Assignments for the course
Computational Chemistry and Classical Molecular Dynamics (CCCMD):
Lectures 11 to Lecture 15 Week - 3

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.

11.1) What is the difference between a truncation error and a round off error?

11.2) What is the difference between interpolation and curve fitting?

11.3) What is the difference between mathematical analysis and numerical analysis?

12.1) Distinguish between single precision, double precision and quadruple precision. When do you need double precision?

12.2) What are the Taylor expansions for the functions $\log(1+x)$, $\tan(x)$, $\sinh(x)$ and $\tanh(x)$? You may need to know about Bernoulli numbers and Euler numbers for this purpose. If these are difficult to program, you treat this exercise and a process to familiarise with these numbers and do only those problems that do not involve Bernoulli or Euler numbers.

13.1) Write functions to estimate $\log(1+x)$ and $\tanh(x)$ in single precision. Use 30 terms.

13.2) When you execute the same functions in double precision, what are the differences between the values of the function in the two cases for $x = 1.0$ and 2.0?

14.1) What is the difference between forward interpolation and backward interpolation? Will the results in the two cases be the same?

14.2) Are the results of a third order Newton's interpolation and a third order Lagrange interpolation identical? Demonstrate your answer with your programs.

15.1) What are the advantages of an interpolating polynomial?

15.2) How do the errors in the interpolation change when the order of interpolation is increased?

15.3) When there are a large number of data points $\{y_i\}$ between a given set of closely spaced values of $\{x_i\}$, will you use interpolation of curve fitting?