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Department of Engineering Sciences
IKC-MH.55
Scientific Computing with Python
Take-home Midterm Examination
April 07, 2023 14:00 – May 01, 2023 23:59
Good Luck!

NAME-SURNAME:

SIGNATURE:

ID:

DEPARTMENT:

DURATION: Due to May 01, 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
TOTAL		

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PartI Numerical Techniques: Root Searching

A) **(20pts)** Write a program that finds the roots of the following functions in the given intervals using the interval halving, secant and Newton-Raphson methods:

$$x tan x - 1 = 0 \qquad [0,1]$$
$$e^x - x^2 + 3x - 2 = 0 \qquad [0,1]$$

B) **(40pts) 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 $Pv = RT$.

C) **(40pts) Bond Length of Diatomic Molecules** In the NaCl molecule, the interaction potential between the Na^+ ion and the Cl^- ion is :

$$V(r) = -\frac{e^2}{r} + \alpha e^{-r/\rho}$$

Here, the first term is the attractive Coulomb potential, and the second term is due to the distribution of other electrons in the system. The equilibrium position between the two ions is where the potential is minimum:

$$f(r) = -\frac{dV}{dr} = \frac{e^2}{r^2} - \frac{\alpha}{\rho}e^{-r/\rho} = 0$$

The root of this equation gives the bond length r_0. Write a program that calculates the bond length in Å using the experimental values of $\alpha = 1.09\times10^3\ eV$, $\rho = 0.33$ Å and the constant $e^2 = 14.4$ ÅeV for NaCl.

PartII Numerical Techniques: Numerical Differentiation and Integration

A) **(20pts)** 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:

$$\begin{aligned} f(x) &= xlnx, \; (at\ x = 8) \\ f(x) &= xcosx - x^2 sinx, \; (at\ x = 3) \end{aligned}$$

B) **(30pts)** 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 $f''(x) = -1/x^2$.

C) **(20pts)** Calculate the following integrals with the trapezoidal formula at N=4,8,16 points and compare with their exact value.

$$\begin{aligned} \int_0^1 (3x^3 + 5x - 1)dx &= \frac{9}{4} \\ \int_0^1 e^{-x} dx &= 1 - \frac{1}{e} \end{aligned}$$

D) **(40pts) Debye Model** Molar specific heat of solids is given by the following expression:

$$c_V = 9k_B \left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx$$

Here $k_B = 1.3 \times 10^{-23}\ J/K$ is Boltzmann constant and θ_D is Debye temperature. This integral has no analytical solution. Write a program that calculates this integral for copper ($\theta_D = 300\ K$) at the temperature of each $T = 0, 5, 10, \ldots 100\ K$ by using the trapezoidal rule with N=100 points. Plot $c_V(T)\ vs\ T$ graph(s). (Hint: This integral has singularity at x=0. Taking $e^x \approx 1 + x$ for small x will simplify the integrand.)

E) **(40pts) Blackbody Radiation** Planck proposed the following integral expression for the total radiation power of a blackbody:

$$u(T) = \frac{8\pi k_B^4 T^4}{h^3 c^3} \int_0^\infty \frac{x^3 dx}{e^x - 1}$$

Write a program that calculates that integral. (Hint: This integral has singularity at x=0. Taking $e^x \approx 1 + x$ for small x will simplify the integrand.)

PartIII Numerical Techniques: Differential Equations - Initial Value Problems

A) **(20pts)** 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.

$$\begin{aligned} xy' &= (1+x)y \ \& \ 1 \le x \le 2, y(1) = 1, h = 0.1 \\ y' &= 1 + (x-y)^2 \ \& \quad 2 \le x \le 3, y(2) = 1, h = 0.2 \end{aligned}$$

The analytical solutions of these equations are:

$$\begin{aligned} y(x) &= xe^{x-1} \\ y(x) &= x + \frac{1}{1-x} \end{aligned}$$

B) **(30pts)** 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:

$$\begin{aligned} y'' &= yy' \& \ 0 \le x \le 1, y(0) = 1, y'(0) = -1; h = 0.1 \\ y'' - 2y' + y &= e^x \ \& \ 0 \le x \le 1, y(0) = y'(0) = 0; h = 0.1 \end{aligned}$$

C) **(40pts) Logistics Equation** Let $P(t)$ be the population of people in a country at time t. If the country's birth rate b is constant, then population growth increases by $bP(t)$. If the mortality rate as being proportional to the population and is taken as $k[P(t)]^2$, the population change at any time is given by the logistic equation:

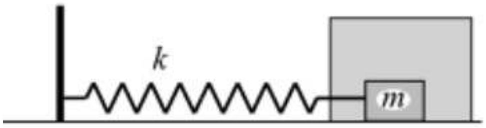
$$\frac{dP}{dt} = bP(t) - k[P(t)]^2$$

Let $b = 0.03\ year^{-1}$ and $k = 0.000002\ year^{-2}$. Write a program that calculates the population of a country after 5 years with current population of 1000 people.

D) **(40pts) Damped Harmonic Motion** For the mechanical system shown in the figure:

$$y'' + by' + \omega^2 y = 0 \ \& \ y(0) = 1,\ y'(0) = 1$$

This differential equation represents damped harmonic motion with decreasing amplitude.



i First convert this equation to a linear system, then write a program that solves it with Runge-Kutta method. Take the numerical data $h = 0.01, \omega = 1$ and $b = 0.5$.

ii Test that simple harmonic motion occurs for b=0.