M. TECH. (NANO TECHNOLOGY) SEM-II (CBCS – 2015 COURSE) : SUMMER - 2018

SUBJECT : NANO COMPUTING

Day : **Monday**
Date : **11/06/2018**

S-2018-2944

Time : **11.00 AM TO 02.00 PM**
Max. Marks : 60

N.B.:

1) All questions are **COMPULSORY**.
2) Figures to the right indicate **FULL** marks.
3) Use of non programmable **CALCULATOR** is allowed.
4) Answers to both the sections should be written in **SEPARATE** answer books.

SECTION – I

Q.1 Describe algorithm to implement Bisection method. Solve equation **[10]**

$f(c)=\frac{gm}{c}\left[1-e^{-\frac{c}{m}t}\right]-V=0$. To arrive at value of 'c' given m = 68.1, t = 10, V = 40 and g = 9.8 start with values of 'c' between interval 12 and 16.

OR

Use Gauss-Jordan method to solve the system of equations. **[10]**

$15x_1-3x_2-x_3=3800$

$-3x_1+18x_2-6x_3=1200$

$-4x_1-x_2+12x_3=2350$

Q.2 Find the maximum and minimum values of the following functions using analytical method. **[10]**

i) $f(x)=\sin(2x+3)$

ii) $f(x)=e^{-2x}$

iii) $f(x)=3(x-4)^2+6$

OR

For the function $f(x)=x^5-3.14x^3+3x^2+2x+10$ approximate value of its derivative at $x=1$. **[10]**

i) Using Forward difference formula.
ii) Using Backward difference formula.
iii) Using Central difference formula.
iv) Which of the above three is better approximation to the real answer?

Q.3 Using Laplace Transform solve the initial value problem. **[10]**

$\frac{d^2y}{dt^2}+5\frac{dy}{dt}+6y=u(t-1)+\delta(t-2),\ y(0)=0,\ y'(0)=1.$

OR

Find the Fourier series for the function f(x) defined by **[10]** $f(x)=x+\pi,\ if\ -\pi<x<\pi$ and $f(x+2\pi)=f(x)$.

P.T.O.

SECTION – II

Q.4 Discuss any solution methodology for wave equation in 2D. **[10]**

OR

Explain D'Almbert principle with suitable example and its use in nano comupting. **[10]**

Q.5 State difference between molecular dynamics and Monte Carlo dynamics. **[10]**

OR

What is simulation? Discuss various algorithms related to Monte-Carlo simulation. **[10]**

Q.6 i) Explain molecular dynamics assuming that the particles in the system interact via the Leonard Jones potential **[05]**

ii) How does one calculate measurable quantities in Leonard Jones molecular dynamics **[05]**

OR

What is MATLAB? Discuss in detail with respect to Nano Modelling. **[10]**

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