Atomistic Homework 1

(1) Write a simple **two-dimensional (2D)** "MD code" for particles interacting through Lennard-Jones potential. In the 2D system all atoms are moving on the same plane – you create the system by defining x and y coordinates of particle only and solve the equations of motion for x and y coordinates/velocities. Attach listing of your code to your homework report. You can use any of the languages you studied/used in other sections of CS6014.

(2) Create an initial system that consists of 50 atoms arranged into square 5×10 lattice as shown in the figure below. Choose the "lattice parameter" (distance between the nearest atoms) to correspond to the minimum of the Lennard-Jones potential (list the value in your report). You can assume that the initial velocities of all atoms are zero.

(3) Define the parameters of your model to be that of Ar (mass of 40 amu, parameters for Lennard-Jones potential: ε = 0.0103 eV and σ = 3.405 Å). Define timestep of integration, Δt=0.01ps. Use an appropriate unit conversion to ensure that all parameters of your system are in the same system of units, e.g. SI units.

(4) Perform MD simulation for the system you created in step (2) using the code you wrote. The total time of the simulation should be 50 ps or more. Make plots of the kinetic, potential, and total energies versus time for the duration of the simulations. Please show energies in eV and time in ps in your plots.

(5) Make plots of the initial and final atomic configuration that you obtained in the simulation. You can use your favorite plotting program to plot data points for x and y coordinates (do not connect points by lines). Or use "scatter plot" option if your graphic program has one. Or download one of the available free

visualization packages for atomic structures. Please use Angstroms as units of coordinates in your plots.

(6) **Provide a physical discussion/explanation** of the final atomic structure and the time dependences of the total, potential, and kinetic energies. Try to be quantitative in your discussion of the values of energies.

Your code can have the following structure:

Define the parameters of the system (mass of an atom m), initial coordinates and velocities of the particles in the system (x_i^0, y_i^0, $v_i^{x,0}$, $v_i^{y,0}$), set initial time $t^0 = 0$, total time of the simulation, timestep of integration, Δt.

Calculate the two components of the initial force $F_i^{x,init}$, $F_i^{y,init}$ for each particle *i*

$F_i^{x,old} = F_i^{x,init}$, $F_i^{y,old} = F_i^{y,init}$, $x_i^{old} = x_i^0$, $y_i^{old} = y_i^0$, $v_i^{x,old} = v_i^{x,0}$, $v_i^{y,old} = v_i^{y,0}$

- use a subroutine for calculation of forces

Time loop:

Loop over all atoms:

1. Calculate position at the current time

$$x_i^{new} = x_i^{old} + \Delta t\, v_i^{x,old} + \Delta t^2 F_i^{x,old}/2m$$

$$y_i^{new} = y_i^{old} + \Delta t\, v_i^{y,old} + \Delta t^2 F_i^{y,old}/2m$$

End loop for atoms

2. Calculate new forces, $F_i^{x,new}$, $F_i^{y,new}$ (*and potential energy of the system*) **– use a subroutine**

Loop over all atoms:

3. Calculate new velocities (*and kinetic energy of the system*)

$$v_i^{x,new} = v_i^{x,old} + \Delta t(F_i^{x,old} + F_i^{x,new})/2m \qquad v_i^{y,new} = v_i^{y,old} + \Delta t(F_i^{y,old} + F_i^{y,new})/2m$$

4. Copy new variables to old ones (actually, you do not need to store the values of coordinates and velocities at two different times, you can use the same variables and write new values over the old ones at steps 1 and 3).

End loop for atoms

5. Write potential, kinetic, and total energies of the system to disc for further analysis.

6. Update time ($t_n = t_{n-1} + \Delta t$). If t_n is less than the time of the simulation, continue with the time loop

End of the time loop, write the final atomic configuration to the disc and stop of simulation

---

Note that the potential energy given by Lennard-Jones interatomic potential is for a pair of atoms (*i* and *j*) – you should divide it between the two atoms.

Figure: