BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI

COMPUTATIONAL PHYSICS (**PHY F313**)

Date: 15-12-2023 **Max Time:** 90 min **Max Marks**: 50

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. **[10M]** Consider the standing waves forming in a string with both ends fixed ($x = 0,\ x = L$). The wave equation is,
$$\frac{\partial^2 u(x,t)}{\partial t^2} - c^2 \frac{\partial^2 u(x,t)}{\partial x^2} = 0$$
Using the finite difference method, find out the iterative equation (in terms of time) that can be used to find the solutions.

2. **[10M]** The function describes the current through a resistor in a hypothetical circuit,
$$I(t) = (36 - t)^2 + (32 - t)\sin(\sqrt{t})$$
while the resistance is a function of current, as,
$$R = 15I + I^{2/3}.$$
Using the 10-point Gauss Legendre formula, compute the average voltage over $t = 0$ to 36.

3. **[5M]** The initial guess is very important to find out the roots of any equation by the Newton-Raphson method. Find out the most probable guess (with proper justification) to find out the roots of the Legendre polynomial, $P_8(x)$, that is given as
$$P_8(x) = \frac{6435x^8 - 12012x^6 + 6930x^4 - 1260x^2 + 35}{128}$$

4. **[15M]** The following equation can describe the dynamics of an object's motion,
$$\frac{dx}{dt} = x + 2y \qquad \frac{dy}{dt} = 3x + 2y; \qquad x(0) = 2,\ y(0) = 3$$
How will the system evolve as a time function from $t = 0$ to $t = 1$ at an interval of 0.2? Use the Euler's method to solve. *Distances are in meters while time is in seconds.*

5. **[10M]** In most molecular dynamics (MD) simulations, we adopt a classical approach and simulate the process in 2-dimensions.
   (a) [7M] In a few points, justify these approaches. Any reason for working in a reduced unit?
   (b) [3M] List the parameters in which all the simulations are performed.

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Given:

Abscissas = $\{\pm 0.9739065285, \pm 0.8650633667, \pm 0.6794095683, \pm 0.4333953941, \pm 0.148874339\}$
Weights = $\{0.0666713443, 0.1494513492, 0.2190863625, 0.2692667193, 0.2955242247\}$

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

BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI
COMPUTATIONAL PHYSICS (**PHY F313**)

Date: 15-12-2023 **Max Time:** 90 min **Max Marks**: 55

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1. **[15M]** The elastic curve for a cantilever is given by and differential equation:

$$EI\frac{d^2y}{dx^2} = -P(L-x),$$

where E is the modulus of elasticity and I is the moment of inertia.

(a) [6M] Solve the given differential equation using the RK-4 method. Take: $E = 3 \times 10^4,\ I = 800,\ P = 1,\ L = 10$ (in arbitrary units).

(b) [3M] Plot y as a function of x and discuss the obtained plot.

(c) [6M] Make a table showing the step size and output, and comment on the results. Compare your results with the analytical solution:

$$y = -\frac{PLx^2}{2EI} + \frac{Px^3}{6EI}$$

2. **[20M]** In a simple random walk, a walker may cross the walk an infinite number of times. In 1-dimension, the end-to-end distance varies with the number of steps, as,

$$R_{EE} = \sqrt{R^2(N)} \propto N^{\nu}$$

where $\nu = 0.5$ for simple random walk.

(a) [10M] Take at least 10 different values of N between 100 & 10,000 to estimate the value of ν for a simple random walk on a square lattice. Show the error bars and compare your results with the exact results.

(b) [10M] Now consider a self-avoiding walk in which a site that is occupied can not be occupied by the next step. Estimate the value of ν for the self-avoiding walk on a square lattice. Show the error bars and compare your results with the exact results.

3. **[20M]** Consider a system of 16 particles (in a 4×4 box) that are interacting with each other by a potential,

$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

where ϵ represents the energy while σ is hard-core repulsion. At the beginning of the simulation, all the particles are at rest. Use Verlet equations to find out the evolution of the system with time. Simulate the system using your MD simulation code(s) by assigning a random fluctuation in the position and velocity.

(a) [10M] Show the change in the energy with time at low temperatures.

(b) [10M] Show the snapshots of the change in the displacement of the particles. For a better visualization, plot y vs x for three different times ($t = 0 - 15$).

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