



DF-1520

M. Sc. (Sem. III) Examination

March / April – 2016

Physics : PH(T) - 534

(Computational & Simulation Methods In Physics)

Time : 3 Hours]

[Total Marks : 70

Instruction :

नीचे दशांशवैध निशानोंवाणी विगतो उत्तरवही पर अवश्य लपवी.  
 Fillup strictly the details of signs on your answer book.

Seat No. :

Name of the Examination :

Name of the Subject :

Subject Code No. :     Section No. (1, 2,.....):

Student's Signature

- (2) Attempt all four questions.
- (3) Symbols used have their usual meaning.
- (4) Figures to the right indicate marks.
- (5) Non-programmable scientific calculator may be used.

1 Attempt any two questions.

(i) (a) Explain how Gauss elimination method can be implemented through LU 3 decomposition method.

(b) Fit the data points given below using cubic spline and determine the value of the function at x= 7 4

X <sub>i</sub>	4	9	16
F <sub>i</sub>	2	3	4

(ii) (a) What is the difference between polynomial interpolation, least-square fit, and spline interpolation? 3

(b) Find the Cholesky decomposition of the matrix  $\begin{bmatrix} 4 & 1 & 1 \\ 1 & 5 & 2 \\ 1 & 2 & 3 \end{bmatrix}$  4

(iii) (a) Describe essential features of cubic spline fit. 3

(b) Fit a straight line to the following set of data: 4

x	1	2	3	4	5
y	3	4	5	6	8

**2 Attempt any two questions.**

- (i) (a) Explain the concepts employed in Gauss quadrature. 3  
(b) For the tabular values 4

$x$	1.0	1.2	1.4	1.6	1.8
$f(x)$	1.543	1.811	2.151	2.577	3.107

find  $O(h^4)$  value of  $\int_1^{1.8} f(x)dx$  using Romberg's integration method, starting with the  $O(h^2)$  values obtained using Trapezoidal rule calculations with  $h = 0.4$  and  $h = 0.2$ .

- (ii) (a) Explain the essential improvement of the Romberg method over the Trapezoidal method for numerical integration. 3

(b) Compute  $\int_{-1}^1 e^x dx$  using two point Gauss quadrature method. 4

- (iii) (a) What is meant by improper integrals? How are they evaluated? 3

(b) Find the largest eigenvalue and corresponding eigenvector of the matrix 4  
$$\begin{bmatrix} 1 & -3 & 2 \\ 4 & 4 & -1 \\ 6 & 3 & 5 \end{bmatrix}$$
 by Power method upto four iterations.

**3 Attempt any two questions.**

- (i) (a) Develop FFT for the case, when  $N$  is the product of two integers,  $t_1$  and  $t_2$ . 3

(b) Derive the finite difference formula corresponds to the Poisson equation in two dimensions. 4

- (ii) (a) Describe Sande-Tukey algorithm for FFT. 3

(b) Establish the heat conduction equation and discuss an explicit finite difference method for its solution. 4

- (iii) (a) Explain the advantage of the Fast Fourier Transforms over the Discrete Fourier Transforms. 3

(b) Use the explicit method to find the temperature distribution at  $t=0.1$  s. and  $0.2$  s. 4  
of a long, thin rod with a length of 10 cm and the following values:  $k=0.49$  cal/(s.cm. $^{\circ}$ C),  $\Delta x=2$  cm, and  $\Delta t=0.1$  s. At  $t=0$ , the temperature of the rod is zero and the boundary conditions are fixed for all times at  $T(0)=100$   $^{\circ}$ C and  $T(10)=50$   $^{\circ}$ C. The rod is of Aluminium with  $C=0.2174$  cal/(g. $^{\circ}$ C) and  $\rho=2.7$  g/cm $^3$ ,  $k=0.835$  cm $^2$ /s and  $\lambda=0.020875$ .

**4 Attempt any two questions.**

- (i) (a) Find out acceleration formula when an object is tied on the end of a spring. 3  
Using this acceleration formula write an algorithm for motion of an object on a spring.
- (b) Apply Kirchhoff's loop rule to a LR circuit and write an algorithm to determine current  $i(t)$  in the loop. 4
- (ii) (a) Discuss the problem and a simulation algorithm of a realistic car moving in one-dimension with air resistance and rolling friction 3
- (b) Write an algorithm for finding the horizontal range of a projectile fired with an initial velocity  $v_0$  at an angle  $\theta$  with the horizontal. Neglect air-resistance. 4
- (iii) (a) Write an algorithm to simulate the motion of a simple pendulum with damping. 3
- (b) Apply Kirchhoff's loop rule to a RC circuit and write an algorithm to determine current  $i(t)$  in the loop. 4

**5 Attempt any two questions.**

- (i) (a) Discuss the Verlet algorithm for solution of 2<sup>nd</sup> order differential equations. 2
- (b) Discuss the Euler-Cromer algorithm for finding energy eigen values and eigen functions for a particle in a one-dimensional harmonic oscillator potential using time-independent Schrödinger equation 5
- (ii) (a) What is Lennard-Jones interaction potential used in the molecular dynamics method for simulation of classical many particle systems? 2
- (b) Write a FORTRAN subprogram to evaluate temperature of a classical gas in *Molecular Dynamics* simulation after equilibrium has been reached. 5
- (iii) Discuss a mathematical model of radioactivity and a simulation algorithm for the same. 7