

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 $\text{root1} = (\text{real1}, \text{aimag1})$ and $\text{root2} = (\text{real2}, \text{aimag2})$.

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.