Can you see the melting occur? This is best seen if you view along the y-axis. Is it at roughly the same time as seen in the graphs? Can you see something about the mechanism? It appears to be a two-step process. Can you understand this from the interactions?

h) This was a bulk simulation, with no surfaces or clear nucleation points for the phase transition. In the next part we go to another extreme: a small, isolated sphere which has a very large surface/volume ratio. Run `lmp_serial < md-sphere.in`. This will again take a while.

i) Open the `md-sphere.in` file. Here first a $4 \times 4 \times 4$ cell is created and then only the molecules inside a sphere are left. There are two mean differences in the set-up between this and the previous simulation: Ewald summation is not used and the simulation is in the NVT ensemble. Why?

j) Repeat e-g for the new simulation.