Project 0: Programms

Download and install LAMMPS from:
https://rpm.lammps.org/windows/32bit/
https://rpm.lammps.org/windows/64bit/

After the installation, you can run LAMMPS by double clicking the mybatch file in each folder.
You can edit the files using a notepad (I suggest Notepad++) and change the name of the executable or the input file.

Download and install Ovito from:
https://www.ovito.org/windows-downloads/

READ THE MANUAL:
https://docs.lammps.org/Manual.html
https://docs.lammps.org/fix_nh.html

Always pay attention to the commands and the parameters you are using!
Check the manual to see what every little command and parameter does.

Project 1: Checking the perfect gas law with MD

The purpose is to run a simple simulation to check the perfect gas law. You can use the in.ar.lj.lp.txt input file, which automatically creates a 3D box and fills it with atoms and performs a NVE run for a fixed temperature. Visualise your results with Ovito (drag and drop the trajectory file produced by the dump command after the run is done).

After each simulation you should get the value of the temperature and the pressure of the system vs the timestep. Since you know the volume and the number of atoms then you can check the perfect gas law:

$$PV = nRT$$

where P, V and T are the pressure, volume and temperature respectively; n is the amount of substance; and R is the ideal gas constant.

Remember: $n = \frac{N}{6.022\times10^{23}}$

where N is the number of atoms.
Check if R and the pressure, volume and temperature are in the correct units! The units of a specific run can be found next to the `units` command in the input file. A list of the different units LAMMPS accepts as input and prints as output can be found here: https://docs.lammps.org/units.html

Repeat the process for a different temperature. What happens if the temperature is too low?

Project 2: Choosing the right parameters for a MD simulation

The purpose is to see how the $timestep$ parameter affects the simulation. Using the project's files, Set an initial velocity field to get a temperature of 600 K. Then vary the $timestep$ from 0.1 fs to 100 fs (e.g. 0.1, 0.5, 1, 5, 10, 50, and 100 fs) and execute NVE ensemble runs with a fixed temperature.
Plot the kinetic, potential and total energy vs the timestep and check for energy conversion (all info is in the log.lammps file).
After each run, produce the temperature vs timestep plot. The relative variance of the temperature deviation must be within:

$$\frac{\sigma_T}{\langle T \rangle} = \sqrt{\frac{2}{3N}}$$

where σ_T is the standard deviation of the temperature, T is the temperature of the run and N is the number of atoms in the model. For example, for a model with 1000 atoms you should see an average deviation of about 3%. Details of how this fraction is derived can be found in the presentation Temperature fluctuations in canonical ensemble.pdf. You can calculate the standard deviation in Excel using the STDEVA function. Repeat the process for a temperature of 1200 K. Does anything change?

The second part is to look at the effect of the temperature damping parameter of the Nose-Hoover thermostat $Tdamp$. A Nose-Hoover thermostat will **not** work well for arbitrary values of $Tdamp$. If $Tdamp$ is too small, the temperature can fluctuate wildly; if it is too large, the temperature will take a very long time to equilibrate.
A simple way to calibrate $Tdamp$ is via using an immediate variable expression accessing the thermo property dt, which is the length of the time step. Example: `$(50.0*dt)`.

You will follow the same procedure as previously using the ideal timestep you found, but simulating a NVT ensemble this time. In the $Tdamp$ parameter you can give values `$(50.0*dt)`, `$(100.0*dt)`, `$(200.0*dt)` and `$(500.0*dt)`, produce the temperature vs step plots and calculate the standard deviation of the temperature for each case.

What are the optimal $timestep$ and $Tdamp$ parameters for your runs?

Run the exercise twice: once for a light material (e.g. Ni or Cu) and then for a heavy material (e.g. Pt or Au).
Is there a difference?

Notes:

- ✓ At the beginning of each run you will see an area that has sharp temperature changes and then the situation normalizes. This is the part where the program tries to equilibrate. This part is OK to ignore.

- ✓ You can use different seeds each time (the `12345` in the file) to get a variety of results as well.
- ✓ You can use different temperatures than the ones suggested, which ideally should be in the 300-1200K range. Remember that the runs will be under constant temperature, so `Tstart` and `Tstop` will be the same.
- ✓ You have about 10 runs to do, so adjust the `run` command accordingly. Remember: we want them to last **as long as possible**, but we don't want your computers to catch fire either. You can do an initial run to see how much real time e.g. 10,000 steps take you, and then proceed accordingly. **DO YOUR TESTS!**
- ✓ If you run LAMMPS serially you can run several at once! If e.g. your computer has an 8-core processor, you can run 8 runs at the same time!

Project 3: NP melting

Melt the NPs with the optimized timestep and Tdamp values you selected from the previous steps! Start at 300K and stop at 1000K. Temperature should rise at rates of 10-20K/ns.
Watch your NP melt in Ovito (drag and drop the file produced by the `dump` command after the run is done). Your file should be large enough to provide detail, but not huge so that Ovito can still handle it. Control the size via the parameters of the `dump` command.
Produce the step vs potential energy graph and notice the jump in potential energy when the NP melts. Define the melting point from the potential energy vs timestep plot and/or the crystallization degree from the CNA analysis in Ovito (Add modification > Common neighbor analysis), which allows you to see how many atoms are recognized as crystalline and how many as amorphous.
Find the melting temperature of the 309-, 561-, and 923-atom NPs and produce the melting temperature vs NP size plot. Does it look like the one expected from theory (https://en.wikipedia.org/wiki/Melting-point_depression)?

Project 4: Monte Carlo vs Molecular Dynamics

The purpose is to work with the Monte Carlo method and see how it differs from molecular dynamics. We will perform 2 simulations on an amorphous metallic alloy nanoparticle of 923 atoms. The runs will be under a constant temperature of 400K and we will see what result each method comes up with after the same number of steps. It is advisable to make the runs last as long as you can.

The command we call Monte Carlo with is `fix atom swap` in addition to the `fix nvt` command. For its syntax you can see here: https://docs.lammps.org/fix_atom_swap.html. For a theoretical introduction to Monte Carlo, you can see the attached presentations.

The creation of amorphous nanoparticles can be done with the `create atoms` command of LAMMPS. Alternatively, if you are lazy, you can use the files in the project folder.

Can md jump over the obstacles that MC jumps over? Can MC give the time evolution of the system?