ChE-312 Numerical methods April 16th, 2024

Part I exam

Solutions should be provided with **detailed calculus and expressions**. You should **discuss your choice** whenever it is required to choose an appropriate method.

1. **(10 points)** Consider a general linear system $Ax = b$. Discuss which method you would choose to solve the system for the cases below.

   a) A is very large and has the following form:

$$A = \begin{pmatrix} a_{11} & 0 & 0 & 0 & 0 & 0 & \cdots & \\ a_{21} & a_{22} & a_{23} & 0 & 0 & 0 & \cdots & \\ 0 & a_{32} & a_{33} & a_{34} & 0 & 0 & \cdots & \\ \vdots & 0 & a_{43} & a_{44} & a_{45} & 0 & \cdots & \\ 0 & \vdots & 0 & \ddots & \ddots & \ddots & \cdots & \\ 0 & 0 & 0 & 0 & \vdots & \vdots & \vdots & \end{pmatrix}$$

   b)

$$A = \begin{pmatrix} 5 & 3 & 2 \\ 0 & -1 & 2 \\ 0 & 0 & 3 \end{pmatrix}$$

   c) b can take multiple values and

$$A = \begin{pmatrix} 5 & 3 & 2 \\ 4 & -1 & 2 \\ 2 & 1 & 3 \end{pmatrix}$$

   d) b can take multiple values and

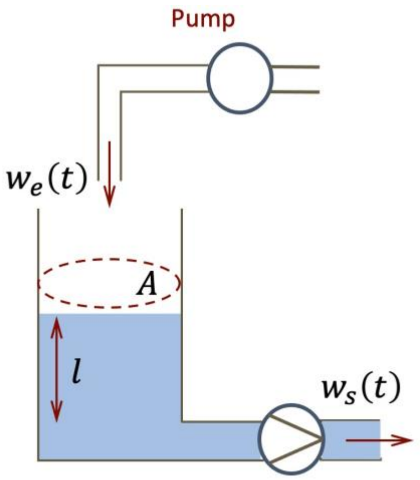
$$A = \begin{pmatrix} 5 & 2 & 2 \\ 2 & 1 & 2 \\ 2 & 2 & 3 \end{pmatrix}$$

   e) b can take multiple values and

$$A = \begin{pmatrix} 5 & 2 & 2 \\ 2 & 3 & 2 \\ 2 & 2 & 3 \end{pmatrix}$$

2. **(20 points)** The volume of water in the tank with the variable volume shown below evolves according to the following equation:

$$\rho \frac{dV(t)}{dt} = w_e(t) - w_s(t)$$



The following quantities are known: the water density $\rho = 1000\ kg/m^3$, the cross-section of the tank $A = 2\ m^2$, the output mass flow $w_s(t) = 600\ kg/s$, and the initial volume of the water in the tank $V(0) = 3\ m^3$. The measured values of the input mass flow, $w_e(t)$, are provided in the table below:

Student name: Sciper no:

Time (s)	0	60	120	180	240
w_e (kg/s)	602	604	598	601	597

a) Integrate the equation given above to obtain the evolution of the tank's water level, $l(0), l(60), l(120), l(180), l(240)$, over the observed period. Provide a rationale for selecting the specific method utilized for these calculations.
b) Compute the rate of the input mass flow variations $a = \frac{dw_e}{dt}$. Justify the method(s) used for calculations.
c) Which method would you employ to compute an improved estimate of a, $\hat{a}$, such that $a = \hat{a} + O(h^4)$? Use the chosen method to compute $\hat{a}$ with the given accuracy at $t = 120s$.

3. **(20 points)** Consider the following system of nonlinear equations

$$f_1(x,y) = x^3 - y + 0.25 = 0$$
$$f_2(x,y) = x^2 + y^2 - 1 = 0$$

   a) Compute approximately the solution of this system using the Newton-Raphson formula in two iterations starting at $x_0 = 1, y_0 = 1$. What are the obtained values of $f_1(x_1, y_1)$, $f_2(x_1, y_1)$, $f_1(x_2, y_2)$, and $f_2(x_2, y_2)$?
   b) The Damped Newton method is favored over the Newton-Raphson method for solving which categories of systems? Would it make sense to apply the Damped Newton's method to the system solved in a)? Explain your answer.

4. **(20 points)** The following SIR model depicts the spread of an infectious disease

$$\frac{dS}{dt} = -\beta SI$$
$$\frac{dI}{dt} = (\beta S - \nu)I$$

where $S(t)$ denotes the number of individuals that are part of a population that is susceptible to catching the disease because they have never been infected, $I(t)$ denotes infected individuals who can spread the disease to the susceptible individuals, β is infectivity parameter, and ν is the recovery rate modeling a fraction of infected individuals that recovered. Knowing the nature of the epidemics, we can consider that the underlying system of ODEs is non-stiff.
   a) Consider that one person was infected in a population of 1000 individuals with a disease characterized by $\beta = 0.003$ and $\nu = 1$. Use the simplest method suitable for solving these ODEs with a step size of $h = 0.25$ to determine the values for $S(0.5)$ and $I(0.5)$. Discuss your choice of method.
   b) Repeat a) with Heun's method.
   c) Compare the solutions obtained in a) and b) and explain which should be closer to the true solution. If you could solve this system on a computer, which method would you use and why? Which type of methods are suitable for solving non-stiff systems? Can you name a few of these methods?