ESS 524 Class #5

Highlights from last Wednesday – Shashank
Today's highlights report on Wednesday – Surabhi

- Highlights reporters – please send me your report by email.
- Great Week 1 journals.
- HW #1 on Matlab (or python or java)   Good work!
- HW #2 on Matlab (Finite Difference code) due Wednesday

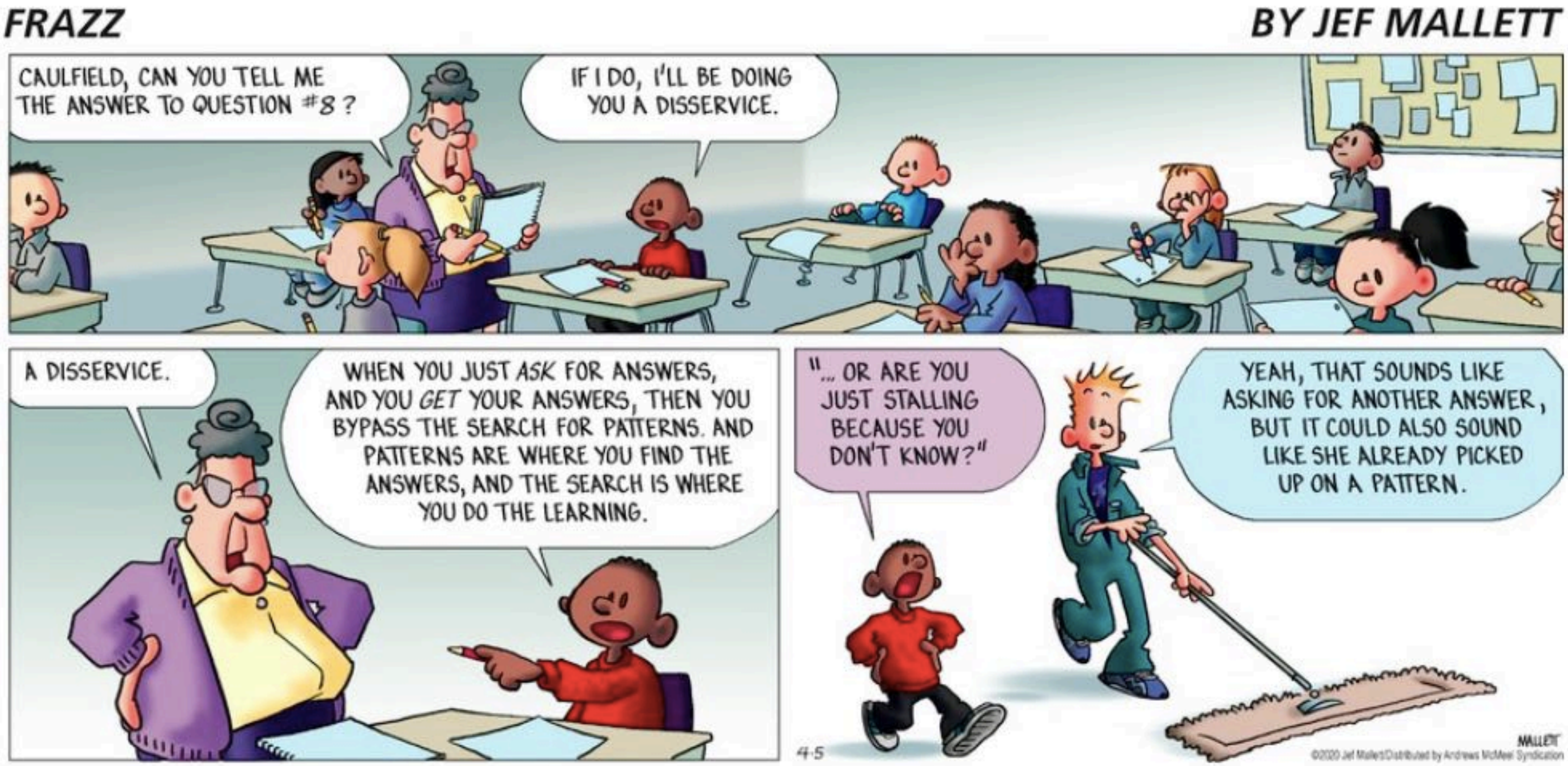
Today

- Project updates
- Discussion points about reading materials?
- Interpolation fns; Weighting fns; Integration by Parts
- Finite Element Method (FEM)

Next Week

- Finite Volume Method (FVM)

Caulfield Prepares for Grad School



Homework #2 Analytical Solution

2020-04-09

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

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

Integrate once

$$\left(k(x)\frac{d\phi}{dx}\right) = -\int_{x_0}^{x_1} S(x')\,dx' = \text{a polynomial}$$

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

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

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

a polynomial

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

gradient BC is embedded here

HW #2

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

$$\frac{\partial}{\partial x}\left(k(x)\frac{\partial \phi}{\partial x}\right) + S(x) = 0 \quad (*)$$

Product Rule

$$k(x)\frac{\partial^2 \phi}{\partial x^2} + \frac{dk}{dx}\frac{\partial \phi}{\partial x} + S(x) = 0$$

$$\rightarrow \quad k_j\left(\frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{\Delta x^2}\right) + \left(\frac{k_{j+1} - k_{j-1}}{2\Delta x}\right)\left(\frac{\phi_{j+1} - \phi_{j-1}}{2\Delta x}\right) + S_j = 0$$

Collect terms -

$$\phi_{j-1}\left[\frac{k_j}{\Delta x^2} - \frac{(k_{j+1} - k_{j-1})}{4\Delta x^2}\right]$$

$$-\phi_j\left[\frac{2k_j}{\Delta x^2}\right]$$

$$+\phi_{j+1}\left[\frac{k_j}{\Delta x^2} + \frac{(k_{j+1} - k_{j-1})}{4\Delta x^2}\right] \qquad + S_j = 0$$

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. $k_{j+1/2} = \frac{(k_{j+1}+k_j)}{2}$

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

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

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

HW #2

- FDM - Handling the second derivative (diffusion term)
- Evaluate first derivatives at midpoints

$$\frac{\partial}{\partial x}\left(k(x)\frac{\partial \phi}{\partial x}\right) + S(x) = 0 \quad (*)$$

Mid-Point First Derivatives

$$\rightarrow \left[k_{j+1/2}\frac{(\phi_{j+1} - \phi_j)}{\Delta x} - k_{j-1/2}\frac{(\phi_j - \phi_{j-1})}{\Delta x} \right] \Big/ \Delta x + S(x) = 0$$

$$\rightarrow \left(\frac{k_j + k_{j+1}}{2\Delta x^2}\right)(\phi_{j+1} - \phi_j) - \left(\frac{k_{j-1} + k_j}{2\Delta x^2}\right)(\phi_j - \phi_{j-1}) + S(x) = 0$$

HW #2

- FDM - Handling the second derivative (diffusion term)
- Evaluate first derivatives at midpoints

$$\frac{\partial}{\partial x}\left(k(x)\frac{\partial \phi}{\partial x}\right) + S(x) = 0 \quad (*)$$

$$\rightarrow \phi_{j-1}\left[\frac{k_{j-1}+k_j}{2\Delta x^2}\right]$$

$$-\phi_j\left[\left(\frac{k_j+k_{j+1}}{2\Delta x^2}\right)+\left(\frac{k_{j-1}+k_j}{2\Delta x^2}\right)\right] \quad \left(\rightarrow \left[\frac{k_{j-1}}{2}+k_j+\frac{k_{j-1}}{2}\right]\Big/\Delta x^2\right)$$

$$+\phi_{j+1}\left[\frac{k_{j-1}+k_j}{2\Delta x^2}\right] \qquad +S(x)$$

Product Rule and Integration by Parts

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

or $$\frac{d}{dx}\Big[u(x)v(x)\Big] = u\frac{dv}{dx} + v\frac{du}{dx} \qquad (2)$$

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

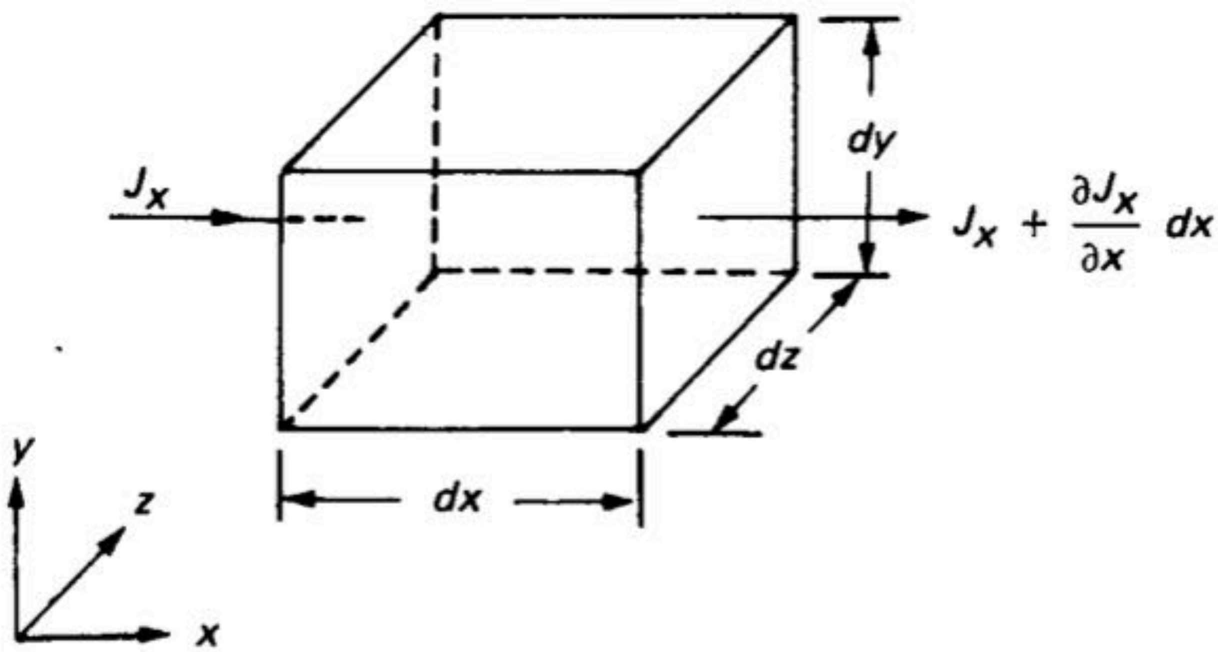


Figure 2.1 Flux balance over a control volume.

Which equation to solve?

Solving $\frac{d\phi}{dx} = -q/k$ is easy $\quad k =$ uniform.

$\phi(0) = \phi_B \quad q =$ uniform.

So Why did we go to solve

$$k\frac{d^2\phi}{dx^2} = \rho c \frac{\partial \phi}{\partial t} = 0 \text{ instead?} \quad \begin{cases} \phi(0) = \phi_B \\ \left.\frac{d\phi}{dx}\right|_{x_N} = -q/k \end{cases}$$

(We needed to invert a matrix.)

Because source terms also need to be accounted for.

$$\frac{d}{dx}\left(k\frac{d\phi}{dx}\right) + S(x) = 0 \qquad \begin{aligned} \phi(0) &= \phi_B \\ \frac{d\phi}{dx} &= -q^N/k \end{aligned}$$

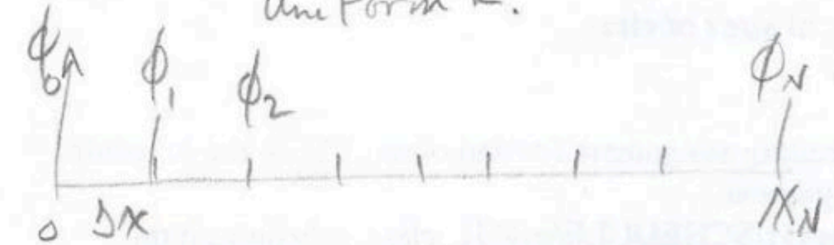
k can still be uniform but q cannot.

Finite Differences with uniform *k*, non-uniform source *S*(*x*)

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

uniform k.

$$\left.\frac{d\phi}{dx}\right|_{x_N} = -\left(\frac{g_N}{k_N}\right) = \phi'_N$$



$$\phi_0 = 1$$

$$\frac{k}{\Delta x^2}\left(\phi_0 - 2\phi_1 + \phi_2\right) = -S_1$$

$$\frac{k}{\Delta x^2}\left(\phi_1 - 2\phi_2 + \phi_3\right) = -S_2$$

$$\frac{k}{\Delta x^2}\left(\phi_2 - 2\phi_3 + \phi_1\right) = -S_3$$

$$\vdots$$

$$\frac{k}{\Delta x^2}\left(\phi_{N-2} - 2\phi_{N-1} + \phi_N\right) = -S_{N-1}$$

$$\frac{1}{\Delta x}\left(-\phi_{N-1} + \phi_N\right) = \phi'_N$$

Finite Differences equation matrix

$$
\begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & \cdots \\
1 & -2 & 1 & 0 & 0 & 0 & \cdots \\
0 & 1 & -2 & 1 & 0 & 0 & \cdots \\
0 & 0 & 1 & -2 & 1 & 0 & \cdots \\
 & & \ddots & \ddots & \ddots & & \\
\cdots & & & 0 & 1 & -2 & 1 \\
\cdots & & & 0 & 0 & 0\ \ -1 & 1
\end{bmatrix}
\begin{bmatrix}
\phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \\ \phi_{N-2} \\ \phi_{N-1} \\ \phi_N
\end{bmatrix}
=
\begin{bmatrix}
1 \\ -S_1 \frac{\Delta x^2}{k} \\ -S_2 \frac{\Delta x^2}{k} \\ -S_3 \frac{\Delta x^2}{k} \\ \vdots \\ -S_{N-1} \frac{\Delta x^2}{k} \\ \phi_N' \Delta x
\end{bmatrix}
$$

$$\underline{\underline{A}}\,\underline{\phi} = \underline{B}$$

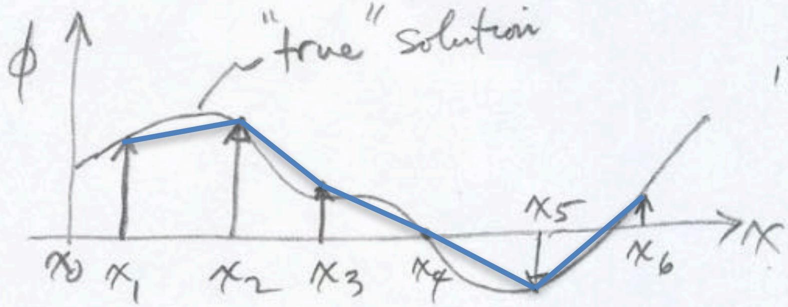
Finite Differences vs Finite elements

- F.D. - just approximated derivatives in Diff. Eq.
  - hoped they adequately represented behavior between nodes (true derivatives smoothly varying)

F.E.M - find approximating functions determined by nodal values
  - approximations are constrained to satisfy Diff Eq as closely as possible over entire domain (not just at nodes).

Finite Differences vs Finite elements

with Finite Differences, we estimated values of solution at a few points



in 1-D $\quad \mathcal{L}(\phi) - g(x) = 0$

$\mathcal{L}(\ )$ differential operator

e.g. $\mathcal{L}(\ ) = a\frac{\partial^2(\ )}{\partial x^2} + b\frac{\partial(\ )}{\partial x} + c\frac{\partial(\ )}{\partial y}$

Now let's look at a different class of approximations where we find some function that approximates $\phi(\vec{x})$ everywhere.

low-order polynomial $\tilde{\phi}(x)$

$$\hat{\phi}(x) = a_0 + a_1 x + a_2 x^2 + \dots + a_m x^m$$

Now all we need to do is to find the m parameters a_i $i=1:m$

Variational Method (in 1-D)

$$I(\phi) = \int_{x_0}^{x_{end}} F\left(x, \phi, \frac{d\phi}{dx}, \frac{d\phi}{dx^2} \ldots\right) dx$$

F is a functional (function of functions) chosen so
that the $\phi(x)$ that minimizes (or maximizes) its integral over
the domain is equivalent to solving $\mathcal{L}(\phi) - g(x) = 0$
with the same boundary conditions e.g. $\phi(x_0) = \phi_0$
$\phi(x_{end}) = \phi_{end}$

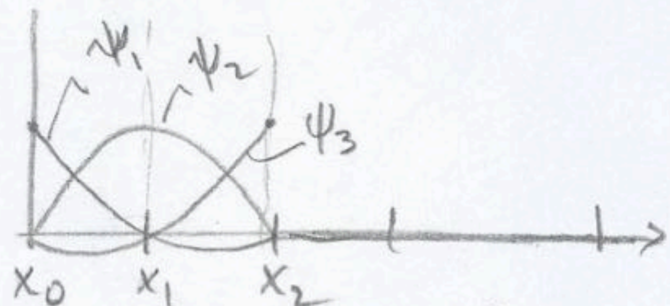
Weighted Residuals in FEM

$\mathcal{L}(\phi) - g(x) = 0$

Assume an approximate solution that is a sum of simple functions $\tilde{\phi}(x) = \sum_{j=1}^{J} a_j \psi_j(x)$.

In practice, each $\psi_j(x)$ is nonzero on only a small part of the domain

e.g. ψ_1, ψ_2, ψ_3 are nonzero only between x_0 & x_2



Substitute $\tilde{\phi}(x)$ into $\left[\mathcal{L}\{\tilde{\phi}\} - g(x)\right] = R(x)$.

Unless we made a really lucky guess, $\tilde{\phi}$ was not the exact solution, and RHS $\neq 0$. There is a residual $R(x)$.

Weighted Residuals

To keep the residuals small, we choose J weighting functions $W_j(x)$ and require that

$$\int W_j(x') R(x') dx' = 0 \qquad (J \text{ equations}).$$

To get J equations to solve for a_j $j = 1, \ldots J$ expand the integrals, which contain only simple (known) functions $\psi_j(x)$, $W_j(x)$ $g(x)$ and the a_j (unknown)

To keep the residuals small locally, make sure that the weight functions $W_j(x)$ peak locally, & all localities are "covered".