Assignments for the course
Computational Chemistry and Classical Molecular Dynamics (CCCMD):
Lectures 21 to Lecture 25 Week - 5

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.

21.1) Obtain 100 random numbers between 0.0 and 1.0. Among these, determine how many of these lie in the range (0.0, 0.25), (0.25, 0.5), (0.5, 0.75) and (0.75, 1.0). From your result, what do you conclude about the uniformity of your random number generator? Extend the same calculation by considering 1000 and 10000 random numbers and see to what extent your conclusion changes.

21.2) (You may do this problem after watching the videos on numerical integration and submit the solution to this assignment in the next week) Obtain the integrals of the function given in problem 20.1 using the trapezoidal rule and the Simpson's rule. How much do these two values differ from the integral over the fitted function, ax + b (by using the values of a and b obtained from the linear least square fit program)?

22.1) Integrate dy/dx = cos x using the Eulers' method in the range of x = (0.0, $\pi/2$) using an interval of 0.01. Compare this result with the analytical result of y = sin (x), which is the analytical solution.

22.2) Repeat the process for the function

$dy/dx = \cos x / (x^{4/7} + \cos x + \sqrt{(x)}\, e^{x})$.

The analytical solution of the second case would be difficult to find.

22.3) In the two problems discussed above, after finding a numerical solution for y, test its accuracy by obtaining its numerical derivative at each relevant value of x by taking its numerical derivative as follows.

Numerical derivative dy_i/dx at $x = x_i$ equals

$0.5\,[\,(y_{i+1} - y_i)/(x_{i+1} - x_i) + (y_i - y_{i-1})/(x_i - x_{i-1})$.

Compare this numerical derivative with the original analytical value given by the function.

23.1) Execute the program that contains Simpson's rule as a subroutine for odd and even numbered points. Use 1000 or 1001 points for the function f(x) = exp $(-x)$ and, f(x) = exp $(-x^2)$, in the range [0, 3.0]. First determine all points in the range with a spacing of 3/1000 using a dimension statement F(1000) or F(1001). For the function exp $(-x)$, compare the numerical and the analytical integral. Familiarise yourself with a function called the error function for which tables are available.

23.2) Generate Gaussian random numbers between [–3.0, 3.0] at intervals of 0.2. Use the mean = 0 and variance = 1.0.

24.1) Using Scilab, obtain the transpose, inverse and the diagonal form for the matrix given in problem 18.3. Obtain the eigenvectors of the matrix.

24.2) For the functions given in problem 23.1, obtain the integrals using the trapezoidal rule in Scilab.

25.1) Find the roots of the equation, $10\,x^5 + 4\,x^4 + 3\,x^2 - 9x + 3 = 0$, using a suitable command in Scilab.

25.2) Solve the ordinary differential equation (ode),

$dy/dx = 4 \sin x + \cosh x + e^{-\sqrt{x}}$, using Scilab. Use the range for x as $[0, \pi/2]$.