PH-566: Midsem
21/02/2022

TIME: 2 Hrs 30 mins

(Full Marks – 30)

Name	
Roll No.	

Q. No.	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**Total**
Marks									

Instructions:

- **Questions to PART A should purely be answered on paper (no coding) while PART B needs writing program on the computer.**
- **Answers to PART A needs to be sent via text email for online participants. For PART B, you need to write and send codes corresponding to each question (code name should be as per question number e.g. Q6.f90, Q7.f90 etc…..)**
- **Internet(google) is NOT allowed for any search related to code syntaxes etc.**

PART – A (Each question carries 2 marks)

1. For what range of values of variable x does the following code segment print the letter 'C'?

```
IF (x .LE. 200) THEN
    IF (x .LT. 100) THEN
       IF (x .LE. 0) THEN
           print *, 'A'
       ELSE
           print *, 'B'
       ENDIF
    ELSE
       print *, 'C'
    ENDIF
ELSE
     print *, 'D'
ENDIF
```

Answer :

2. What is the output by the following code? Assume sum and i are integer variables.

```
sum = 0
i = 1
do while (i .le. 15)
     if (i .lt. 5) then
          sum = sum + 1
          end if
       if (i .lt. 10) then
          sum = sum + 2
       end if
       if (i .lt. 15) then
          sum = sum + 3
       end if
     i = i + 3
end do
print *, sum
```

Answer :

3. How many times (or lines) does this code prints ?

```
program codes
integer P,Q
Do P=1,3
    Do Q=P,3
       Print*, "P-Q"
    Enddo
Enddo
End program
```

Answer :

4. What will be the output of the following code:

```
          program format1
          integer :: i,j,k,v4,v5
          real:: a,b,c,d,v1,v2,v3
          i=1
          j=1
          k=3
          a=2.5831
          b=3.52302
          c=1.51
          d=2.0004
          v1=i+j+d
          v2=a+b+j
          v3=d+k+c
          v4=a+b+c
          v5=i*j*k
          write(*,20)v1,v2,v3,v4,v5
20        FORMAT(E10.4,2F10.2,I2,I3)
          end
```

Answer :

5. What will be the output of the following code :

```
     program chk
     real X1,DY,DX,SL,FUN
     integer X
     X1=1
     Do X=2,3
     DY=FUN(float(X))-FUN(X1)
     DX=float(X)-X1
     SL=DY/DX
     PRINT*,X,DX,SL
     X1=X
     ENDDO
     END

     REAL FUNCTION FUN(Z)
     REAL Z
     FUN=Z**2+1
     RETURN
     END
```

Answer :

PART – B (To be programmed on computer)

6. Write a Fortran program which lists all the prime factors of a given natural number greater than one. The output must be written both in terminal as well as into a file named '**PrimeFactors.dat**'.

e.g. for the natural number 2000, the output should look like :-

The prime factors of the natural number 2000 are:
Factor # 1 : 2
Factor # 2 : 2
Factor # 3 : 2
Factor # 4 : 2
Factor # 5 : 5
Factor # 6 : 5
Factor # 7 : 5

[5 marks]

7. For a quantum mechanical problem, an electron in a symmetric square well potential governs the following transcendental equation for the quantized energies,

$$\cos(\kappa L) = 0.226(\kappa L)$$

where L=0.2nm is the width of the well, $\kappa = \sqrt{\frac{2mE}{\hbar^2}}$, m=9.1×10^{-31} Kg is the mass of electron, and $\hbar$ =6.58 x 10^{-16} eV.s. Solve the above transcendental equation using Newton Raphson method to calcualte the ground state (lowest) energy (E) in eV.

[7 marks]

8. The Debye Temperature T_D for an element at a particular temperature (T) is related to its molar heat capacity C_V by the following equation-

$$\frac{C_V}{R} = 9\left(\frac{T}{T_D}\right)^3 \int_0^{\left(\frac{T_D}{T}\right)} \frac{x^4 e^x}{(e^x - 1)^2}\, dx$$

Here R = 8.3144598 (in SI unit), is the well known Gas constant.

From the C_V *vs* T data given below, calculate Debye temperature (T_D) at each temperature (T) by solving the above integration using Simpson's 1/3rd rule. Print the T_D's at those T's in an output file named 'Debye_T'. (All data are in SI unit.)

T(K)	C_V (SI)
300	20.04
400	21.95
500	22.95
600	23.53
700	23.89

Hint: Use T_D values between 600K and 700K with steps of 0.5 K.

[8 Marks]