IISER THIRUVANANTHAPURAM

# PHY 423/623: Computational Techniques & Programming languages

*School of Physics, IISER Thiruvananthapuram*

*Vasanth, 2018*

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## Problem Set 3: Due Mar 05, 2018

**Note:** Name the programs as 'qnxx_yourname.py' where 'xx' is the question number and 'yourname' is your own name. Put all the files a folder named as your name and upload it in the shared google drive folder.

1. Use the Bisection Method to find the root to eight correct decimal places of (a) $x^5 + x = 1$ (b) $\sin x = 6x + 5$ and (c) $\ln x + x^2 = 3$.

2. The van der Waals equation is

$$\left(P + \frac{n^2 a}{V^2}\right)(V - nb) = nRT$$

where $P$, $V$, $T$ are pressure, volume and temperature. $R$ is gas constant. Use Newton's method to find the volume of $n = 1$ mole of oxygen at $T = 325$ K and $P = 15$ atm. For $O_2$, $a = 1.36 \text{L}^2\text{-atm/mole}^2$ and $b = 0.003138$ L/mole. Make your initial guess using the ideal gas law equation.

3. Apply the Secant method to solve the function $e^x + \sin x = 4$ with initial guess $x_0 = 1$.

4. Apply the *Regula falsi* method to solve the function $e^x + \sin x = 4$ with initial guess $x_0 = 1$.

5. Let H denote the $n \times b$ Hilbert matrix, whose $(i, j)$ entry is $1/(i + j - 1)$. Write a function to LU factorise the matrix. Write another function which takes the LU factors and the right hand side vector as argument to solve Hx = b, where b is the vector of all ones. $n$ can take variable values, say, $n = 10, 100$.

6. Write a function to implement 'Gaussian Elimination with Partial Pivoting' to solve a system of liner equations $Ax = b$. Apply the function to solve

$$\begin{aligned} x_1 - x_2 + 3x_3 &= -3 \\ -x_1 - 2x_3 &= 1 \\ 2x_1 + 2x_2 + 4x_3 &= 0 \end{aligned}$$

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