Molecular dynamics for the formation of a material

We will use Fortran code to simulate the formation of a lattice structure in two dimension and three dimensions. You should be able to access it on the Globex website (Tutorial 8: MD code).

(a) **Download** the Fortran code, and open it with simplyFortran. Familiarize yourself with the code. We use here the main programme (it starts with "program MD", and ends with "end program"). You will find also subroutines, below "end program". Those subroutine execute specific operations and return new values for the arguments. Locate in the program where you can change the main parameters: LBOX is the size of the periodic box, "np" is the number of particles, "nd" is the dimension, "step_num" is the number of steps for the MD simulation, "dt" is the time step inbetween two iterations. "imode" allows to choose two different type of simulations: if imode=1, the simulation tries to find the lowest energy structure, typically this will be the stable form of the crystal. This is done by periodically reducing the velocity of the particles, which reduces the kinetic energy. It is a "thermal" drift (like cooling a gaz of particles). If "imode=2", you will do a real molecular simulation where the energy is conserved. Note that the energy is given by your choice if initial configuration. By default, the code starts from a random configuration (random particles in the box) , zero acceleration , and random velocities with maximum random amplitude "amplitude_init_vel", if it is set to zero, the programme starts from zero initial velocities.

(b) **Download and Install VESTA**:

http://jp-minerals.org/vesta/en/download.html.

Vesta will be useful to plot the final obtained configuration. Your programme will produce a file called "final_configuration.xyz". You can double click the obtained file and observe the obtained crystal

(c) **Your programme has the wrong potential V(r),** please find where the potential is used in the programme, and replace V (r)

with the Lennard-Jones potential. The equation for the force also needs to be updated.

(d) Set the dimension nd=2. Set the width of the box to LBOX=4, the number of particle to np=20, the number of steps to 80'000 step_num=80000, the time step to dt=0.0001. Execute the simulation with imode=1. You will obtain a final_configuration.xyz, have a look at it. Which crystal did you obtain? How can you explain this?

(e) Now copy final_configuration.xyz to initial_configuration.xyz. The programme will restart from this obtained configuration. Change imode=1 to imode=2. Do the simulation again, did the final configuration change? Now we will increase temperature, and repeat the same experiment a few time. To increase the temperature, we need to increase the initial kinetic energy. To do this, you can increase the value of amplitude_init_vel, try 0.3, 0.5, 1.0, 1.8. What do you observe?

(f) Now we set the dimension to nd=3 (three dimension). Set the programme back to imode=1, and erase the initial and final_configuration.xyz files. We will use np=50 particles. Run the simulation with amplitude_init_vel=0. Plot the final configuration. Which crystal do you obtain? How can you explain it?

(g) Repeat now the calculation but change to imode=2. Rename final_configuration.xyz to initial_configuration.xyz. Start with amplitude_init_vel=0, and increase gradually to 6.0. What do you observe?