ESS 524 Class #6

Highlights from last Monday – Surabhi
Today's highlights report on next Monday – Erich
Highlights reporters – please send me your report by email.

- Great Week 2 journals. You are all doing some good thinking.

Today

- HW #2 on Matlab (Finite Difference code) due today
  Are there challenges to discuss now?   More time needed?
- Class organization – how is it going with Zoom?
- If you get stuck on HW assignments, please feel free to contact me and/or classmates directly with your questions.
- It's great to work together on problems, just prepare your own answers in the end.
- Zoom study sessions for you to interact, compare approaches and answers?

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Today
- Project updates
- Continuing with Finite Element Method (FEM)

Next Week
- Finite Volume Method (FVM)
- We will follow Patankar fairly closely, Ch 3 and Ch 4

HW #2

Getting the analytical solution?

- FDM - Handling the second derivative (diffusion term)
- Expand with Product Rule, or not?

$$\frac{\partial}{\partial x}\left(k(x)\frac{\partial \phi}{\partial x}\right) \quad (*) \text{ when } k(x) \text{ varies with } x.$$

① Product Rule Approach

$$(*) = k(x)\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial k}{\partial x}\frac{\partial \phi}{\partial x}$$

$$\rightarrow k_j\left(\frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{\Delta x^2}\right) + \left(\frac{k_{j+1} - k_{j-1}}{\Delta x}\right)\left(\frac{\phi_{j+1} - \phi_{j-1}}{\Delta x}\right)$$

Problem - First derivatives span $2\Delta x$

HW #2

- FDM − Evaluate the slope at midpoints, so that all first derivatives are taken over span Δx rather than 2Δx

(2) Evaluate slopes at mid points. I assume $k(x)$ is known at mid points or can be estimated there e.g. $k_{j+1/2} = \frac{(k_{j+1} + k_j)}{2}$

$$(*) \longrightarrow \frac{\left[k\frac{\partial\phi}{\partial x}\right]_{j+1/2} - \left[k\frac{\partial\phi}{\partial x}\right]_{j-1/2}}{\Delta x}$$

$$= \left[k_{j+1/2}\left(\frac{\phi_{j+1} - \phi_j}{\Delta x}\right) - k_{j-1/2}\left(\frac{\phi_j - \phi_{j-1}}{\Delta x}\right)\right] \Big/ \Delta x$$

$$= \frac{k_{j+1/2}\,\phi_{j+1} - k_{j+1/2}\,\phi_j - k_{j-1/2}\,\phi_j + k_{j-1/2}\,\phi_{j-1}}{\Delta x^2}$$

<u>HW 2</u>

2020-04-09

$$S(x) = P_N^{(s)}(x) = \sum_{n=0}^{N} a_n x^n \qquad \frac{1}{k(x)} = P_M^{(k)}(x) = \sum_{m=0}^{M} b_m x^m$$

$$\frac{d}{dx}\left(k(x)\frac{d\phi}{dx}\right) + S(x) = 0 \quad (1)$$

Integrate once

$$\left(k(x)\frac{d\phi}{dx}\right) = -\int_{x_0}^{x} S(x')dx' = \text{a polynomial}$$

$$= k(x_0)\frac{d\phi}{dx}\bigg|_{x_0} + \sum_{n=0}^{N}\frac{1}{n+1}a_n x^{n+1} = R(x)$$

$$\frac{d\phi}{dx} = R(x)\,P_M^{(k)}(x) = \text{a polynomial } T(x)$$

$$\int_{x_1}^{x_0}\frac{d\phi}{dx'}dx' = \phi(1) - \phi(x) = \int_{x_0}^{x} T(x)dx = U(x)$$

a polynomial

$$\phi(x) = \phi_1 - U(x)$$

gradient BC is embedded here

Product Rule and Integration by Parts

$$\int_{v(a)}^{v(b)} u(x)\,dv(x) = \left[u\,v \right]_a^b - \int_{u(a)}^{u(b)} v(x)\,du(x) \qquad (1)$$

$$\text{or} \quad \frac{d}{dx}\left[u(x)\,v(x)\right] = u\,\frac{dv}{dx} + v\,\frac{du}{dx} \qquad (2)$$

Integrate (2) from *a* to *b* to get (1)

Product Rule and Integration by Parts

$$\int_{v(a)}^{v(b)} u(x)\,dv(x) = \Big[u\,v\Big]_a^b - \int_{u(a)}^{u(b)} v(x)\,du(x) \qquad 1$$

When $v(x)$ is the 2nd derivative term, and $u(x)$ does not include a derivative, after integration by parts,

- both $u(x)$ and v(x) appear with first derivatives in the new integral term.
- In general, v(x) is differentiated one time less, and $u(x)$ is differentiated one time more.
- boundary conditions show up naturally in the new constant term.

The challenge –

- How to represent a 2nd order differential equation with piecewise 1st order functions?
- The 2nd derivative is identically zero everywhere
- except at the nodes, where it can be infinite.

The Solution - The weak form of the differential equation

- The weak form is a weighted-integral statement that is equivalent to the governing differential equation combined with its natural boundary conditions.
- The original equation is satisfied in an average sense, rather than point by point.
- The weak form is derived from the strong form by an integration by parts.
- After integration by parts, the 2nd derivative has been replaced by a 1st derivative, which is nonzero for a piecewise linear representation.

With Equation (17), the algebraic equations (12) and (13) in element j reduce to

$$\begin{aligned} -k_j \left[\frac{\mathrm{d}\tilde{\phi}}{\mathrm{d}x}\right]^{(j)}_{x_{j-1}} - \frac{k_j}{\Delta x_j}\phi_{j-1} + \frac{k_j}{\Delta x_j}\phi_j + S_j\frac{\Delta x_j}{2} &= 0 \\ k_j \left[\frac{\mathrm{d}\tilde{\phi}}{\mathrm{d}x}\right]^{(j)}_{x_j} + \frac{k_j}{\Delta x_j}\phi_{j-1} - \frac{k_j}{\Delta x_j}\phi_j + S_j\frac{\Delta x_j}{2} &= 0 \end{aligned} \tag{18}$$

Note that if these two equations were added together, we would get an expected finite-volume expression for conservation of ϕ in element j, , i.e.

$$k_j \left[\frac{\mathrm{d}\tilde{\phi}}{\mathrm{d}x}\right]^{(j)}_{x_j} - k_j \left[\frac{\mathrm{d}\tilde{\phi}}{\mathrm{d}x}\right]^{(j)}_{x_{j-1}} = S_j\,\Delta x_j \tag{19}$$

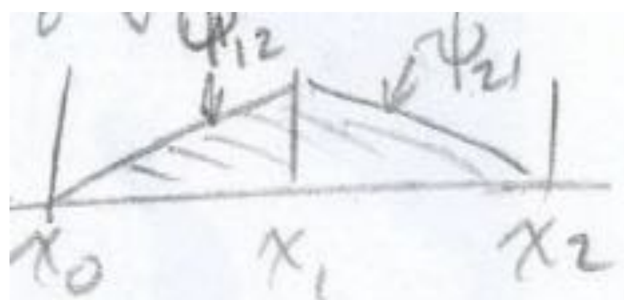
i.e. the difference in fluxes across the boundaries must equal the integrated production rate inside element j.

Equations for 3 linear elements, with 4 nodes

We have 6 weighting equations for 4 nodes.

- We need only 4 equations.
- The first and last equations are just the boundary conditions
- Add together the two equations that apply to the same boundary, but from the elements on opposite sides.
- This effectively isolates the residuals around that node
- Combining the equations at nodes 2 and 3 reduces the number of equations by 2
- We are left with 4 equations.

$$\begin{bmatrix} a_{11} & a_{12} & 0 & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & a_{32} & a_{33} & 0 \\ 0 & a_{42} & a_{43} & 0 \\ 0 & 0 & a_{53} & a_{54} \\ 0 & 0 & a_{63} & a_{64} \end{bmatrix} \begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix}$$



- The flux terms will also cancel and vanish.