Course: CD61004 **Date: 29.09.2020**
Duration = 90 min **Marks: 30**

Answer any three of the following questions and each carry equal marks. Use the proper filenames for writing the programs/answers such as Q1a.f90, Q1b.f90, Q4.f90, etc.

1. Write an Fortran code to read the given file 'co2.xyz' (enclosed) and calculate the average and minimum distance between C and O atoms (intra-molecular). Here, 'intra-molecular' means the atoms belong to the same molecule. CO_2 molecule has three atoms, hence calculate two distances (C-O1 & C-O2), and repeat the same over all molecules (1000 CO_2 molecules in each snapshot/repetition) and all snapshots (total 10 snapshots). Please check the following link to know the xyz file format.
   https://openbabel.org/docs/dev/FileFormats/XYZ_cartesian_coordinates_format.html

   Contents of the file, co2.xyz

   3000
   generated by VMD

C	-0.755834	-33.262402	26.253700
O	-0.152550	-32.439400	26.781300
O	-1.484310	-33.973499	25.721100
C	10.719000	20.118601	-5.849830
O	10.496500	20.867701	-4.984430
O	10.956100	19.364000	-6.719820
C	-20.893900	-15.312300	-1.797260
O	-20.950800	-14.227400	-1.419060
O	-20.687099	-16.365700	-2.207300

   Here, each color represents one CO_2 molecule.

2. A) Write a program to solve the quadratic equation $ax^2+bx+c=0$. The program should ask to input a, b and c from standard input. Then, the program should check whether the roots are real or not (check for $b^2-4ac>=0$). If they are real, it should proceed to calculate the roots using,

$$\frac{-b \pm \sqrt{(b^2-4ac)}}{2a}$$

   If the roots are not real, then the program should output a message to inform this and exit the program.

B) Write a FORTRAN program to calculate the number of odd numbers and even numbers in the range of 2 and N.

3.

A) Which flags do you use for gfortran compiler to check array bounds during the run-time/execution?

B) fix-errors.f90: Fix errors during compilation and execution. Required input files are enclosed.

C) Write a Fortran program to remove duplicate numbers from input ‘N’ numbers.

4.

A) Write a Fortran program to sort the ‘N’ numbers in descending order

B) Write a program to generate ‘N’ random numbers and find the average value (Use rand() internal function)