Name: key

ChBE 2120, Numerical Methods, Paravastu Section, Fall 2015
Exam 1: 100 points possible, time: 70 min

Problem 1 (40 points total): In a journal article, you find the following data. These data were calculated using a theoretical model and the values are known precisely (no error).

x	y
-1	0
1	2
2	4.5

You would like to use interpolation in order to calculate y values for intermediate values of x (e.g., between 1 and 2). The variables are expected to obey the relationship, $y = ax + \frac{b}{x} + c$, where a, b, and c are constants.

a. (10 points) Set up a linear system of equations which could be used to find the values of a, b and c. Write your system in matrix form.

$$-a - b + c = 0$$
$$a + b + c = 2$$
$$2a + \tfrac{1}{2}b + c = 4.5$$

(+7)

$$\Longrightarrow \begin{bmatrix} -1 & -1 & 1 \\ 1 & 1 & 1 \\ 2 & 0.5 & 1 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 2 \\ 4.5 \end{bmatrix}$$

(+3)

If you are unable to do part (a), complete the rest of this problem using the alternative linear system: $\begin{bmatrix} 1 & 1 & 4 \\ 4 & 2 & 6 \\ 3 & 8 & 9 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$

b. (7.5 points) Calculate the determinant of the coefficient matrix and evaluate whether or not this system has a unique solution. Please explain your answer. If a unique solution does not exist, use the alternative linear system (has a unique solution) for the rest of the problem.

(+5)

$$\begin{vmatrix} -1 & -1 & 1 \\ 1 & 1 & 1 \\ 2 & 0.5 & 1 \end{vmatrix} = -1\underbrace{\begin{vmatrix} 1 & 1 \\ 0.5 & 1 \end{vmatrix}}_{-0.5} + 1\underbrace{\begin{vmatrix} 1 & 1 \\ 2 & 1 \end{vmatrix}}_{-1} + 1\underbrace{\begin{vmatrix} 1 & 1 \\ 2 & 0.5 \end{vmatrix}}_{-1.5}$$

$= -3 \neq 0 \Rightarrow$ There is a unique solution (+2.5)

$$\begin{vmatrix} 1 & 1 & 4 \\ 4 & 2 & 6 \\ 3 & 8 & 9 \end{vmatrix} = 1\underbrace{\begin{vmatrix} 2 & 6 \\ 8 & 9 \end{vmatrix}}_{18-48=-30} - 1\underbrace{\begin{vmatrix} 4 & 6 \\ 3 & 9 \end{vmatrix}}_{-(36-18)=-18} + 4\underbrace{\begin{vmatrix} 4 & 2 \\ 3 & 8 \end{vmatrix}}_{4(32-6)=4\cdot 26=104}$$

$= -48 + 104 = 56 \neq 0$

c. (7.5 points) Use Gaussian elimination to convert your linear system to a system with an upper triangular coefficient matrix.

(+1.5)

$$\left[\begin{array}{ccc|c} -1 & -1 & 1 & 0 \\ 1 & 1 & 1 & 2 \\ 2 & 0.5 & 1 & 4.5 \end{array}\right] \xrightarrow[R_3 \to 2R_1 + R_3 \ (+2)]{R_2 \to R_1 + R_2 \ (+2)} \left[\begin{array}{ccc|c} -1 & -1 & 1 & 0 \\ 0 & 0 & 2 & 2 \\ 0 & -1.5 & 3 & 4.5 \end{array}\right] \xrightarrow{R_2 \leftrightarrow R_3 \ (+2)} \left[\begin{array}{ccc|c} -1 & -1 & 1 & 0 \\ 0 & -1.5 & 3 & 4.5 \\ 0 & 0 & 2 & 2 \end{array}\right]$$

$$\left[\begin{array}{ccc|c} 1 & 1 & 4 & 1 \\ 4 & 2 & 6 & 2 \\ 3 & 8 & 9 & 3 \end{array}\right] \xrightarrow[R_2 \to R_2 - 4R_1]{R_3 \to R_3 - 3R_1} \left[\begin{array}{ccc|c} 1 & 1 & 4 & 1 \\ 0 & -2 & +10 & -2 \\ 0 & 5 & -3 & 0 \end{array}\right] \xrightarrow{R_3 \to R_3 + \frac{5}{2}R_2} \left[\begin{array}{ccc|c} 1 & 1 & 4 & 1 \\ 0 & -2 & -10 & -2 \\ 0 & 0 & -28 & -5 \end{array}\right]$$

d. (15 points) Write a Matlab function which could be used to determine the solution (e.g., a, b, and c) of a linear system with an upper triangular coefficient matrix such as the one you calculated in part c. Do not worry about potential division by 0 errors. Although this specific problem involves 3 equations and unknowns, your function should work for problems with any number of equations (and an equal number of unknowns). Your function should accept an upper triangular augmented matrix (n rows by $n + 1$ columns) as the sole input.

```
function [ xSolution ] = BackSubstitution( UDMatrix )
%In: Upper diagonal augmented matrix for a linear system (number of columns should be one more than the number of rows)
%Out: The x values that solve the linear system, as a column vector
  [nRows, ~] = size(UDMatrix);
  xSolution = zeros(nRows, 1);
  for i = nRows:-1:1
    xSolution(i, 1) = (UDMatrix(i, end) - UDMatrix(i, i:end-1) * xSolution(i:end, 1)) / UDMatrix(i, i);
  end
end
```

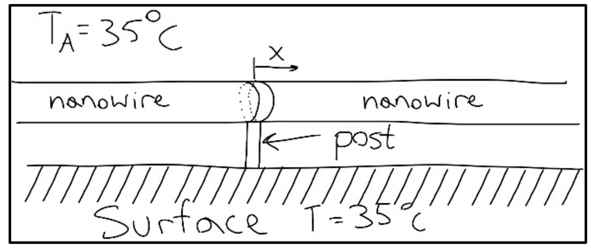
```
function [ xSolution ] = RecursiveBackSubstitution( UDMatrix )
%In: Upper diagonal augmented matrix for a linear system (number of columns should be one more than the number of rows)
%Out: The x values that solve the linear system, as a column vector
  [nRows, ~] = size(UDMatrix);
  lastXvalue = UDMatrix(end, end) / UDMatrix(end, end-1);
  if nRows == 1
    xSolution = lastXvalue;
  else
    xSolution = [RecursiveBackSubstitution([UDMatrix(1:end-1, 1:end-2) UDMatrix(1:end-1, end) - UDMatrix(1:end-1, end-1) * lastXvalue]); lastXvalue];
  end
end
```

(+5): idea/basic approach

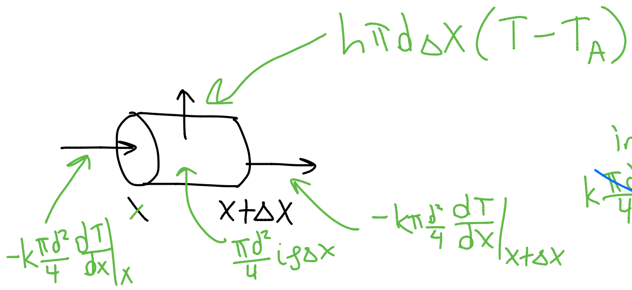
(+5): execution/details

(+5): Works for arbitrary # of unknowns

Problem 2 (45 points total): A nanowire is held just above a surface by a post ($x = 0$) as shown in the drawing. A current, $i = 0.1$, is running through the wire, generating heat at a rate of $i\rho$ per unit volume within the wire. The wire's resistivity, ρ, is 0.3. The post is connected to a surface with a large heat capacity, such that the post and the surface have a fixed temperature of 35 °C. Therefore: $T|_{x=0} = 35$°C. The temperature profile along the nanowire is assumed to be symmetric about the position of the post. Thus, $\left.\frac{dT}{dx}\right|_{x=0} = 0$. The nanowire has a thermal conductivity, k, of 0.5. Exchange of heat between the wire and the surrounding air is governed by a heat transfer coefficient, h, of 1.1. The ambient temperature, T_A, is 35 °C. The nanowire has a circular cross section and a constant dimeter of 0.01.



a) (10 points) Perform a differential energy balance to formulate a differential equation for temperature within the nanowire, T, as a function of x at steady state. Assume that T depends only on x; in other words, temperature does not depend on position within the nanowire's cross section. Current does not need to be directly considered in the energy balance. However, heat generated due to the wire's resistance to current does need to be considered.



in − out + gen − ~~cons~~ = ~~accum~~

$$k\frac{\cancel{\pi} d^2}{4}\frac{\left(\frac{dT}{dx}\Big|_{x+\Delta x} - \frac{dT}{dx}\Big|_x\right)}{\Delta x} - h\cancel{\pi} d(T-T_A) + \frac{\cancel{\pi} d^2}{4} i\rho = 0$$

+3 +5

$$\frac{d^2T}{dx^2} = \frac{4h}{kd}(T-T_A) - \frac{i\rho}{k}$$

+2

b) (5 points) Put the differential equation you derived in (a) into standard form necessary for obtaining a numerical solution to an initial value problem. If you are unable to do part (a), proceed with the differential equation $\frac{d^2T}{dx^2} = 3 - \sin x$.

$y = \frac{dT}{dx}$ +2

$\frac{dy}{dx} = \frac{d^2T}{dx^2}$

$$\boxed{\begin{aligned}\frac{dT}{dx} &= y \\ \frac{dy}{dx} &= \frac{4h}{kd}(T-T_A) - \frac{i\rho}{k}\end{aligned}}$$

+3

$$\boxed{\begin{aligned}\frac{dT}{dx} &= y \\ \frac{dy}{dx} &= 3 - \sin x\end{aligned}}$$

c) (10 points) Perform one step of Euler's method on the differential equation you obtained in (b). Use a step size, Δx, of 0.1.

+3

$T|_{x=0} = 35 \Rightarrow \frac{dy}{dx}\Big|_{x=0} = \frac{4h}{kd}(35-35) - \frac{i\rho}{k} = -0.06$

$y|_{x=0} = 0 \Rightarrow \frac{dT}{dx}\Big|_{x=0} = 0$ +4

$$\begin{bmatrix} T \\ y \end{bmatrix}\Bigg|_{x=0+\Delta x=0.1} = \begin{bmatrix} 35 \\ 0 \end{bmatrix} + 0.1\begin{bmatrix} 0 \\ -0.06 \end{bmatrix} = \begin{bmatrix} 35 \\ -0.006 \end{bmatrix}^3$$

+3

$\frac{dy}{dx}\Big|_{x=0} = 3$

$\frac{dT}{dx}\Big|_{x=0} = 0$

$$\begin{bmatrix} T \\ y \end{bmatrix}\Bigg|_{x=0+\Delta x=0.1} = \begin{bmatrix} 35 \\ 0 \end{bmatrix} + 0.1\begin{bmatrix} 0 \\ 3 \end{bmatrix} = \begin{bmatrix} 35 \\ 0.3 \end{bmatrix}$$

d) (10 points) The following Matlab function is intended to implement the Midpoint method. However, it contains 2 mistakes. Correct these mistakes.

```
function [ tSolution, Ysolution ] = ODEMidpoint( Yprime, tRange, Y0, h )
   tSolution = tRange(1):h:tRange(2);
   [numberOfEquations, ~] = size(Y0);
   Ysolution = zeros(numberOfEquations, length(tRange));
   Ysolution(:, 1) = Y0;
   for (i = 2:length(tSolution))
      y12 = Ysolution(:, i-1) + h * Yprime(tSolution(i-1), Ysolution(:, i-1));
      Ysolution(:, i) = Ysolution(:, i-1) + h * Yprime(tSolution(i-1), y12);
   end
end
```

h/2 (+5)

+h/2 (+5)

e) (5 points) Write a Matlab function that could be passed to the Yprime variable in ODEMidpoint in order to define the differential equation obtained in part b.

```
function [Yprime]=NanowireIVP(x, Y)   (+1)
   k=0.5;
   d=0.1;
   TA=35;
   h=1.1;
   i=0.1;
   rho=0.3;
   T=Y(1,1);
   y=Y(2,1);
   Yprime=[y; 4*h/k/d*(T-TA)-i*rho/k];
end
```

(+1)

(+3)

alternative: 3-sinx

f) (5 points) Write the Matlab code necessary to execute ODEMidpoint in order to numerically solve the differential equation defined in part b. Your code must define the initial conditions and the desired step size ($\Delta x = 0.1$) and use the function defined in part e (after corrections). The domain of interest is $0 \le x \le 10$.

```
[xSolution,ySolution]=ODEMidpoint(@NanowireIVP, [0 10], [35; 0], 0.1);
```

(+1) (+1) (+2) (+1)

Problem 3 (15 points total): You are designing a plant to produce a generic version of a widely used cancer drug.

a) (5 points) Calculate the expected venture profit using the figures below.
   tax rate: 28% $\rightarrow t = 0.28$
   annual sales in the third year = 100,000 grams
   drug price = \$1000/gram
   production cost = \$500/gram
   total capital investment = \$100,000,000 $\rightarrow C_{TCI}$
   minimum desired return = 20% $\rightarrow i_{min} = 0.20$

$$S = \frac{\$1000}{\text{gram}}(100{,}000 \text{ grams}) = \$100{,}000{,}000 \quad (+1)$$

$$C = \$500(100{,}000) = \$50{,}000{,}000 \quad (+1)$$

$$VP = (1-0.28)(\$100{,}000{,}000 - \$50{,}000{,}000) - 0.20(\$100{,}000{,}000) = \$16{,}000{,}000$$

(+3)

b) (5 points) Five years after starting production, the price of the drug has fallen to \$680/gram because of competition from other manufacturers. Assuming that the drug price depreciated a constant annual fractional rate (or percentage) since you started your manufacturing, setup an equation that could be used to determine this depreciation rate.

$$1000(1-d)^5 = 680 \Rightarrow f(d) = 1000(1-d)^5 - 680 = 0$$

(+5)

c) (5 points) Using initial guesses of 5% and 10%, perform one iteration of the Bisection Method on the equation you setup in part b. If were unable to do part b, use the equation $p = 1000 - 3500\,d$, where p is the drug price (\$/gram) and d is the fractional annual depreciation rate.

$f(d) = 1000(1-d)^5 - 680 = 0$ (+1)

$d_L = 0.05,\ f(d_0) = 1000(0.95)^5 - 680 = 93.78$ (+1)

$d_u = 0.10,\ f(d_1) = 1000(0.90)^5 - 680 = -89.51$ (+1)

$d_r = \frac{0.05+0.10}{2} = 0.075 \quad f(d_2) = -2.82 \Rightarrow \text{new } d_u$

(+2)

new bracket = [0.05, 0.075]

$f(d) = 1000 - 3500d - 680 = 0$

$f(d_L) = f(0.05) = 145$

$f(d_u) = f(0.10) = -30$

$f(d_r) = f(0.075) = 57.5$

new bracket: [0.05, 0.075]