

$$\frac{1}{h_e} \sum (\bar{J}_{l+\frac{1}{2},mn}^{ug} - \bar{J}_{l-\frac{1}{2},mn}^{ug}) + \sum_{l,m,n}^g \phi_{l,m,n}^g$$

$$= \sum_{h=1}^G \sum_{l,m,n}^{h \rightarrow g} \phi_{l,m,n}^h + \frac{1}{k} \sum_{h=1}^G \sum_{l,m,n}^{h \rightarrow g} \phi_{l,m,n}^h$$

Balance over cell

Inside a cell

$$\nabla \cdot \bar{J}^g + \sum_{l,m,n}^g \bar{J}_{l,m,n}^g(\vec{r}) = \sum_{h=1}^G \sum_{l,m,n}^{h \rightarrow g} \bar{J}_{l,m,n}^h(\vec{r}) + \frac{1}{k} \sum_{h=1}^G \sum_{l,m,n}^{h \rightarrow g} \bar{J}_{l,m,n}^h(\vec{r})$$

Diffusion Approx.

$$\bar{J}^g = -D^g(\vec{r}) \nabla \phi^g(\vec{r})$$

3-D

$$-D_{l,m,n}^g \frac{\partial^2 \phi^g}{\partial x^2} - D_{l,m,n}^g \frac{\partial^2 \phi^g}{\partial y^2} - D_{l,m,n}^g \frac{\partial^2 \phi^g}{\partial z^2} + \sum_{l,m,n}^g \bar{J}_{l,m,n}^g(\vec{r}) =$$

$$\sum_{h=1}^G \sum_{l,m,n}^{h \rightarrow g} \bar{J}_{l,m,n}^h(\vec{r}) + \frac{1}{k} \sum_{h=1}^G \sum_{l,m,n}^{h \rightarrow g} \bar{J}_{l,m,n}^h(\vec{r})$$

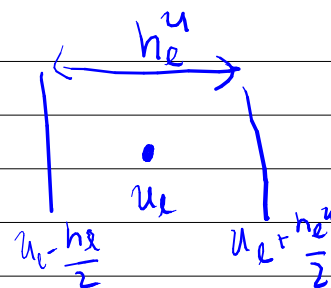
Integrate over transverse directions (v,w) - switch roles

$$-D_{l,m,n}^g \frac{\partial^2}{\partial u^2} \int_{v_m - \frac{h}{2}}^{v_m + \frac{h}{2}} \int_{w_n - \frac{h}{2}}^{w_n + \frac{h}{2}} \phi(u,v,w) dv dw + -D_{l,m,n}^g \frac{\partial^2}{\partial v^2} \int du \int dw \phi(u,v,w)$$

$$+ -D_{l,m,n}^g \frac{\partial^2}{\partial w^2} \int du \int dv \phi(u,v,w) + \sum_{l,m,n}^g \int \phi(u,v,w) = \sum_{l,m,n}^g \int \phi^h + \frac{1}{k} \sum_{l,m,n}^g \int \phi$$

Define

Coordinates inside a cell: $\frac{u - u_c}{h_x^u} \equiv u'$



Transverse Integrated Flux:
$$\int_{v_m - \frac{h_m^v}{2}}^{v_m + \frac{h_m^v}{2}} dv \int_{w_n - \frac{h_n^w}{2}}^{w_n + \frac{h_n^w}{2}} dw \phi(u', v', w') \frac{1}{h_m^v h_n^w} = \bar{\phi}_{lmn}^{ug}(u')$$

Transverse Integrated Ledge (around one of the ints)

$$\underbrace{L_{lmn}^{ug}(u)}_{\substack{\uparrow \\ \text{divide} \\ \text{thru} \\ \text{eqn.}}} \frac{D_{lmn}^2}{h_m^v h_n^w} \left[\int_{w_n - \frac{h_n^w}{2}}^{w_n + \frac{h_n^w}{2}} dw \frac{\partial \phi^2}{\partial v} \bigg|_{v_m - \frac{h_m^v}{2}}^{v_m + \frac{h_m^v}{2}} + \int_{v_m - \frac{h_m^v}{2}}^{v_m + \frac{h_m^v}{2}} dv \frac{\partial \phi^2}{\partial w} \bigg|_{w_n - \frac{h_n^w}{2}}^{w_n + \frac{h_n^w}{2}} \right]$$

from transverse flux

Equation Becomes (now eqs are decoupled)

$$\begin{aligned} & -D_{lmn}^2 \frac{d^2}{du^2} \bar{\phi}_{lmn}^{ug}(u) + \sum_t \bar{\phi}_{lmn}^{tg}(u') \\ &= \sum_{h=1}^G \sum_{s_{lmn}}^{h \rightarrow s} \bar{\phi}_{lmn}^{us}(u) + \frac{1}{k} \sum_{h=1}^G \sum_{f_{lmn}}^{h \rightarrow f} \bar{\phi}_{lmn}^{uf}(u') + L_{lmn}^{us}(u) \end{aligned}$$

Expand Transverse Integrated Flux

$$\bar{\Phi}_{lmn}^{ug}(u) = \bar{\Phi}_{lmn}^g \left[1 + \sum_{t=1}^5 a_{t,lmn}^{ug} P_t(u) \right]$$

Quadratic Transverse Leakage Approximate

$$L_{lmn}^{ug} \left(\frac{u-u_c}{h_c^u} \right) = L_{0,lmn}^{ug} + L_{1,lmn}^{ug} \frac{u-u_c}{h_c^u} + L_{2,lmn}^{ug} \left(\frac{u-u_c}{h_c^u} \right)^2$$

Define average transverse leakage in cell:

$$\bar{L}_{lmn}^{ug} = \frac{1}{h_c^u} \int_{u_c - \frac{h_c^u}{2}}^{u_c + \frac{h_c^u}{2}} L_{lmn}^{ug} \left(\frac{u-u_c}{h_c^u} \right) du$$

Integrate polynomial over adjacent cells:

$$\bar{L}_{lmn}^{ug} = \frac{1}{h_c^u} \int_{u_c - \frac{h_c^u}{2}}^{u_c + \frac{h_c^u}{2}} \left(L_{0,lmn}^{ug} + L_{1,lmn}^{ug} \left(\frac{u-u_c}{h_c^u} \right) + L_{2,lmn}^{ug} \left(\frac{u-u_c}{h_c^u} \right)^2 \right) du$$

$$\bar{L}_{l-1,m,n}^{ug} = \frac{1}{h_{c-1}^u} \int_{u_{c-1} - \frac{h_{c-1}^u}{2}}^{u_c - \frac{h_c^u}{2}} \left(L_{0,lmn}^{ug} + L_{1,lmn}^{ug} \left(\frac{u-u_c}{h_c^u} \right) + L_{2,lmn}^{ug} \left(\frac{u-u_c}{h_c^u} \right)^2 \right) du$$

$$\bar{L}_{l+1,m,n}^{ug} = \frac{1}{h_{c+1}^u} \int_{u_c + \frac{h_c^u}{2}}^{u_{c+1} + \frac{h_{c+1}^u}{2}} \left(L_{0,lmn}^{ug} + L_{1,lmn}^{ug} \left(\frac{u-u_c}{h_c^u} \right) + L_{2,lmn}^{ug} \left(\frac{u-u_c}{h_c^u} \right)^2 \right) du$$

3 previous equations are solved simultaneously

This was done with Mathematica

The results are below (file saved in code folder)

$$L_{0,lmn}^{ug} = \bar{L}_{lmn}^{ug} - \frac{1}{12} L_{2,lmn}^{ug}$$

$$L_{1,lmn}^{ug} = \frac{h_l^u}{h_{l-1}^u + h_l^u + h_{l+1}^u} \left[\left(\bar{L}_{l-1,mn}^{ug} - \bar{L}_{lmn}^{ug} \right) \frac{2h_{l-1}^u + h_l^u}{h_l^u + h_{l+1}^u} - \left(\bar{L}_{lmn}^{ug} - \bar{L}_{l+1,mn}^{ug} \right) \frac{h_l^u + 2h_{l+1}^u}{h_{l-1}^u + h_l^u} \right]$$

$$L_{2,lmn}^{ug} = \frac{3(h_l^u)^2}{h_{l-1}^u + h_l^u + h_{l+1}^u} \left[\left(\bar{L}_{l-1,mn}^{ug} - \bar{L}_{lmn}^{ug} \right) \frac{1}{h_l^u + h_{l+1}^u} + \left(\bar{L}_{lmn}^{ug} - \bar{L}_{l+1,mn}^{ug} \right) \frac{1}{h_{l-1}^u + h_l^u} \right]$$

The average transverse load can be backed out from nodal balance:

$$\bar{L}_{lmn}^{ug} = \frac{\bar{J}_{l,m-k_2,n}^{vg} - \bar{J}_{l,m+k_2,n}^{vg}}{h_m^v} + \frac{\bar{J}_{l,m,n-1/2}^{wg} - \bar{J}_{l,m,n+1/2}^{wg}}{h_n^w}$$

Polynomials for 5th order NEM:

$$P_0(\xi) = 1 \quad P_1(\xi) = \xi \quad P_2(\xi) = \xi^2 - \frac{1}{12}$$

$$P_3(\xi) = \xi^3 - \frac{\xi}{4} \quad P_4(\xi) = \xi^4 - \frac{3\xi^2}{10} + \frac{1}{80}$$

$$P_5(\xi) = \xi^5 - \frac{\xi^3}{3} + \frac{\xi}{48}$$

Note 10 eqs. per group are needed for a two node problem - 5 expansion coeffs per node per group

Constraint #2 - Longitudinal Leakage

$$Q_{lmn}^{ug} = \frac{\overline{J}_{L+1/2, mn}^{ug} - \overline{J}_{L-1/2, mn}^{ug}}{h_L^u}$$

Net current

$$\overline{J}_{lmn}^{ug} \left(\frac{u - u_L}{h_L^u} \right) = -D_{lmn}^g \frac{d\overline{\phi}_{lmn}^{us}}{du'} \frac{du'}{du}$$

we know expansion from before
need chain rule here for coordinate system change $\Rightarrow \frac{d\phi}{du}$

$$\overline{J}_{lmn}^{ug} \left(\frac{u - u_L}{h_L^u} \right) = \frac{-D_{lmn}^g}{h_L^u} \overline{\phi}_{lmn}^g \sum_{t=1}^5 a_{t,lmn}^{us} P_t' \left(\frac{u - u_L}{h_L^u} \right)$$

from chain \uparrow

$$P_0'(\xi) = 0 \quad P_1'(\xi) = 1 \quad P_2'(\xi) = 2\xi \quad P_3'(\xi) = 2\xi^2 - \frac{1}{4}$$

$$P_5'(\xi) = 5\xi^4 - \xi^2 + \frac{1}{48} \quad P_4'(\xi) = 4\xi^3 - \frac{3}{5}\xi$$

Right Face: $u = \frac{u_e + h_e^u/2 - u_e}{h_e^u} = \frac{1}{2}$

$$P'_0(\frac{1}{2})=0 \quad P'_1(\frac{1}{2})=1 \quad P'_2(\frac{1}{2})=1 \quad P'_3(\frac{1}{2})=\frac{1}{2}$$

$$P'_4(\frac{1}{2})=\frac{1}{5} \quad P'_5(\frac{1}{2})=\frac{1}{12}$$

Left Face: $u = \frac{u_e - h_e^u/2 - u_e}{h_e^u} = -\frac{1}{2}$

$$P'_0(-\frac{1}{2})=0 \quad P'_1(-\frac{1}{2})=1 \quad P'_2(-\frac{1}{2})=-1 \quad P'_3(-\frac{1}{2})=\frac{1}{2}$$

$$P'_4(-\frac{1}{2})=-\frac{1}{5} \quad P'_5(-\frac{1}{2})=\frac{1}{12}$$

Thus we can express longitudinal current as:

$$\overline{J}_{l \pm \frac{1}{2} m, n}^{u, g} = -\frac{D_{lm}^g}{h_e^u} \overline{\Phi}_l^g \left[q_{1,lm}^{u, g} - q_{2,lm}^{u, g} + \frac{1}{2} q_{3,lm}^{u, g} + \frac{1}{5} q_{4,lm}^{u, g} + \frac{1}{12} q_{5,lm}^{u, g} \right]$$

Substituting these values into the net longitudinal current over a cell in u -direction: (only - ions remain)

$$Q_{lm}^{u, g} = \frac{\overline{J}_{l+1/2 m, n}^{u, g} - \overline{J}_{l-1/2 m, n}^{u, g}}{h_e^u} = -2 \frac{D_{lm}^g}{h_e^u} \overline{\Phi}_l^g \left[q_{2,lm}^{u, g} + \frac{1}{5} q_{4,lm}^{u, g} \right]$$

$$Q_{lm}^{u, g} = -2 \frac{D_{lm}^g}{h_e^u} \overline{\Phi}_l^g \left[q_{2,lm}^{u, g} + \frac{1}{5} q_{4,lm}^{u, g} \right]$$

Constraint 1

Smoot said others use node average flux here.

Constraint 3 Net Current Contin

$$-\frac{D_{lmn}^g}{h_l^u} \bar{\Phi}_{lmn}^g \left[a_{1,lmn}^{ug} + a_{2,lmn}^{ug} + \frac{1}{2} a_{3,lmn}^{ug} + \frac{1}{5} a_{4,lmn}^{ug} + \frac{1}{12} a_{5,lmn}^{ug} \right]$$

$$= -\frac{D_{l+1,m,n}^g}{h_{l+1}^u} \bar{\Phi}_{l+1,m,n}^g \left[a_{1,l+1,m,n}^{ug} - a_{2,l+1,m,n}^{ug} + \frac{1}{2} a_{3,l+1,m,n}^{ug} - \frac{1}{5} a_{4,l+1,m,n}^{ug} + \frac{1}{12} a_{5,l+1,m,n}^{ug} \right]$$

Constraint 4 $\bar{\Phi}$ Continuity

Note all
polynomials >
order 2 = 0
at $\pm 1/2$

$$P_0(\pm 1/2) = 1 \quad P_1(\pm 1/2) = \pm \frac{1}{2} \quad P_2(\pm 1/2) = 1/6$$

$$\frac{1}{f_{lmn}^{ug}} \bar{\Phi}_{lmn}^g \left[1 + \frac{1}{2} a_{1,lmn}^{ug} + \frac{1}{6} a_{2,lmn}^{ug} \right] =$$

$$\frac{1}{f_{l+1,m,n}^{ug}} \bar{\Phi}_{l+1,m,n}^g \left[1 - \frac{1}{2} a_{1,l+1,m,n}^{ug} + \frac{1}{6} a_{2,l+1,m,n}^{ug} \right]$$

Weighted Residual Constraint

Start w/ Transverse Integral

$$\begin{aligned}
 & -D_{lmn}^g \frac{d^2}{du^2} \bar{\Phi}_{lmn}^{ug} \left(\frac{u-u_L}{h_L^u} \right) + \sum_{l \neq m}^g \bar{\Phi}_{lmn}^{ug} \left(\frac{u-u_L}{h_L^u} \right) \\
 & = \sum_h \sum_{s \neq lmn}^{h \rightarrow g} \bar{\Phi}_{lmn}^{uh} \left(\frac{u-u_L}{h_L^u} \right) + \frac{1}{k} \sum_h v \sum_{s \neq lmn}^{h \rightarrow g} \bar{\Phi}_{lmn}^{uh} \left(\frac{u-u_L}{h_L^u} \right) + L_{lmn}^{ug} \left(\frac{u-u_L}{h_L^u} \right)
 \end{aligned}$$

Pull summation out + write in general:

$$\begin{aligned}
 & \sum_h \left(-D_{lmn}^h \frac{d^2}{du^2} \sigma_{gh} + \sum_{l \neq m}^h \sigma_{gh} - \sum_{s \neq lmn}^{h \rightarrow g} \frac{1}{k} v \sum_{s \neq lmn}^{h \rightarrow g} \right) \bar{\Phi}_{lmn}^{uh} \left(\frac{u-u_L}{h_L^u} \right) \\
 & = L_{lmn}^{ug} \left(\frac{u-u_L}{h_L^u} \right) \quad \text{Desire: } \gamma_{lmn}^{h \rightarrow g} = \sum_{l \neq m}^h \sigma_{gh} - \sum_{s \neq lmn}^{h \rightarrow g} - \frac{1}{k} v \sum_{s \neq lmn}^{h \rightarrow g}
 \end{aligned}$$

Rewrite Equation:

$$\sum_h \left(-D_{lmn}^h \frac{d^2}{du^2} \sigma_{gh} + \gamma_{lmn}^{h \rightarrow g} \right) \bar{\Phi}_{lmn}^{uh} \left(\frac{u-u_L}{h_L^u} \right) = L_{lmn}^{ug} \left(\frac{u-u_L}{h_L^u} \right)$$

Write Flux out:

$$\bar{\Phi}^g(\xi) = \bar{\Phi}_{lmn}^g \left[1 + a_{1lmn}^{ug} \xi + a_{2lmn}^{ug} \left(\xi^2 - \frac{1}{2} \right) + a_{3lmn}^{ug} \left(\xi^3 - \frac{3}{4} \xi \right) + a_{4lmn}^{ug} \left(\xi^4 - \frac{3}{10} \xi^2 + \frac{1}{40} \right) + a_{5lmn}^{ug} \left(\xi^5 - \frac{1}{3} \xi^3 + \frac{1}{40} \xi \right) \right]$$

Derivative:

$$\frac{d\bar{\Phi}^{ug}}{d\xi} = \bar{\Phi}_{lmn}^g \left[a_{1lmn}^{ug} + a_{2lmn}^{ug} (2\xi) + a_{3lmn}^{ug} (3\xi^2 - \frac{1}{4}) + a_{4lmn}^{ug} (4\xi^3 - \frac{3}{10}\xi) + a_{5lmn}^{ug} (5\xi^4 - \xi^2 + \frac{1}{40}) \right]$$

2nd Derivative

$$\frac{d^2 \bar{\Phi}^{ug}}{d\xi^2} = \bar{\Phi}_{lmn}^g \left[2a_{2lmn}^{ug} + 6a_{3lmn}^{ug} \xi + a_{4lmn}^{ug} (12\xi^2 - \frac{3}{5}) + a_{5lmn}^{ug} (20\xi^3 - 2\xi) \right]$$

Substitute flux expansion + flux derivative:

$$\sum_h \left(-D_{lm}^h \left(2a_{2lm}^{nh} + 6a_{3lm}^{nh} \xi + a_{4lm}^{nh} (12\xi^2 - 3/5) + a_{5lm}^{nh} (20\xi^3 - 2\xi) \right) \right. \\ \left. + \tau_{lm}^{h \rightarrow g} \left(1 + a_{1lm}^{nh} \xi + a_{2lm}^{nh} (\xi^2 - 1/2) + a_{3lm}^{nh} (\xi^3 - \xi/4) + a_{4lm}^{nh} (\xi^4 - 3/10 \xi^2 + 1/80) \right. \right. \\ \left. \left. + a_{5lm}^{nh} (\xi^5 - 1/3 \xi^3 + 1/48 \xi) \right) \right) \bar{\Phi}_{lm}^{nh} = L_{0lm}^{ng} + L_{1lm}^{ng} \xi + L_{2lm}^{ng} \xi^2$$

Multiply by ξ + integrate over $-1/2$ to $1/2$: 5+6

$$\sum_h \left[\tau_{lm}^{h \rightarrow g} a_{1lm}^{nh} - \left(\frac{1}{10} \tau_{lm}^{h \rightarrow g} + \delta_{gh} 6 \frac{D_{lm}^h}{h_l^{n+2}} \right) a_{3lm}^{nh} - \left(\frac{1}{420} \tau_{lm}^{h \rightarrow g} + \delta_{gh} \frac{D_{lm}^h}{h_l^{n+2}} \right) a_{5lm}^{nh} \right] \bar{\Phi}_{lm}^{nh} = L_{2lm}^{ng}$$

Multiply by $(\xi^2 - 1/2)$ + integrate over $-1/2$ to $1/2$: 7+8

$$\sum_h \left[\tau_{lm}^{h \rightarrow g} a_{2lm}^{nh} - \left(\frac{3}{35} \tau_{lm}^{h \rightarrow g} + \delta_{gh} 12 \frac{D_{lm}^h}{h_l^{n+2}} \right) a_{4lm}^{nh} \right] \bar{\Phi}_{lm}^{nh} = L_{2lm}^{ng}$$

Multiply by $(\xi^3 - \xi/4)$ + integrate over $-1/2$ to $1/2$: 9+10

$$\sum_h \left[\tau_{lm}^{h \rightarrow g} a_{1lm}^{nh} - \left(\frac{1}{7} \tau_{lm}^{h \rightarrow g} + \delta_{gh} 6 \frac{D_{lm}^h}{h_l^{n+2}} \right) a_{3lm}^{nh} - \delta_{gh} \frac{1}{7} \frac{D_{lm}^h}{h_l^{n+2}} a_{5lm}^{nh} \right] \bar{\Phi}_{lm}^{nh} = L_{1lm}^{ng}$$

$$\tau_{lm}^{h \rightarrow g} = \sum_{l' \neq l}^h \delta_{gl'} - \sum_{s \neq l}^{h \rightarrow g} - \frac{1}{k} \nu \sum_{s \neq l}^{h \rightarrow g}$$