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IKC-MH.55
Scientific Computing with Python
Take-home Midterm Examination
Nov 24, 2023 14:00 – Dec 18, 2023 23:59
Good Luck!

NAME-SURNAME:

SIGNATURE:

ID:

DEPARTMENT:

DURATION: Due to Dec 18, 2023

◇ **Answer at least 1 question from each parts.**
◇ **Prepare your report/codes.**
◇ **Copy your files into a directory named as your ID.**
◇ **Upload a single file by compressing this directory to UBYS.**

Question	Grade	Out of
1		25
2		25
3		25
4		25
TOTAL		100

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Part I

Numerical Techniques: Root Searching

Choose only one question.

A) **(25pts)** Write a program that finds the roots of the following functions in the given intervals using the interval halving, secant and Newton-Raphson methods:

$$lnx + \sqrt{x} - 2 = 0 \qquad [1, 2]$$
$$2x - e^{-x} = 0 \qquad [0, 1]$$

B) **(25pts) van der Waals Equation** The equation of state $PV = nRT$ for ideal gases approximates the state of real gases. A more accurate equation for real gases stated by van der Waals as:

$$(P + \frac{a}{v^2})(v - b) = RT$$

Here, $v = V/n$ is the molar volume, $R = 0.08207\ liter.atm/mol.K$ is the ideal gas constant, and a and b parameters change as depending on the gas. For carbon monoxide (CO), $a = 3.592$ and $b = 0.04267$. Write a program that finds the volume v of 1 mole of CO gas at a temperature of $T = 320\ K$ and at a pressure of $P = 2.2\ atm$ and compares it with the ideal gas equation $Pv = RT$.

Part II

Numerical Techniques: Numerical Differentiation and Integration

Choose only one question.

A) **(25pts)** Write a program that calculates the 1st derivatives with central-, forward- and backward-difference approximations at the given points and compares them with the exact value:

$$f(x) = xe^x \ (at\ x = 2)$$

B) **(25pts)** Investigate the effect of the the step length as $h = 0.1, 0.01, 0.001$ on the central-, forward- and backward-difference approximations of the 2nd derivative of the function $f(x) = lnx$ at the point $x = 1$. Compare with the analytic solution of $f''(x) = -1/x^2$.

Choose only one question.

C) **(25pts)** Calculate the following integrals with the trapezoidal formula at N=4,8,16 points and compare with their exact value.

$$\int_1^{10} \frac{dx}{x} = ln10$$
$$\int_0^1 \frac{dx}{2+x} = ln\frac{3}{2}$$

D) **(25pts) Area of the ellipse**. Equation of an ellipse with long axis a and short axis b is given as:

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$$

By considering the surface area in the first quadrant, the area of this ellipse is S and

$$S = 4\int_0^a y(x)dx$$

Write a program that calculates this expression using the Trapezoidal formula for the values a=2, b=1, and compare it with the exact result, $S = \pi ab$.

Part III

Numerical Techniques: Differential Equations - Initial Value Problems

Choose only one question.

A) **(25pts)** Write a program that solves the following initial value problems for the given range, initial condition and step length using the

Euler and fourth order Runge-Kutta methods. Compare your results with the analytical solution.

$$y' = -y cos x \qquad 0 \leq x \leq 1, \qquad y(0) = 1, h = 0.05$$
$$y' = cos 2x + sin 3x \qquad 0 \leq x \leq 1, \qquad y(0) = 1, h = 0.01$$

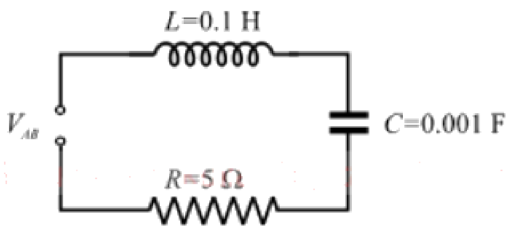
The analytical solutions of these equations are:

$$\begin{aligned} y(x) &= xe^{-sinx} \\ y(x) &= \frac{1}{2}sin2x - \frac{1}{3}cos3x + \frac{4}{3} \end{aligned}$$

B) **(25pts)** First convert the following quadratic differential equations into a linear system of equations and write a program that solves them using the Runge-Kutta method:

$$y'' = yy' \qquad 0 \leq x \leq 1, \qquad y(0) = 1, y'(0) = -1; h = 0.1$$
$$y'' - 2y' + y = e^x \qquad 0 \leq x \leq 1, \qquad y(0) = y'(0) = 0; h = 0.1$$

C) **(25pts) RLC circuits.** In the alternating current circuit shown in the figure, the voltage on each circuit element occurs as follows: Ri on the resistor R, $L(di/dt)$ on the inductor L and q/C on the capacitor C. Accordingly, a voltage applied between terminals AB would be:



$$L\frac{di}{dt} + Ri + \frac{q}{C} = V_{AB}$$

Let's take the derivative of this equation according to the variable t and use the relation $dq/dt = i$:

$$L\frac{d^2i}{dt^2} + R\frac{di}{dt} + \frac{i}{C} = \frac{dV_{AB}}{dt}$$

This differential equation is a driven damped harmonic equation of motion.

A voltage of $V_{AB} = 10sin(\omega t)$ is applied to the circuit with $R = 5\ \Omega$, $L = 0.1\ H$, $C = 0.001\ F$. First convert this equation into a linear system, then write a program to solve it by using Runge-Kutta method for the frequency $\omega = 300\ Hz$. Take the numerical data as $h = 0.01, \omega = 1$ and $b = 0.5$ and test that simple harmonic motion occurs at $b = 0$ (where b=R/L).