

Hands-On-Session –V (05/03/12) Time 2-4pm

Complete the lab assignments of sessions-IV.

(Perform 1000 MD steps; with the particle positions, Potential Energy and Total Energy written at intervals of 10 MD steps; and demonstrate energy conservation.)

Use the positions to calculate the Radial Distribution Function
(averaged over all particles and over 100 MD steps.)

Compare the same with the RDF of the static-FCC lattice.

Bring Your Notebooks/C/Fortran- books;

Do not use internet!