Self Assessment Test - Computational Chemistry

1) What are the major numerical methods that are useful in chemical computations? Which methods require extensive memory and which methods require extensive CPU time?

2) Two particles interact via the potential $4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^{6}] - 0.01e^2/(4\pi\varepsilon_o r)$. The values of ε, σ, e and $4\pi\varepsilon_o$ are 120 k_B K (k_B = 1.38 10^{-23}J/K), 3.4 Å, 1.6 x 10^{-19} C, and 1.11263 x 10^{-10} C^2/N m^2 (ε_o = 8.854 x 10^{-12} C^2/N m^2) respectively. Write a program to calculate the potential from 0.1 Å to 10 Å in Joules/mol. Also convert the energy values into eV, kcal/mol, hartree, a.u. and cm^{-1}.

3) Write a program in C/C++ to multiply tow 3x3 matrices. The purpose of this is to show that the programming language is a means rather than the end. We used the compiler f77 in the chapters. Your PC/Server may have gfortran or gcc.

4) Demonstrate that the 3rd order Lagrange interpolation for a set of equidistant points x_i for which y_i are known gives the same values as the Newton's third order interpolating polynomial. For the data, use the function $y = 0.5\ x^2$ to calculate (x_i, y_i) at x_i = 0.5,1.0,1.5 and 2.0.

5) Find the largest eigehvalue and its corresponding eigenvector for the following matrix.

1.0	2.0	3.2	4.5
-0.3	0.0	42.3	9.8
0.0	23.0	3.8	-6.8
22.0	17.3	0.2	50.0

6) For the function $y = 0.5\ x^2$ to calculate (x_i, y_i) at x_i = 0.0 to 10.0 at an interval of 0.01. Obtain the integral of this set of data by using Trapezoidal rule as well as Simpson's rule and compare both these values with the analytical result.

7) Solve problem 6) using a set of random numbers generated from the gfortran library. Generate a set of 10000 pairs of random numbers in the range between 0 and 10 by simply scaling the random number of pairs (x_i, y_i) between 0 and 1 by a factor of 10. Among these pairs which are now between 1 and 10, count the number of pairs for which y_i is less than $(x_i)^2$. This fraction multiplied by 100/3 is the value of the integral. Check how much the accuracy of the extimate changes by increasing the random number set to 100000.

8) Use Scilab to sole the problems 5) and 6) above.

9) Use the Plotdigitizer software to digitize a repulsive potential energy curve given in Chapter 9. Use Gnuplot software to plot the function

$e^2 \exp(-\kappa r)/r$ where e is the electronic charge and κ is the ionic strength. Use κ of NaCl solution of 1M. Use r in Å. If e is in esu and r in cm, then, use $(esu)^2/cm = 1$ erg. Use Scilab software to compute the Fourier transform of the function $\exp(-2 r) + \exp (-3 r^2)$.

10) Calculate the overlap integral between two 1s orbitals on H atoms separated by 1Å, numerically as well as by the analytical formula as a function of r from r = 0Å to 10Å. Also calculate the Coulomb integral at 1Å. Write two Slater determinants for Li atom using the 1s, 2s and $2p_x$ orbitals of Li.