EXAM 3 - BIOE 391 Take Home – 2022

This portion of the exam is **open book/open notes**. Any other resources used <u>must be acknowledged</u>. Please **READ ALL INSTRUCTIONS**, manage your time effectively and answer the questions concisely but completely. Please upload a hard copy of the exam as a single PDF or Word file to Canvas. Handwritten formulas (equations) and diagrams are OK if the files are clearly scanned. Please make sure your file is clearly readable before uploading it. The <u>recommended</u> time investment in this take-home exam should be of no more than **5 hours**, although you are allowed to use more.

On my honor, I have neither given nor received any unauthorized aid on this exam.
Signature:
Read Carefully!

Please comment your code as much as possible. This will help us to grade and give YOU partial credit.

Problem 1 (60 pts). A bioengineering team designed a microfluidic chamber to test cell migration in the presence of a nutrient gradient. The reaction-diffusion equation describing the steady state distribution C(x) of the nutrient is:

$$D\frac{d^2C}{dx^2} - kC + F\frac{1}{x^2 + x_0^2} = 0$$

Here, the first term is the diffusion flux along the length of the chamber, the second term accounts for nutrient consumption by the cells, and the final term represents influx of nutrients through the sides of the chamber. At one end of the tube (x = 0), there is another large source of nutrients that results in a fixed concentration of 30 mM. On the other end of the tube (x = 1.5mm) there is an absorbing reservoir that keeps the concentration at 0 mM. Thus, we have boundary conditions C(0) = 30 mM and C(1.5) = 0 mM.

- a) Use the parameters $F = 0.8 \text{ mM s}^{-1}$, $x_0 = 0.4 \text{ mm}$, $k = 3 \times 10^{-3} \text{ s}^{-1}$, and $D = 2.5 \times 10^{-4} \text{ mm}^2 \text{ s}^{-1}$ to determine the concentration C(x) within the tube using the shooting method and the ode45 solver. Assume tube dimensions 0 < x < 1.5 mm. Please plot the concentration C(x) vs position x in tube as obtained by the shooting method.
- b) The team concluded that the results of the model (Eq. 1) did not fit their measurements, and that the nutrient consumption is best described by Hill-type kinetics resulting in a modified model

$$D\frac{d^2C}{dx^2} - \frac{kC}{1 + \frac{C}{K_M}} + F\frac{1}{x^2 + x_0^2} = 0$$

where $K_M = 2.5$ mM. Determine the concentration C(x) within the tube 0 < x < 1.5 mm in this non-linear case. Please plot the concentration C(x) vs position x in tube for the nonlinear case as obtained by the shooting method.

Problem 2 (40 pts). As a part of another bioengineering team, you now investigate the diffusion of fluorescent dye in a 2D chamber as a function of space and time. You argue that the dye concentration obeys the following conditions:

PDE	Boundary Conditions	Initial Conditions
$\frac{\partial^2 C}{\partial x^2} + b \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}$	C(0,t)=0	C(x,0)=0
$\frac{\partial x^2}{\partial x} + D \frac{\partial x}{\partial x} - \frac{\partial t}{\partial t}$	C(1,t)=1	$0 \le x \le 1$

- a) Discretize the given PDE using second-order accurate finite-difference analogues for the derivatives with a Crank-Nicolson formulation to solve the problem, given that $\mathbf{b} = 6$.
- b) Implement the Crank-Nicolson formulation on MATLAB.
- c) Utilize an appropriate method to solve the equation system. Increase the value of Δt by 10% for each time step to more quickly obtain the steady state solution and select values of Δx and Δt for good accuracy.
- d) Plot C versus x for various values of t.
- e) Repeat the solution process for different values of the dispersion term. Solve for these values of **b**: 4, 2, 0, -2, -4. Again, plot **C** versus **x** for various values of **t**.
- f) **BONUS** (5pts): Explain what the influence of the dispersion term **b** is, and what is changing in the solution.