

2063

M.Tech. (Material Science and Technology)

Second Semester

MT-204: Computational Tool and Techniques

Time allowed: 3 Hours

Max. Marks: 50

NOTE: Attempt five questions in all, including Question No. 1 which is compulsory and selecting two questions from each Part.

x-x-x

1. (a) How complex number is presented in python environment?
- (b) Which command is used to calculate square root of integer "a" in python?
- (c) Write a command to plot 2d graph, considering $y = \sin(x)$ as function in python?
- (d) What is a LaTeX package? How can it enhance document formatting?
- (e) Which are the different types of force fields used in molecular dynamics simulations?

(2 X 5 = 10)

PART A

2. Explain the components, terminology and working of the following operating systems:
 - (a) Windows and DOS operating system (5)
 - (b) Linux operating system (5)
3. (a) Explain forward, backward and central differentiations with its mathematical interpretation. Also discuss which one is a more accurate approach and why? (7)
- (b) Internet in present times is a boon as well as has its own disadvantages. Discuss. (3)
4. Which mathematical method is used to evaluate area under curve? Write a python program for the given functions. (10)

(a) Weighted Sum

$$A = \int_a^b f(x)dx \approx \frac{b-a}{n-1} \sum_{i=1}^n f(x_i)$$

(b) Trapezoidal method

$$A = \int_a^b f(x)dx \approx \sum_{i=1}^{n-1} \frac{f(x_{i+1}) + f(x_i)}{2} (x_{i+1} - x_i)$$

PART B

5. (a) What is Monte Carlo simulation? Mention various steps used in the process of Monte Carlo estimating. (5)
- (b) How Monte Carlo method can be used it to evaluate the value of pi(π), by using area of square and circle, where circle lies in a square and having radius $r = a/2$, and 'a' is side of square. (5)
6. (a) What is Fourier Transform? How can it be used to extract characteristic frequency from noise in computational environment? The provided function is, (6)

$$\tilde{y}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} y(t)e^{i\omega t} dt$$

Take $\omega_1 = 2$, $\omega_2 = 0.3$ and $\omega_3 = 3.5$, $y(t) = \frac{1}{2} \cos(\omega_1 t) + 2 \sin(\omega_2 t) + \cos \sin(\omega_3 t)$

- (b) What is Simpson Rule? Derive an expression for Simpson Rule. (4)

7. (a) What do you mean by Molecular Dynamics simulations? Explain some of the properties of materials which can be investigated by using Molecular Dynamics? (7)
- (b) Discuss any one approach to solve a system of linear equations. (3)

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