



Savitribai Phule Pune University

Department of Physics

Departmental Semester-End Examinations: December, 2021

M. Sc. (Physics) [Academic Flexibility]

Methods of Computational Physics, Section - II

Date: 10 December, 2021 Time: 4:15 p.m. – 05:15 p.m.

Maximum Marks: 20

Answer any ONE of the questions Q1 and Q2. Usual notation is used. Name the files exactly as mentioned in each question and upload only these files. Screenshots or hand-written page images are not allowed. In program source file mention your name, PRN number, and the question number as comment at the top.

Q1 Write a program to calculate the area of an ellipse with semi-major axis 4 and semi-minor axis 3 using Monte Carlo sample mean method. Name the program ‘Q1.f90’. Use this program to calculate the area for sample sizes $n = 2000, 4000, 8000, 16000, 32000, 64000, 128000, 256000, 512000$. The program should also calculate the absolute value of the error ϵ in the estimated value of the area for each value of n . The output should be a table with four columns giving values of n , $|\epsilon|$, $\log n$ and $\log |\epsilon|$ respectively. Write this output to a file named ‘Q1output.dat’. Make a plot (only points, no connecting line) of $\log |\epsilon|$ Vs $\log n$ and save it as ‘Q1.png’ (or some other format such as pdf). Upload the files ‘Q1.f90’, ‘Q1output.dat’ and ‘Q1.png’. **(20)**

Q2 Write a program to generate random numbers which are distributed according to the probability density using Metropolis Monte Carlo method:

$$\rho(x) = \begin{cases} ax(x-1), & \text{if } 0 \leq x \leq 1; \\ 0 & \text{otherwise} \end{cases}$$

where $a > 0$ is a constant. Name the program ‘Q2.f90’. Take the initial value $x_0 = 0.5$, step size $\Delta x \in [-\delta, \delta]$ with $\delta = 0.3$. Use $n = 55000$ Monte Carlo steps. Discard the first 5000 random values generated and save rest 50000 random values to a file named ‘Q2output.dat’. Obtain the probability density distribution of the numbers in this file. Use a binsize of 0.01. Plot the probability density $\rho(x)$ Vs x . Also plot the exact probability density curve (which is given above, but you need to determine the value of a) on the same plot. Save this plot as ‘Q2.png’ (or in any other format such as pdf). Upload the files ‘Q2.f90’, ‘Q2output.dat’ and ‘Q2.png’. **(20)**