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Department of Engineering Sciences
IKC-MH.55
Scientific Computing with Python
Take-home Final Examination
June 09, 2023 16:00 –June 16, 2023 23:59
Good Luck!

NAME-SURNAME:

SIGNATURE:

ID:

DEPARTMENT:

DURATION: Due to June 16, 2023

◇ **Answer at least 1 question from each parts and at most 5 questions.**
◇ **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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Part I

Numerical Techniques: Differential Equations - Boundary Value & Eigenvalue Problems

A) **(20pts)** Compute the following boundary value problems with the boundary conditions given next to them, and Write a program that compares it to analytical solutions:

$$\begin{aligned} y'' + 2y' + y &= (x+2)^2 - 2 \quad with \;\; y(0) = 0, \;\; y(1) = 2, \\ y'' &= y^3 - yy' \quad with \;\; y(1) = 1/2, \;\; y(2) = 1/3 \end{aligned}$$

The analytical solutions of these equations are:

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

B) **(30pts)** Write a program that solve the following eigenvalue problems with the given boundary conditions and find the smallest two eigenvalues:

$$\begin{aligned} y'' - 3y' + 2k^2 y &= 0 \quad with \;\; y(0) = 0, \;\; y(1) = 0, \\ y'' + k^2x^2 y &= 0 \quad with \;\; y(0) = 0, \;\; y(1) = 0 \end{aligned}$$

C) **(30pts) Lennard-Jones potential** It is a widely used potential for the interaction potential between inert gas atoms or neutral molecules. In one-dimensional space, this potential is given by the following expression:

$$V(x) = 4\epsilon \left[\left(\frac{\sigma}{x}\right)^{12} - \left(\frac{\sigma}{x}\right)^{6} \right]$$

Where, ϵ is the intensity of the potential, and σ is the equilibrium distance parameters. Take the constants in the Schrödinger equation $\hbar = m = 1$ and the potential parameters $\epsilon = 10$ and $\sigma = 1$. Write a program to find the ground state energy by solving the Schrödinger equation with the boundary conditions $\psi(0) = \psi(5) = 0$ in the range x : [0, 5].

Part II

Numerical Techniques: Linear Algebra and Matrix Computing

A) **(20pts)** Write a program that solves the following systems of linear equations using Gaussian elimination:

a)

$$\begin{aligned} 2x_1 + x_2 - 3x_3 &= -1 \\ -x_1 + 3x_2 + 2x_3 &= 12 \\ 3x_1 + x_2 - 3x_3 &= 0 \end{aligned}$$

b)

$$\begin{aligned} x_1 + 2x_2 + 4x_3 &= 11 \\ 4x_1 - x_2 + x_3 &= 8 \\ 2x_1 + 5x_2 + 2x_3 &= 3 \end{aligned}$$

B) **(30pts)** Write a program that first checks that the determinants of the matrices given below are as being nonzero and then calculates their inverses. (There is a simple way to check your results: Multiply each matrix by its inverse and it should result as a unit matrix.)

a)

$$\begin{pmatrix} 1 & 2 & 0 \\ 2 & 1 & -1 \\ 3 & 1 & 1 \end{pmatrix}$$

b)

$$\begin{pmatrix} 1 & 1 & -1 & 1 \\ 1 & 2 & -4 & -2 \\ 2 & 1 & 1 & 5 \\ -1 & 0 & -2 & -4 \end{pmatrix}$$

C) **(30pts)** Set up a system of equations that give the currents with Kirchhoff's rules for the direct current circuit given in the figure and write a program that calculates these currents.