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BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI

(I Semester 2023-24)

Assignment

Computational Physics (PHY F313) **Date: 28-10-2023**

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Important:

1. It is expected that each group will work on the assignment independently. *Learning is more important than copying!*
2. Submit your assignment by 15-11-23 at the latest. Submission after this date will be treated as late submission. In any case after 20-11-23, the codes will not be executed.
3. Upload the assignments on link shared with you. Do not send through email.
4. Compress all the files in one directory as *grpxx_asgtyy.zip*, where, *xx* is the group number, *yy* is the assignment number.

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1. Find the root of the following equations by Newton-Raphson Method. (10 iterations)
   - $f(x) = x^x + x - 4$
   - $f(x) = 3x - \cos(x) - 1$
   - $f(x) = x^2 - \ln(x) - 2$
   - $f(x) = x^3 + x^2 + x + 7$

2. Approximate the Integral
$$I = \int_e^{e+1} \frac{dx}{x\ln(x)}$$
using the trapezoidal rule (use 5 points). Also solve it using 5 point Gauss-Legendre method. Use following data for Gauss-Legendre Method:
Weights: $w_1 = 0.23692689, w_2 = 0.47862867, w_3 = 0.56888889, w_4 = 0.47862867, w_5 = 0.23692689$
Abscissas: $x_1 = -0.90617985, x_2 = -0.53846931, x_3 = 0, x_4 = 0.53846931, x_5 = 0.90617985$

3. Approximate the following integral
$$I = \int_0^{\frac{\pi}{2}} \ln(\cos x)e^{\sin x}dx$$
using the trapezoidal rule (use 5-points). Also solve it using 5 point Gauss-Legendre method. Use the weights and abscissas from question 2.

4. Approximate the integral
$$I = \int_{-1}^{1} \frac{\exp(-\cos(x)^2)}{\sqrt{1-x^2}}$$
using 5-point Gauss-Legendre method, and also using Monte-Carlo method(generate 10 randmon points). Compare the results from two methods and find out why Gauss-Legendre method is accurate in this case. what should be the sample size for the Monte-Carlo method to obtain accurate answers ?

5. Solve the differential equation $y\prime = xy + y^2 - 2$ using RK-4 method and Euler's method with step size of $h = 0.2$ and estimate the value of $y(1)$. Given $y(0) = 1$.

6. Consider a simple mass-spring system :
$$m\frac{d^2x}{dt^2} + kx = 0$$
where, m is the mass of the object ($m = 1$), k is the spring constant ($k = 10$ N/m), x is the position of mass as a function of time. The initial conditions are given as: $x(0)$= 1 m, $v(0) = 0$ m/s. Use Euler's method and RK-4 method to estimate the values of $x(1)$ and $v(1)$ with step size of $h = 0.2$

7. Write a program to understand the process of nuclear decay through Monte Carlo simulation. Consider $N_0 = 100,500$ (the initial number of unstable nuclei), the probability to decay, $p = 0.01$, the maximum time for the simulation, $t_{max} = 100$. Show the process through a plot.

8. Choose the importance function $p(x) = Ae^{-x}$ and evaluate the integrals:

$$\text{(a)} \int_0^3 x^{3/2} e^{-x} dx \qquad \text{(b)} \int_0^{\pi} \frac{dx}{x^2 + \cos^2 x}$$

9. The Lorenz model is used to study the climate change and is given by

$$\frac{dx}{dt} = a(y - x) \qquad \frac{dy}{dt} = -xz + bx - y \qquad \frac{dz}{dt} = xy - cz$$

where $a = 10,\ c = 8/3$ are some constants. b denotes the temperature difference between the top and bottom surfaces of the fluid. Solve the equations with RK-4 method with $a = 10,\ c = 8/3$ and $b = 5,\ 10,\ 25$. Plot the following:

   (a) z as a function of time for $b = 5, 10, 25$ for $x = 1,\ y = z = 0$. You can move from $t = 0$s to $t = 50$s. Is there any stricking difference at $b = 25$?

   (b) The trajectory of Lorenz model (for $b = 25$) in $x - z$ plane with initial condition as $x = 1,\ y = z = 0$.

   (c) The trajectory in yz plane when $x = 0$ with $b = 25$.

   (d) The trajectory in xz plane when $y = 0$ with $b = 25$.

10. The equipartition theoram states that for a classical system the average energy of each quadratic degree of freedom is $\frac{k_B T}{2}$. Consider the speed of a particle in a classical gas. The distributions of velocity is given by Maxwell distribution as,

$$P(v) = C \frac{v^2}{k_B T} \exp\left(-\frac{mv^2}{k_B T}\right)$$

where $P(v)$ is the probability per unit v of finding a particle with speed v, and C is a constant that depends on the mass of the particle. It is said that if the molecular dynamic method describes the behaviour of a real gas, it should yield velocity and speed distributions that have Maxwell form.

Calculate the speed distributions for a dilute gas and compare your results with the Maxwell distributions. Follow the steps:

   (a) Consider all particles with initial speed as $v = 1$ (in reduced units).

   (b) Run your simulation and after every 10 time steps record the speed distribution by dividing the v range into bins.

   (c) Tabulate the number of atoms whose speed is in the range corresponding to each bin.