(1)

Ch-6 lec - 2

Review Spatial diffusion of @

Consider steady state @ balance. ϕ & xs are averaged over energy - one group.

Neutron balance (steady state)

Loss rate = production rate

→ leakage + absorption rate = source emission + fission @ gen. rate

↳ $\underline{\nabla} \cdot \underline{J}(\underline{r}) + \Sigma_a(\underline{r})\phi(\underline{r}) = S'''(\underline{r}) + \nu\Sigma_f(\underline{r})\phi(\underline{r})$

Fick's law: $\underline{J}(\underline{r}) = -D(\underline{r})\underline{\nabla}\phi(\underline{r})$

Diffusion Equation.

$$\boxed{\underline{\nabla}\cdot D(\underline{r})\underline{\nabla}\phi(\underline{r}) + \Sigma_a(\underline{r})\phi(\underline{r}) = S'''(\underline{r}) + \nu\Sigma_f(\underline{r})\phi(\underline{r})}$$

→ $D(\underline{r})$?

Use 1D transport equation with isotropic scattering.

$$\mu\frac{\partial}{\partial x}\psi(x,\mu) + \Sigma_t(x)\psi(x,\mu) = \frac{1}{2}\Sigma_s(x)\phi(x) + \frac{1}{2}S(x)$$

$$\phi(x) = \int_{-1}^{1} d\mu\, \psi(x,\mu)$$

$$\phi_1(x) = J(x) = \int_{-1}^{1} d\mu\, \mu\, \psi(x,\mu)$$

Take 0^{th} & 1^{st} legendre moment of transport equation re arrange * combine to get a diffusion equation. Finally,

$$\boxed{D = \frac{1}{3\sigma_t}}$$

just normalization can be defined as $(2l+1)$ if we define $\Phi_l(x) = \frac{\Phi}{2}$

In general

$$\psi(x,\mu) = \sum_{l=0}^{L} \frac{2l+1}{2} P_l(\mu)\phi_l(x),$$

$$\phi_l(x) = \int_{-1}^{1} d\mu\, P_l(\mu)\,\psi(x,\mu).$$

For diffusion, because we get diffusion equation just by taking 0^{th} & 1^{st} moment of transport equation, ψ only depends on Φ & J.

$$\Rightarrow \psi(x,\mu) \approx \sum_{l=0}^{l=1} \frac{2l+1}{2} P_l(\mu)\,\phi(x,\mu)$$

$$\boxed{\psi(x,\mu) = \frac{1}{2}\phi(x) + \frac{3}{2}\mu J(x)}$$

1D Diffusion Equation:

$$-\frac{\partial}{\partial x} D(x) \frac{\partial}{\partial x} \phi(x) + \Sigma_a(x)\phi(x) = S(x) + \nu \Sigma_f(x)\phi(x).$$

Boundary conditions:

1 Reflecting / symmetric boundary.

Net current at boundary = 0.
$\Rightarrow$ no n cross boundary.

Suppose we consider 1D system

$$J_x(\text{boundary}) = -D \frac{\partial \phi}{\partial x}\Big|_{x_{\text{boundary}}} = 0$$

$$\Rightarrow \quad \frac{\partial}{\partial x}\phi\Big|_{x_{\text{boundary}}} = 0.$$

2 Vacuum boundary.

Nothing comes in from boundaries.

$\longrightarrow |$ $| \longleftarrow$

n carrying in = 0   # n carrying in = 0

In order to mathematically represent we introduce partial currents.

$$\text{Current} = J(x) \xrightarrow{\text{represent by}} J(x) = \int_{-1}^{1} d\mu\, \mu\, \psi(x,\mu)$$

Decompose current into partial currents in +ve & -ve directions: $J^+(x)$ $J^-(x)$

$$J(x) = \int_{-1}^{1} d\mu\, \mu\, \psi(x,\mu) = \int_{-1}^{0} d\mu\, \mu\, \psi(x,\mu) + \int_{0}^{1} d\mu\, \mu\, \psi(x,\mu)$$

$J^-(x)$ $\qquad$ $J^+(x)$.

$$\Rightarrow J(x) = \int_{0}^{1} d\mu\, \mu\, \psi(x,\mu) - \int_{-1}^{0} d\mu\, |\mu|\, \psi(x,\mu)$$

-ve sign because -ve angles from -1 to 0.

$$J^+(x) = \int_0^1 \mu\, \psi(x,\mu)\, d\mu$$

$$= \int_0^1 \mu \left[\frac{1}{2}\phi(x) + \frac{3}{2}\mu J(x)\right] d\mu$$

$$= \frac{\phi(x)}{2}\int_0^1 \mu\, d\mu + \frac{3}{2} J(x) \int_0^1 \mu^2\, d\mu$$

$$\boxed{J^+(x) = \frac{\phi(x)}{4} + \frac{1}{2} J(x)}$$

Now $J(x) = -D \frac{\partial}{\partial x} \phi(x)$.

$\Rightarrow$ ~~$J^{+}(x)$~~

$\Rightarrow$ $$\boxed{J^{+} = \frac{1}{4}\phi(x) - \frac{1}{2} D \frac{\partial}{\partial x}\phi(x)}$$

Similarly, $J^{-}(x) = \int_{-1}^{0} d\mu \, |\mu| \, \psi(x,\mu)$

$$J^{-} = \frac{1}{4}\phi(x) - \frac{1}{2} J(x)$$

$$\boxed{J^{-} = \frac{1}{4}\phi(x) + D\frac{\partial}{\partial x}\phi(x)}$$

for vacuum boundaries then, $\quad x_L \longleftrightarrow x_R$

$$J^{+}(x_L) = 0 \quad \& \quad J^{-}(x_R) = 0$$

$$J^{+}(x_L) = 0 = \frac{\phi(x)}{4} - \frac{1}{2} D \frac{d}{dx}\phi$$

$$\Rightarrow D\frac{\partial}{\partial x}\phi\Big|_{x=x_L} = \frac{\phi(x)}{2}$$

At right boundary,

$$J^{-}(x_R) = 0 = \frac{1}{4}\phi(x_R) - \frac{1}{2} D \left|\frac{d}{dx}\phi(x)\right|_{x_R}$$

on right derivative is $-ve$ thus can write without abs. value & + sign

So now, how do we solve diffusion equation?

Different methods:

① finite difference,
finite volume,
finite element
mesh free methods - Peridynamic differential operator etc

- In general finite volume & discontinuous fem used in neutronics.

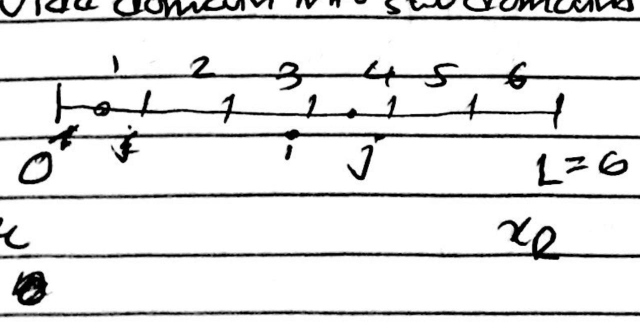
Finite element method:

In general never write your own code unless that is your job. Several free packages exist

- ANSYS
- Comsol
- Moose
- DEAL II
- FENICS
- XFEM
- ADINA

General procedure for FEM.

① Divide domain into subdomains called "elements"



(2) ~~Develop~~ Write equation in weighted residual form & develop weak form of diff. eqn. over each element.

(3) Assume ~~test~~ weight & trial functions.

(4) Find matrix equation for each element.

(5) Assemble global matrix eqn by combining eqn. for each element.

(6) Solve matrix eqn. using direct / indirect methods.

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(1) ~~Write equation in weighted residual form.~~

DISCRETISE

Each element is represented by discrete set of points called nodes with unique coordinates on coordinate system.

In the domain in fig. on prev page,

element #	node i	coord	node j	coord.
1	1	(0,0)	2	(1,0)
2	2	(1,0)	3	(2,0)
3	3	(2,0)	4	(3,0)
4	4	(3,0)	5	(4,0)
5	5	(4,0)	6	(5,0)
6	6	(5,0)	7	(6,0)

Consider generic element starting at i & ending at j

~~Depend on the type of element, each~~

(2) WEIGHTED RESIDUAL & WEAK FORM OVER ELEMENT

diffusion eqn: $-\frac{\partial}{\partial x} D \frac{\partial}{\partial x}\phi + \Sigma_a \phi = S$

residual form: $-\frac{\partial}{\partial x} D \frac{\partial}{\partial x}\phi + \Sigma_a \phi - S = 0.$

must be minimized.

weighted residual: $\int_{x_i}^{x_j} dx\, \omega \left(-\frac{\partial}{\partial x} D \frac{\partial}{\partial x}\phi + \Sigma_a \phi - S\right) = 0$

Weak form: To get weak form, we integrate weighted residual eqn. by parts.

$x_j = x_{i+1}$

$$= \int_{x_i} \left(-\frac{\partial}{\partial x} D \frac{\partial \phi}{\partial x} + \Sigma_a \phi - S\right)\omega \; dx$$

$$= \underbrace{\int_{x_i}^{x_{i+1}} \left(-\frac{\partial}{\partial x} D \frac{\partial}{\partial x}\phi\right)\omega\, dx}_{I_1} + \underbrace{\int_{x_i}^{x_{i+1}} \Sigma_a \phi\, \omega\, dx}_{I_2} + \underbrace{\int_{x_i}^{x_{i+1}} -S\, \omega\, dx}_{I_3}.$$

$\Rightarrow I = I_1 + I_2 + I_3$

$$I_1 = \int_{x_i}^{x_{i+1}} \left(\frac{-d}{dx} D \frac{d\phi}{dx} \right) w \, dx$$

Integrate by parts:

$$I_1 = \int_{x_i}^{x_{i+1}} \left(-\frac{d}{dx} D \frac{d\phi}{dx} \right) w \, dx$$

$$= -\left[\int_{x_i}^{x_{i+1}} -\frac{dw}{dx} D \frac{d\phi}{dx} \, dx + \left[w D \frac{d\phi}{dx} \right]_{x_i}^{x_{i+1}} \right]$$

$$I_1 = D_i \underbrace{\int_{x_i}^{x_{i+1}} \frac{dw}{dx} \frac{d\phi}{dx} \, dx}_{I_{1,1}} - \underbrace{\left[w D_i \frac{d\phi}{dx} \right]_{x_i}^{x_{i+1}}}_{I_{1,2}}$$

assume constant over each element i

$$I = I_1 + I_2 + I_3$$

weighted residual

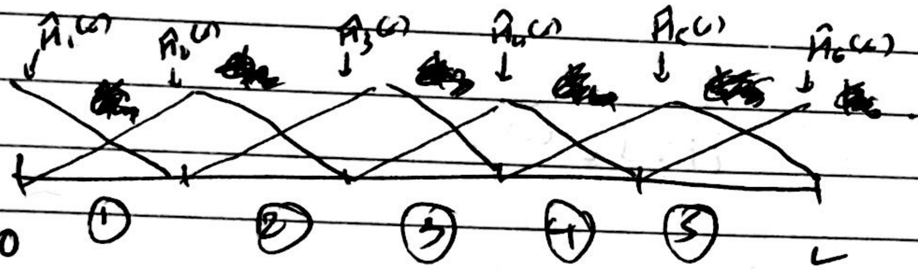
$\Rightarrow$ Equation is $\quad I_1 + I_2 + I_3 = 0$

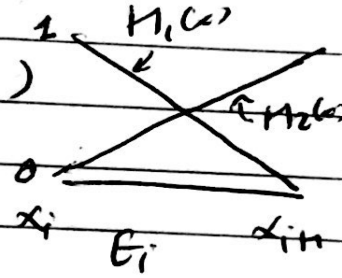
$$\Rightarrow \boxed{D_i \int_{x_i}^{x_{i+1}} \frac{\partial w}{\partial x} \frac{\partial \phi}{\partial x} \, dx - \left[w D_i \frac{d\phi}{dx} \right]_{x_i}^{x_{i+1}} + \Sigma_{a_i} \int_{x_i}^{x_{i+1}} \phi w \, dx = \int_{x_i}^{x_{i+1}} S w \, dx}$$

- weak Form as $\frac{d^2\phi}{dx^2}$ reduced to $d\phi/dx$

③ WEIGHT & TRIAL f^n

Here, we choose linear elements (hat functions)





Over element,

$$\Phi = H_1(x)\,\phi_i + H_2(x)\,\phi_{i+1}$$ ⇐ Trial function

Galerkin Method: Weight function has the same form as trial function.

Petrov Galerkin when weight f^n & trial f^n do not have the same form.

We will do Galerkin ⇒ $\omega = H_1(x)\,\omega_1 + H_2(x)\,\omega_2$.

(4) Find matrix equation for each element.

First thing we do is write ϕ & ω as matrices.

$$\phi = H_1(x)\,\phi_i + H_2(x)\,\phi_{i+1}$$

$$= \begin{bmatrix} H_1(x) & H_2(x) \end{bmatrix} \begin{bmatrix} \phi_i \\ \phi_{i+1} \end{bmatrix}$$

$$= [H][\Phi]$$

$$\omega = H_1(x)\,\omega_i + H_2(x)\,\cancel{\phi_{i+1}}\,\omega_{i+1}$$

$$\boxed{\omega = \cancel{[H][\tilde{\omega}]} \begin{bmatrix} H_1(x) & H_2(x) \end{bmatrix} \begin{bmatrix} \omega_1 \\ \omega_2 \end{bmatrix}}$$

$$= \cancel{\omega} \; [H][\tilde{\omega}]$$

Now ω is a scalar.

$$\Rightarrow \omega = \omega^T$$

$$\Rightarrow \omega = \omega^T = \cancel{[H]}\,[\tilde{\omega}]^T [H]^T$$

$$= \cancel{\begin{bmatrix} H_1(x) \\ H_2(x) \end{bmatrix}} \begin{bmatrix} \omega_1 & \omega_2 \end{bmatrix} \begin{bmatrix} H_1(x) \\ H_2(x) \end{bmatrix}$$

Now, lets look at $I = I_1 + I_2 + I_3$

Now, the equation becomes

$$I_1 + I_2 + I_3 = 0$$

$$\Rightarrow D_i \int_{x_i}^{x_{i+1}} \frac{dw}{dx}\frac{d\phi}{dx}\,dx - \left[w\, D_i \frac{d\phi}{dx}\right]_{x_i}^{x_{i+1}} + \Sigma_{a_i}\int_{x_i}^{x_{i+1}} w\,\phi\, dx$$

$$= \int_{x_i}^{x_{i+1}} S\, w\, dx.$$

$$\hookrightarrow D_i \int_{x_i}^{x_{i+1}} \frac{d}{dx}[\tilde{w}]^T [H]^T \frac{d}{dx}[H][\tilde{\phi}]\, dx$$

I

$$- \cancel{[\tilde{w}]^T} \left[D_i\, [\tilde{w}]^T [H]^T \frac{\partial \phi}{\partial x}\right]_{x_i}^{x_{i+1}}$$

II

Boundary condition will apply here so keep it like that for now.

$$+ \Sigma_{a_i} \int_{x_i}^{x_{i+1}} [\tilde{w}]^T [H]^T [H][\phi]\, dx$$

III

$$= S_i \int_{x_i}^{x_{i+1}} [\tilde{w}]^T [H]^T dx.$$

IV

Now note that $[\tilde{w}]^T$ is arbitrary and does not depend on x. Moreover all terms have it. We cancel $[\tilde{w}]^T$ from all terms. We get:

$$\boxed{D_i \int_{x_i}^{x_{i+1}} \frac{d}{dx}[H]^T \frac{d}{dx}[H]\,dx \,[\tilde{\phi}] - \left[D_i [H]^T \frac{\partial \phi}{\partial x}\right]_{x_i}^{x_{i+1}} + \Sigma_{a_i} \int_{x_i}^{x_{i+1}} [H]^T [H]\, dx\, [\tilde{\phi}] = S_i \int_{x_i}^{x_{i+1}} [H]^T dx.}$$

Now let's substitute $[H]$, $[H]'$ & $[\hat{\Phi}]$ in the weak form equation from last page.

$$I_{1,1} = D_i \int_{x_i}^{x_{i+1}} \frac{d}{dx}[H]' \frac{d}{dx}[H]\, dx\, [\tilde{\Phi}]$$

$$= D_i \int_{x_1}^{x_{i+1}} \begin{pmatrix} \frac{d}{dx} H_1(x) \\ \frac{d}{dx} H_2(x) \end{pmatrix} \begin{bmatrix} \frac{d}{dx} H_1(x) & \frac{d}{dx} H_2(x) \end{bmatrix} dx \begin{bmatrix} \phi_i \\ \phi_{i+1} \end{bmatrix}$$

$$\frac{d}{dx} H_1(x) = \frac{d}{dx} \left(\frac{x_{i+1} - x}{x_{i+1} - x_i} \right) = \frac{-1}{h_i} \quad //$$

$$\frac{d}{dx} H_2(x) = \frac{d}{dx} \frac{(x - x_i)}{x_{i+1} - x_i} = \frac{1}{h_i} \quad //$$

$$\Rightarrow I_{1,1} = D_i \int_{x_i}^{x_{i+1}} \begin{bmatrix} -1/h_i \\ 1/h_i \end{bmatrix} \begin{bmatrix} -1/h_i & 1/h_i \end{bmatrix} dx \begin{bmatrix} \phi_i \\ \phi_{i+1} \end{bmatrix}$$

$$= \frac{D_i}{h_i^2} \int_{x_i}^{x_{i+1}} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \begin{bmatrix} -1 & 1 \end{bmatrix} dx \begin{bmatrix} \phi_i \\ \phi_{i+1} \end{bmatrix}$$

$$= \frac{D_i}{h_i^2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \int_{x_i}^{x_{i+1}} dx \begin{bmatrix} \phi_i \\ \phi_{i+1} \end{bmatrix}$$

$$= \frac{D_i}{h_i}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} \phi_i \\ \phi_{i+1} \end{bmatrix} //$$

$$I_{1,2} = \left[D_i \, [H]^T \frac{\partial \Phi}{\partial x} \right]_{x_i}^{x_{i+1}}$$ ← more on this later.

$$I_2 = \Sigma_{a_i} \int_{x_i}^{x_{i+1}} [H]^T [H] \, dx \, [\tilde{\Phi}]$$

on simplification / evaluation

$$= \Sigma_{a_i} \int_{x_i}^{x_{i+1}} \begin{bmatrix} H_1(x) \\ H_2(x) \end{bmatrix} \begin{bmatrix} H_1(x) & H_2(x) \end{bmatrix} dx \begin{bmatrix} \phi_i \\ \phi_{i+1} \end{bmatrix}$$

$$= \Sigma_{a_i} \begin{bmatrix} h_i/3 & h_i/6 \\ h_i/6 & h_i/3 \end{bmatrix} \begin{bmatrix} \phi_i \\ \phi_{i+1} \end{bmatrix} //$$

$$I_3 = S_i \int_{x_i}^{x_{i+1}} [H]^T \, dx = S_i \int_{x_i}^{x_{i+1}} \begin{bmatrix} H_1(x) \\ H_2(x) \end{bmatrix} dx$$

$$= S_i \int_{x_i}^{x_{i+1}} \begin{bmatrix} \frac{x_{i+1} - x}{h_i} \\ \frac{x - x_i}{h_i} \end{bmatrix} dx$$

upon evaluation

$$= S_i \begin{bmatrix} h_i/2 \\ h_i/2 \end{bmatrix}$$

//

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Now lets come to $I_{1,2}$

$$I_{1,2} = \left[D_i [H]^T \frac{\partial \phi}{\partial x}\right]_{x_i}^{x_{i+1}}$$

when we are at interfaces / interior of slab, interface condition states that both ϕ & J must be continuous.

That means at x_{i+1} & x_i (except at slab boundaries, where ϕ conditions will be prescribed),

$$\cancel{\phi(x_-) = \phi(x_+) \Rightarrow \frac{\partial \phi}{\partial x}} \qquad \phi(x_-) = \phi(x_+)$$

This will be taken care of naturally when we do global matrix assembly later.

$$I_{1,2} = \begin{bmatrix} \left[D_i H_1(x) \frac{\partial \phi}{\partial x}\right]_{x_{i+1}} - \left[D_i H_1(x) \frac{d\phi}{dx}\right]_{x_i} \\ \left[D_i H_2(x) \frac{\partial \phi}{\partial x}\right]_{x_{i+1}} - \left[H_2(x) D_i \frac{d\phi}{dx}\right]_{x_i} \end{bmatrix}$$

Now, we know that $H_1(x_{i+1}) = 0$ & $H_2(x_i) = 0$

moreover, $H_1(x_i) = 1$ & $H_2(x_{i+1}) = 1$

$\Rightarrow$

$$I_{1,2} = \begin{bmatrix} -D_i \left.\frac{d\phi}{dx}\right|_{x_i} \\ +D_i \left.\frac{d\phi}{dx}\right|_{x_{i+1}} \end{bmatrix}$$

~~Specifically for boundary elements.~~

Then ~~total~~ we put I_1, I_2 & I_3 together to obtain a matrix equation for a generic element:

we have

$$I_1 + I_2 = I_3.$$

$$\therefore \begin{bmatrix} D_i/h_i + \Sigma a_i h_i/3 & -D_i/h_i + \Sigma a_i h_i/6 \\ -D_i/h_i + \Sigma a_i h_i/6 & D_i/h_i + \Sigma a_i h_i/3 \end{bmatrix} \begin{bmatrix} \phi_i \\ \phi_{i+1} \end{bmatrix}$$

$$- \begin{bmatrix} -D_i \frac{d\phi}{dx}\Big|_{x_i} \\ D_i \frac{d\phi}{dx}\Big|_{x_{i+1}} \end{bmatrix} = s_i \begin{bmatrix} h_i/2 \\ h_i/2 \end{bmatrix}$$

Now, let us look at ~~Bound~~ specific boundary conditions.

<u>Reflecting boundary</u>:

$D \frac{\partial \phi}{\partial x} = 0.$ $\Rightarrow$ for left reflecting boundary we have

$$I_{1,2} = \begin{bmatrix} 0 \\ D\frac{d\phi}{dx}\Big|_{x_{i+1}} \end{bmatrix}.$$

Similarly for Right reflecting boundary,

$$I_{1,2} = \begin{bmatrix} -D_i \frac{d\Phi}{dx}\Big|_{x_i} \\ 0 \end{bmatrix}.$$

For vacuum boundary condition.

$$J_x^{\pm}(x) = \frac{1}{4}\phi(x) \mp \frac{1}{2} D \frac{d\Phi}{dx}$$

for left vacuum boundary

$$J^{+} = 0 \Rightarrow \frac{1}{4}\phi(x) = \frac{1}{2}\frac{d}{dx}\Phi(x)$$

$$\Rightarrow +D \frac{d}{dx}\Phi(x) = \frac{1}{2}\Phi(x).$$

$$\Rightarrow I_{1,2}^{left,vac} = \begin{bmatrix} -\frac{\Phi(x)}{2}\Big|_{x_1} \\ +D\frac{d\Phi}{dx}\Big|_{x_{i+1}} \end{bmatrix}$$

for Right ~~b~~ vacuum boundary,

$$-D\frac{d\Phi}{dx} = \frac{\Phi(x)}{2} \Rightarrow I_{1,2} = \begin{bmatrix} -D\frac{d\Phi}{dx}\Big|_{x_i} \\ -\frac{\Phi(x)}{2}\Big|_{x_{i+1}} \end{bmatrix}$$