

Hand-On-Session: 1 (Today! 2-4 pm)

Name your codes as "loginid_xy.c".

Name the output files of the code as "loginid_xy.out".

Have your **name, rollno, date of the session, and title of the assignment** as the first four lines of your code.

You may bring with you programming books.

- **Assignment a)**

Title: Generation of FCC lattice

Make 4x4x4 unit cells of the FCC lattice of Argon. Unit cell parameters 5.26 Å (angstrom).

- **Assignment b)**

Title: Calculation of total potential energy

Argon atoms interact through Lennard-Jones potential with $\epsilon = 119.8 \text{ kB}$ (kB - Boltzmann constant). Convert ϵ to eV before using it in the code (electron Volts). $\sigma = 3.4 \text{ angstrom}$.

Read the positions of the Ar atoms from the output of a) and calculate the total potential energy of the system (without any periodic boundary conditions or cut of distances imposed).