**PRACTICAL 1**

For the practical, please use the online MD tool developed by Daniel V. Schroeder, University of Weber State University:

http://physics.weber.edu/schroeder/md/InteractiveMD.html

The associated paper:

Schroeder, Daniel V. "Interactive molecular dynamics." American Journal of Physics 83.3 (2015): 210-218.

There are numerous exercises one can do using this tool, if you are interested see:

http://physics.weber.edu/schroeder/md/exercises.html

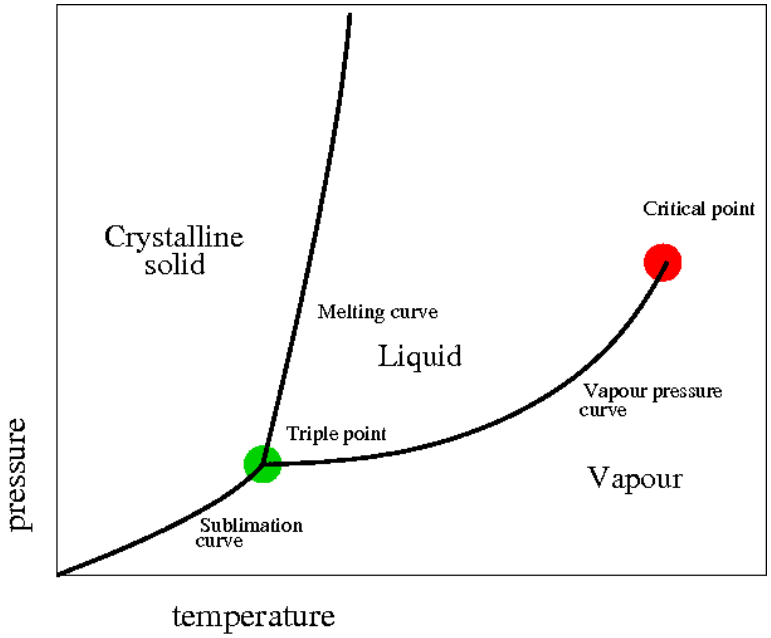
For the practical session within this course, please model and discuss the following:

1. How timestep size affects simulation? Can you run with a bigger timestep? What determines a suitable timestep?

2. Set up a few equilibrium systems, such as gas, liquid, solid, and their interfaces (gas/liquid, liquid/solid). How do you know systems are at equilibrium?

3. As in exercise 2, while keeping particle number constant, record temperature and pressure. Now you can build a phase diagram of your system.

4. On you phase diagram, can you find the triple point and the critical point?




5. Within the tool, there are pre-sets for non-equilibrium systems.

How do you know the system is not at equilibrium?
Can you build your own non-equilibrium system, such as a meta-stable crystal?

This is a good place to try the 'reverse' button – if the system is near equilibrium will it be able to trace back to its original non-equilibrium state?

6. Model gas expansion (*example: set up a small box of gas, then pause and expand the simulation box*). Record changes in T, P and energy. How do they change?

7. Will the ideal gas relation (*PV = nkT*, in natural units *k=1*) hold for the gas in the box? Why?

8. Track the position of a particle in the box, then calculate its mean squared displacement, *MSD*.:

$$MSD = \langle \Delta x^2 + \Delta y^2 \rangle$$

Plot *MSD* vs $\Delta t$. The graph should be approximately linear, characteristic of a random walk (i.e. diffusive motion).

Calculate the diffusion constant, *D:*

$$MSD = 4D\Delta t$$