Hands-On-Session –IV (13/2/12) Time 2-4pm

Demonstrate the lab assignments of sessions-I, II, III.

Make a new copy of your Force Calculation Program &

Name it **"loginid_4a.c"** (retain your older version!!)

1. Read the fcc (4x4x4) positions (*x, y, z -already generated*)
   Keep (0, 0, 0) particle displaced at (-0.2, 0.3, 0.5).
2. Impose PBC & Minimum Image Convention (Rcut = 10A)
3. Use the forces to integrate the equations of motion using "velocity Verlet" algorithm. Use time step, dt = 1 fs.

   mass- that of argon. **(Workout the unit system!!!)**

   Perform 100 MD steps.

   Bring Your Notebooks/C/Fortran- books;

   Do not use internet!