Assignments for the course
Computational Chemistry and Classical Molecular Dynamics (CCCMD):
Lectures 5 to Lecture 10 Week-2

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.

6.1) What are the advantages of an array variable that is declared by a dimension statement?

6.2) List two common mistakes that can occur when you use an array variable.

6.3) What are the differences between the declaration statements for a one dimensional array, a two dimensional array and a three dimensional array? Give an example each when you will need a two dimensional array and a three dimensional array.

7.1) Extend the Fibonacci number sequence to another sequence wherein, \( f(1) = 1, \ f(2) = 1, \ f(3) = 2, \ f(4) = f(1) + f(2) + f(3) \) and \( f(n) = f(n-1) + f(n-2) + f(n-3), \) for all \( n > 4. \) Calculate the first 15 numbers of this new series.

7.2) Using your own program, calculate the sum of numbers \( 1/n^2, \) for \( n \) going from 1 to 100. Extend the calculation to the sum of \( 1/n^3. \)

8.1) What is the difference between a formatted statement and an unformatted statement? Illustrate with an example of your own program.

8.2) What is the significance or the use of line numbers in Fortran?

8.3) Write a program to calculate the largest and the smallest number in an array of 15 numbers. You may choose any 15 numbers of your liking.

9.1) What is the difference between a function and a subroutine?

9.2) Convert the program that you studied for solving a quadratic equation into a subroutine and obtain the solution of the quadratic equation by providing the
coefficients a, b and c of the quadratic equation to the subroutine. The subroutine should provide the roots of the equation as root1 = (real1, aimag1) and root2 = (real2, aimag2).

10.1) What are the advantages of a common statement?
10.2) Write a program wherein different common statements are used to call different subroutines.