a) VMD visualization of crystal structures

1) creation of a crystal using the script lattice (./lattice 3 > crystal.xyz)
2) visualization with VMD (vmd crystal.xyz)
. CPK drawing method (Graphics-> Representation-> Drawing Method CPK)
. changing visualization options (radius,colors..)

b) VMD visualization of trajectories

1) MD trajectory of 3000 steps (T=1,gamma=1)
2) visualization with VMD of the trajectory
3) what changes using "wrapatoms True" in the input file
4) multiple frames visualization (Graphics-> Representation-> Trajectory -> Selected Atoms "index 1" -> draw multiple frames "0:30:300")

c) BLOCK ANALYSIS of MD traj

1) calculation of avarage and standard deviation of total energy of previous MD traj
2) discard the first part of trajectory (relaxation of the system)
3) blocks analysis on this trajectory (does this trajectory reached equilibrium?)
4) repeat blocks analysis with longer trajectories (nstep=5000,10000,20000)
5) calculate correlation time