Assignments for the course
Computational Chemistry and Classical Molecular Dynamics (CCCMD):
Lectures 31 to Lecture 35 Week - 7

The assignments are listed lecture-wise and weekly. For example, Assignment (5.1) will be the first assignment after lecture 5. There are a total of 41 lectures.

31.1) Define the radial distribution function and outline the algorithm to calculate this function from a molecular dynamics trajectory or the position data from a Monte Carlo algorithm.

31.2) How do you calculate the internal energy of a system or its pressure from the radial distribution function?

32.1) How many subroutines are there in the program argon.f?

32.2) How many files are generated when you execute the program argon.f?

32.3) Can you calculate the diffusion coefficient of the particles from a Monte Carlo simulation?

33.1) What is the full form of mdp in full.mdp ?
33.2) Which is the software used to generate the initial configuration?
33.3) Name the command used to view all the files in a particular directory.
33.4) What is the unit of the coordinates for x, y and z in a pdb file?
33.5) What is the unit of the coordinates for x, y and z in a gro file?

34.1) What is the unit of sigma in a topology file?
34.2) Which algorithm is used for energy minimization of liquid argon?
34.3) What is the information contained in a .tpr file?
34.4) Which command is used to read a .tpr file?
34.5) Which command is used for final MD run?

35.1) Which is the command used to calculate radial distribution functions between two argon atoms?

35.2) What is the command used to create an index file?

35.3) What is the flag used to specify an output file?

35.4) Which plotting software is used to plot radial distribution functions between two argon atoms?

35.5) Which is the property calculated by using the command g_msd?