NE336 Assignment 3 Due Nov 8^{th}

Instructions

You know what to do at this point...

Systems of ODEs

Question 1

This is a classic problem called Gear's Chemistry Problem. The kinetics of a batch reaction are described by the following system of ODE IVPs:

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} = -0.013x_1 - 1000x_1x_3$$
$$\frac{\mathrm{d}x_2}{\mathrm{d}t} = -2500x_2x_3$$
$$\frac{\mathrm{d}x_3}{\mathrm{d}t} = -0.013x_1 - 1000x_1x_3 - 2500x_2x_3$$

Subject to initial conditions: $x_1(t=0)=1$, $x_2(t=0)=1$ and $x_3(t=0)=0$.

Integrate (solve) this system of equations over $t=[0,50]$. Try using different solvers (you could do this by changings methods in `solve_ivp`) and print the time it takes for each to see how the solution time varies.

Please explain the reason behind this variance.

Submit in a file called `system_ODEs_question1.py`.

> **Note** :
> Gear was a mathematician and not an engineer, so these equations are not of practical interest but have become a classic problem for testing ode solvers; note they do contain a typo making the results physically meaningless.

Question 2

Consider a narrow cylindrical pore of length L = 1.0 cm. At the entrance to the pore, the concentration of species A is $C_{A,0}$ = 1.0 $\times 10^{-3}$ mol/cm^3. Species A diffuses into the pore and reacts according to the following reaction:

$$A \rightarrow B \;\text{ with } r = kC_A^2 \;\text{ where } k = 10 \text{ cm}^3\text{/mol s}$$

Neglecting radial terms gives the following differential equation:

$$D_A \frac{d^2C_A}{dx^2} = kC_A^2$$

With $D_A = 1.0 \times 10^{-3} \mathrm{cm}^2/s$. Assuming that the end of the pore (x = L) is closed off, the BCs are:

$$C_A(x = 0) = C_{A,0}$$
$$\left.\frac{\mathrm{d}C_A}{\mathrm{d}x}\right|_{x=L} = 0$$

Find $C_A(x)$ by using the shooting method with (a) `solve_ivp` and (b) `solve_bvp`.

Include both approaches in one file and plot the results ($C_A(x)$ vs x) for both methods on one figure with labels to distinguish between them.

Submit in a file called `system_ODEs_question2.py`.

Question 3 (BONUS)

Solve the previous problem using a FD approach.

i) (On paper) Set up finite difference equations. Maintain second order accuracy.
Explain how the boundary conditions can be implemented.

ii) Solve the system in python. How do you know your answer has converged?

iii) Plot $C_A(x)$ vs x and compare to the results from Question 2 (comment in code).

Submit in a file called `system_ODEs_question3.py`.

Elliptic PDEs

Given the following PDE:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \sigma(T_a - T^4) = 0$$

with the following boundary conditions:

$$\begin{aligned} T(x, 0) &= 20 \quad 0 \leq x \leq 0.3 \\ T(0, y) &= 50 \quad 0 \leq y \leq 0.3 \\ \frac{\partial T}{\partial y}(x, 0.3) &= 0 \quad 0 \leq x \leq 0.3 \\ \frac{\partial T}{\partial x}(0.3, y) &= 0 \quad 0 \leq y \leq 0.3 \end{aligned}$$

Determine the temperature distribution T(x,y) using centered finite differences under the following conditions:

a) $\sigma = 1e - 4$ (**BONUS**)

b) $\sigma = 0$

Assume $T_a = 25$ and $\Delta x = \Delta y = 0.1$ for both conditions. Please include the setup steps on paper and submit along your code.

Submit in a file called `elliptic_PDE.py`.