LECTURE 5

THE MD PROJECT:

The experimental lattice parameter of Argon is 5.26 Angstroms = 1.5471 (σ), corresponding to a density ρ = 1.0803 (σ^{-3}) in LJ units. The experimental melting point T_M = 84 K, corresponding to T_M^* = 0.696 (ε) in LJ units. (Temperature is in units of energy, the scaled T_M^* = $k_B T_M / \varepsilon$, k_B = 8.617 x 10^{-5} eV / K). For Argon, σ = 3.40 A and ε = 0.0104 eV.

Simulate the dynamics of LJ lattice in a few thermodynamical points (ρ,T) at low temperatures, where you should observe just vibrations of atoms around their equilibrium fcc lattice positions, and at high temperatures where the lattice melts. Implement the calculation of order parameter $|S_k|$ (Lecture 4) and the so-called mean square displacement (MSD, defined below) and monitor their behaviour as a function of simulation time. From the MSD(t) one can calculate the diffusion constant in the liquid phase.

MSD is defined as

$$MSD(t) = (1/N) \sum_{i=1,N} | r_i(t) - r_i(0) |^2$$

where $r_i(t)$ is the position vector of atom i at time t and $r_i(0)$ is the initial position of atom i at time origin (e.g. the beginning of the simulation or the beginning of the "production" run after an initial equilibrium period to the desired T).

In the bulk liquid phase the MSD(t) will approach a linear behaviour as a function of time, and the diffusion constant can be calculated from the slope as follows:

$$MSD(t) \rightarrow 6Dt, \quad when\ t \rightarrow \infty$$

Typical values of D in liquids are of order 10^{-5} to 10^{-4} cm^2 / s (note the unit!)
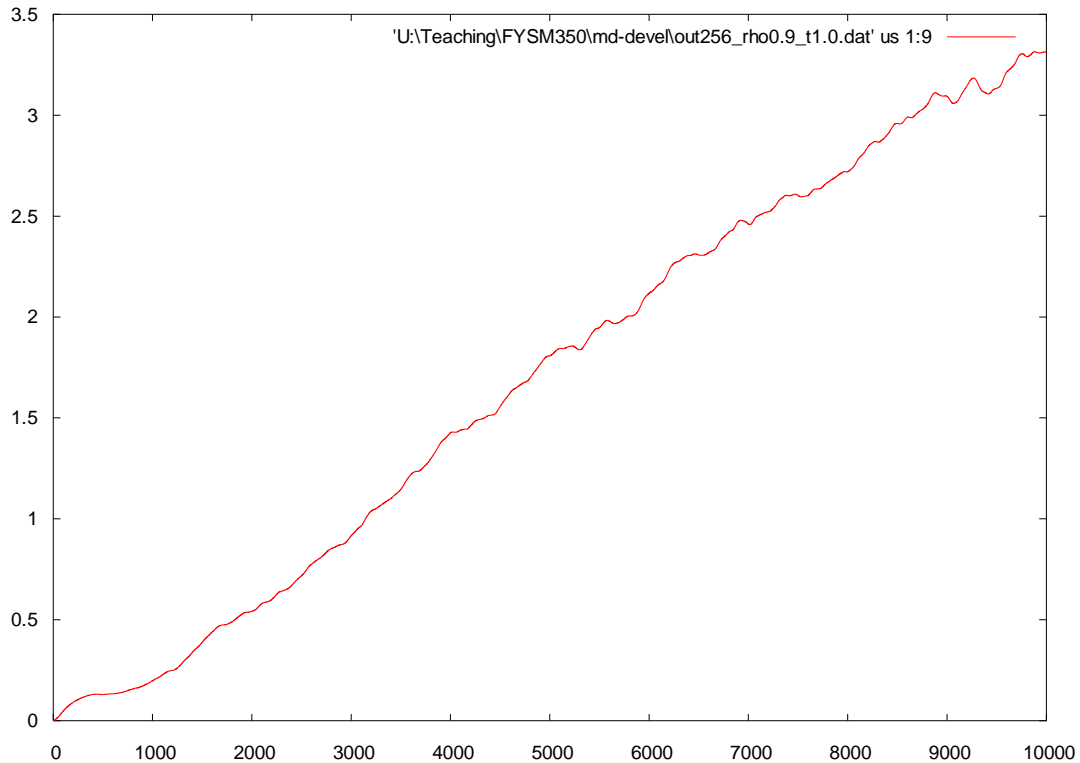
y-axis, MSD in units of σ^2 , x-axis, time in MD time steps. 256 atoms, T* = 1.0, ρ* = 0.9

To equilibrate your system to the desired T you can use the rough velocity scaling method discussed in lecture 4. Another crude way: If you start from the ordered fcc lattice and want to have your system equilibrate around $T_{desired}$, "kick" it in the beginning of run by kinetic energy which is twice as much, i.e. set the initial velocities to correspond to temperature 2 $T_{desired}$. The equipartition between the potential energy and kinetic energy will take your system in the right ballpark close to $T_{desired}$ after some time.

NOTE1: If you have persistent technical difficulties e.g. in getting the periodic boundaries to work, or are using MATLAB and want to avoid long simulation times with big lattices, it is OK to take one of the smaller samples and treat the system as a finite "cluster". See in what temperature range your cluster seems to be "solid" and where it "melts". Note that melting transition is not just a well defined transition in a small finite system but you should observe signatures that are reminiscent to bulk transition. Also, even in the "solid" phase the cluster most likely will deform away from the fcc structure (it is known to be not a preferred

structure for small LJ clusters) and the order parameter $|S_k|$ will drift to values significantly below 1.

NOTE2: An additional project to those who are quick: Introduce a defect in your periodic crystal, e.g. by removing one atom. Repeat some of the runs at high temperatures. What can you say about the effect of the defect on the "melting temperature"?

PRESENTATION OF YOUR PROJECT THURSDAY 20.4.:

Each work group will be given max 10 minutes to present their work, which includes a short discussion of the main structure of the code, and showing a couple of representative results of the simulations. You can present your work either in Finnish or in English, as you wish.