ChE-312 Numerical methods May 29th, 2023

Part II – Take home exam

All submitted solutions to exam problems have to be **handwritten** (either written on paper and scanned or handwritten on a tab/pad), except for when a MATLAB file/Python script is required. Written solutions without **detailed calculus and expressions** used to obtain them are not enough.

1. **Finite Difference Method (20 points, Written response).** In many cases even non-linear differential equations can be solved with Finite Difference methods. While the matrix method cannot be used, a different non-linear solving algorithm can be used (for example "fsolve" in Matlab). Consider the Kidder equation for flow in porous media:

$$\sqrt{1-\alpha u}\frac{d^2u}{dx^2} + 2x\frac{du}{dx} = 0$$

where $u = u(x)$, α is a constant, and with the boundary conditions : $u(0) = 0$, $\left.\frac{du}{dx}\right|_{x=1} = 0$ (over the domain from 0 to 1). Using the finite difference approach with 5 (equally spaced) discretized points over the domain, can you write the system of equations that would need to be solved to find the $u_i's$ for i =1 to 5? You do not need to solve these equations, just write them down.

2. **Fourier transform second derivative (20 points, Written response).** Using your preferred calculator or software, compute the discrete Fourier transform for the following three arrays:

$$\begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 3 \\ 2 \\ 1 \end{bmatrix} \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ -1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \begin{bmatrix} 0 \\ 0 \\ -1/2 \\ 0 \\ 0 \\ 0 \\ 1/2 \\ 0 \end{bmatrix}$$

Please explain your results in terms of "frequency space".

3. **Crank–Nicolson method (40 points, Written response and MATLAB/python file)**

Consider the transient boundary value problem given as:

$$\frac{\partial u}{\partial t} = \alpha\frac{\partial^2 u}{\partial x^2} - \beta(u - u_0) + \gamma$$

Where α, β, γ, and u_0 are constants and $u = u(x,t)$. The boundary and initial conditions are given as:

$$\left.\frac{\partial u}{\partial x}\right|_{x=0} = 0, \;\; u(x=1,t) = u_0\,, \;\; u(x,t=0) = u_0.$$

a) Using the Crank–Nicolson method, with N discrete points with spacing Δx over the x domain from 0 to 1, and N_t time steps with spacing Δt, write the terms of the linear matrix problem needed to solve for the non-dimensional, discrete u values at an arbitrary next time point: $\boldsymbol{u}^{n+1} = [u_1^{n+1} \;\cdots\; u_{i-1}^{n+1} \;\; u_i^{n+1} \;\; u_{i+1}^{n+1} \;\cdots\; u_N^{n+1}]$. That is, what terms belong in place of the question marks in the following matrix equation? (remember: the elements of $\boldsymbol{u}^n$ are known)

$$\begin{bmatrix} ? & ? & & & & & \\ \ddots & \ddots & \ddots & & & & \\ & ? & ? & ? & & & \\ & & ? & ? & ? & & \\ & & & ? & ? & ? & \\ & & & & \ddots & \ddots & \ddots \\ & & & & & ? & ? \end{bmatrix} \begin{bmatrix} u_1^{n+1} \\ \vdots \\ u_{i-1}^{n+1} \\ u_i^{n+1} \\ u_{i+1}^{n+1} \\ \vdots \\ u_N^{n+1} \end{bmatrix} = \begin{bmatrix} ? \\ \vdots \\ ? \\ ? \\ ? \\ \vdots \\ ? \end{bmatrix}$$

b) Create a MATLAB function (problem3.m) or python script to solve this system where N, Δt, the number of time steps (N_t), and the other constants, α, β, γ, u_0, of the system are input arguments and the output is $\boldsymbol{u}^{N_t}$ (also plotting the solution for the last time point). Upload this script to Moodle.

c) If $u_0 = 0, \alpha = 1, \beta = 300000/\gamma$ and $\gamma =$ your EPFL SCIPER number (which is found on your EPFL identity CAMIPRO card), can you use your numerical solution to find the value for $u(x=0,t=1)$?

4. Finite Element approach (20 points, Written response). In the Finite element approach, it is also possible to use parabolic basis functions. Consider the example from the course where three "hat"-shaped basis functions were used that were generally defined as:

$$\phi_j(x) = \begin{Bmatrix} \dfrac{x - x_{j-1}}{h_j} \text{ for } x_{j-1} \le x \le x_j \\ \dfrac{x_{j+1} - x}{h_{j+1}} \text{ for } x_j \le x \le x_{j+1} \\ 0 \quad \text{for } x < x_{j-1}, x > x_{j+1} \end{Bmatrix}$$

Can you propose new general forms of $\phi_j(x)$ and $\phi_j'(x)$ if parabolic basis functions are chosen without equal spacing between the nodes, h_j ?