Lecture Note 2

I-2. Power Method and Wielandt Shift
II. Multigroup Neutron Diffusion

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Power Method

- Eigenvalue problem

$$M\phi = \lambda F\phi = \frac{1}{k}F\phi \qquad k\phi = M^{-1}F\phi \qquad 0 \le k_i \le k_1 = k$$

$\uparrow$ (Largest eigenvalue corresponding to fundamental eigen vector (=1st harmonics))

minimum adjustment of ν

$\rightarrow$ minimum λ

$\rightarrow$ maximum k

$$A\phi = k\phi \quad \left(A = M^{-1}F\right)$$

– Iterative scheme to find the fundamental eigenvector of $A(\mathit{largest}\,k)$

$$\phi^{(l)} = A\phi^{(l-1)} = A^l\phi^{(0)} \rightarrow \text{Power method}$$

let $\phi^{(0)} = c_1u_1 + c_2u_2 + \cdots\cdots + c_Nu_N$ (Let u_i be the i-th normalized eigenVector of A and corresponding to k_i)

$$\phi^{(l)} = A^l\phi^{(0)} = A^l\left(c_1u_1 + c_2u_2 + \cdots\cdots + c_Nu_N\right)$$

$$= c_1 \cdot k_1^l u_1 + c_2 \cdot k_2^l u_2 + \cdots\cdots + c_N \cdot k_N^l u_N$$

$$= k_1^l\left(c_1u_1 + \sum_{i=2}^{N}\left[\left(\frac{k_i}{k_1}\right)^l c_iu_i\right]\right) \qquad \left(\because \frac{k_i}{k_1} < 1\right)$$

$$\approx k_1^l c_1u_1 \qquad (\text{as } l \rightarrow \infty)$$

– How to obtain $k^{(l)}$?

For sufficiently large l

$$\phi^{(l)} = A\phi^{(l-1)} = k\phi^{(l-1)}$$

$$\left\langle \phi^{(l)}, \phi^{(l)} \right\rangle = k\left\langle \phi^{(l)}, \phi^{(l-1)} \right\rangle$$

$$k^{(l)} = \frac{\left\langle \phi^{(l)}, \phi^{(l)} \right\rangle}{\left\langle \phi^{(l)}, \phi^{(l-1)} \right\rangle}$$

Power Method with Scaling

- The problem of power method

  $\left\| \vec{\phi} \right\| \uparrow$ as $l \uparrow \Rightarrow$ Scaling is needed (if $k > 1$)

- Scaling

  $$\hat{\phi}^{(l)} = \frac{1}{k^{(l-1)}} \phi^{(l-1)}$$ $\leftarrow$ Divide in advance anticipating mutiplication by k

  $$\phi^{(l)} = A\hat{\phi}^{(l-1)} = k\hat{\phi}^{(l-1)} = \frac{k}{k^{(l-1)}} \phi^{(l-1)}$$

  $$k = k^{(l-1)} \frac{\left\langle \phi^{(l)}, \phi^{(l)} \right\rangle}{\left\langle \phi^{(l)}, \phi^{(l-1)} \right\rangle} = k^{(l)}$$

- Power Iteration Scheme with Scaling
  - From known $k^{(l-1)}$ and $\phi^{(l-1)}$

1) $\phi^{(l)} = A\hat{\phi}^{(l-1)} = \frac{1}{k^{(l-1)}} A\phi^{(l-1)}$

2) $k^{(l)} = k^{(l-1)} \frac{\left\langle \phi^{(l)}, \phi^{(l)} \right\rangle}{\left\langle \phi^{(l)}, \phi^{(l-1)} \right\rangle}$

3) Repeat

c.f) Power method Only

$$\phi^{(l)} = A\phi^{(l-1)}$$

$$k^{(l)} = \frac{\left\langle \phi^{(l)}, \phi^{(l)} \right\rangle}{\left\langle \phi^{(l)}, \phi^{(l-1)} \right\rangle}$$

Convergence of Power Method with Scaling

$$\phi^{(l)} = \frac{1}{k^{(l-1)}} \cdot \frac{1}{k^{(l-2)}} \cdots \frac{1}{k^{(0)}} A^l \phi^{(0)}$$

$$= \left(\prod_{i=0}^{l-1} \frac{1}{k^{(i)}} \right) k_1^l \left[c_1 u_1 + \sum_{i=2}^{n} \left(c_i u_i \left(\frac{k_i}{k_1} \right)^l \right) \right] \qquad \leftarrow A^l \phi^{(0)} = k_1^l \left[c_1 u_1 + \sum_{i=2}^{n} \left(c_i u_i \left(\frac{k_i}{k_1} \right)^l \right) \right]$$

$$= \left(\prod_{i=0}^{l-1} \frac{k_1^l}{k^{(i)}} \right) \left[c_1 u_1 + \sum_{i=2}^{n} \left(c_i u_i \left(\frac{k_i}{k_1} \right)^l \right) \right]$$

$$\approx \left(\prod_{i=0}^{l-1} \frac{k_1^l}{k^{(i)}} \right) c_1 u_1 \qquad (\text{as } l \to \infty) \qquad \left(\because \frac{k_i}{k_1} < 1 \right)$$

Inverse Power method

$$\phi^{(l)} = \frac{1}{k^{(l-1)}} A\phi^{(l-1)} \qquad \left(A = M^{-1}F\right)$$

$$\phi^{(l)} = \frac{1}{k^{(l-1)}} M^{-1}F\phi^{(l-1)}$$ $\rightarrow$ Difficult to obtain M^{-1}

$$M\phi^{(l)} = \frac{1}{k^{(l-1)}} F\phi^{(l-1)} = b$$: Inverse power method requiring solution of a linear system except for 1D problems

$M\phi^{(l)} = b$ $\rightarrow$ need to be solved iteratively in practical cases

$\rightarrow$ another level of iteration $\rightarrow$ outer and inner iteration (nested loop)

LU factorization

- For 1-D Problems

$$M\phi^{(l)} = b \quad (M = LU)$$

$$LU\phi^{(l)} = b$$

$M = LU$

$$\begin{bmatrix} d_1 & -u_1 & 0 & & 0 \\ -l_2 & d_2 & -u_2 & 0 & \\ 0 & \ddots & \ddots & \ddots & 0 \\ & 0 & \ddots & \ddots & \ddots \\ 0 & & 0 & -l_N & d_N \end{bmatrix} = \begin{bmatrix} 1 & 0 & & & 0 \\ -l_2 & 1 & 0 & & \\ 0 & \ddots & \ddots & 0 & \\ & 0 & \ddots & \ddots & 0 \\ 0 & & 0 & -l_N & 1 \end{bmatrix} \begin{bmatrix} \tilde{d}_1 & -u_1 & 0 & & 0 \\ 0 & \tilde{d}_2 & -u_2 & 0 & \\ 0 & 0 & \ddots & \ddots & 0 \\ & 0 & 0 & \ddots & \ddots \\ 0 & & 0 & 0 & \tilde{d}_N \end{bmatrix}$$

$$\tilde{d}_1 = d_1; \ m_i = \frac{l_i}{\tilde{d}_{i-1}}; \ \tilde{d}_i = d_i - m_i u_{i-1}; l_i = m_i$$

– Foward Substitution

$$LU\phi^{(l)} = b$$

$$Ly = b \quad \left(\text{substitute } y = U\phi^{(l)}\right)$$

$L\,y = b$

$$\begin{bmatrix} 1 & 0 & & & 0 \\ -l_2 & 1 & 0 & & \\ 0 & \ddots & \ddots & 0 & \\ & 0 & \ddots & \ddots & 0 \\ 0 & & 0 & -l_N & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ \vdots \\ y_N \end{bmatrix} = \begin{bmatrix} b_1 \\ b_1 \\ \vdots \\ \vdots \\ b_N \end{bmatrix}$$

$$y_1 = b_1 \Rightarrow y_1 = b_1$$

$$-l_2 y_1 + y_2 = b_2 \Rightarrow y_2 = b_2 + l_2 y_1$$

$$\downarrow \qquad \downarrow$$

$$-l_i y_{i-1} + y_i = b_i \Rightarrow y_i = b_i + l_i y_{i-1}$$

– Backward Substitution

$$U\phi^{(l)} = y$$

$U\phi^{(l)} = y$

$$\begin{bmatrix} \tilde{d}_1 & -u_1 & 0 & & 0 \\ 0 & \tilde{d}_2 & -u_2 & 0 & \\ 0 & 0 & \ddots & \ddots & 0 \\ & 0 & 0 & \ddots & \ddots \\ 0 & & 0 & 0 & \tilde{d}_N \end{bmatrix} \begin{bmatrix} \phi_1^{(l)} \\ \phi_2^{(l)} \\ \vdots \\ \vdots \\ \phi_N^{(l)} \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ \vdots \\ y_N \end{bmatrix}$$

$$\phi_1^{(l)} = \frac{1}{\tilde{d}_1}\left(y_1 + u_1\phi_2^{(l)}\right)$$

$$\uparrow$$

$$\phi_i^{(l)} = \frac{1}{\tilde{d}_i}\left(y_i + u_i\phi_{i+1}^{(l)}\right)$$

$$\uparrow$$

$$\phi_N^{(l)} = \frac{y_N}{\tilde{d}_N}$$

store inverse of $\tilde{d}_i$

Convergence of Power method

$$\phi^{(l)} = \tilde{c}_1 u_1 + \tilde{c}_2 \left(\frac{k_2}{k_1}\right)^l u_2 + \cdots\cdots \quad \leftarrow \quad \tilde{c}_k = \left(\prod_{i=0}^{l-1}\left[\frac{k_1}{k^{(i)}}\right]\right) c_k \quad \rightarrow \left\|\phi^{(l)}\right\| \cong \left|\tilde{c}_1\right| \quad \because \left|\tilde{c}_2\left(\frac{k_2}{k_1}\right)^l\right| << 1$$

$$\frac{\phi^{(l)}}{\tilde{c}_1} = u_1 + \frac{\tilde{c}_2}{\tilde{c}_1}\left(\frac{k_2}{k_1}\right)^l u_2 + \cdots\cdots \quad (u_1 \ : \text{Normalized eigenvector})$$

– Error vector

$$e_1^{(l)} = \frac{\phi^{(l)}}{\tilde{c}_1} - u_1 = \frac{\tilde{c}_2}{\tilde{c}_1}\sigma^l u_2 + \cdots\cdots \quad \left(\sigma = \frac{k_2}{k_1} < 1 : \text{Dominace ratio}\right)$$

– How to find σ ?

As σ becomes smaller, problem converges FASTer.

As σ becomes close to 1, problem converges SLOWer.

$$\begin{cases} e^{(l)} = \dfrac{\phi^{(l)}}{\tilde{c}_1} - u_1 = \dfrac{\tilde{c}_2}{\tilde{c}_1}(\sigma)^l u_1 + \cdots\cdots \\ e^{(l-1)} = \dfrac{\phi^{(l-1)}}{\tilde{c}_1} - u_1 = \dfrac{\tilde{c}_2}{\tilde{c}_1}(\sigma)^{l-1} u_1 + \cdots\cdots \end{cases}$$

$$\left\|e^{(l)}\right\| = \sigma \left\|e^{(l-1)}\right\|$$

$$\sigma = \frac{\left\|e^{(l)}\right\|}{\left\|e^{(l-1)}\right\|}$$

Practical Method to determine σ

$$e^{(l)} = \sigma e^{(l-1)} \rightarrow \phi^{(l)} - \phi^* = \sigma\left(\phi^{(l-1)} - \phi^*\right)$$

$$\phi^{(l-1)} - \phi^* = \sigma\left(\phi^{(l-2)} - \phi^*\right)$$

$$\phi^{(l)} - \phi^{(l-1)} = \sigma\left(\phi^{(l-1)} - \phi^{(l-2)}\right)$$

$$\rightarrow \tilde{e}^{(l)} = \sigma \tilde{e}^{(l-1)} : \text{pseudo error}$$

$$\sigma = \frac{\left\|\tilde{e}^{(l)}\right\|}{\left\|\tilde{e}^{(l-1)}\right\|}$$

Wielandt Eigenvalue Shift Method

- How to obtain smaller σ? $\left(= \text{How to make it converge FASTer}\right)$?

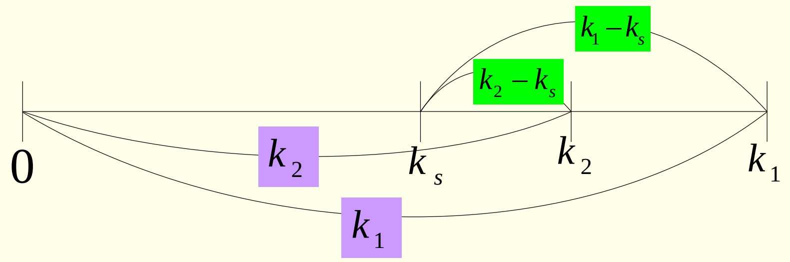
$$A\phi = k\phi$$

$$A\phi - k_s\phi = k\phi - k_s\phi$$

$$\left(A - k_s I\right)\phi = \left(k - k_s\right)\phi \qquad \left[\text{Condition: } \max\left(k_s\right) < k_2\right]$$

$$\tilde{A}\phi = \tilde{k}\phi$$

$$\therefore \quad \tilde{\sigma} = \frac{\tilde{k}_2}{\tilde{k}_1} = \frac{k_2 - k_s}{k_1 - k_s}$$



- through eigenvalue shift, σ is smaller than before

$\rightarrow$ improved convergence $\rightarrow$ Wielandt shift method

$$A\phi = k\phi \quad \Leftrightarrow \quad \tilde{A}\phi = \tilde{k}\phi$$

$$\sigma\left(= \frac{k_2}{k_1}\right) \quad > \quad \tilde{\sigma}\left(= \frac{\tilde{k}_2}{\tilde{k}_1} = \frac{k_2 - k_s}{k_1 - k_s}\right)$$

$$\text{ex.)} \ \sigma = \frac{k_2}{k_1} = \frac{0.99}{1.00} = 0.99 \ \rangle \ \tilde{\sigma} = \frac{0.99 - 0.9}{1.00 - 0.9} = 0.90$$

Wielandt Shift Method for Neutronic EigenValue Problem

$$M\phi = \frac{1}{k}F\phi \quad \leftrightarrow M\phi = \lambda F\phi$$

$$\left(M - \frac{1}{k_s}F\right)\phi = \left(\frac{1}{k} - \frac{1}{k_s}\right)F\phi$$

$\leftrightarrow \ (M - \lambda_s F)\phi = (\lambda - \lambda_s)F\phi,$

$\lambda > \lambda_s$ to retain RHS positive

$$\tilde{M}\phi = \frac{1}{\tilde{k}}F\phi \qquad \left(\frac{1}{\tilde{k}} = \frac{1}{k} - \frac{1}{k_s}\right)$$

$$\left[k_s = k + \delta k \quad ,\delta k > 0\right]$$

$$\tilde{k}\phi = \tilde{M}^{-1}F\phi$$

– How to obtain $\phi^{(l)}$ at the l-th step?

$$\tilde{M}^{(l-1)}\phi^{(l)} = \frac{1}{\tilde{k}^{(l-1)}}F\phi^{(l-1)} \quad \rightarrow \begin{pmatrix} \text{Power method with Scaling} \\ \text{Solve with LU fact.} \end{pmatrix}$$

$$\begin{bmatrix} \tilde{M}^{(l-1)} = M - \dfrac{1}{k_s^{(l-1)}}F \\ k_s^{(l-1)} = k^{(l-1)} + \delta k \quad ,\delta k > 0 \end{bmatrix}$$

Determination of Eigenvalue in Wielandt Shift

– How to obtain $k^{(l)}$?

$$\phi^{(l)} = \frac{1}{\tilde{k}^{(l-1)}} \underbrace{\left[\tilde{M}^{(l-1)}\right]^{-1} F\phi^{(l-1)}}_{=\tilde{k}\phi^{(l-1)}\text{(for large } l)} \quad \text{: Power method with Scaling}$$

$$\frac{1}{\tilde{k}}\phi^{(l)} = \frac{1}{\tilde{k}^{(l-1)}}\phi^{(l-1)}$$

$$\left(\frac{1}{k} - \frac{1}{k_s^{(l-1)}}\right)\phi^{(l)} = \left(\frac{1}{k^{(l-1)}} - \frac{1}{k_s^{(l-1)}}\right)\phi^{(l-1)}$$

$$\left(\frac{1}{k} - \frac{1}{k_s^{(l-1)}}\right)\left\langle\phi^{(l)},\phi^{(l)}\right\rangle = \left(\frac{1}{k^{(l-1)}} - \frac{1}{k_s^{(l-1)}}\right)\left\langle\phi^{(l)},\phi^{(l-1)}\right\rangle$$

$$\frac{1}{k} = \left(\frac{1}{k^{(l-1)}} - \frac{1}{k_s^{(l-1)}}\right)\frac{\left\langle\phi^{(l)},\phi^{(l-1)}\right\rangle}{\left\langle\phi^{(l)},\phi^{(l)}\right\rangle} + \frac{1}{k_s^{(l-1)}}$$

☞ $\gamma = \frac{\left\langle\phi^{(l)},\phi^{(l-1)}\right\rangle}{\left\langle\phi^{(l)},\phi^{(l)}\right\rangle}$

$$= \left(\frac{1}{k^{(l-1)}} - \frac{1}{k_s^{(l-1)}}\right)\gamma + \frac{1}{k_s^{(l-1)}} = \frac{\gamma}{k^{(l-1)}} + (1-\gamma)\frac{1}{k_s^{(l-1)}}$$

$$\therefore k = \frac{1}{\frac{\gamma}{k^{(l-1)}} + (1-\gamma)\frac{1}{k_s^{(l-1)}}} = k^{(l)}$$

Reduction in Dominance Ratio with Inverse Wielandt Shift

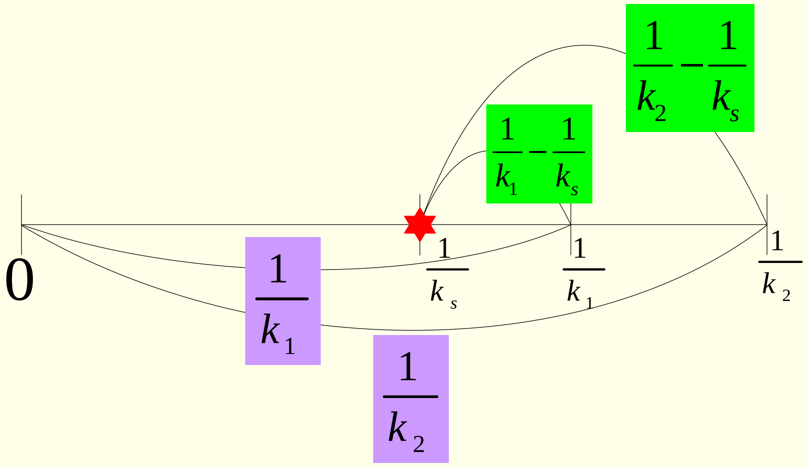
- Dominance ratio σ
  - Original dominance ratio

$$\sigma = \frac{k_2}{k_1} = \frac{\frac{1}{k_1}}{\frac{1}{k_2}} = \frac{\lambda_1}{\lambda_2}$$

smallest eigenvalue

  - New dominance ratio

$$\tilde{\sigma} = \frac{\tilde{k}_2}{\tilde{k}_1} = \frac{\frac{1}{\tilde{k}_1}}{\frac{1}{\tilde{k}_2}} = \frac{\frac{1}{k_1} - \frac{1}{k_s}}{\frac{1}{k_2} - \frac{1}{k_s}}$$



As $\frac{1}{k_s}\left(= \frac{1}{k_1 + \delta k}\right)$ is close to $\frac{1}{k_1}$, converge FAST.

$\rightarrow$ As δk is close to 0, Converge FAST.

II. 1-D, Multigroup Neutron Diffusion Problem

$$-\frac{d}{dx}\left(D_g^k \frac{d\phi_g^k}{dx}\right) + \Sigma_{tg}^k \phi_g^k = \lambda \chi_g^k \left(\sum_{g'=1}^{G} \nu\Sigma_{fg'}^k \phi_{g'}^k\right) + \left(\sum_{g'=1}^{G} \Sigma_{g'g}^k \phi_{g'}^k\right)$$

Node index: k (*not* k-th power), Group index: g

Total unknowns: $N = K \times G$

$$-\frac{d}{dx}\left(D_g^k \frac{d\phi_g^k}{dx}\right) + \Sigma_{rg}^k \phi_g^k = \lambda \chi_g^k \left(\sum_{g'=1}^{G} \nu\Sigma_{fg'}^k \phi_{g'}^k\right) + \left(\sum_{\substack{g'=1 \\ g' \neq g}}^{G} \Sigma_{g'g}^k \phi_{g'}^k\right)$$

$$\Sigma_{tg}^k = \Sigma_{ag}^k + \Sigma_s^k = \Sigma_{ag}^k + \sum_{g'=1}^{G} \Sigma_{gg'}^k$$

$$= \Sigma_{ag}^k + \Sigma_{gg}^k + \sum_{\substack{g'=1 \\ g' \neq g}}^{G} \Sigma_{gg'}^k$$

$\Sigma_{rg}^k = \Sigma_{tg}^k - \Sigma_{gg}^k \Leftarrow$

Removal Xsec

- Discretization (Assume same node size (h))

$$-\tilde{D}_g^{k-1}\phi_g^{k-1} + (\tilde{D}_g^{k-1} + \tilde{D}_g^k + \Sigma_{r,g}^k h)\phi_g^k - \tilde{D}_g^k \phi_g^{k+1} = \lambda \chi_g^k \left(\sum_{g'=1}^{G} \nu\Sigma_{fg'}^k \phi_{g'}^k\right) h + \left(\sum_{\substack{g'=1 \\ g' \neq g}}^{G} \Sigma_{g'g}^k \phi_{g'}^k\right) h$$

$$-l_g^k \phi_g^{k-1} + d_g^k \phi_g^k - u_g^k \phi_g^{k+1} = q_g^k$$

$\leftarrow$ *Nodal balance Eq. after dividing by mesh width h!*

$$\begin{cases} l_g^k = \dfrac{\tilde{D}_g^{k-1}}{h} = \dfrac{2}{h^2} \dfrac{D_g^{k-1} D_g^k}{D_g^{k-1} + D_g^k} \\ u_g^k = \dfrac{\tilde{D}_g^k}{h} = \dfrac{2}{h^2} \dfrac{D_g^k D_g^{k+1}}{D_g^k + D_g^{k+1}} \\ d_g^k = l_g^k + u_g^k + \Sigma_{r,g}^k \end{cases}$$

$$q_g^k = \lambda \chi_g^k \left(\sum_{g'=1}^{G} \nu\Sigma_{fg'}^k \phi_{g'}^k\right) + \left(\sum_{\substack{g'=1 \\ g' \neq g}}^{G} \Sigma_{g'g}^k \phi_{g'}^k\right)$$

Discretization at boundary

At $\phi = \phi_g^1$ (Left side albedo)

$$\left(l_g^1 + u_g^1 + \Sigma_{r,g}^1\right)\phi_g^1 - u_g^1\phi_g^2 = q_g^1$$

$Note$: superscript is for node index, not exponent

$$l_g^1 = \frac{\tilde{D}_g^0}{h} = \frac{1}{h}\frac{2\beta_g^0\beta_g^1}{\beta_g^0 + \beta_g^1};\ \beta_g^0 = \frac{\alpha_g^L}{2},\ \beta_g^1 = \frac{D_g}{h}$$

At $\phi = \phi_g^K$ (Right side albedo)

$$-l_g^K\phi_g^{K-1} + \left(l_g^K + u_g^K + \Sigma_{rg}^K\right)\phi_g^K = q_g^K$$

Ordering scheme

① Group Major Ordering

primary sort variable : Group (g)

secondary sort variable : Node (k)

$$\begin{bmatrix} \begin{bmatrix} \phi_1^1 \\ \vdots \\ \phi_1^k \\ \vdots \\ \phi_1^K \end{bmatrix} \\ \vdots \\ \begin{bmatrix} \phi_G^1 \\ \vdots \\ \phi_G^k \\ \vdots \\ \phi_G^K \end{bmatrix} \end{bmatrix}$$

② Node Major Ordering

primary sort variable : Node (k)

secondary sort variable : Group (g)

$$\begin{bmatrix} \begin{bmatrix} \phi_1^1 \\ \vdots \\ \phi_g^1 \\ \vdots \\ \phi_G^1 \end{bmatrix} \\ \vdots \\ \begin{bmatrix} \phi_1^K \\ \vdots \\ \phi_g^K \\ \vdots \\ \phi_G^K \end{bmatrix} \end{bmatrix}$$

Matrix Structure with Node Major Ordering Scheme

$$-l_g^k\phi_g^{k-1} + d_g^k\phi_g^k - u_g^k\phi_g^{k+1} = q_g^k = \lambda\chi_g^k \underbrace{\sum_{g'=1}^{G}\nu\Sigma_{fg'}^k\phi_{g'}^k}_{\psi^k} + \sum_{\substack{g'=1\\ g'\neq g}}^{G}\Sigma_{g'g}^k\phi_{g'}^k$$

$$-l_g^k\phi_g^{k-1} + d_g^k\phi_g^k - u_g^k\phi_g^{k+1} - \sum_{\substack{g'=1\\ g'\neq g}}^{G}\Sigma_{g'g}^k\phi_{g'}^k = \lambda\chi_g^k\psi^k$$

$$M\phi = \lambda F\phi$$

$$M = \begin{bmatrix} D_1 & U_1 & 0 & & 0 \\ L_2 & D_2 & U_2 & 0 & \\ 0 & \ddots & \ddots & \ddots & 0 \\ & 0 & L_{K-1} & D_{K\text{-}1} & U_{K-1} \\ 0 & & 0 & L_K & D_K \end{bmatrix}$$

Block Tri-Diagonal $\left[(\mathrm{G}\times\mathrm{K})\times(\mathrm{G}\times K)\right]$

$$D_k = \begin{bmatrix} \Sigma_{r1}^k & & & & & \cdots & \\ -\Sigma_{12}^k & \Sigma_{r2}^k & & & & & \\ & & \ddots & & & \ddots & \vdots \\ -\Sigma_{1g}^k & -\Sigma_{2g}^k & -\Sigma_{g-1,g}^k & \Sigma_{rg}^k & -\Sigma_{g+1,g}^k & & \\ & & & & \ddots & & \\ \vdots & \ddots & & & & \ddots & \\ & \cdots & & & -\Sigma_{G-2,G}^k & -\Sigma_{G-1,G}^k & \Sigma_{rG}^k \end{bmatrix}$$

$$L_k = \begin{bmatrix} -l_1^k & 0 & & & 0 \\ 0 & \ddots & 0 & & \\ & 0 & -l_g^k & 0 & \\ & & 0 & \ddots & 0 \\ 0 & & & 0 & -l_G^k \end{bmatrix} \quad U_k = \begin{bmatrix} -u_1^k & 0 & & & 0 \\ 0 & \ddots & 0 & & \\ & 0 & -u_g^k & 0 & \\ & & 0 & \ddots & 0 \\ 0 & & & 0 & -u_G^k \end{bmatrix}$$

Matrix Structure in Node Major Ordering Scheme

$$
\begin{bmatrix}
\begin{bmatrix} \; \end{bmatrix} & & & & & & \\
& \begin{bmatrix} \; \end{bmatrix} & & & & & \\
\begin{bmatrix} 0 & & & 0 \\ & 0 & 0 & \\ & 0 & 0 & \\ 0 & & & 0 \end{bmatrix} &
\begin{bmatrix} -l_1^{k-1} & 0 & & & 0 \\ 0 & \ddots & 0 & & \\ & 0 & -l_g^{k-1} & 0 & \\ & & 0 & \ddots & 0 \\ 0 & & & 0 & -l_G^{k-1} \end{bmatrix} &
\begin{bmatrix} \Sigma_{r1}^k & & & & & & \\ -\Sigma_{12}^k & \Sigma_{r2}^k & & & & & \\ & & \ddots & & & & \\ -\Sigma_{1g}^k & -\Sigma_{2g}^k & -\Sigma_{g-1,g}^k & \Sigma_{rg}^k & -\Sigma_{g+1,g}^k & & \\ & & & & \ddots & & \\ & & & & & \ddots & \\ & & & & -\Sigma_{G-2,G}^k & -\Sigma_{G-1,G}^k & \Sigma_{rG}^k \end{bmatrix} &
\begin{bmatrix} -u_1^{k-1} & 0 & & & 0 \\ 0 & \ddots & 0 & & \\ & 0 & -u_g^{k-1} & 0 & \\ & & 0 & \ddots & 0 \\ 0 & & & 0 & -u_G^{k-1} \end{bmatrix} &
\begin{bmatrix} 0 & & & 0 \\ & 0 & 0 & \\ & 0 & 0 & \\ 0 & & & 0 \end{bmatrix} \\
& & \begin{bmatrix} \; \end{bmatrix} & & \begin{bmatrix} \; \end{bmatrix} & & \\
& & & & & \begin{bmatrix} \; \end{bmatrix} &
\end{bmatrix}
\begin{bmatrix}
\begin{bmatrix} \phi_1^1 \\ \phi_g^1 \\ \phi_G^1 \end{bmatrix} \\
\begin{bmatrix} \phi_1^k \\ \phi_g^k \\ \phi_G^k \end{bmatrix} \\
\begin{bmatrix} \phi_1^K \\ \phi_g^K \\ \phi_G^K \end{bmatrix}
\end{bmatrix}
$$

Matrix Structure in Node Major Ordering Scheme

$$F=\begin{bmatrix} F^1 & 0 & & & 0 \\ 0 & \ddots & 0 & & \\ & 0 & F^k & 0 & \\ & & 0 & \ddots & 0 \\ 0 & & & 0 & F^K \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} & 0 & 0 \\ 0 & \begin{bmatrix} p & p & p \\ p & p & p \\ 0 & 0 & 0 \end{bmatrix} & 0 \\ 0 & 0 & \begin{bmatrix} p & p & p \\ p & p & p \\ 0 & 0 & 0 \end{bmatrix} \end{bmatrix}$$

Area NOT having Fission

Fission block matrix for node k

$$F^k\phi^k = \underbrace{\overbrace{\begin{bmatrix} \chi_1^k \\ \vdots \\ \chi_g^k \\ \chi_{g'}^k \\ 0 \\ 0 \end{bmatrix}}^{\boldsymbol{\chi}_k} \overbrace{\begin{bmatrix} \nu\Sigma_{f1}^k & \cdots & \nu\Sigma_{fg}^k & \cdots & \nu\Sigma_{fG}^k \end{bmatrix}}^{\mathbf{f}_k^T} \begin{bmatrix} \phi_1^k \\ \vdots \\ \phi_g^k \\ \vdots \\ \phi_G^k \end{bmatrix}}_{\psi} = \overbrace{\begin{bmatrix} \chi_1^k\nu\Sigma_{f1}^k & \cdots & \chi_1^k\nu\Sigma_{fg}^k & \cdots & \chi_1^k\nu\Sigma_{fG}^k \\ \chi_2^k\nu\Sigma_{f1}^k & \cdots & \chi_2^k\nu\Sigma_{fg}^k & \cdots & \chi_2^k\nu\Sigma_{fG}^k \\ \vdots & & \vdots & & \vdots \\ \chi_{g'}^k\nu\Sigma_{f1}^k & \cdots & \chi_{g'}^k\nu\Sigma_{fg}^k & \cdots & \chi_{g'}^k\nu\Sigma_{fG}^k \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}}^{\mathbf{F}_k=\boldsymbol{\chi}_k\mathbf{f}_k^T} \begin{bmatrix} \phi_1^k \\ \vdots \\ \phi_g^k \\ \vdots \\ \phi_G^k \end{bmatrix}$$

Matrix Structure in Group Major Ordering Scheme

$$-l_g^k \phi_g^{k-1} + d_g^k \phi_g^k - u_g^k \phi_g^{k+1} = \lambda \chi_g^k \underbrace{\sum_{g'=1}^{G} \nu\Sigma_{fg'}^k \phi_{g'}^k}_{\psi^k} + \sum_{\substack{g'=1 \\ g'\neq g}}^{G} \Sigma_{g'g}^k \phi_{g'}^k$$

$$M\phi = \lambda F \phi + \Sigma_S \phi$$

$$\mathbf{M}\phi = \begin{bmatrix}
\begin{bmatrix} d_1^1 & -u_1^1 & 0 & & & 0 \\ -l_1^2 & d_1^2 & -u_1^2 & 0 & & \\ 0 & & \dots & & 0 & \\ & 0 & -l_1^k & d_1^k & -u_1^k & 0 \\ & & & & \dots & -u_1^{K-1} \\ 0 & & & 0 & -l_1^K & d_1^K \end{bmatrix} & & 0 & & 0 \\
& \dots & & 0 & \\
0 & & \begin{bmatrix} d_g^1 & -u_g^1 & 0 & & & 0 \\ -l_g^2 & d_g^2 & -u_g^2 & 0 & & \\ 0 & & \dots & & 0 & \\ & 0 & -l_g^k & d_g^k & -u_g^k & 0 \\ & & & & \dots & -u_g^{K-1} \\ 0 & & & 0 & -l_g^K & d_g^K \end{bmatrix} & & 0 \\
& 0 & & \dots & \\
0 & & 0 & & \begin{bmatrix} d_G^1 & -u_G^1 & 0 & & & 0 \\ -l_G^2 & d_G^2 & -u_G^2 & 0 & & \\ 0 & & \dots & & 0 & \\ & 0 & -l_G^k & d_G^k & -u_G^k & 0 \\ & & & & \dots & -u_G^{K-1} \\ 0 & & & 0 & -l_G^K & d_G^K \end{bmatrix}
\end{bmatrix}
\begin{bmatrix}
\begin{bmatrix} \phi_1^1 \\ \dots \\ \phi_1^k \\ \dots \\ \phi_1^K \end{bmatrix} \\ \dots \\
\begin{bmatrix} \phi_g^1 \\ \dots \\ \phi_g^k \\ \dots \\ \phi_g^K \end{bmatrix} \\ \dots \\
\begin{bmatrix} \phi_G^1 \\ \dots \\ \phi_G^k \\ \dots \\ \phi_G^K \end{bmatrix}
\end{bmatrix}$$

Fission Matrix Structure in Group Major

$$\frac{1}{k}\chi\nu\Sigma_f\phi=\frac{1}{k}\begin{bmatrix}\begin{bmatrix}\chi_1^1 & & & 0\\ & \cdots & & \\ & & \chi_1^k & \\ 0 & & & \chi_1^K\end{bmatrix}\\ \cdots \\ \begin{bmatrix}\chi_g^1 & & & 0\\ & \cdots & & \\ & & \chi_g^k & \\ 0 & & & \chi_g^K\end{bmatrix}\\ \cdots \\ \begin{bmatrix}\chi_G^1 & & & 0\\ & \cdots & & \\ & & \chi_G^k & \\ 0 & & & \chi_G^K\end{bmatrix}\end{bmatrix}\underbrace{\begin{bmatrix}\begin{bmatrix}\nu\Sigma_{f1}^1 & & & 0\\ & \cdots & & \\ & & \nu\Sigma_{f1}^k & \\ 0 & & & \nu\Sigma_{f1}^K\end{bmatrix} & \cdots & \begin{bmatrix}\nu\Sigma_{fg}^1 & & & 0\\ & \cdots & & \\ & & \nu\Sigma_{fg}^k & \\ 0 & & & \nu\Sigma_{fg}^K\end{bmatrix} & \cdots & \begin{bmatrix}\nu\Sigma_{fG}^1 & & & 0\\ & \cdots & & \\ & & \nu\Sigma_{fG}^k & \\ 0 & & & \nu\Sigma_{fG}^K\end{bmatrix}\end{bmatrix}\begin{bmatrix}\begin{bmatrix}\phi_1^1\\ \cdots\\ \phi_1^k\\ \cdots\\ \phi_1^K\end{bmatrix}\\ \cdots\\ \begin{bmatrix}\phi_g^1\\ \cdots\\ \phi_g^k\\ \cdots\\ \phi_g^K\end{bmatrix}\\ \cdots\\ \begin{bmatrix}\phi_G^1\\ \cdots\\ \phi_G^k\\ \cdots\\ \phi_G^K\end{bmatrix}\end{bmatrix}}_{\begin{bmatrix}\psi^1\\ \vdots\\ \psi^k\\ \vdots\\ \psi^K\end{bmatrix}}$$

Scattering Matrix Structure in Group Major Ordering

$$
\Sigma_s \phi =
\begin{bmatrix}
\begin{bmatrix} 0 & & & \\ & 0 & & \\ & & 0 & \\ & & & 0 \end{bmatrix} & & & & & \\
\begin{bmatrix} \Sigma_{12}^{1} & & \\ & \Sigma_{12}^{k} & \\ & & \Sigma_{12}^{K} \end{bmatrix} & \begin{bmatrix} 0 & & & \\ & 0 & & \\ & & 0 & \\ & & & 0 \end{bmatrix} & & & & \\
\begin{bmatrix} \Sigma_{13}^{1} & & \\ & \Sigma_{13}^{k} & \\ & & \Sigma_{13}^{K} \end{bmatrix} & \begin{bmatrix} \Sigma_{23}^{1} & & \\ & \Sigma_{23}^{k} & \\ & & \Sigma_{23}^{K} \end{bmatrix} & \begin{bmatrix} 0 & & \\ & 0 & \\ & & 0 \end{bmatrix} & \begin{bmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \end{bmatrix} & & \\
& \begin{bmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \end{bmatrix} & \begin{bmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \end{bmatrix} & \begin{bmatrix} 0 & & \\ & 0 & \\ & & 0 \end{bmatrix} & \begin{bmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \end{bmatrix} & \\
& \begin{bmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \end{bmatrix} & \begin{bmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \end{bmatrix} & \begin{bmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \end{bmatrix} & \begin{bmatrix} 0 & & \\ & 0 & \\ & & 0 \end{bmatrix} & \\
& & & \begin{bmatrix} \Sigma_{gG}^{1} & & \\ & \Sigma_{gG}^{k} & \\ & & \Sigma_{gG}^{K} \end{bmatrix} & \begin{bmatrix} \Sigma_{G-1G}^{1} & & \\ & \Sigma_{G-1G}^{k} & \\ & & \Sigma_{G-1G}^{K} \end{bmatrix} & \begin{bmatrix} 0 & & \\ & 0 & \\ & & 0 \end{bmatrix}
\end{bmatrix}
\begin{bmatrix}
\begin{bmatrix} \phi_1^1 \\ \cdots \\ \phi_1^k \\ \cdots \\ \phi_1^K \end{bmatrix} \\
\cdots \\
\begin{bmatrix} \phi_g^1 \\ \cdots \\ \phi_g^k \\ \cdots \\ \phi_g^K \end{bmatrix} \\
\cdots \\
\begin{bmatrix} \phi_G^1 \\ \cdots \\ \phi_G^k \\ \cdots \\ \phi_G^K \end{bmatrix}
\end{bmatrix}
$$

Matrix Structure According to Ordering Scheme

	Node Major	Group Major
Interior	Scattering Shape	Tri diagonal matrix
Exterior	Tri diagonal matrix	Scattering Shape
Problem to Fit	A Few Group Problem (2G)	Many Group Problem

Ex.) 2-Group Problem with Node Major Ordering Scheme

$$
\begin{bmatrix}
\begin{bmatrix} \bullet & \bullet \\ \bullet & \bullet \end{bmatrix} & \begin{bmatrix} \bullet & \\ & \bullet \end{bmatrix} & & \\
\begin{bmatrix} \bullet & \\ & \bullet \end{bmatrix} & \begin{bmatrix} \bullet & \bullet \\ \bullet & \bullet \end{bmatrix} & \ddots & \\
& \ddots & \ddots & \begin{bmatrix} \bullet & \\ & \bullet \end{bmatrix} \\
& & \begin{bmatrix} \bullet & \\ & \bullet \end{bmatrix} & \begin{bmatrix} \bullet & \bullet \\ \bullet & \bullet \end{bmatrix}
\end{bmatrix}
\begin{bmatrix}
\begin{bmatrix} \phi_1^1 \\ \phi_2^1 \end{bmatrix} \\ \vdots \\ \begin{bmatrix} \phi_1^k \\ \phi_2^k \end{bmatrix}
\end{bmatrix}
=
\begin{bmatrix}
D_1 & U_1 & & \\
L_2 & D_2 & \ddots & \\
& \ddots & \ddots & \ddots \\
& & \ddots & D_K
\end{bmatrix}
\begin{bmatrix}
\begin{bmatrix} \phi_1^1 \\ \phi_2^1 \end{bmatrix} \\ \vdots \\ \begin{bmatrix} \phi_1^k \\ \phi_2^k \end{bmatrix}
\end{bmatrix}
$$

Eigenvalue Update with Fission Source

$$M\phi = \frac{1}{k}F\phi$$

$$\underbrace{M^{-1}F}_{A}\phi = k\phi$$

Power Method with Scaling: $\phi^{(l)} = M^{-1}F\dfrac{\phi^{(l-1)}}{k^{(l-1)}}$

Inverse Power Method: $M\phi^{(l)} = F\dfrac{\phi^{(l-1)}}{k^{(l-1)}} = \dfrac{1}{k^{(l-1)}}\chi\psi^{(l-1)}$, $\chi \in R^{N,K}$, $N = G \times K$

Let $\Gamma = [I_K \cdots I_K] \in R^{K,N}$ with I_K being identity matrix of Rank K ($N = K \times G$)

$$\rightarrow \Gamma\chi = I_K \quad \because \sum_{g=1}^{G}\chi_g^k \equiv 1 \text{ irrespective of } k$$

$$\Gamma M\phi^{(l)} = \frac{1}{k^{(l-1)}}\psi^{(l-1)}$$

For large l, $M\phi^{(l)} = \dfrac{1}{k}\chi\psi^{(l)} \rightarrow \Gamma M\phi^{(l)} = \dfrac{1}{k}\psi^{(l)}$

$$\rightarrow k = \frac{<\psi^{(l)},\psi^{(l)}>}{<\psi^{(l)},\Gamma M\phi^{(l)}>} = \frac{<\psi^{(l)},\psi^{(l)}>}{<\psi^{(l)},\frac{1}{k^{(l-1)}}\psi^{(l-1)}>} = k^{(l-1)}\frac{<\psi^{(l)},\psi^{(l)}>}{<\psi^{(l)},\psi^{(l-1)}>}$$

Source Iteration for Group Major Ordering

- Assume that fission source are known from the flux and eigenvalue of previous step (power iteration)

$$\boldsymbol{\psi} = \begin{bmatrix} \psi^1 \\ \vdots \\ \psi^k \\ \vdots \\ \psi^K \end{bmatrix} = \begin{bmatrix} \sum_{g'=1}^{G} \nu\Sigma^1_{fg'}\phi^1_{g'} \\ \vdots \\ \sum_{g'=1}^{G} \nu\Sigma^k_{fg'}\phi^k_{g'} \\ \vdots \\ \sum_{g'=1}^{G} \nu\Sigma^K_{fg'}\phi^K_{g'} \end{bmatrix}$$

$$\begin{bmatrix} M_1 & & & & \\ -S_{12} & M_2 & & -S_{g'g} & \\ -S_{1g} & -S_{2g} & M_g & \bullet & \\ & \ddots & \ddots & \ddots & \\ & \bullet & \bullet & -S_{G-1,G} & M_G \end{bmatrix} \begin{bmatrix} \boldsymbol{\phi}_1 \\ \vdots \\ \boldsymbol{\phi}_g \\ \vdots \\ \boldsymbol{\phi}_G \end{bmatrix} = \lambda \begin{bmatrix} \chi_1 \boldsymbol{\psi} \\ \vdots \\ \chi_g \boldsymbol{\psi} \\ \vdots \\ \chi_G \boldsymbol{\psi} \end{bmatrix}$$

Iteration Scheme

1. Determine $\phi_1^{(l)}$ (Solve for Group 1) : $M_1 \ \phi_1^{(l)} = S_1^{(l-1)} = \lambda^{(l-1)} \chi_1 \psi^{(l-1)}$ (No upscattering)

2. For g=2:G, solve for $\phi_g^{(l)}$: $M_g \ \phi_g^{(l)} = \lambda^{(l-1)} \chi_g \psi^{(l-1)} + \sum_{g'=1}^{g-1} \Sigma_{g'g} \phi_{g'}^{(l)} + \sum_{g'=g+1}^{G} \Sigma_{g'g} \phi_{g'}^{(l-1)}$ (Gauss-Seidel)

Iterative Multigroup Solution Algorithm

Loop for outer iteration step i

1) Determine fission source at each node and fission source adjustment parameter

    Loop over groups   Wielandt Shift

        2) Determine source at each node for the current group

        3) Solve for flux for the group

4) Determine new fission source

5) Estimate new k

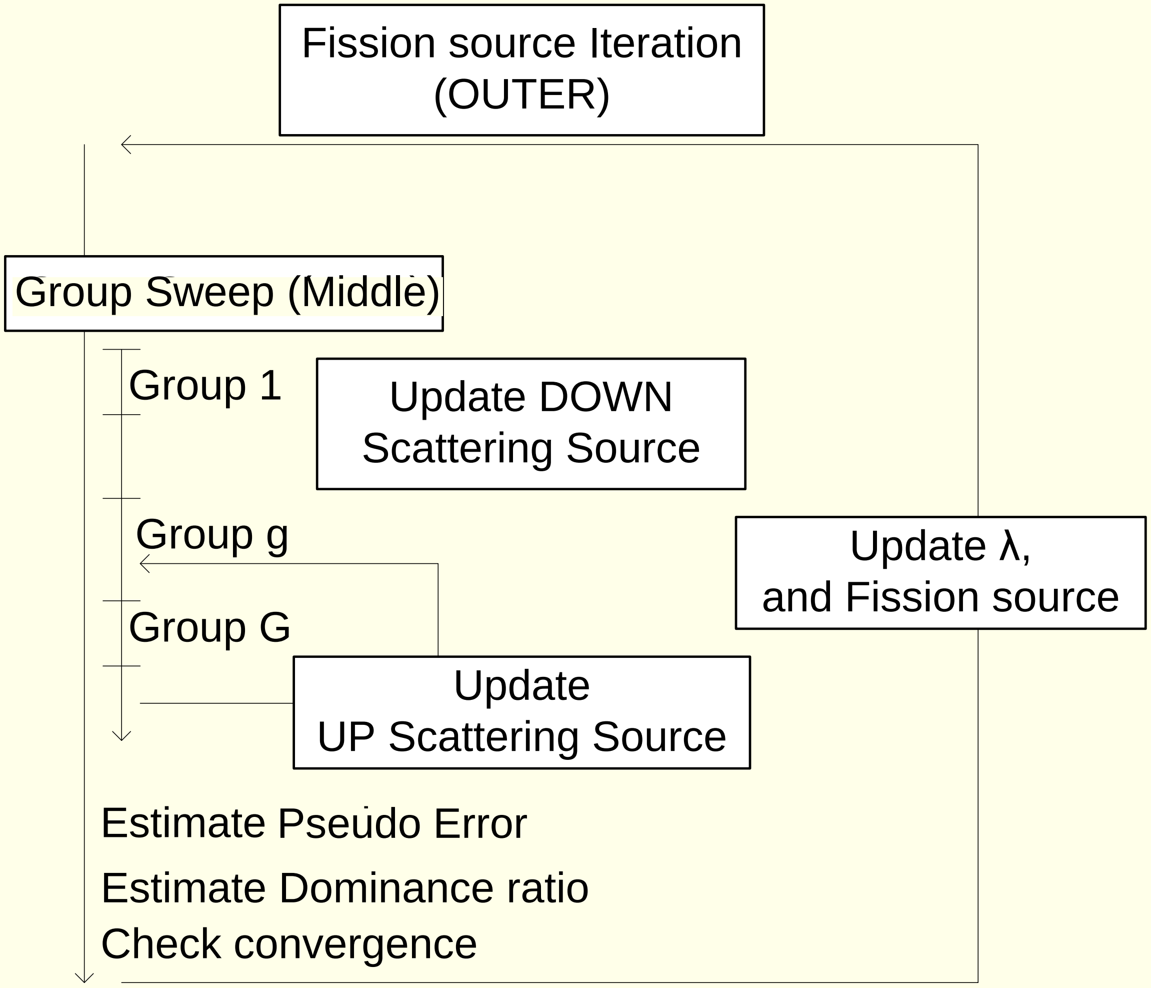
$$k^{(l)} = k^{(l-1)} \frac{<\psi^{(l)}, \psi^{(l)}>}{<\psi^{(l)}, \psi^{(l-1)}>}$$

6) Estimate pseudo error

7) Estimate Dominance Ratio

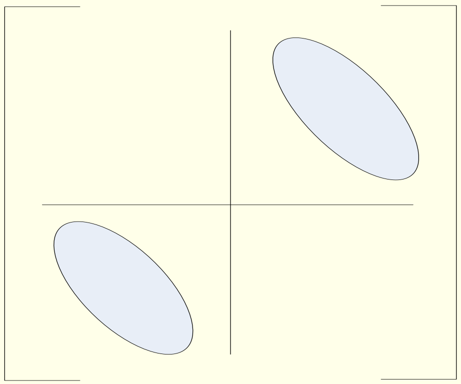
8) Check Convergence and Exit outer if convergence is met else go (1)

Nested Iteration Flow Chart (when upscattering present)



Problem with Wielandt Shift for MG

$$M - \frac{1}{k_s}F =$$



Fill in by moving fission source in case of Wielandt

$\rightarrow$ Additional group sweeps required

The solution is "Chebyshev Polynomial Acceleration Method".