

PHZ4151C, Fall 2019
Homework 4
Due Friday Oct 18th, 11.59PM

Instructions: Solve all four problems. Every problem is worth 10 points. Write your codes following the strategy discussed in the “Structure of the program and program design” video and the format used in the sample programs discussed in the class and lecture videos. Make sure that your code is clear, readable for users other than yourself, and properly commented. Once finished, include all your program files and figures into a zip file named after your last name and homework number (e.g. “Ullah_HW4.zip”) and submit it through canvas. Submitting individual files for each problem or part of the problem will not be accepted and disregarded. There is no need to include big data files generated by your programs unless the data files are read by your programs (that is the program reads data from the file and uses that data). Email me any questions or concerns about the homework either through canvas or directly my email address.

Note: You are allowed to submit incomplete codes for partial credit.

Problem 1: The interaction potential between Na^+ and Cl^- ions when separated by distance r in NaCl molecule is given by

$$V(r) = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{r} + \alpha e^{-r/\rho} \quad (1)$$

Where e is the charge on a proton, $\alpha = 1.09 \times 10^3$ eV, $\rho = 0.330$ angstrom. Use Secant method to find the root of equation (1). Pay attention to the units, otherwise you might end up getting the wrong answer.

Problem 2: Use Gaussian Elimination method to solve the following system of equations

$$\begin{aligned} x_1 + x_2 - x_3 + x_4 - x_5 &= 2 \\ 2x_1 + 2x_2 + x_3 - x_4 + x_5 &= 4 \\ 3x_1 + x_2 - 3x_3 - 2x_4 + 3x_5 &= 8 \\ 4x_1 + x_2 - x_3 + 4x_4 - 5x_5 &= 16 \\ 16x_1 - x_2 + x_3 - x_4 - x_5 &= 32 \end{aligned} \quad (2)$$

Problem 3: Use Gaussian Elimination with Partial Pivoting method to solve the following system of equations

$$\begin{aligned} 3.03x_1 - 12.1x_2 + 14x_3 &= -119 \\ -3.03x_1 + 12.1x_2 - 7x_3 &= 120 \\ 6.11x_1 - 14.2x_2 + 21x_3 &= -139 \end{aligned} \quad (3)$$

Problem 3: Write a program that performs the following matrix operation

$$D = A^{-1}.C$$

Where

$$A = \begin{pmatrix} -11 & -4 & 9 \\ 1 & -8 & 1 \\ 5 & 7 & 5 \end{pmatrix}, C = \begin{pmatrix} 33 & 4 & -9 \\ -9 & 18 & 81 \\ 12 & -17 & -15 \end{pmatrix} \quad (4)$$