ChE-312 Numerical methods

Part 2

Exercises 4-5 solutions.

Ex. 4

Equation:

$$\rho C_p \frac{\partial T(x,t)}{\partial t} = k\frac{d^2T(x,t)}{dx^2} + J^2(\varepsilon T(x,t) + \rho_{ele}^0)$$

Simplify!

$$\frac{\partial T(x,t)}{\partial t} = \frac{k}{\rho C_p}\frac{d^2T(x,t)}{dx^2} + \frac{J^2\varepsilon}{\rho C_p}T(x,t) + \frac{J^2\rho_{ele}^0}{\rho C_p}$$

Assign constants

$$\frac{\partial T(x,t)}{\partial t} = \alpha\frac{d^2T(x,t)}{dx^2} + \beta T(x,t) + \gamma$$

With $\alpha = \frac{k}{\rho C_p}, \beta = \frac{J^2\varepsilon}{\rho C_p}, \gamma = \frac{J^2\rho_{ele}^0}{\rho C_p}$

and $T(x=0,t) = T_0,\ T(x=L,t) = T_L$ and $T(x,t=0) = \frac{T_L - T_0}{L}x + T_0$

Crank-Nicolson equation:

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{1}{2}(F_i^{n+1} + F_i^n)$$

With finite difference approximations:

$$\frac{d^2T(x,t)}{dx^2} = \frac{T_{i+1} - 2T_i + T_{i-1}}{(\Delta x)^2} \quad \Leftrightarrow F_i^n = \alpha\left(\frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta x)^2}\right) + \beta T_i^n + \gamma$$

In to Crank-Nicolson equation:

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{1}{2}\left(\alpha\left(\frac{T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}}{(\Delta x)^2}\right) + \beta T_i^{n+1} + \gamma + \alpha\left(\frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta x)^2}\right) + \beta T_i^n + \gamma\right)$$

Rewrite:

$$T_i^{n+1} - T_i^n = \left(\frac{\alpha\Delta t}{2(\Delta x)^2}(T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}) + \frac{\beta\Delta t}{2}T_i^{n+1} + \frac{\gamma\Delta t}{2} + \frac{\alpha\Delta t}{(\Delta x)^2}(T_{i+1}^n - 2T_i^n + T_{i-1}^n) + \frac{\beta\Delta t}{2}T_i^n + \frac{\gamma\Delta t}{2}\right)$$

Define revised constants:

$$T_i^{n+1} - T_i^n = (\alpha'(T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}) + \beta' T_i^{n+1} + \alpha'(T_{i+1}^n - 2T_i^n + T_{i-1}^n) + \beta' T_i^n + 2\gamma')$$

Where: $\alpha' = \frac{k\Delta t}{2(\Delta x)^2\rho C_p}, \beta' = \frac{J^2\varepsilon\Delta t}{2\rho C_p}, \gamma' = \frac{J^2\rho_{ele}^0\Delta t}{2\rho C_p}$

Move all unknown terms to one side:

$$T_i^{n+1} - \alpha' T_{i+1}^{n+1} + 2\alpha' T_i^{n+1} - \alpha' T_{i-1}^{n+1} - \beta' T_i^{n+1} = T_i^n + \alpha' T_{i+1}^n - 2\alpha' T_i^n + \alpha' T_{i-1}^n + \beta' T_i^n + 2\gamma'$$

Group:

$$(-\alpha')T_{i+1}^{n+1} + (1 + 2\alpha' - \beta')' T_i^{n+1} + (-\alpha')T_{i-1}^{n+1} = T_i^n + \alpha' T_{i+1}^n - 2\alpha' T_i^n + \alpha' T_{i-1}^n + \beta' T_i^n + 2\gamma'$$

At the boundary $i = 1$:

$$T_1 = T_0$$

At the boundary $i = N_x$:

$$T_{N_x} = T_L$$

The matrix can now be written.

$$\begin{bmatrix} 1 & 0 & & & & & \\ \ddots & \ddots & \ddots & & & & \\ & -\alpha' & 1+2\alpha' - \beta' & -\alpha' & & & \\ & & -\alpha' & 1+2\alpha' - \beta' & -\alpha' & & \\ & & & -\alpha' & 1+2\alpha' - \beta' & -\alpha' & \\ & & & & \ddots & \ddots & \ddots \\ & & & & & 0 & 1 \end{bmatrix} \begin{bmatrix} T_1^{n+1} \\ \vdots \\ T_{i-1}^{n+1} \\ T_i^{n+1} \\ T_{i+1}^{n+1} \\ \vdots \\ T_{N_r}^{n+1} \end{bmatrix}$$

$$= \begin{bmatrix} T_0 \\ \vdots \\ T_{i-1}^n + \alpha' T_i^n - 2\alpha' T_{i-1}^n + \alpha' T_{i-2}^n + \beta' T_{i-1}^n + 2\gamma' \\ T_i^n + \alpha' T_{i+1}^n - 2\alpha' T_i^n + \alpha' T_{i-1}^n + \beta' T_i^n + 2\gamma' \\ T_{i+1}^n + \alpha' T_{i+2}^n - 2\alpha' T_{i+1}^n + \alpha' T_i^n + \beta' T_{i+1}^n + 2\gamma' \\ \vdots \\ T_L \end{bmatrix}$$

Where: $\alpha' = \frac{k\Delta t}{2(\Delta x)^2 \rho C_p}, \beta' = \frac{J^2 \varepsilon \Delta t}{2\rho C_p}, \gamma' = \frac{J^2 \rho_{ele}^0 \Delta t}{2\rho C_p}$

Ex. 5

The first one:

$$\hat{f}_k = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & \omega & -i & -i\omega & -1 & -\omega & i & i\omega \\ 1 & -i & -1 & i & 1 & -i & -1 & i \\ 1 & -i\omega & i & \omega & -1 & i\omega & -i & -\omega \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -\omega & -i & i\omega & -1 & \omega & i & -i\omega \\ 1 & i & -1 & -i & 1 & i & -1 & -i \\ 1 & i\omega & i & -\omega & -1 & -i\omega & -i & \omega \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\hat{f}_k = \begin{bmatrix} 1 & +1 & +1 & +1 & +1 & +1 & +1 & +1 \\ 1 & +\omega & -i & -i\omega & -1 & -\omega & +i & +i\omega \\ 1 & -i & -1 & +i & +1 & -i & -1 & +i \\ 1 & -i\omega & +i & +\omega & -1 & i\omega & -i & -\omega \\ 1 & -1 & +1 & -1 & +1 & -1 & +1 & -1 \\ 1 & -\omega & -i & i\omega & -1 & +\omega & +i & -i\omega \\ 1 & +i & -1 & -i & +1 & +i & -1 & -i \\ 1 & +i\omega & +i & -\omega & -1 & -i\omega & -i & +\omega \end{bmatrix}$$

$$\hat{f}_k = \begin{bmatrix} 8 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Only the lowest “frequency” mode has a value.

The second one:

$$\hat{f}_k = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & \omega & -i & -i\omega & -1 & -\omega & i & i\omega \\ 1 & -i & -1 & i & 1 & -i & -1 & i \\ 1 & -i\omega & i & \omega & -1 & i\omega & -i & -\omega \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -\omega & -i & i\omega & -1 & \omega & i & -i\omega \\ 1 & i & -1 & -i & 1 & i & -1 & -i \\ 1 & i\omega & i & -\omega & -1 & -i\omega & -i & \omega \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

$$\hat{f}_k = \begin{bmatrix} 1 & +0 & +1 & +0 & +1 & +0 & +1 & +0 \\ 1 & +0 & -i & +0 & -1 & +0 & +i & +0 \\ 1 & +0 & -1 & +0 & +1 & +0 & -1 & +0 \\ 1 & +0 & +i & +0 & -1 & +0 & -i & +0 \\ 1 & +0 & +1 & +0 & +1 & +0 & +1 & +0 \\ 1 & +0 & -i & +0 & -1 & +0 & +i & +0 \\ 1 & +0 & -1 & +0 & +1 & +0 & -1 & +0 \\ 1 & +0 & +i & +0 & -1 & +0 & -i & +0 \end{bmatrix}$$

$$\hat{f}_k = \begin{bmatrix} 4 \\ 0 \\ 0 \\ 0 \\ 4 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

The mode at $\omega_4 = \pi/L$ is present due to the periodicity of the array

The third one:

$$\hat{f}_k = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & \omega & -i & -i\omega & -1 & -\omega & i & i\omega \\ 1 & -i & -1 & i & 1 & -i & -1 & i \\ 1 & -i\omega & i & \omega & -1 & i\omega & -i & -\omega \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -\omega & -i & i\omega & -1 & \omega & i & -i\omega \\ 1 & i & -1 & -i & 1 & i & -1 & -i \\ 1 & i\omega & i & -\omega & -1 & -i\omega & -i & \omega \end{bmatrix} \begin{bmatrix} 2 \\ 1 \\ 0 \\ 1 \\ 2 \\ 1 \\ 0 \\ 1 \end{bmatrix}$$

$$\hat{f}_k = \begin{bmatrix} 2 & +1 & +0 & +1 & +2 & +1 & +0 & +1 \\ 2 & +\omega & +0 & -i\omega & -2 & -\omega & +0 & +i\omega \\ 2 & -i & +0 & +i & +2 & -i & +0 & +i \\ 2 & -i\omega & +0 & +\omega & -2 & i\omega & +0 & -\omega \\ 2 & -1 & +0 & -1 & +2 & -1 & +0 & -1 \\ 2 & -\omega & +0 & i\omega & -2 & +\omega & +0 & -i\omega \\ 2 & +i & +0 & -i & +2 & +i & +0 & -i \\ 2 & +i\omega & +0 & -\omega & -2 & -i\omega & +0 & +\omega \end{bmatrix}$$

$$\hat{f}_k = \begin{bmatrix} 8 \\ 0 \\ 4 \\ 0 \\ 0 \\ 0 \\ 4 \\ 0 \end{bmatrix}$$

The modes at ω_2 and ω_7 is present due to the periodicity of the array