

# **Assignments for the course Computational Chemistry and Classical Molecular Dynamics (CCCMD): Lectures 1 to Lecture 5    Week-1**

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.

- 1.1) List 2-3 quantities that can be calculated using computational chemistry.
- 1.2) What is the difference between a programming statement  $a = b + c$  and a mathematical statement  $a = b + c$ ?
- 1.3) List the names of three programming languages.
  
- 2.1) What is meant by a file on a computer?
- 2.2) List three types of files.
- 2.3) How do you convert a program file: matrix.f into an executable file: a.out?
- 2.4) List the names of two operating systems.
  
- 3.1) List 4 rules of programming in the Fortran language.
- 3.2) What is meant by an algorithm?
- 3.3) State the steps to calculate  $\cos(x)$  by using its Taylor expansion by considering the first 40 terms of the expansion.
  
- 4.1) Write a do loop for calculating the product of all the odd numbers between 1 and 99 (including 1 and 99). How will you change the do loop to calculate the sum of all even numbers between 2 and 100 (including 2 and 100)?
- 4.2) List 6 functions that are calculated by using a Fortran compiler and compare the values given by your program for a given value of  $x$ , and the values for the same functions given by your calculator or the value that you get from the internet.
- 4.3) When are the roots of a quadratic equation purely imaginary?

- 5.1) List 6 commands of the Linux operating system.
- 5.2) What is the difference between the command 'ls' and the command 'ls -l'?
- 5.3) How do you copy a file a.f to b.f?
- 5.4) How do you concatenate the files a.dat (that contains 4 lines of data) and b.dat (that contains 7 lines of data) using a Linux command?
- 5.5) What are the major errors that you have got in your programming studies so far?