PH442 Hands- On- Session VI (on Monday, 02 April 2012; 2- 4 pm)

Please make a copy of your working MD code and
make suitable modifications for simulation of Ar13 cluster.

Use the initial conditions (positions & velocities) circulated by mail.

Perform 100000 MD steps with a time step of exact 4 fs.
Write Temp, Pot. Energy, and Total energies in to a file at
intervals of 10 MD steps.

Demonstrate Energy conservation plotting E and U in a graph.

Obtain a histogram of the potential energy.