Lecture Note 5

S_N Method

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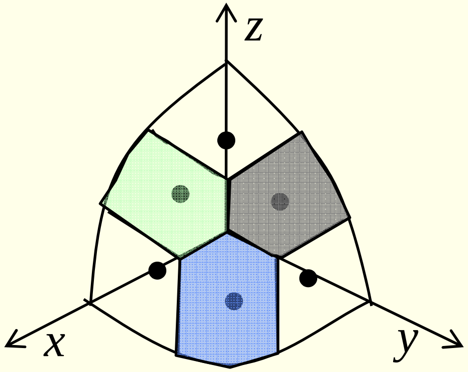
S_N Method

- Drawbacks of P_L Method
  - Complicated
  - Each P_L has its own set of equations

    $\rightarrow$ hard to extend to higher order by a general subroutine



- Outlines of the S_N method

  1)Discretize the solid angle into M segments (S for segment)

$$\hat{\Omega}(\theta,\alpha)\rightarrow\hat{\Omega}_m,\ M=f(N)$$

  2) Represent the angular flux within a segment with a representative value

$$\varphi(\hat{\Omega}_m+\delta\hat{\Omega})=\varphi_m$$

  3) Assume proper weight to each segment such that $\sum_{m=1}^{M}\omega_m=2$

  and represent the angular integral as the following summation:

$$\phi=\int_{4\pi}\varphi(\hat{\Omega})d\hat{\Omega}=C\sum_{m=1}^{M}\omega_m\varphi_m=\sum_{m=1}^{M}\omega_m 2\pi\varphi_m=\sum_{m=1}^{M}\omega_m\tilde{\varphi}_m$$

with $\tilde{\varphi}_m=2\pi\varphi_m$: new variable

Should be valid for isotropic flux $\varphi_m=\dfrac{\phi}{4\pi}\rightarrow C=2\pi$

Discretized Boltzmann Transport Equation

•Discretized Boltzmann Transport Equation (2π timed)

- Construct a balance equation for each φ_m with proper source and B.C.

$$\hat{\Omega}_m \cdot \nabla \tilde{\varphi}_m + \Sigma \tilde{\varphi}_m = \frac{1}{2} \lambda \chi \psi + S_m$$

- Solve for $\tilde{\varphi}_m$ $\forall$m, then determine $\phi = \sum_m \omega_m \tilde{\varphi}_m$ to update the fission source and scattering source

$$S_m = \sum_{l=1}^{M} \int_{E'} \Sigma_s (r, E' \to E, \hat{\Omega}_l \to \hat{\Omega}_m) \tilde{\varphi}_l (r, E') dE' \text{ from all angles}$$

•Simplification of Scattering source

$$S_m = \int_0^\infty \int_{4\pi} \Sigma(\vec{r}, E' \to E, \hat{\Omega}' \cdot \hat{\Omega}_m) \tilde{\varphi}(\vec{r}, E', \hat{\Omega}') d\hat{\Omega}' dE'$$

$$\boxed{\Sigma(\vec{r}, E' \to E, \mu_{s,m}) = \frac{1}{4\pi} \left(\Sigma_0(\vec{r}, E' \to E) + 3\mu_{s,m} \Sigma_1(\vec{r}, E' \to E) \right)}$$

$$= \int_0^\infty \int_{4\pi} \frac{1}{4\pi} \left(\Sigma_0(\vec{r}, E' \to E) + 3\mu_{s,m} \Sigma_1(\vec{r}, E' \to E) \right) 2\pi \varphi(\vec{r}, E', \hat{\Omega}') d\hat{\Omega}' dE'$$

$$= \frac{1}{2} \left[\int_0^\infty \Sigma_0(\vec{r}, E' \to E) \phi(\vec{r}, E') dE' + 3\hat{\Omega}_m \int_0^\infty \Sigma_1(\vec{r}, E' \to E) \vec{J}(\vec{r}, E') dE' \right] \leftarrow Addition\,Theorem$$

Discretized Boltzmann Transport Equation

•Multigroup Form $\boxed{\text{(Represent } \tilde{\varphi}_m (\equiv 2\pi\varphi_m) \text{ simple with } \varphi_m \text{ from now on.} \rightarrow \phi = \sum_{m=1}^{M} w_m \varphi_m)}$

$$\hat{\Omega}_m \cdot \vec{\nabla}\varphi_m + \Sigma\varphi_m = \frac{1}{2}\lambda\chi\psi + \frac{1}{2}\int \Sigma_0(E' \rightarrow E)\phi(E')dE' + \frac{3}{2}\hat{\Omega}_m \int \Sigma_1(E' \rightarrow E)\vec{J}(E')dE'$$

- Apply $\int_{E_g}^{E_{g-1}} dE$ $\qquad \varphi_{mg} = \int_{E_g}^{E_{g-1}} \varphi_m(E)dE \qquad \chi_g = \int_{E_g}^{E_{g-1}} \chi(E)dE$

$$\int_{E_g}^{E_{g-1}} \Sigma(E)\varphi_m(E)dE = \Sigma_{mg}\varphi_{mg} \longrightarrow \Sigma_{mg} = \frac{1}{\varphi_{mg}}\int_{E_g}^{E_{g-1}} \Sigma(E)\varphi_m(E)dE$$

Angle dependent total X-sec

$$\Sigma_{1g'\rightarrow g}^{x} = \frac{\int_{E_g}^{E_{g-1}}\int_{E_g}^{E_{g-1}} \Sigma(E)\varphi_m(E)J_x(E')dE'dE}{J_{gx}} = \Sigma_{1g'\rightarrow g}^{y} = \Sigma_{1g'\rightarrow g}^{z}$$

Neglect direction dependency

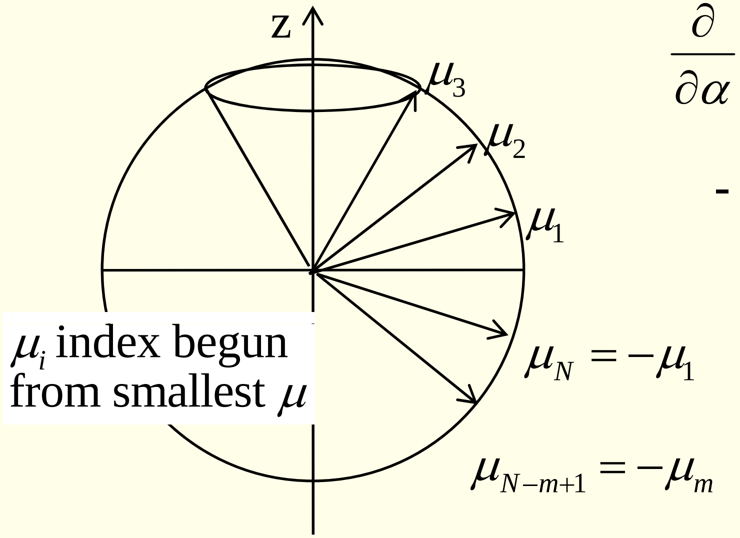
$$\Sigma_{tg} - \Sigma_{mg} = \Delta\Sigma_{mg} \Rightarrow \Sigma_{mg} = \Sigma_{tg} - \Delta\Sigma_{mg}$$

$$\hat{\Omega}_m \cdot \nabla\varphi_{mg} + \Sigma_{mg}\varphi_{mg} = s_m \quad \Rightarrow \quad \hat{\Omega}_m \cdot \nabla\varphi_{mg} + (\Sigma_{tg} - \Delta\Sigma_{mg})\varphi_{mg} = s_m$$

$$\underline{\hat{\Omega}_m \cdot \nabla\varphi_{mg} + \Sigma_{tg}\varphi_{mg}} = s_m + \Delta\Sigma_{mg}\varphi_{mg} = \tilde{s}_{mg}$$

Xsec with no angle dependency

Selection of Discretized Angle in 1-D



$$\frac{\partial}{\partial \alpha} = 0, \quad \frac{\partial}{\partial x} = \frac{\partial}{\partial y} = 0 \qquad S_N \to M = N \text{ in 1D}$$

- Suppose a polynomial expansion for true angular flux $\varphi(\mu)$

$$\phi = \int_{-1}^{1} \varphi(\mu) d\mu = \sum_{m=1}^{M} \omega_m \underbrace{\varphi(\mu_m)}_{\varphi_m}$$

$$\varphi(\mu) \cong \sum_{i=0}^{K} a_i \mu^i$$

- In order to have accurate integral upto the $2M$ -1 order: Gaussian Quadrature

$$\int_{-1}^{1} \varphi(\mu) d\mu = \int_{-1}^{1} \sum_{i=0}^{2M-1} a_i \mu^i d\mu = \sum_{i=0}^{2M-1} a_i \int_{-1}^{1} \mu^i d\mu \Leftarrow \int_{-1}^{1} \mu^i d\mu = \sum_{m=1}^{M} \omega_m \mu_m{}^i, \quad i = 0, 1, \cdots 2N-1$$

$$= \sum_{i=0}^{2M-1} a_i \sum_{m=1}^{M} \omega_m \mu_m^i = \sum_{m=1}^{M} \omega_m \sum_{i=0}^{2M-1} a_i \mu_m^i = \sum_{m=1}^{M} \omega_m \varphi(\mu_m)$$

$$\int_{-1}^{1} \mu^i d\mu \Longrightarrow \quad i = 0: \quad 2 = \sum_{m=1}^{M} \omega_m \qquad i = 1: \quad 0 = \sum_{m=1}^{M} \omega_m \mu_m \to \mu_m = -\mu_{N-m+1} = \mu_{-m}, \omega_{-m} = \omega_m$$

$\to \mu_m$: Roots of $(2M-1)$th order Lengendre Polynomials

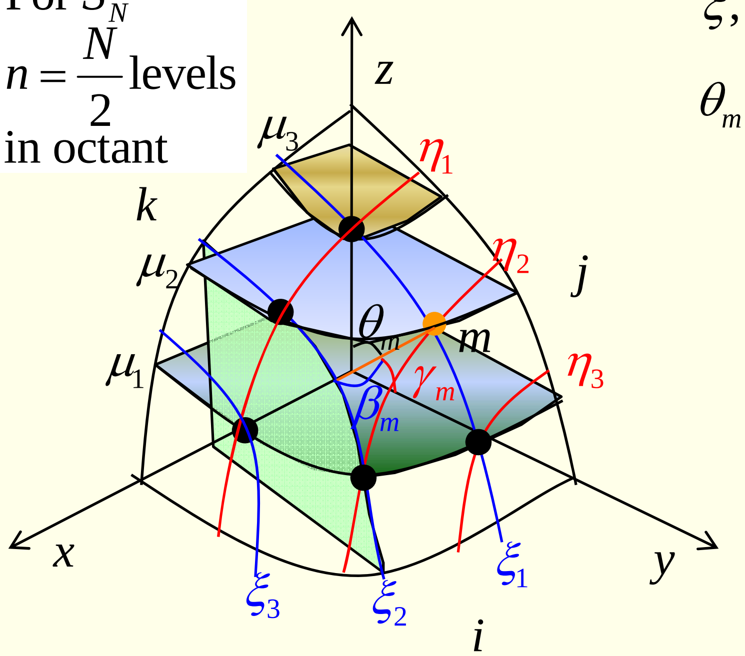
Determination of the angles and weights in 3D

- Consideration of Symmetry in Angle

For S_N

$n = \dfrac{N}{2}$ levels

in octant



$\xi,\ \eta,\ \mu \qquad \xi_i = \eta_i = \mu_i \quad \Rightarrow$ Only one set of μ_i's required

θ_m:Polar angle, a_m:Azimuthal angle

$$\begin{cases} \Omega_x^m = \sin\theta_m \cos\alpha_m = \cos\beta_m = \xi_i \\ \Omega_y^m = \sin\theta_m \sin\alpha_m = \cos\gamma_m = \eta_j \\ \Omega_z^m = \cos\theta_m = \mu_k \end{cases}$$

$m \rightarrow i(m),\ j(m), k(m) \qquad \rightarrow i + j + k = n + 2$

If $i \rightarrow i+1 \quad \Rightarrow j \rightarrow j-1$ *or* $k \rightarrow k-1$

$$\Omega_x^{m2} + \Omega_y^{m2} + \Omega_z^{m2} = \xi_{i(m)}^2 + \eta_{j(m)}^2 + \mu_{k(m)}^2 = 1$$

$$\xi_i^{\ 2} + \eta_j^{\ 2} + \mu_k^{\ 2} = 1 = \mu_i^{\ 2} + \mu_j^{\ 2} + \mu_k^{\ 2}$$

$$= \mu_{i+1}^{\ \ 2} + \mu_{j-1}^{\ \ 2} + \mu_k^{\ 2}$$

$\Rightarrow \quad \mu_{i+1}^2 - \mu_i^{\ 2} = \mu_i^{\ 2} - \mu_{j-1}^2 = \Delta$ for any i, j, k

$\Rightarrow \quad \mu_i^{\ 2} = \mu_1^{\ 2} + (i-1)\Delta$

Determination of the angles and weights in 3D

$$\mu_i^2 = \mu_1^2 + (i-1)\Delta$$

$$\mu_i^2 + \mu_j^2 + \mu_k^2 = 3\mu_1^2 + (\overbrace{i+j+k}^{n+2}-3)\Delta$$

$$= 3\mu_1^2 + (n-1)\Delta = 1$$

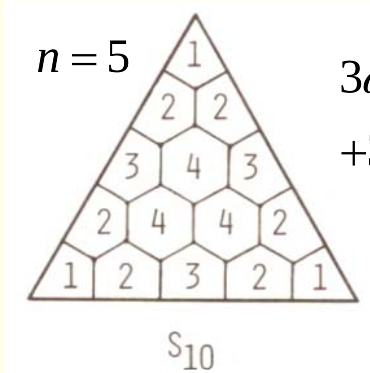
$$\Rightarrow \quad \Delta = \frac{1-3\mu_1^2}{n-1}$$

Only μ_1 need to be determined!

- For n levels, segments in octant

$$M_8 = 1+2+\cdots+n = \frac{n(n+1)}{2}$$

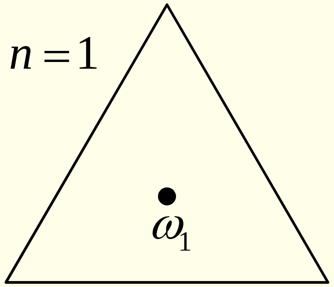
$$M = 8\cdot M_8 = 4n(n+1) = 4\cdot\frac{N}{2}\left(\frac{N}{2}+1\right) = N(N+2)$$



$3\omega_1 + 6\omega_2 + 3\omega_3 + 3\omega_4 = 1$

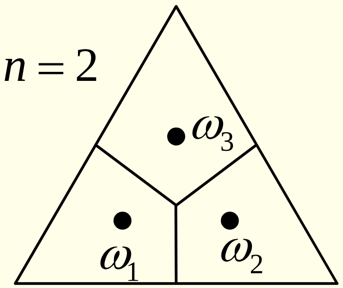
- Symmetry in ω_i

$n=1$



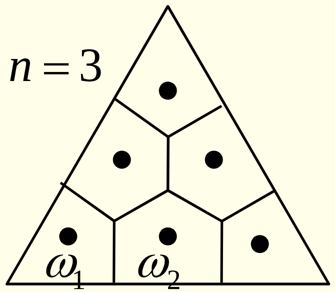
ω_1

$n=2$

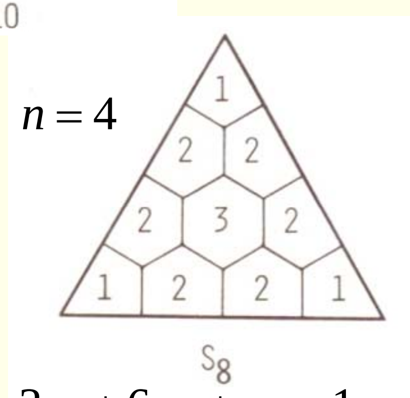


$\omega_1 = \omega_2 = \omega_3$

$n=3$



$3(\omega_1 + \omega_2) = 1$



$3\omega_1 + 6\omega_2 + \omega_3 = 1$

Determination of μ by Level Symmetry

- How to determine μ_i and ω_i (l=1, $\cdots$, L), L=f(n)
  - Impose even moment conservation

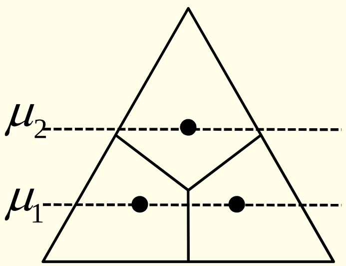
$$\Delta = \frac{1-3\mu_1^2}{n-1}$$

(old moment conservation already holds by choosing $\mu_{-m} = -\mu_m$)

$$\frac{1}{2k+1} = \int_0^1 \mu^{2k} d\mu = \sum_{i=1}^{M_8} \omega_i \mu_i^{2k}$$

$-\ n = 1\ (S_2)$ $\qquad \omega_1 = 1,\ \frac{1}{3} = \mu_1^2 \rightarrow \mu_1 = \frac{1}{\sqrt{3}}$

$-n = 2\ (S_4)$ $\qquad \sum_{m=1}^{3} \omega_m = 3\omega_1 = 1 \rightarrow \omega_1 = \frac{1}{3}$



2nd moment

$$\mu_2^2 = \mu_1^2 + \Delta = \mu_1^2 + (1-3\mu_1^2) = 1-2\mu_1^2$$

$$\frac{1}{3} = \sum_{m=1}^{M_8} \omega_m \mu_m^2 = \frac{2}{3}\mu_1^2 + \frac{1}{3}\mu_2^2 = \frac{2}{3}\mu_1^2 + \frac{1}{3}(1-2\mu_1^2) = \frac{1}{3}$$

Valid!

4th moment

$$\frac{1}{5} = \sum_{m=1}^{M_8} \omega_m \mu_m^4 = \frac{2}{3}\mu_1^4 + \frac{1}{3}\mu_2^4 = \frac{2}{3}\mu_1^4 + \frac{1}{3}(1-2\mu_1^2)^2$$

choose the lowest

$$\mu_1 = \begin{cases} 0.350021 \\ 0.737666 \end{cases}$$

$$\mu_2 = 0.868890$$

Determination of μ by Level Symmetry

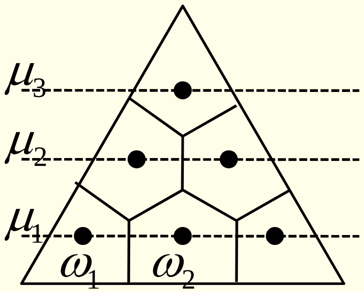
- $n = 3\ (S_6)$

$$3(\omega_1+\omega_2)=1 \rightarrow \omega_1+\omega_2=\frac{1}{3} \quad \cdots ①$$

$$\Delta = \frac{1-3\mu_1^{\ 2}}{n-1}$$

2nd moment $\mu_2^{\ 2} = \mu_1^{\ 2} + \Delta = \mu_1^{\ 2} + \frac{1}{2}(1-3\mu_1^{\ 2})$

$$\mu_3^{\ 2} = \mu_1^{\ 2} + 2\Delta = 1-2\mu_1^{\ 2}$$



$$(2\omega_1+\omega_2)\mu_1^{\ 2} + 2\omega_2\mu_2^{\ 2} + \omega_1\mu_3^{\ 2}$$

$$= (2\omega_1+\omega_2+2\omega_2+\omega_1)\mu_1^{\ 2} + 2(\omega_1+\omega_2)\Delta \quad = \mu_1^{\ 2} + \frac{2}{3}\frac{1-3\mu_1^{\ 2}}{2} = \frac{1}{3} : hold$$

4th moment

$$\frac{1}{5} = (2\omega_1+\omega_2)\mu_1^{\ 4} + 2\omega_2\left(\frac{1}{2}-\frac{1}{2}\mu_1^{\ 2}\right)^2 + \omega_1(1-2\mu_1^{\ 2})^2 \quad \cdots ②$$

6th moment

$$\frac{1}{7} = (2\omega_1+\omega_2)\mu_1^{\ 6} + 2\omega_2\left(\frac{1}{2}-\frac{1}{2}\mu_1^{\ 2}\right)^3 + \omega_1(1-2\mu_1^{\ 2})^3 \quad \cdots ③$$

$$①, ②, ③ \Rightarrow \begin{cases} \omega_1 = 0.176126 \\ \omega_2 = 0.157207 \\ \mu_1 = 0.266636 \end{cases}$$

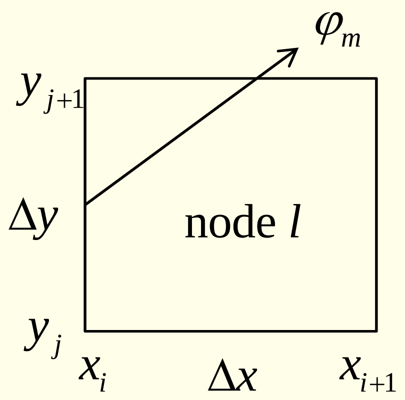
Finite Difference Scheme

- In 2D

$$\varphi_m(x,y) : \text{dependent on } x, y$$

$$\varphi_m = 2\pi\varphi(x,y,\hat{\Omega})$$

$$\underbrace{\boxed{\Omega_x^m}}_{\xi_m}\frac{\partial\varphi_m}{\partial x} + \underbrace{\boxed{\Omega_y^m}}_{\eta_m}\frac{\partial\varphi_m}{\partial y} + \Sigma_t\varphi_m = s_m$$



Appply $\int_{y_j}^{y_{j+1}}\int_{x_i}^{x_{i+1}} \cdot dxdy \Rightarrow \xi_m\int_{y_j}^{y_{j+1}}\left(\varphi_m(x_{i+1},y)-\varphi_m(x_i,y)\right)dy + \eta_m\int_{x_i}^{x_{i+1}}\left(\varphi_m(x,y_{j+1})-\varphi_m(x,y_j)\right)dy$

$$+\Sigma_t\int_{y_j}^{y_{j+1}}\int_{x_i}^{x_{i+1}}\varphi_m(x,y)dxdy = \int_{y_j}^{y_{j+1}}\int_{x_i}^{x_{i+1}} s_m dxdy$$

$$\varphi_m = \frac{1}{\Delta x\Delta y}\int_{y_j}^{y_{j+1}}\int_{x_i}^{x_{i+1}}\varphi_m(x,y)dxdy$$

$$\varphi_{m,i+1} = \frac{1}{\Delta y}\int_{y_j}^{y_{j+1}}\varphi_m(x_{i+1},y)dy$$

$$\varphi_{m,j} = \frac{1}{\Delta x}\int_{x_i}^{x_{i+1}}\varphi_m(x,y_j)dx$$

$\Rightarrow$

$$\xi_m\Delta y(\varphi_{m,i+1}-\varphi_{m,i}) + \eta_m\Delta x(\varphi_{m,j+1}-\varphi_{m,j}) + \Sigma_t\varphi_m\Delta x\Delta y = s_m\Delta x\Delta y$$

$$\xi_m\frac{\varphi_{m,i+1}-\varphi_{m,i}}{\Delta x} + \eta_m\frac{\varphi_{m,j+1}-\varphi_{m,j}}{\Delta y} + \Sigma_t\varphi_m = s_m\varphi_m$$

Finite Difference Scheme

- Incoming flux condition given

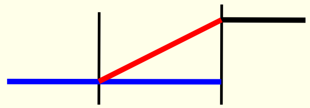
  $\varphi_{m,i}$ and $\varphi_{m,j}$ given for $\xi_m > 0$ and $\eta_m > 0$

- Unknowns

  $\varphi_{m,i+1}, \varphi_{m,j+1}, \varphi_m$

- Weighted Difference

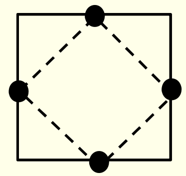
$$\varphi_m = \omega\varphi_{m,i} + (1-\omega)\varphi_{m,i+1} = \omega\varphi_{m,j} + \underbrace{\boxed{(1-\omega)}}_{\bar{\omega}}\varphi_{m,j+1}$$



$\omega = 1$: Step differencing

$\omega = \frac{1}{2}$: Diamond differencing (Linear Approximation of Angular Flux)

$$\varphi_m = \frac{1}{4}\left[\varphi_{m,i} + \varphi_{m,j} + \varphi_{m,i+1} + \varphi_{m,j+1}\right]$$



$$\varphi_{m,i+1} = \frac{1}{\bar{\omega}}(\varphi_m - \omega\varphi_{m,i})$$

$$\varphi_{m,i+1} - \varphi_{m,i} = \frac{1}{\bar{\omega}}\varphi_m - \left(\frac{\omega}{\bar{\omega}} + 1\right)\varphi_{m,i} = \frac{1}{\bar{\omega}}\varphi_m - \frac{1}{\bar{\omega}}\varphi_{m,i} = \frac{\varphi_m - \varphi_{m,i}}{\bar{\omega}}$$

$$\Rightarrow \quad \xi_m \Delta y(\varphi_m - \varphi_{m,i}) + \eta_m \Delta x(\varphi_m - \varphi_{m,j}) + \Sigma_t \Delta x \Delta y \bar{\omega}\varphi_m = s_m \Delta x \Delta y \bar{\omega}$$

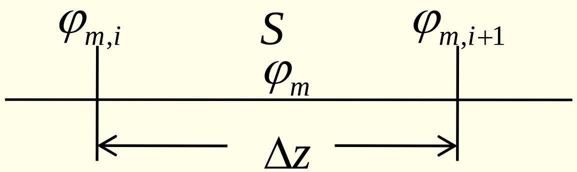
$$\varphi_m = \frac{s_m V\bar{\omega} + \xi_m \Delta y \varphi_{m,i} + \eta_m \Delta x \varphi_{m,j}}{\xi_m \Delta y + \eta_m \Delta x + \bar{\omega} V \Sigma_t}$$

ω=1: $\varphi_m = \dfrac{\xi_m \Delta y \varphi_{m,i} + \eta_m \Delta x \varphi_{m,j}}{\xi_m \Delta y + \eta_m \Delta x}$, weighted average ?

In fact, $\varphi_{m,i+1}$ & $\varphi_{m,j+1}$ first from 1-D, then φ_m from 2-D balance.

Analysis of Difference Scheme

- 1D, Flat Source



$$\mu_m \frac{d\varphi_m}{dz} + \Sigma_t \varphi_m = s_m$$

$$\frac{d\varphi_m}{dz} + \frac{\Sigma_t}{\mu_m}\varphi_m = \frac{s_m}{\mu_m} \quad \rightarrow \frac{d}{dz}\left(e^{\frac{\Sigma_t}{\mu_m}z} \varphi_m(z) \right) = \frac{s_m}{\mu_m} e^{\frac{\Sigma_t}{\mu_m}z} \quad \rightarrow e^{\frac{\Sigma_t}{\mu_m}z}\varphi_m(z) - \varphi_m(0) = \frac{s_m}{\mu_m}\frac{\mu_m}{\Sigma_t}(e^{\frac{\Sigma_t}{\mu_m}} - 1)$$

$$\Rightarrow \varphi_m(z) = \varphi_{m,i} e^{-\frac{\Sigma_t}{\mu_m}z} + \frac{s_m}{\Sigma_t}(1 - e^{-\frac{\Sigma_t}{\mu_m}z}) \qquad \varphi_{m,i+1} = \varphi_{m,i}e^{-\tau} + \frac{s_m}{\Sigma_t}(1 - e^{-\tau}) \cdots (1) \quad where\ \tau = \Sigma_t \frac{\Delta z}{\mu_m}$$

- Balance equation to find the average flux

$$\mu_m(\varphi_{m,i+1} - \varphi_{m,i}) + \Delta z \cdot \Sigma_t \varphi_m = s_m \cdot \Delta z$$

$$\frac{s_m}{\Sigma_t} = \frac{\mu_m}{\Delta z \Sigma_t}(\varphi_{m,i+1} - \varphi_{m,i}) + \varphi_m = \frac{1}{\tau}(\varphi_{m,i+1} - \varphi_{m,i}) + \varphi_m \cdots (2)$$

(2) in (1): $\varphi_{m,i+1} = \varphi_{m,i}e^{-\tau} + \left(\frac{1}{\tau}(\varphi_{m,i+1} - \varphi_{m,i}) + \varphi_m \right)(1 - e^{-\tau})$

$$\varphi_m = \underbrace{\boxed{(\frac{1}{\tau} - \frac{e^{-\tau}}{1 - e^{-\tau}})}}_{\omega}\varphi_{m,i} + (\frac{1}{1 - e^{-\tau}} - \frac{1}{\tau})\varphi_{m,i+1}$$

$$1 - \omega = 1 - \frac{1}{\tau} + \frac{e^{-\tau}}{1 - e^{-\tau}} = \frac{1}{1 - e^{-\tau}} - \frac{1}{\tau}$$

for large τ $\qquad \omega = 0$

small τ $\qquad \omega = \frac{1}{2}$?

Analysis of Difference Scheme

$$\omega = \frac{1-e^{-\tau}-\tau e^{-\tau}}{\tau(1-e^{-\tau})} = \frac{1-(1-\tau+\frac{\tau^2}{2}-\frac{\tau^3}{6}+\cdots)-\tau+\tau^2-\frac{\tau^3}{2}+\frac{\tau^4}{6}+\cdots}{\tau(1-(1-\tau+\frac{\tau^2}{2}-\frac{\tau^3}{6}+\cdots))}$$

$$\boxed{\omega = \frac{1}{\tau} - \frac{e^{-\tau}}{1-e^{-\tau}}}$$

$$\cong \frac{\frac{\tau^2}{2}-\frac{\tau^3}{3}}{\tau(\tau-\frac{\tau^2}{2})} = \frac{\frac{1}{2}-\frac{1}{3}\tau}{1-\frac{1}{2}\tau}$$

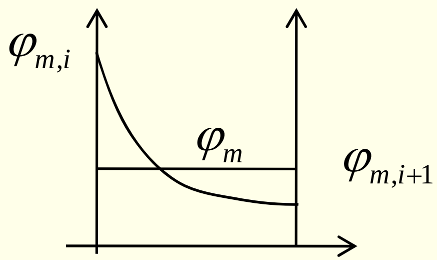
$$\cong (\frac{1}{2}-\frac{1}{3}\tau)(1+\frac{1}{2}\tau) = \frac{1}{2}+\frac{1}{4}\tau-\frac{1}{3}\tau-\cancel{\frac{\tau^2}{12}} = \frac{1}{2}-\frac{1}{12}\tau$$

$\therefore 0 \le \omega \le \frac{1}{2} - \frac{\tau}{12} \rightarrow$ more weighting on $\varphi_{m,i+1}$!

$\rightarrow$ step differencing ($\omega = 1$) not reasonable!

- For Left Direction

$$\varphi_m = \omega \cdot \varphi_{m,i+1} + (1-\omega)\varphi_{m,i}$$



Average shifted toward $\varphi_{m,i+1}$

Error Estimation

$$\varphi(z) = \varphi(0) + \varphi'(0)z + \frac{1}{2}\varphi''(0)z^2 + \frac{1}{6}\varphi^{(3)}(0)z^3 + \frac{1}{24}\varphi^{(4)}(0)z^4 + \cdots$$

$$\bar{\varphi} = \frac{1}{h}\int_{-\frac{2}{h}}^{\frac{2}{h}} \varphi(z)dz \; = \varphi(0) + \frac{1}{h}\frac{1}{2}\varphi''(0)\cdot 2\cdot\frac{h^3}{3\cdot 8} + \frac{1}{h}\frac{1}{24}\varphi^{(4)}(0)2\cdot\frac{h^5}{5\cdot 32} + \cdots$$

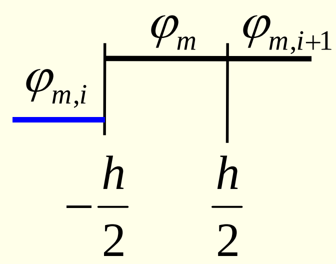
$$= \varphi(0) + \varphi''(0)\frac{h^2}{24} + \varphi^{(4)}(0)\frac{h^4}{60\cdot 32} + \cdots \; = \varphi^*$$

$\varphi_{m,i+1}, \varphi_{m,j+1}$ first from 1D,
then φ_m from 2D

- Backward (Implicit) Step Difference (ω=0)

$$\bar{\varphi}_{SD} = \varphi(\frac{h}{2}) = \varphi(0) + \varphi'(0)\frac{h}{2} + \frac{1}{2}\varphi''(0)\frac{h^2}{4} + \cdots$$

$$\bar{\varphi}_{SD} - \varphi^* = \varphi'(0)\frac{h}{2} + \cdots \qquad \Rightarrow \qquad O(h)$$



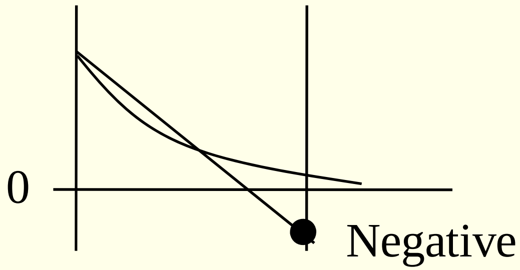
- Diamond Difference (ω=$\frac{1}{2}$)

$$\bar{\varphi}_{DD} = \frac{1}{2}(\varphi(\frac{h}{2}) + \varphi(-\frac{h}{2})) = \varphi(0) + \frac{1}{2}\varphi''(0)(\frac{h}{2})^2 + \frac{1}{24}\varphi^{(4)}(0)(\frac{h}{2})^2 + \cdots$$

$$\bar{\varphi}_{DD} - \varphi^* = \varphi''(0)(\frac{1}{8} - \frac{1}{24})h^2 + \cdots \qquad \Rightarrow \qquad O(h^2)$$

Negative Flux

- A weak point of Diamond Difference $\rightarrow$ Negative Flux



- Negative Flux

$$\varphi_m = \omega\varphi_{m,i} + (1-\omega)\varphi_{m,i+1} = \omega\varphi_{m,i} + \bar{\omega}\varphi_{m,i+1}$$

$$\mu_m(\varphi_{m,i+1} - \varphi_{m,i}) + \Sigma_t \Delta z \varphi_m = s_m \Delta z$$

$$(\mu_m + \bar{\omega}\Sigma_t\Delta z)\varphi_{m,i+1} + (-\mu_m + \omega\Sigma_t\Delta z)\varphi_{m,i} = s_m\Delta z \quad \Rightarrow \quad \varphi_{m,i+1} = \frac{(\mu_m - \omega\Sigma_t\Delta z)\varphi_{m,i} + s_m\Delta z}{\mu_m + \bar{\omega}\Sigma_t\Delta z}$$

- For Positivity

$$(\mu_m - \omega\Sigma_t\Delta z)\varphi_{m,i} + s_m\Delta z > 0$$

$$\Rightarrow \quad \mu_m - \omega\Sigma_t\Delta z > 0$$

$$\Sigma_t\Delta z < \frac{\mu_m}{\omega}$$

For step diff. ω=0. *RHS* $\rightarrow \infty \Rightarrow$ Always satisfy

For $\omega = \frac{1}{2}$, if $\Sigma_t\Delta z > 2\mu_m$ $\varphi_{m,i+1}$ can be negative

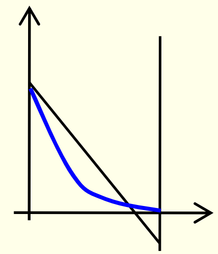
$\Rightarrow$ for various angles $\rightarrow$ more fine meshes

Negative Flux Fix-up & Ray Effect

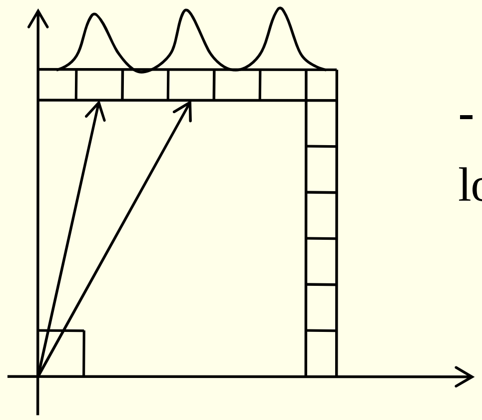
- Negative Flux Fix-up

If $\varphi_{m,i+1} < 0$, set $\varphi_{m,i+1}$ to zero.

$$\mu_m(\varphi_{m,i+1} - \varphi_{m,i}) + \Sigma_t \Delta z(\varphi_m) = \mu_m(0 - \varphi_{m,i}) + \Sigma_t \Delta z\underbrace{\left(\frac{\mu_m}{\Sigma_t \Delta z}\overset{\text{Negative}}{\varphi_{m,i+1}} + \varphi_m\right)}_{=\varphi'_m \;\to\; \varphi'_m < \varphi_m} = s_m \Delta z$$



- Ray Effect

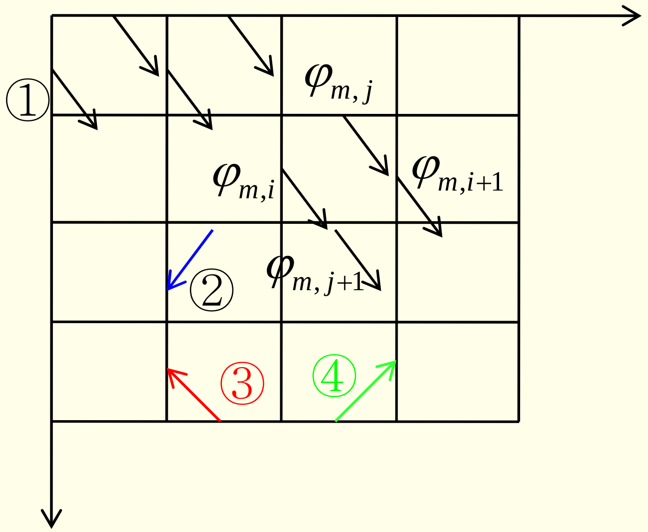


- Shielding problems due to limited number of discrete ordinate low scattering, low density, localized source.

Sweeping Strategy

- Sweeping for inner iteration

$$\xi_m(\varphi^g_{m,i+1}-\varphi^g_{m,i})\Delta y+\eta_m(\varphi^g_{m,j+1}-\varphi^g_{m,j})\Delta x+\Sigma_t\Delta x\Delta y\varphi^g_m=\frac{1}{2}\underbrace{\left(\overbrace{\chi_g\psi\Delta V+\underbrace{\boxed{\sum_{g'\neq g}\Sigma_{g'g}\phi_g}}_{\text{In-scattering}}}^{\tilde{Q}^g_m}+\underbrace{\Sigma_{gg}\phi_g}_{\text{Self-scattering}}\right)}_{Q^g_m}$$



$$\varphi_m=\frac{Q_m V\bar{\omega}+\xi_m\Delta y\varphi_{m,i}+\eta_m\Delta x\varphi_{m,j}}{\xi_m\Delta y+\eta_m\Delta x+\bar{\omega}V\Sigma_t}$$

$$\varphi_{m,i+1}=\frac{1}{\bar{\omega}}(\varphi_m-\omega\varphi_{m,i})$$

- Inner iteration
  - Find φ^g_m and ϕ^g_m for given fission and in-scattering source
  - Multiple spatial sweeps are necessary depending of angular directions
  - Need to update self-scattering

Inner Iteration Strategy

For iin=1 : Nin

For q=1 : 4

For j=jb(q) : je(q)

For i=ib(q) : ie(q)

$l = l(\text{i,j})$

For m=1 :M_8

$$\varphi_m^{g,l} = f(Q_m^g, \varphi_{m,x}^{g,l,in}, \varphi_{m,y}^{g,l,in})$$

$$\varphi_{m,x}^{g,l,out} = f(\omega, \varphi_{m,x}^{g,l,in}, \varphi_m^{g,l})$$

$$\text{or } \varphi_{m,y}^{g,l,out} = f(\omega, \varphi_{m,y}^{g,l,in}, \varphi_m^{g,l})$$

$$\phi_g^l = \phi_g^l + \omega_m^{g,l} \varphi_m^{g,l}$$

end ! of m

end ! of i

end ! of j

end ! of g

$$Q_l^g = \tilde{Q}_l^g + \Sigma_{gg} \phi_g$$

end ! of iin

q	j		i	
	begin	end	begin	end
1	1	Ny	1	Nx
2	1	Ny	Nx	1
3	Ny	1	Nx	1
4	Ny	1	1	Nx

Acceleration of S_N iteration

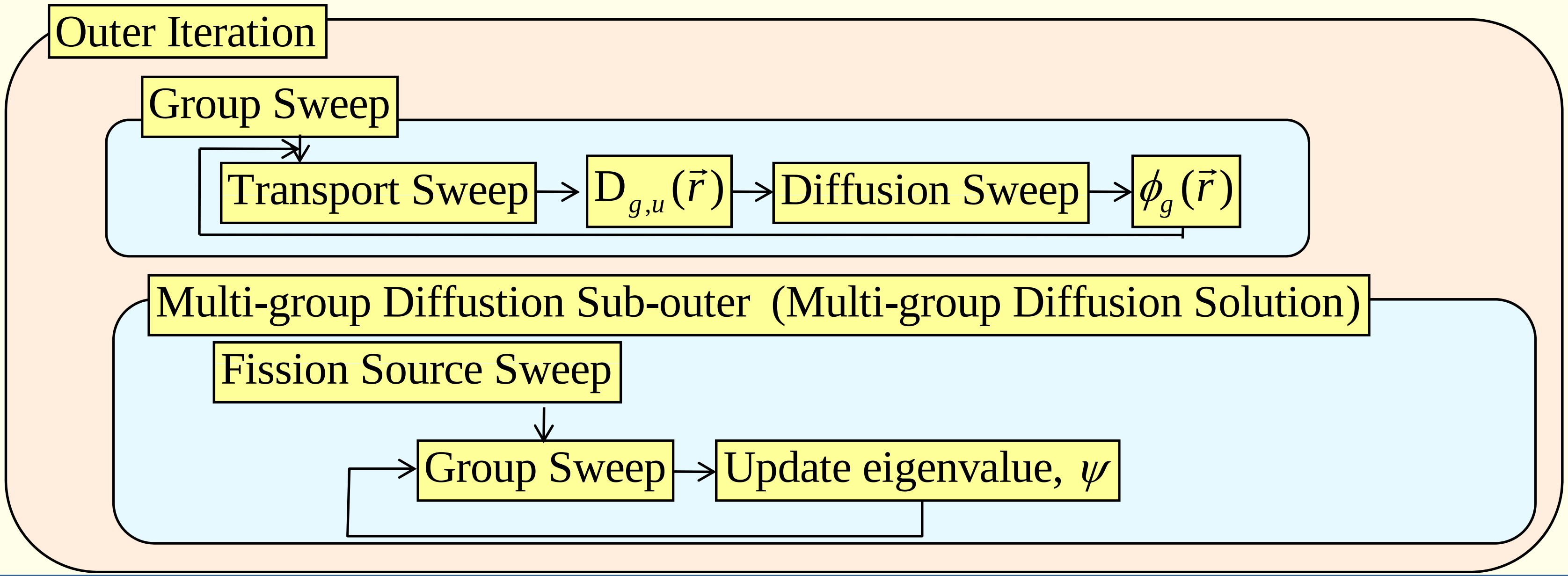
- Diffusion Synthetic Method

  - Construct diffusion equation equivalent to the transport equation.

$$-\vec{\nabla} \cdot D_g \nabla \phi_g + \Sigma_{rg} \phi_g = \lambda \chi_g \psi + \sum_{g' \neq g} \phi_{g'}$$

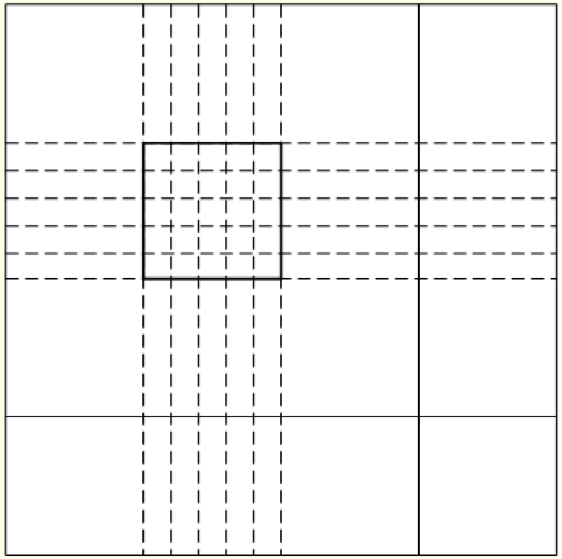
$$-D_g \nabla \phi_g = J_g^{S_N} \qquad D_g = -\frac{J_g^{S_N}}{\nabla \phi_g} \Rightarrow D_{g,u} = \frac{J_g^{S_N}}{-\nabla_u \phi_g}$$: Direction Diffusion Coefficient

- Iteration strategy for D.S. Method



Coarse Mesh Finite Difference

- CMFD Acceleration



$$J_C^{S_N} = -\tilde{D}(\bar{\phi}_r - \bar{\phi}_l) + \hat{D}(\bar{\phi}_r + \bar{\phi}_l)$$

$$\hat{D} = \frac{-J_C^{S_N} - \tilde{D}(\bar{\phi}_r - \bar{\phi}_l)}{\bar{\phi}_r + \bar{\phi}_l}$$

$$J_C^{S_N} = \frac{\sum_{s=1}^{N_s} J_{f,s}^{S_N} \Delta h_s}{\sum_{s=1}^{N_s} \Delta h_s} \qquad \bar{\phi}_l = \frac{\sum_i \phi_{f,i}^{l} A_{il}}{\sum_i A_{il}}$$

- Prolongation

$$\phi_{f,i,l}^{g} = \frac{\phi_{f,i,l}^{g}}{\bar{\phi}_{l,g}^{prv}} \times \bar{\phi}_{l,g}^{CMFD}$$

- Faster Convergence
  - Global coupling between distant nodes or with boundary can be resolved quickly by solving CMFD which is an elliptic problem
  - Source convergence is accelerated as a result