BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI

COMPUTATIONAL PHYSICS (**PHY F313**)

Date: 28-12-2022 **Max Time:** 60 min **Max Marks**: 40

IMPORTANT:
Finding numerical answer is good but weightage will be given for correct procedure. Blindly finding the answer has no meaning.

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1. [**Finding the roots**] Consider a particle in a finite square well. The Schrödinger equation that represents the partice position in the well is,

$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi = 0$$

   On solving the equation we get the solution for even states as, $\alpha \tan\alpha = \beta$ with $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$, $\beta = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$.

   (a) (5 marks) How the above equation can be solved using the method of Newton Raphson? Write down the algorithm.

   (b) (5 marks) The method fails at a specific point. Can you identify the problem in finding the roots of the above equation using Newton Raphson's method? If yes, how can the issue be solved?

2. [**Monte Carlo method**]

   (a) (5 marks) Consider a box divided into two halves separated by a wall. In the beginning, time t_0, there are M particles on the right side. By creating a small hole in the wall, we allow one particle to pass through the hole per unit of time. After some time, the system reaches equilibrium. Through a proper algorithm, simulate the problem.

   (b) (10 marks) Using the linear congruential method, find the 10 random numbers with $a = 6,\ c = 7,\ M = 5$ and initial seed as 2. Convert the obtained numbers in the range of $0 - 1$.

3. [**Partial Differential Equation**, 15 marks] Write the algorithm to find the solution to the Laplace equation, $\nabla^2 V = 0$ (*Jacobi relaxation* method).

========================== ALL THE BEST ==========================

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COMPUTATIONAL PHYSICS (**PHY F313**)

Date: 28-12-2022 **Max Time:** 120 min **Max Marks**: 80

1. Finding the roots using Newton Raphson method:
   (a) (5 marks) $f(x) = x - \cos(x)$
   (b) (5 marks) $f(x) = 2^x - 5 + \sin(x)$
   (c) (5 marks) Any special observation in finding the roots of the equation $f(x) = x^3 - x - 3$ with initial guess, $x_0 = 0$?

   Show your answers through appropriate plots.

2. [10 marks] Use 10-point Gaussian formula to find out the RMS value of current, given by the formula

$$I_{\text{rms}} = \int_0^{0.5} [A_0 e^{-t} \sin(2\pi t)]^2 dt$$

   Take $A_0 = 5$.

3. [10 marks] Water is drained from a vertical cylindrical tank by opening a valve at the base. The rate with which the water will be drained is given by,

$$\frac{dx}{dt} = -\alpha\sqrt{x}$$

   where α is a constant depending on the shape of the hole and the cross-sectional area of the tank and drain hole. The depth of the water x is measured in meters, and the time t in minutes. If $\alpha = 0.05$, determine how long it takes the tank to drain if the fluid level is initially 7 m. Solve by **RK-4** method using a time step of 0.1 minutes. Show the water level as a time function with a suitable plot.

4. [15 marks] Consider a pendulum with mass m at the end of a rigid rod of length l attached to, say, a fixed frictionless pivot which allows the pendulum to move freely under gravity in the vertical plane, as shown in Fig. 01. in the presence of drag and periodic forces, the equation of motion is,

$$ml\frac{d^2\theta}{dt^2} + v\frac{d\theta}{dt} + mg\sin\theta = A\cos(\omega t)$$

   where, A represents the amplitude and ω represents the angular frequency of the motion. The natural frequency of the pendulum is $\omega_0 = \sqrt{\frac{g}{l}}$. If we introduce the dimensionless quantities as,

$$\hat{t} = \omega_0 t, \qquad \hat{\omega} = \frac{\omega}{\omega_0}, \qquad \hat{A} = \frac{A}{mg}, \qquad Q = \frac{mg}{\omega_0 v}$$

   where Q is the quality factor. Solve the equation of motion with the help of Euler's, modified Euler's, and RK-4 methods with 100 grid points. Take the constants of the motion as $Q = 2,\ \hat{\omega} = 2/3,\ \hat{A} = 0.5,\ m = 1,\ l = 1\ \hat{v_0} = 0,\ \theta_0 = 0.01$. How will the pendulum move between a time interval $t = 0, 10\pi$? Show your results through a labelled plot.

5. [10 marks] Write a computer code to investigate the random walk of a particle. Plot the distance traveled versus the number of steps taken.

6. [20 marks] Consider a protein on a simple square lattice. The energy of the model is defined as,

$$E = \sum_{\langle i,j \rangle} \delta_{ij} J_{A(i),A(j)}$$

   where, the sum is over all pairs of proteins $\langle i,j \rangle$ in the chain. Whether a hydrogen bond is formed is taken care of by $\delta_{i,j}$; it is 1 if a direct covalent bond does not connect amino acids. Consider 25 amino acids and assume that energy is measured in units of k_B and the system is at a temperature of 10. Using your Monte Carlo codes (Metropolis based), simulate the different protein structures. Show the results through an appropriate plot.

========================== ALL THE BEST ==========================

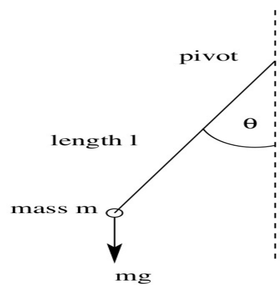

Figure 1: For Q4