Name:

Enrolment No:

UPES
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UNIVERSITY OF PETROLEUM AND ENERGY STUDIES
End Semester Examination, December 2021

Course: Introduction to Computational Physics **Semester: I**
Program: M. Sc. Physics

Time 03 hrs.
Course Code: PHYS7016 **Max. Marks: 100**

SECTION A

1. **Each Question will carry 4 Marks**
2. **Instruction: Complete the statement / Select the correct answer(s)/Write short answers**

S. No.	**Question**	**CO**
Q1	Write down the syntax of "CASE" construct in FORTRAN 90. Write a small program using CASE construct in FORTRAN 90, which outputs "even" or "odd" based on the number entered by the user.	**CO1**
Q2	Why pointers are very important in computing? Write a program to in C++ to add the elements of the following array {0,-11,13,3,15,21,16,-19,20}. You should not hard code the array in the code. The user should provide the elements of the array. In addition, the size of the array should be taken from the user during run time.	**CO2**
Q3	What is simple regression? How this can be done in Gnuplot?	**CO3**
Q4	Discuss briefly how bibliography is handled in LaTeX. Write the steps of compilation and execution of the LaTeX file containing the bibliography.	**CO1**
Q5	Write following equations in LaTeX: a) $y = x\tan(\cos x) + \log(\sin x) + 5$ b) $\phi = e^{i\theta} + m\cosh x + \log(\tan\gamma)$ c) $M = N\mu\frac{\int_{-1}^{1} xe^{ax}dx}{\int_{-1}^{1} e^{ax}dx} + \sum_{M_j=-j}^{j} e^{g\mu_B M_j B/k_B T}$	**CO1**

SECTION B

1. **Each question will carry 10 marks**
2. **Instruction: Write short / brief notes**

Q6	Discuss Newton Raphson method of finding the roots of an equation $f(x) = 0$. Write a code in C++ to implement Newton's method in finding the roots of following equation: $e^x + 2^{-x} + 2\cos x - 6 = 0$ in the interval $1 \leq x \leq 2$. The maximum accuracy needed in the root estimation 10^{-5}.	**CO4**
Q7	What are various techniques available in Gnuplot for curve smoothing? Considering a data file "example.txt", write a Gnuplot script, which plots the data along with the smoothed curve in an output image file, named "example-graph.png".	**CO3**
Q8	What do you mean by function approximation? Using Lagrange interpolation, approximate the average weight curve of the sample given in the following table: **Day** | **Sample Average Weight (mg)** 0 | 6.67 6 | 17.33	**CO4**

10	42.67
13	37.33
17	30.10
20	29.31

[Hint: you need to find $P(x)$ which will approximate the data.]

Q9 Write following in LaTeX. Please consider the name of the figure as "reaction.jpg". Make sure that you are citing the paper, and referring the figure in the text body. **CO1**

Section 1: Introduction

The reaction boundary condition equates the normal component of the defect fluxes at the boundary to the rate of reaction of these defects with the surface. Such reactions result in the motion of the surface either by adding to or removing atoms from the surface. For instance, the reaction of a vacancy moves the surface inwards by removing an atom from the surface, while a dumbbell interstitial moves the surface outwards by adding an atom to the surface. Therefore, depending on the rate of reaction of defects with the surface, some atomic components enrich at the expense of the others at the boundary. The consequence of reaction of both the vacancy and interstitial with the surface is schematically displayed in Fig. 1. In this figure, a boundary node is magnified to show the reaction of the defects with the surface.

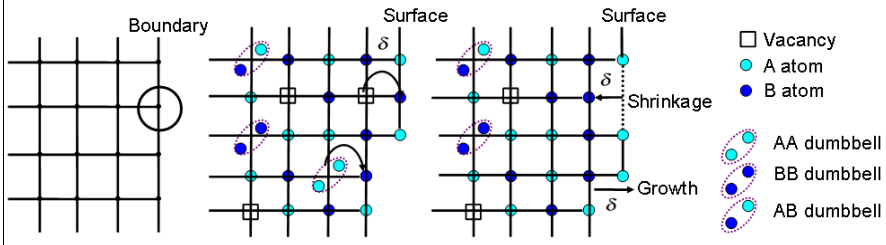

Fig 1: Reaction of vacancies and dumbbell interstitials with the surface

Vacancies may react with either A or B atoms at the surface. The forward reaction of vacancies corresponds to the removal of the atoms from the surface; its rate is given by

$$\psi_v^{\rightarrow}(\mathrm{A}) = C_v(r_s)C_A(r_s)\nu_{Av}^{\rightarrow}\exp\left(-\frac{E_s(v,\mathrm{A})}{k_BT}\right) \qquad (1)$$

$$\psi_v^{\rightarrow}(\mathrm{B}) = C_v(r_s)C_B(r_s)\nu_{Bv}^{\rightarrow}\exp\left(-\frac{E_s(v,\mathrm{B})}{k_BT}\right) \qquad (2)$$

where r_s is the location of the boundary node, E_s the surface activation barrier, and ν a vibration factor. In the reverse jump, the curvature of the surface plays an important role in defining the jump rate [1]. A reverse vacancy jump is equivalent to creating a vacancy in the material by placing an atom from the interior at the surface.

References:

[1]. Y. Grandjean, P. Bellon and G. Martin, Physical Review B 50 (1994) 4228.

Section C

1. **Each Question carries 20 Marks.**
2. **Instruction: Write long answer.**

Q10 Using Forward Euler's method of integrating ODEs, solve following initial value problem:

$$\frac{dy}{dt} = \frac{y}{t} - \left(\frac{y}{t}\right)^2 \qquad 1 \le t \le 2, \;\; y(t=1) = 1$$

CO4

You may take $h = 0.1$ and 0.02. Prepare following table for both values of h:

t_i	y_i

In the above table, t_i and y_i represent time and solution after i^{th} step. In this, you do not need to write the code. You have to calculate the solution using Euler's method and populate the table. Get the solution for at least 7 time steps.

Q11 (**10+10**) **CO2**

a) The cost of sending a package by an express delivery service is 50 Rs for the first 2 kg, and 20 Rs for each kg or fraction thereof over 2 kg. If the package weighs more than 70 kg, a 100 Rs excess weight surcharge is added to the cost. No package over 100 kg will be accepted. Write a program in FORTRAN 90 that accepts the weight of a package in grams and computes the cost of mailing the package. Be sure to handle the case of overweight packages. The program should be modular.

b) Write a program in FORTRAN 90 that computes the tax and tip on a restaurant bill for a patron with a $44.50 meal charge. The tax should be 6.75 percent of the meal cost. The tip should be 15 percent of the total after adding the tax. Display the meal cost, tax amount, tip amount, and total bill on the screen. Use functions to calculate the tax and tip.

OR

a) Write a program in FORTRAN 90 to evaluate the function

$$f(x) = \ln\frac{1}{1-x}$$

For any user-specified value of x, where ln is natural logarithm (logarithm to the base *e*). Write the program using a *while* loop so that the program repeats the calculation for each legal value of x entered into the program. When an illegal value of x is entered, terminate the program.

b) Radioactive elements decay at a rate characterized by their "half-life," defined as the time required for the original amount of radioactive material to decrease by half. For example, radon has a half-life of 3.8 days. If there are originally 100 mg of radon gas in an enclosed container, there will be 50 mg after 3.8 days, 25 mg after 7.6 days, and so forth. The process of radioactive decay can be described by the formula

$$A(t) = A_0 \exp(-t/\tau_0)$$

where A_0 is the initial amount, $A(t)$ is the amount after time t, t_0 is proportional to half-life t_{half}

$$t_0 = -\frac{t_{\text{half}}}{\ln(1/2)}$$

For Radon, $t_0 = 5.48$ days. Write a program in FORTRAN 77 that calculates and prints the amount of radon remaining from a given original sample mass after a specified number of days (print this for several intervals). This program should have provision to output the data in an external file, which should contain two columns: time and amount of radon remaining.