Lab Assignment – 3 (2022)
PH-566

1. Write a function subprogram for the function defined as:

$f(x) = 5x^2+3x+2$ for $x<2$
$=0$ for $x=2$
$=5x^2-3x+1$ for $x>2$

Hence, calculate the value of the function at x=-0.5, 0.1 and 2.5 in the main program. You should print your answer with REAL format F15.4.

2. Given a 5 digit integer, write a function subprogram which will return its modulus 11 check digit.
Modulus 11 check digit is defined as follows:
For a number N=36532, Calculate 2×2 + 3×3 + 5×4 + 6×5 + 3×6 =81,
Now, 81/11 gives 7 as quotient and remainder 4.
Modulus 11 check digit of N will be = (11-remainder) = 7

3. Write a program with two subroutines to find the average and root mean square (rms) of a set of 'n' numbers. First subroutine finds the average and second the root mean square value. Print your answers with REAL format F12.4.
[N.B. The set of 'n' numbers should be declared as a one dimensional array]

4. In this exercise, you need to calculate the radial distribution function (RDF) for ls, 2s and 2p orbitals of a Hydrogen-atom. The RDF is $4\pi r^2$ times the square of the wave function. The wave functions themselves are given by:

- $\Psi_{1s}(r)= e^{-r/2}$
- $\Psi_{2s}(r)= 32^{-1/2} (2 -r) e^{-r/2}$
- $\Psi_{2p}(r)= 972^{-1/2} (6 - 6r + r^2) e^{-r/2}$

Write a subroutine to evaluate the RDFs and hence calculate their numerical values at r=0.5, 1.0 and 2.5 in a main program. Print your answer in REAL format F15.5