b.	Explain about the basic concept of C++, create a program for the following cases (i) Control statement (ii) Input / output statement (iii) Looping statement	12	3	2	1
30. a.	Derive the Schrodinger wave equation for particle in one dimensional box.	12	3	3	1
	(OR)				
b.	Write a short notes on the following (i) Kohn-Sham equation (ii) Hohenberg-Kohn theorem	12	3	3	1
31. a.	Briefly describe the following methods (i) Limitation of molecular dynamics (ii) Verlet algorithm	12	3	4	1
	(OR)				
b.	Explain the temperature variation effect in molecular dynamics. Highlight the benefits and demerits.	12	3	4	1
32. a.	Write a brief notes on (i) Metropolis algorithm (ii) Limitations of Monte-Carlo method	12	3	5	1
	(OR)				
b.	Analyze in detail about the kinetic Monte-Carlo methods along with its advantages and disadvantages.	12	3	5	1

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Reg. No.														

B.Tech. DEGREE EXAMINATION, MAY 2023

Fourth Semester

18NTC108T – MODELING AND COMPUTATIONAL TOOLS

(For the candidates admitted during the academic year 2018-2019 to 2021-2022)

Note:

(i) **Part - A** should be answered in OMR sheet within first 40 minutes and OMR sheet should be handed over to hall invigilator at the end of 40th minute.

(ii) **Part - B & Part - C** should be answered in answer booklet.

Time: 3 hours Max. Marks: 100

PART – A (20 × 1 = 20 Marks)

Answer **ALL** Questions

		Marks	BL	CO	PO
1.	If A is a square matrix, then inverse of A is given by (A) inv (A) (B) A' (C) A^(–1) (D) A*(–1)	1	1	1	3
2.	While defining an array ';' indicates (A) End of a column (B) End of a row (C) Don't display the operation (D) End of the array	1	2	1	3
3.	If P = [1 2 3] and Q = [4 5 6]. Then R = P.* Q gives (A) Error (B) R = [15 30 45] (C) R = [4 10 18] (D) R = [32]	1	2	1	1
4.	If X = [1 4 9]. Then Y = X^2 gives (A) Error (B) Y = [1 16 81] (C) Y = [1 2 3] (D) R = [42]	1	1	1	1
5.	Which of the following is not an arithmetic symbol in MATLAB? (A) + (B) * (C) / (D) !=	1	1	2	1
6.	If A = [9] and B = [10]. Then A = = B gives (A) A = [10] (B) A = [0] (C) Logical 0 (D) B = [9]	1	2	2	3
7.	Which of the following statement is not true? (A) There can be multiple decision variables for a while loop (B) A for loop can have multiple index (C) Break statement will not come out from the outer loop (D) A for loop can have multiple index values	1	2	2	3
8.	Consider the command: plot (x, y, 'g'). Here g indicates (A) X axis label (B) Y axis label (C) Green color (D) Gray color	1	1	2	3

9. Which of the following command will not give a 3D plot? 1 2 3 3
   (A) Surf (x, y, z) (B) Plot (x, y, z)
   (C) Plot3 (x, y, z) (D) Grid (x, y, z)

10. Which operator can not be overloaded? 1 1 3 3
   (A) + (B) -
   (C) * (D) : :

11. What is the output of the following code? 1 1 3 1
   Error {"404"}
   (A) 404 (B) Error in the command
   (C) Error 404 (D) Syntactical error

12. What is the output of the following code? 1 2 3 3
   ver Simulink
   (A) Shows the version of MATLAB (B) Shows the version of MATLAB and the Simulink toolbox
   (C) Shows the version of the Simulink toolbox (D) Shows the contents of Simulink toolbox

13. In density functional theory (DFT) the basic variable is 1 1 4 1
   (A) Electron density (B) Spin density
   (C) Charge density (D) Atomic density

14. The electron, being much lighter than ion core, moves much faster in solid than ion due to this the 1 2 4 3
   (A) Motion of electrons and ions cannot be decoupled (B) Motion of electrons and ions cannot be coupled
   (C) Nuclei cannot be held fixed with respect to the electron motion (D) Motion of electrons and ions can be decoupled

15. The ground-state energy and ground state wave function are determined by the minimization of the 1 1 4 1
   (A) Energy functional (B) Potential functional
   (C) Electrostatic potential (D) Exchange-correlation functional

16. DFT originates from the query 1 1 4 1
   (A) Can we arrive at a potential uniquely, given the charge density? (B) Can we arrive at a charge density uniquely, given the atomic density?
   (C) Can we arrive at a potential uniquely, given the atomic density? (D) Can we arrive at a charge density uniquely, given the potential?

17. W.Kohn, one of the DFT creators, received the Nobel prize 1 2 5 1
   (A) In Physics in 1998 (B) In Chemistry in 1998
   (C) In Physics in 2002 (D) In Chemistry in 2002

18. "The external potential $V_{ext}(r)$ is determined, within a trivial additive constant, by the electron density $\rho(r)$ ". This is statement of the 1 1 5 1
   (A) Hohenberg-Kohn theorem I (B) Hohenberg-Kohn theorem II
   (C) Kohn-Sham equation (D) Dirac equation

19. The net spin density is 1 1 5 3
   (A) The difference between up-spin and down-spin density (B) The sum between up-spin and down-spin density
   (C) The average between up-spin and down-spin density (D) The multiplication of up-spin and down-spin density

20. In an approximation, only the valence electrons are explicitly considered, the effect of the core electrons beings integrated within an equivalent ionic potential. The method is known as 1 1 5 3
   (A) The pseudo potential method (B) The Jellium model
   (C) All electron method (D) LMTO method

PART – B (5 × 4 = 20 Marks) Marks BL CO PO
Answer **ANY FIVE** Questions

21. Explain what is MATLAB? Where MATLAB can be applicable? 4 3 1 1

22. Write about MATLAB application program interface (API). 4 3 2 1

23. What do you know about 3D-visulization elements in MATLAB? 4 3 3 1

24. Justify the short range and long range interaction in molecular dynamics. 4 3 4 3

25. What is the difference between classical and quantum mechanics based on the applications area? 4 3 5 3

26. Comment on the concept of Born-oppenheimer approximation. 4 3 4 1

27. Justify the advantages and disadvantages of rejection sampling. 4 3 1 1

PART – C (5 × 12 = 60 Marks) Marks BL CO PO
Answer **ALL** Questions

28. a. Write a program for the following (using MATLAB)? 12 3 1 1
   (i) Compute the Fibonacci series
   (ii) Compute the perfect number
   (iii) Compute a program for loop and double loop

(OR)

   b. Explain in detail about the step by step procedure to solve ordinary differential equation using MATLAB. Give its applications area. 12 3 1 1

29. a. Write a program and draw a flow chart for following (using MATLAB) 12 3 2 1
   (i) Using "if loop" find are you adult or not?
   (ii) Using "else if loop" find the category
   New-born 0-1, toddlers 1-5, kids 5-13, teenager 13-18 and adult 18+.

(OR)