Assignments for the course
Computational Chemistry and Classical Molecular Dynamics (CCCMD):
Lectures 26 to Lecture 30 Week - 6

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.

26.1) Fit a straight line through the data given in problem (20.1) using Scilab commands.

26.2) Write the output of the above result into a file using a Scilab command.

27.1) Plot the first three Laguerre polynomials in the same plot, in the range of x = [0.0, 10.0] angstroms, using Scilab commands.

27.2) For the following data,

X_i =		0.0	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0
Y_i =	$f(X_i)$	7.01	15.1	38.9	79.2	135.1	206.9	294.8	398.9	520.1

Fit a quadratic function $ax^2 + b$ using Scilab. Find the values of a and b. You may try other fitting functions too and see if the quadratic is the best fit.

28.1) Distinguish between (a) a Fourier transform and a Laplace transform, (b) a discrete sine transform and a Fourier sine transform.

28.2) What are the basic equations of classical mechanics? Rewrite them in the Lagrangian form using the Lagrangian, L = T – V, where T and V are respectively, the kinetic and the potential energies of the system. Use a one particle system and a two particle system as examples.

29.1) Plot the Lennard-Jones potential $U(r) = 4 \varepsilon [(\sigma / r)^{12} – (\sigma / r)^{6}]$ for the range r = [3.0, 10.0] angstroms, where the values of ε/Boltzmann constant (epsilon/k_B) and σ (sigma) are 120 K and 3.4 angstroms respectively.

29.2) What is the difference between the NVE and NVT ensembles?

29.3) List the parameters for different models of water.

30.1) What is the need for using periodic boundary conditions (PBC)?

30.2) What is the difference between the Verlet algorithm and the velocity Verlet algorithm?