Hands-On-session –III on Monday 30/01/12 **Time 2-4pm**

Complete the assignments of Lab Session-I & II.

Make a new copy of your Pot. Energy Program & name it "loginid_3.c" (retain your older version!!)

1. Read the fcc (4x4x4) positions *(**x, y, z** -already generated)*
2. Use a **fixed** cut_off distance of 10 A.
3. Impose PBC & Minimum Image Convention
4. Modify the code to calculate the forces on each atom due to the rest.

Please be prepared with the force expression between a pair of atoms for the Lennard-Jones Potential. Note that force being a vector need be dealt with component wise.

Bring Your Notebooks/C/Fortran- books;

Strictly do not open internet/ email accounts!