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Introduction to Neutron Transport Equation and Overview of Solution Methodologies

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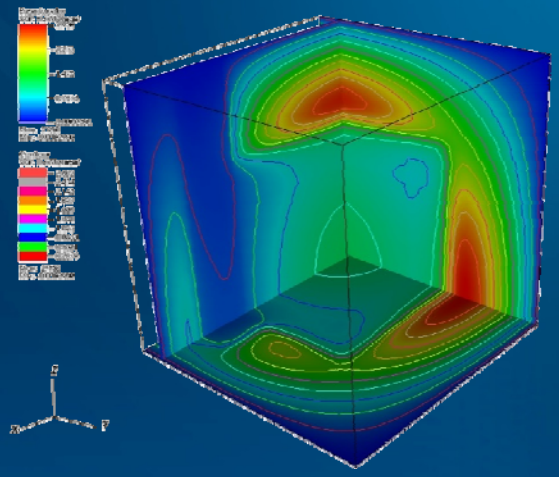

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Summary

- *We will recall briefly the transport equation*
- *The multi-group transport equation and the power and outer iteration schemes*
- *The expansion of the scattering kernel in spherical harmonics*
- *The first order and second order spherical harmonics methods (PN)*
- *The general scheme of the discrete ordinate methods SN*
- *A deeper analysis of the method of characteristics MOC*

The Steady State Neutron Transport Equation

$$\left(\vec{\Omega}\cdot\vec{\nabla}+\Sigma_T\left(\vec{r},E\right)\right)\psi\left(\vec{r},E,\vec{\Omega}\right)=\int_E dE'\int_{4\pi} d\vec{\Omega}'\left[\psi\left(\vec{r},E',\vec{\Omega}'\right)\Sigma_s\left(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega}\right)\right]+$$

$$+\int_E dE'\left[\chi\left(E'\to E\right)\frac{\nu\Sigma_F\left(\vec{r},E'\right)}{K}\frac{1}{4\pi}\int_{4\pi} d\vec{\Omega}\,\psi\left(\vec{r},E',\vec{\Omega}\right)\right]+S_{ext}\left(\vec{r},E,\vec{\Omega}\right)$$

$\Sigma_T\left(\vec{r},E\right)$: Total X-section: neutron interaction probability by unit length

$\psi\left(\vec{r},E,\vec{\Omega}\right)$: Number of neutron crossing the surface unit at the following coordinate

$\Sigma_s\left(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega}\right)$: Scattering X-section Pb by unit length of a neutron in $\left(\vec{r},E',\vec{\Omega}'\right)$ to $\left(\vec{r},E,\vec{\Omega}\right)$

$\chi\left(E'\to E\right)$: Fission spectrum: pb. of a fission in E' to lead neutrons in E

ν: Number of secondary by fission

$\Sigma_F\left(\vec{r},E'\right)$: Fission X-section: fission pb. by unit length

K: Fundamental eigenvalue (K=1 if $S_{ext}\left(\vec{r},E,\vec{\Omega}\right)$)

$S_{ext}\left(\vec{r},E,\vec{\Omega}\right)$: External source

Operator Definition

$\left(\vec{\Omega}\cdot\vec{\nabla}+\Sigma_T\left(\vec{r},E\right)\right)=A[*]$: Stremaing-Removal

$\int_E dE'\int_{4\pi} d\vec{\Omega}'\left[\Sigma_s\left(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega}\right)\right]=H[*]$: Scattering operator

$\left(\vec{\Omega}\cdot\vec{\nabla}+\Sigma_T\left(\vec{r},E\right)\right)-\int_E dE'\int_{4\pi} d\vec{\Omega}'\left[\Sigma_s\left(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega}\right)\right]=A[*]-H[*]=\mathrm{T}[*]$: Transport oprator

$\int_E dE'\left[\chi\left(E'\to E\right)\nu\Sigma_F\left(\vec{r},E'\right)\frac{1}{4\pi}\int_{4\pi} d\vec{\Omega}\right]=F[*]$: Fission operator

$$A[\psi]\left(\vec{r},E,\vec{\Omega}\right)=H[\psi]\left(\vec{r},E,\vec{\Omega}\right)+\frac{F}{K_{eff}}[\psi]\left(\vec{r},E,\vec{\Omega}\right)+S_{ext}\left(\vec{r},E,\vec{\Omega}\right)$$

$$T[\psi]\left(\vec{r},E,\vec{\Omega}\right)=\frac{F}{K_{eff}}[\psi]\left(\vec{r},E,\vec{\Omega}\right)+S_{ext}\left(\vec{r},E,\vec{\Omega}\right)$$

if $S_{ext}\left(\vec{r},E,\vec{\Omega}\right)=0$

$$T[\psi]\left(\vec{r},E,\vec{\Omega}\right)=\frac{F}{K_{eff}}[\psi]\left(\vec{r},E,\vec{\Omega}\right)$$ generalized eigenvalue problem

The Inverse Power Iteration

- We focus for the moment on the fundamental eigenvalue search.
- The reason is that when we can adjust the composition and the geometry such as $K_{eff} = 1$ the reactor is self sustained, it is capable to persevere the same neutron population over time, the homogenous equation has a not null solution, the transport equation has ∞^1 solutions.
- The uniqueness of the solution is achieved imposing the total reactor power.

$$\psi^{P} = T^{-1}\left[\frac{F\left[\psi^{P-1}\right]}{K_{eff}^{p-1}}\right]$$

$$K_{eff}^{p} = \frac{K_{eff}^{p-1} F\left[\psi^{P}\right]}{F\left[\psi^{P-1}\right]}$$

$$\psi^{P+1} = T^{-1}\left[\frac{F\left[\psi^{P}\right]}{K_{eff}^{p}}\right]$$

$$K_{eff}^{p+1} = \frac{K_{eff}^{p} F\left[\psi^{P+1}\right]}{F\left[\psi^{P}\right]}$$

We need to solve the following problem for each inverse power iteration

$$T\left[\psi^{P}\right] = \frac{1}{K_{eff}^{p-1}} F\left[\psi^{P-1}\right]$$

The Multi-Group Approach

- If the solution and the parameters in the transport equation could be considered almost constant within sufficient small energy steps we could define the following multi-group quantities:

$$\Sigma_{T,g}\left(\vec{r}\right)=\Sigma_{T}\left(\vec{r},E_{g}\right)$$

$$\psi_{g}\left(\vec{r},\vec{\Omega}\right)=\psi\left(\vec{r},E_{g},\vec{\Omega}\right)$$

$$\Sigma_{s,g}\left(\vec{r},\vec{\Omega}'\cdot\vec{\Omega}\right)=\Sigma_{s}\left(\vec{r},E_{g'}\rightarrow E_{g},\vec{\Omega}'\cdot\vec{\Omega}\right)$$

$$\chi_{g'\rightarrow g}=\chi\left(E'\rightarrow E_{g}\right)$$

$$\Sigma_{F,g}\left(\vec{r}\right)=\Sigma_{F}\left(\vec{r},E_{g'}\right)$$

$$S_{ext,g}\left(\vec{r},\vec{\Omega}\right)=S_{ext}\left(\vec{r},E_{g},\vec{\Omega}\right)$$

$$E_{1}>\ldots>E_{g}>\ldots>E_{G}$$

g energy index

•In practice we apply a little more sophisticated treatment: we somehow compute a *representative* flux $\tilde{\psi}\left(\vec{r},E_{g},\vec{\Omega}\right)$ and we compute the zero order approximation of the parameters energy values as follows:

$$f_{g}\left(\vec{r},\vec{\Omega}\right)=\frac{\int_{E_{g-1}}^{E_{g}}dEf_{g}\left(\vec{r},E,\vec{\Omega}\right)\tilde{\psi}\left(\vec{r},E_{g},\vec{\Omega}\right)}{\int_{E_{g-1}}^{E_{g}}dE\tilde{\psi}\left(\vec{r},E_{g},\vec{\Omega}\right)}$$

The Multi-Group Transport Equation

$$\left(\vec{\Omega}\cdot\vec{\nabla}+\Sigma_{T,g}\left(\vec{r}\right)\right)\psi_g\left(\vec{r},\vec{\Omega}\right)=\int_{4\pi}d\vec{\Omega}\left[\psi\left(\vec{r},\vec{\Omega}'\right)\Sigma_{s,g\to g}\left(\vec{r},\vec{\Omega}'\cdot\vec{\Omega}\right)\right]+$$

$$+\sum_{\substack{g'=1\\g'\neq g}}^{G}\int_{4\pi}d\vec{\Omega}\left[\psi_{g'}\left(\vec{r},\vec{\Omega}'\right)\Sigma_{s,g'\to g}\left(\vec{r},\vec{\Omega}'\cdot\vec{\Omega}\right)\right]+\frac{1}{K}\sum_{g'=1}^{G}\left[\chi_{g'\to g}\nu\Sigma_{F,g'}\left(\vec{r}\right)\frac{1}{4\pi}\int_{4\pi}d\vec{\Omega}\,\psi_{g'}\left(\vec{r},\vec{\Omega}\right)\right]+S_{ext,g}\left(\vec{r},\vec{\Omega}\right)$$

$\left(\vec{\Omega}\cdot\vec{\nabla}+\Sigma_{T,g}\left(\vec{r}\right)\right)=A_g\left[*\right]$: Streaming-Removal group g

$\int_{4\pi}d\vec{\Omega}\left[\Sigma_{s,g\to g}\left(\vec{r},\vec{\Omega}'\cdot\vec{\Omega}\right)\right]=H_{g\to g}\left[*\right]$: Within-group scattering operator

$\sum_{g'=1}^{G}H_{g'\to g}\left[*\right]$: Multi-group scattering operator

$=A_g\left[*\right]-H_{g\to g}\left[*\right]=\mathrm{T}_g\left[*\right]$: Within-group transport operator

$\chi_{g'\to g}\nu\Sigma_{F,g'}\left(\vec{r}\right)\frac{1}{4\pi}\int_{4\pi}d\vec{\Omega}=F_{g'\to g}\left[*\right]$: Group-g' to g fission operator

$\sum_{g'=1}^{G}\left[F_{g'}\right]=F\left[*\right]$: Fission operator

The Matrix Multi-Group Structure

- First let's assume that the have just solved the last power iteration and so we can define (good to drop the power iteration index from now on):

$$S_g = \frac{1}{K^{p-1}} \sum_{g'=1}^{G} \left[\chi_{g' \to g} \nu \Sigma_{F,g'}(\vec{r}) \frac{1}{4\pi} \int_{4\pi} d\vec{\Omega} \psi_{g'}^{p-1}(\vec{r}, \vec{\Omega}) \right] + S_{ext,g}$$

- In a Matrix (energy discretized) the multi-group equation will look like:

$$\begin{bmatrix} A_1 - H_{1\to1} & & & & & & \\ \cdot & \cdot & & & 0 & & \\ -H_{g-1\to g} & -H_{g-1\to g} & A_g - H_{g\to g} & & & & \\ & & & \cdot & & & \\ -H_{1\to T} & \cdot & \cdot & -H_{T-1\to T} & A_T - H_{T\to T} & \cdot & -H_{G\to G} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & A_G - H_{G\to G} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \cdot \\ \psi_g \\ \cdot \\ \psi_T \\ \cdot \\ \psi_G \end{bmatrix} = \begin{bmatrix} S_1 \\ \cdot \\ S_g \\ \cdot \\ S_T \\ \cdot \\ S_G \end{bmatrix}$$

≠0 only if H is present

Always ≠ from 0

Thermal up-scattering

The Thermal Iterations

- Very simple: Gauss Seidel

$$\begin{bmatrix} A_T - H_{T\to T} & 0 & . & . & 0 \\ -H_{T\to T+1} & A_{T+1} - H_{T+1\to T+1} & 0 & . & . \\ . & . & . & 0 & . \\ . & . & . & A_{G-1} - H_{G-1\to G-1} & 0 \\ -H_{T\to G} & . & . & -H_{G-1\to G} & A_G - H_{G\to G} \end{bmatrix} \begin{bmatrix} \psi_T \\ \psi_T \\ \\ \psi_{G-1} \\ \psi_G \end{bmatrix}^{O+1} =$$

$$= \begin{bmatrix} 0 & H_{T+1\to T} & . & . & H_{G\to T} \\ . & 0 & . & . & . \\ . & . & 0 & . & . \\ . & . & . & 0 & H_{G\to G-1} \\ 0 & . & . & . & 0 \end{bmatrix} \begin{bmatrix} \psi_T \\ \psi_T \\ . \\ \psi_{G-1} \\ \psi_G \end{bmatrix}^{O} + \begin{bmatrix} S_T \\ S_T \\ . \\ S_{G-1} \\ S_G \end{bmatrix} + \begin{bmatrix} H_{1\to T} & . & . & H_{T-1\to T} \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \\ H_{1\to G} & . & . & H_{T-1\to G} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \\ \\ \psi_{T-1} \end{bmatrix}$$

The Within-Group Equation

- Finally, we define a source for each groups that takes care everything happens outside the group and is sending neutron in (the sink is already in the total)

$$S_g^{in} = S_g + \sum_{\substack{g'=1 \\ g' \neq g}}^{T<G} \int_{4\pi} d\vec{\Omega} \left[\psi_{g'}^{O+1}\left(\vec{r},\vec{\Omega}'\right) \Sigma_{s,g' \to g}\left(\vec{r},\vec{\Omega}' \cdot \vec{\Omega}\right) \right] + \sum_{\substack{g'=T<G \\ g' \neq g}}^{G} \int_{4\pi} d\vec{\Omega} \left[\psi_{g'}^{O}\left(\vec{r},\vec{\Omega}'\right) \Sigma_{s,g' \to g}\left(\vec{r},\vec{\Omega}' \cdot \vec{\Omega}\right) \right]$$

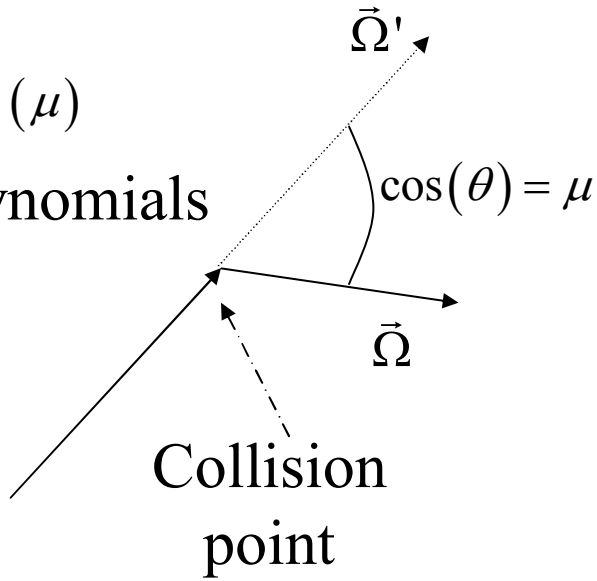
- Let's drop the *O* and g indexes for the outer and we focus on:

$$\left(\vec{\Omega} \cdot \vec{\nabla} + \Sigma_T\left(\vec{r}\right)\right) \psi\left(\vec{r},\vec{\Omega}\right) = \int_{4\pi} d\vec{\Omega} \left[\psi\left(\vec{r},\vec{\Omega}'\right) \Sigma_s\left(\vec{r},\vec{\Omega}' \cdot \vec{\Omega}\right) \right] + S_{in}\left(\vec{r},\vec{\Omega}\right)$$

  - Energy is gone!

The Angular Scattering Kernel (1)

- Under the assumption of isotropic medium $\Sigma_s\left(\vec{r},\vec{\Omega}'\cdot\vec{\Omega}\right)=\Sigma_s\left(\vec{r},\mu\right)$
- We can therefore use an expansion in Legendre polynomials: $\Sigma_s\left(\vec{r},\vec{\Omega}'\cdot\vec{\Omega}\right)=\sum_{k=0}^{\infty}\Sigma_{s,k}\left(\vec{r}\right)P_k\left(\mu\right)$
- The addition theorem for the Legendre polynomials allows: $\Sigma_s\left(\vec{r},\vec{\Omega}'\cdot\vec{\Omega}\right)=\sum_{k=0}^{\infty}\Sigma_{s,k}\left(\vec{r}\right)\sum_{|l|\le k}Y_{k,l}\left(\vec{\Omega}'\right)Y_{k,l}\left(\vec{\Omega}\right)$
- The $Y_{k,l}\left(\vec{\Omega}'\right)$ are the *real* spherical harmonics
- The spherical harmonics are a complete set over the sphere 4π



$$\Sigma_{s,k}\left(\vec{r},\mu\right)=\int_{-1}^{1}d\mu P_k\left(\mu\right)\Sigma_s\left(\vec{r},\mu\right)$$

$$\int_{-1}^{1}d\mu P_k\left(\mu\right)P_{k'}\left(\mu\right)=\delta_{k,k'}$$

$$\int_{4\pi}d\vec{\Omega}Y_{k,l}\left(\vec{\Omega}\right)Y_{k',l'}\left(\vec{\Omega}\right)=\delta_{k',k}\delta_{l',l}$$

The Angular Scattering Kernel (2)

- Since the spherical harmonics are a complete set it holds:

$$\psi\left(\vec{r},\vec{\Omega}\right)=\sum_{k=0}^{\infty}\sum_{|l|\le k}\psi_{k,l}\left(\vec{r}\right)Y_{k,l}\left(\vec{\Omega}\right)$$

$$\psi_{k,l}\left(\vec{r}\right)=\int_{4\pi}d\vec{\Omega}\,\psi\left(\vec{r},\vec{\Omega}\right)Y_{k',l'}\left(\vec{\Omega}\right)$$

- …but then…

$$\int_{4\pi}d\vec{\Omega}\left[\psi\left(\vec{r},\vec{\Omega}'\right)\Sigma_s\left(\vec{r},\vec{\Omega}'\cdot\vec{\Omega}\right)\right]=\int_{4\pi}d\vec{\Omega}\left[\sum_{k'=0}^{\infty}\sum_{|l'|\le k'}\psi_{k',l'}\left(\vec{r}\right)Y_{k',l'}\left(\vec{\Omega}'\right)\sum_{k=0}^{\infty}\Sigma_{s,k}\left(\vec{r}\right)\sum_{|l|\le k}Y_{k,l}\left(\vec{\Omega}'\right)Y_{k,l}\left(\vec{\Omega}\right)\right]=$$

$$=\sum_{k=0}^{\infty}\Sigma_{s,k}\left(\vec{r}\right)\sum_{|l|\le k}\psi_{k,l}Y_{k,l}\left(\vec{\Omega}\right)$$

- …and finally:

$$\left(\vec{\Omega}\cdot\vec{\nabla}+\Sigma_T\left(\vec{r}\right)\right)\psi\left(\vec{r},\vec{\Omega}\right)=\sum_{k=0}^{\infty}\Sigma_{s,k}\left(\vec{r}\right)\sum_{|l|\le k}\psi_{k,l}Y_{k,l}\left(\vec{\Omega}\right)+S_{in}\left(\vec{r},\vec{\Omega}\right)$$

- Usually we are lucky and the expansion could end for k~1, max 5
- k=0 is the isotropic scattering assumption for diffusion

The Spherical Harmonics Projection (1)

- The scattering term is now in terms of angular moments, can we get the all equation in in angular moments?
- We project the transport equation over the spherical harmonics and lets see…

$$\int_{4\pi} d\vec{\Omega} Y_{k.l}\left(\vec{\Omega}\right)\left(\vec{\Omega}\cdot\vec{\nabla}+\Sigma_T\left(\vec{r}\right)\right)\psi\left(\vec{r},\vec{\Omega}\right)=\int_{4\pi} d\vec{\Omega} Y_{k.l}\left(\vec{\Omega}\right)\sum_{k=0}^{\infty}\Sigma_{s,k}\left(\vec{r}\right)\sum_{|l|\le k}\psi_{k,l}Y_{k.l}\left(\vec{\Omega}\right)+\int_{4\pi} d\vec{\Omega} Y_{k.l}\left(\vec{\Omega}\right)S_{in}\left(\vec{r},\vec{\Omega}\right)$$

$$\int_{4\pi} d\vec{\Omega}\left[Y_{k.l}\left(\vec{\Omega}\right)\vec{\Omega}\cdot\vec{\nabla}\psi\left(\vec{r},\vec{\Omega}\right)\right]+\Sigma_T\left(\vec{r}\right)\psi_{k,l}\left(\vec{r}\right)=\Sigma_{s,k}\left(\vec{r}\right)\psi_{k,l}\left(\vec{r}\right)+S_{in,k,l}\left(\vec{r},\vec{\Omega}\right)$$

???

$$S_{in,k,l}\left(\vec{r},\vec{\Omega}\right)=\int_{4\pi} d\vec{\Omega} Y_{k.l}\left(\vec{\Omega}\right)S_{in}\left(\vec{r},\vec{\Omega}\right)$$

The Spherical Harmonics Projection (2)

- Well… $\vec{\Omega} = \frac{1}{\sqrt{3}}\left(Y_{1,-1}\left(\vec{\Omega}\right) \quad Y_{1,1}\left(\vec{\Omega}\right) \quad Y_{1,0}\left(\vec{\Omega}\right)\right)$
- Then there is a recursion law that express the product $Y_{k,l}\left(\vec{\Omega}\right)Y_{\substack{1,-1\\1,1\\1,0}}\left(\vec{\Omega}\right)$

$$
\begin{aligned}
Y_{k,l}\left(\vec{\Omega}\right)Y_{1,0}\left(\vec{\Omega}\right) &= \beta_{k+1,l}Y_{k+1,l}\left(\vec{\Omega}\right) + \beta_{k,l}Y_{k-1,l}\left(\vec{\Omega}\right) \\
Y_{k,l}\left(\vec{\Omega}\right)Y_{1,1}\left(\vec{\Omega}\right) &= \gamma_{k,l}Y_{k+1,l+1}\left(\vec{\Omega}\right) + \varepsilon_{k,l}Y_{k-1,l+1}\left(\vec{\Omega}\right) \\
Y_{k,l}\left(\vec{\Omega}\right)Y_{1,-1}\left(\vec{\Omega}\right) &= -\lambda_{k,l}Y_{k+1,l-1}\left(\vec{\Omega}\right) + \varepsilon_{k,l}Y_{k-1,l-1}\left(\vec{\Omega}\right)
\end{aligned}
\Bigg\} l \geq 0
$$

$$
\begin{aligned}
Y_{k,l}\left(\vec{\Omega}\right)Y_{1,1}\left(\vec{\Omega}\right) &= -\lambda_{k,l}Y_{k+1,l+1}\left(\vec{\Omega}\right) + \varepsilon_{k,l}Y_{k-1,l+1}\left(\vec{\Omega}\right) \\
Y_{k,l}\left(\vec{\Omega}\right)Y_{1,-1}\left(\vec{\Omega}\right) &= \gamma_{k,l}Y_{k+1,l-1}\left(\vec{\Omega}\right) + \varepsilon_{k,l}Y_{k-1,l-1}\left(\vec{\Omega}\right)
\end{aligned}
\Bigg\} l < 0
$$

- Bottom line we a have system of coupled equations.
- Angle is gone, in space we can do FEM, DFM, hybrid DFM, or whatever you like more ☺

The second Order Formulation (1)

- Lets make it simpler and use the isotropic scattering approximation:

$$\int_{4\pi} d\vec{\Omega}\left[\psi\left(\vec{r},\vec{\Omega}'\right)\Sigma_s\left(\vec{r},\vec{\Omega}'\cdot\vec{\Omega}\right)\right]=\sum_{k=0}^{\infty}\Sigma_{s,k}\left(\vec{r}\right)\sum_{|l|\le k}\psi_{k,l}Y_{k.l}\left(\vec{\Omega}\right)\approx\Sigma_{s,0}\left(\vec{r}\right)\psi_{0,0}=\Sigma_{s,0}\left(\vec{r}\right)\phi$$

- We write the transport equation for $\vec{\Omega}$, $-\vec{\Omega}$

$$\begin{cases}\left(\vec{\Omega}\cdot\vec{\nabla}+\Sigma_T\left(\vec{r}\right)\right)\psi\left(\vec{r},\vec{\Omega}\right)=\Sigma_{s,0}\left(\vec{r}\right)\phi+S_{in}\left(\vec{r},\vec{\Omega}\right)\\ \left(-\vec{\Omega}\cdot\vec{\nabla}+\Sigma_T\left(\vec{r}\right)\right)\psi\left(\vec{r},-\vec{\Omega}\right)=\Sigma_{s,0}\left(\vec{r}\right)\phi+S_{in}\left(\vec{r},-\vec{\Omega}\right)\end{cases}$$

- Once sum once subtract the two equation

$$\begin{cases}\vec{\Omega}\cdot\vec{\nabla}\left(\psi\left(\vec{r},\vec{\Omega}\right)-\psi\left(\vec{r},-\vec{\Omega}\right)\right)+\Sigma_T\left(\vec{r}\right)\left(\psi\left(\vec{r},\vec{\Omega}\right)+\psi\left(\vec{r},-\vec{\Omega}\right)\right)=2\Sigma_{s,0}\left(\vec{r}\right)\phi_{0,0}+S_{in}\left(\vec{r},\vec{\Omega}\right)+S_{in}\left(\vec{r},-\vec{\Omega}\right)\\ \vec{\Omega}\cdot\vec{\nabla}\left(\psi\left(\vec{r},\vec{\Omega}\right)+\psi\left(\vec{r},-\vec{\Omega}\right)\right)+\Sigma_T\left(\vec{r}\right)\left(\psi\left(\vec{r},\vec{\Omega}\right)-\psi\left(\vec{r},-\vec{\Omega}\right)\right)=S_{in}\left(\vec{r},\vec{\Omega}\right)-S_{in}\left(\vec{r},-\vec{\Omega}\right)\end{cases}$$

The Second Order Formulation (2)

- We define:

$$\begin{cases} \psi^e(\vec{r},\vec{\Omega}) = \frac{1}{2}\left(\psi(\vec{r},\vec{\Omega}) + \psi(\vec{r},-\vec{\Omega})\right) \\ \psi^o(\vec{r},\vec{\Omega}) = \frac{1}{2}\left(\psi(\vec{r},\vec{\Omega}) - \psi(\vec{r},-\vec{\Omega})\right) \end{cases} \qquad \begin{cases} S_{in}^e(\vec{r},\vec{\Omega}) = \frac{1}{2}\left(S_{in}(\vec{r},\vec{\Omega}) + S_{in}(\vec{r},-\vec{\Omega})\right) \\ S_{in}^o(\vec{r},\vec{\Omega}) = \frac{1}{2}\left(S_{in}(\vec{r},\vec{\Omega}) - S_{in}(\vec{r},-\vec{\Omega})\right) \end{cases}$$

- We solve for the *e*ven component

$$-\vec{\Omega}\cdot\vec{\nabla}\frac{1}{\Sigma_T(\vec{r})}\vec{\Omega}\cdot\vec{\nabla}\psi^e(\vec{r},\vec{\Omega}) + \Sigma_T(\vec{r})\psi^e(\vec{r},\vec{\Omega}) = \Sigma_{s,0}(\vec{r})\phi + S_{in}^e(\vec{r},\vec{\Omega}) + \vec{\Omega}\cdot\vec{\nabla}\frac{1}{\Sigma_T(\vec{r})}S_{in}^o(\vec{r},\vec{\Omega})$$

The Second Order Formulation (3)

- To make it simpler let's say the source is isotropic, and lets put back our expansion in spherical harmonics

$$\vec{\Omega}\cdot\vec{\nabla}\frac{1}{\Sigma_T(\vec{r})}\vec{\Omega}\cdot\vec{\nabla}\sum_{\substack{k=0\\K\ \text{even}}}^{\infty}\sum_{|l|\le k}\psi_{k,l}(\vec{r})Y_{k.l}(\vec{\Omega})+\Sigma_T(\vec{r})\sum_{\substack{k=0\\K\ \text{even}}}^{\infty}\sum_{|l|\le k}\psi_{k,l}(\vec{r})Y_{k.l}(\vec{\Omega})=\Sigma_{s,0}(\vec{r})\phi+S_{in}(\vec{r})$$

- What we did is to solve analytically for half of the space of the solution and so we reduced by half the unknown.
- Last point is a good one but this equation is not defined in void region!!

The Second Order Formulation (2)

- The problem is not yet over we should still solve for the moments, we need to perform a projection on the even spherical harmonics

$$-\int_{4\pi\pi} d\vec{\Omega} Y_{k'.l'}\left(\vec{\Omega}\right)\left(\vec{\Omega}\cdot\vec{\nabla}\frac{1}{\Sigma_T\left(\vec{r}\right)}\vec{\Omega}\cdot\vec{\nabla}\sum_{\substack{k=0\\K\ \text{even}}}^{\infty}\sum_{|l|\le k}\psi_{k,l}\left(\vec{r}\right)Y_{k.l}\left(\vec{\Omega}\right)\right)+\Sigma_T\left(\vec{r}\right)\psi_{k,l}=\Sigma_{s,0}\left(\vec{r}\right)\phi+S_{in}\left(\vec{r}\right)$$

- Once more this terms couple different moments together
- What if $\sum_{\substack{k=0\\K\ \text{even}}}^{\infty}\sum_{|l|\le k}\psi_{k,l}\left(\vec{r}\right)Y_{k.l}\left(\vec{\Omega}\right)\approx\phi\left(\vec{r}\right)$ then DIFFUSION!

$$-\vec{\nabla}\frac{1}{3\Sigma_T\left(\vec{r}\right)}\vec{\nabla}\phi\left(\vec{r}\right)+\Sigma_T\left(\vec{r}\right)\phi\left(\vec{r}\right)=\Sigma_{s,0}\left(\vec{r}\right)\phi\left(\vec{r}\right)+S_{in}\left(\vec{r}\right)$$

The Angular Collocative methods First Order SN

- Going back to the original problem after the representation of the scattering kernel in spherical harmonics can we do something different?

$$\left(\vec{\Omega}\cdot\vec{\nabla}+\Sigma_T(\vec{r})\right)\psi\left(\vec{r},\vec{\Omega}\right)=\sum_{k=0}^{\infty}\Sigma_{s,k}(\vec{r})\sum_{|l|\le k}\psi_{k,l}Y_{k.l}\left(\vec{\Omega}\right)+S_{in}\left(\vec{r},\vec{\Omega}\right)$$

- What we really need is to compute the $\psi_{k,l}(\vec{r})$ up the scattering order. If we recall its definition we might think of a sort of angular quadrature (cubature)..

$$\psi_{k,l}(\vec{r})=\int_{4\pi}d\vec{\Omega}\,\psi\left(\vec{r},\vec{\Omega}\right)Y_{k'.l'}\left(\vec{\Omega}\right)=\sum_{n=1}^{N}\omega_n\psi\left(\vec{r},\vec{\Omega}_n\right)Y_{k'.l'}\left(\vec{\Omega}_n\right)$$

- Now the problem is to find the values of $\psi_n(\vec{r})=\psi\left(\vec{r},\vec{\Omega}_n\right)$ fore each direction of the angular cubature

$$\left(\vec{\Omega}\cdot\vec{\nabla}+\Sigma_T(\vec{r})\right)\psi_n(\vec{r})=\sum_{k=0}^{\infty}\Sigma_{s,k}(\vec{r})\sum_{|l|\le k}\psi_{k,l}Y_{k.l}\left(\vec{\Omega}\right)+S_{in}\left(\vec{r},\vec{\Omega}_n\right)$$

The Angular Collocative methods Second Order SN (1)

- We can start directly from the second order form before the projection over the even spherical harmonics (isotropic scattering already assumed)

$$-\vec{\Omega}\cdot\vec{\nabla}\frac{1}{\Sigma_T(\vec{r})}\vec{\Omega}\cdot\vec{\nabla}\psi^e(\vec{r},\vec{\Omega})+\Sigma_T(\vec{r})\psi^e(\vec{r},\vec{\Omega})=\Sigma_{s,0}(\vec{r})\phi+S^e_{in}(\vec{r},\vec{\Omega})+\vec{\Omega}\cdot\vec{\nabla}\frac{1}{\Sigma_T(\vec{r})}S^o_{in}(\vec{r},\vec{\Omega})$$

- Isotropic source assumption (not needed but easier)

$$-\vec{\Omega}\cdot\vec{\nabla}\frac{1}{\Sigma_T(\vec{r})}\vec{\Omega}\cdot\vec{\nabla}\psi^e(\vec{r},\vec{\Omega})+\Sigma_T(\vec{r})\psi^e(\vec{r},\vec{\Omega})=\Sigma_{s,0}(\vec{r})\phi$$

- Lets examine the computation of the scalar flux

$$\int_{4\pi}d\vec{\Omega}\psi(\vec{r},\vec{\Omega}')=\int_{2\pi^+}d\vec{\Omega}\psi(\vec{r},\vec{\Omega}')+\int_{2\pi^-}d\vec{\Omega}\psi(\vec{r},\vec{\Omega}')=$$

$$=\int_{2\pi^+}d\vec{\Omega}\psi(\vec{r},\vec{\Omega}')+\int_{2\pi^+}d\vec{\Omega}\psi(\vec{r},-\vec{\Omega}')=2\int_{2\pi^+}d\vec{\Omega}\psi^e(\vec{r},\vec{\Omega}')$$

The Angular Collocative methods Second Order SN (2)

- Once more we use a quadrature formula to perform the integral but this time the domain is halved

$$\int_{4\pi} d\vec{\Omega}\psi\left(\vec{r},\vec{\Omega}'\right)=2\int_{2\pi^+} d\vec{\Omega}\psi^e\left(\vec{r},\vec{\Omega}'\right)=2\sum_{n=1}^{N/2}\omega_n\psi^e\left(\vec{r},\vec{\Omega}_n\right)$$

- Once more the problem is reduced to the computation of

$$\psi_n^e\left(\vec{r}\right)=\psi^e\left(\vec{r},\vec{\Omega}_n\right)$$

- By the solution of:

$$-\vec{\Omega}_n\cdot\vec{\nabla}\frac{1}{\Sigma_T\left(\vec{r}\right)}\vec{\Omega}_n\cdot\vec{\nabla}\psi_n^e\left(\vec{r}\right)+\Sigma_T\left(\vec{r}\right)\psi_n^e\left(\vec{r}\right)=\Sigma_{s,0}\left(\vec{r}\right)\phi$$

- By direction is equivalent to the diffusion equation!!

Scattering Iterations for First Order Sn

- Let's write the transport equation for each of the *N* directions:

$$\left(\vec{\Omega}_n \cdot \vec{\nabla} + \Sigma_T(\vec{r})\right)\psi_n(\vec{r}) = \sum_{k=0}^{\infty}\Sigma_{s,k}(\vec{r})\sum_{|l|\le k}\sum_{n'=1}^{N}\omega_{n'}\psi_{n'}(\vec{r})Y_{k,l}\left(\vec{\Omega}_{n'}\right)Y_{k,l}\left(\vec{\Omega}_n\right) + S_{in,n}(\vec{r})$$

- Now it is this term that couple all the N equations together
- Well lets just iterate on it…

$$\left(\vec{\Omega}_n \cdot \vec{\nabla} + \Sigma_T(\vec{r})\right)\psi_n^{i+1}(\vec{r}) = \sum_{k=0}^{\infty}\Sigma_{s,k}(\vec{r})\sum_{|l|\le k}\sum_{n'=1}^{N}\omega_{n'}\psi_{n'}^{i}(\vec{r})Y_{k,l}\left(\vec{\Omega}_{n'}\right)Y_{k,l}\left(\vec{\Omega}_n\right) + S_{in,n}(\vec{r})$$

- The last equation is a partial differential equation in space only (the integral in angle is gone…), so once more pick the solver that you like more
- Form of DFM are probably the most diffused
- Usually the equation in space is solved by a *sweeping* method

What I did not show you

- Methods based on the integral formulation of the transport equation integrated over angle have been largely used in the past but nowadays are deemed to be too memory intensive for large calculation

- Monte Carlo Methods: are used mainly for reference calculation due to the long running time

QUESTIONS?

Lets Get the Way Cleared First

- Lets start back from the scattering source iteration equation

$$\left(\vec{\Omega}_n \cdot \vec{\nabla} + \Sigma_T(\vec{r})\right)\psi_n^{i+1}(\vec{r}) = \sum_{k=0}^{\infty}\Sigma_{s,k}(\vec{r})\sum_{|l|\le k}\sum_{n'=1}^{N}\omega_{n'}\psi_{n'}^{i}(\vec{r})Y_{k.l}\left(\vec{\Omega}_{n'}\right)Y_{k.l}\left(\vec{\Omega}_n\right) + S_{in,n}(\vec{r})$$

- Lets make it simple and assume scattering and source isotropic

$$\left(\vec{\Omega}_n \cdot \vec{\nabla} + \Sigma_T(\vec{r})\right)\psi_n^{i+1}(\vec{r}) = \Sigma_{s,0}(\vec{r})\sum_{n'=1}^{N}\omega_{n'}\psi_{n'}^{i}(\vec{r}) + S_{in}(\vec{r})$$

- We define the emission density at iteration i+1:

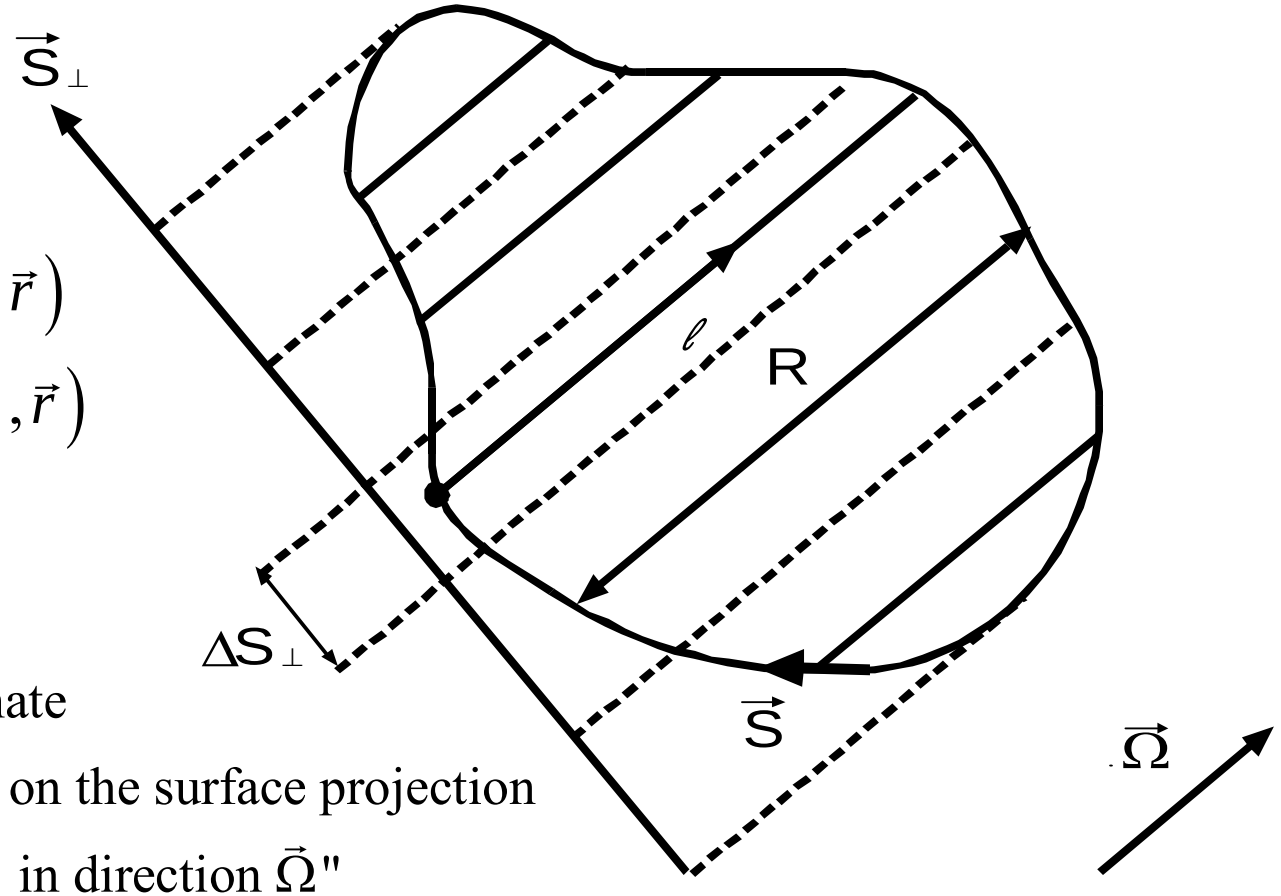
$$Q^{i+1}(\vec{r}) = \Sigma_{s,0}(\vec{r})\sum_{n'=1}^{N}\omega_{n'}\psi_{n'}^{i}(\vec{r}) + S_{in}(\vec{r})$$

- Iteration index over the scattering source could be dropped since all quantity are at the same iteration index

$$\left(\vec{\Omega}_n \cdot \vec{\nabla} + \Sigma_T(\vec{r})\right)\psi_n(\vec{r}) = Q(\vec{r})$$

The Characteristics System of Coordinate

$$\begin{Bmatrix} \vec{r} \\ \vec{\Omega}_n \end{Bmatrix} \rightarrow \begin{cases} \ell = \ell\left(\vec{\Omega}_n, \vec{r}\right) \\ \vec{S} = S\left(\vec{\Omega}_n, \vec{r}\right) \\ \vec{\Omega}''_n = \vec{\Omega}_n \end{cases}$$



$\vec{S}$ = surface coordinate

$\vec{S}_\perp$ = 2D coordinate on the surface projection

ℓ = distance from $\vec{S}$ in direction $\vec{\Omega}''_n$

$\vec{\Omega}_n$ = angular coordinate

The Equation Along the Characteristics

- We write first the equation in the new coordinate system

$$\left(\frac{\partial}{\partial \ell}+\Sigma_T\left(\ell,\vec{S}\right)\right)\psi_n\left(\ell,\vec{S}\right)=Q\left(\ell,\vec{S}\right)$$

- …or in a mixed way…

$$\left(\frac{\partial}{\partial \ell}+\Sigma_T\left(\vec{r}\right)\right)\psi_n\left(\ell,\vec{S}\right)=Q\left(\vec{r}\right)$$

- Remember the coordinate transformation is depended on the direction: essentially this is a different equation for each direction.
- Angle and space are combined together to form a new coordinate system!

The Space Discretization

- The domain is divided into finite elements or "cells" within which the cross sections and the source are assumed to be constant in space:

$$\Sigma_T(\vec{r}) \approx \sum_j \theta_j(\vec{r})\Sigma_{T,j}, \quad Q(\vec{r}) \approx \sum_j \theta_j(\vec{r})Q_j,$$

$$\Sigma_{s,0}(\vec{r}) \approx \sum_j \theta_j(\vec{r})\Sigma_{s,j,0},$$

$$\theta_j(\vec{r}) = \text{ characteristc function of domain } V_j \quad (\bigcup_j V_j = V)$$

- Usually the cells never cross different material therefore having the cross section constant in over V_j is not an approximation as long as we do not consider burn-up problems.
- The approximation so far illustrated involve only the source not the other terms of the equation

Integral Form Along the Characteristics

- Lets' consider a region in space V_i and a trajectory $t_{\vec{S}_n}$ crossing it.
- The intersection of the region with the trajectory happens for

$$R_{\vec{S}}^{j,in} \le \ell \le R_{\vec{S}}^{j,out}$$

$$R_{\vec{S}}^{j} = R_{\vec{S}}^{j,out} - R_{\vec{S}}^{j,in}$$

- Now we integrate along ℓ within this intersection length

$$\psi_n\left(R_{\vec{S}}^{j,out},\vec{S}\right) = \psi_n\left(R_{\vec{S}}^{j,in},\vec{S}\right) e^{-\int_{R_{\vec{S}}^{j,in}}^{R_{\vec{S}}^{j,out}} d\ell \Sigma_T\left(\ell,\vec{S}\right)} + \int_{R_{\vec{S}}^{j,in}}^{R_{\vec{S}}^{j,out}} d\ell Q\left(\ell,\vec{S}\right) e^{\Sigma_T\left(\ell,\vec{S}\right)}$$

The Propagation Equation

- Under the already done assumption that $\Sigma_T\left(\ell,\vec{S}\right)$ and $Q\left(\ell,\vec{S}\right)$ are constant within V_i

$$\psi_n\left(R_{\vec{S}}^{j,out},\vec{S}\right)=\psi_n\left(R_{\vec{S}}^{j,in},\vec{S}\right)e^{-\Sigma_T^j R_{\vec{S}}^j}+\frac{1-e^{-\Sigma_T^j R_{\vec{S}}^j}}{\Sigma_T^j}Q_j$$

- This last equation is known as the propagation equation.

- Given the incoming flux at $\left(0,\vec{S}\right)$ with direction $\vec{\Omega}_n$ in to the domain we will be able to propagate it to the end of the domain

And What About the Source?

- If the source and the boundary conditions are given we know how to propagate the solution through the domain.
- For the moment lets skip the boundary conditions
- As already seen in the general scheme for Sn methods the source for the "scattering iteration" is coming from the previous one

$$Q^{i+2}(\vec{r}) = \Sigma_{s,0}(\vec{r}) \sum_{n'=1}^{N} \omega_{n'} \psi_{n'}^{i+1}(\vec{r}) + S_{in}(\vec{r})$$

- We pose the constant source inside each cell equal to its average value

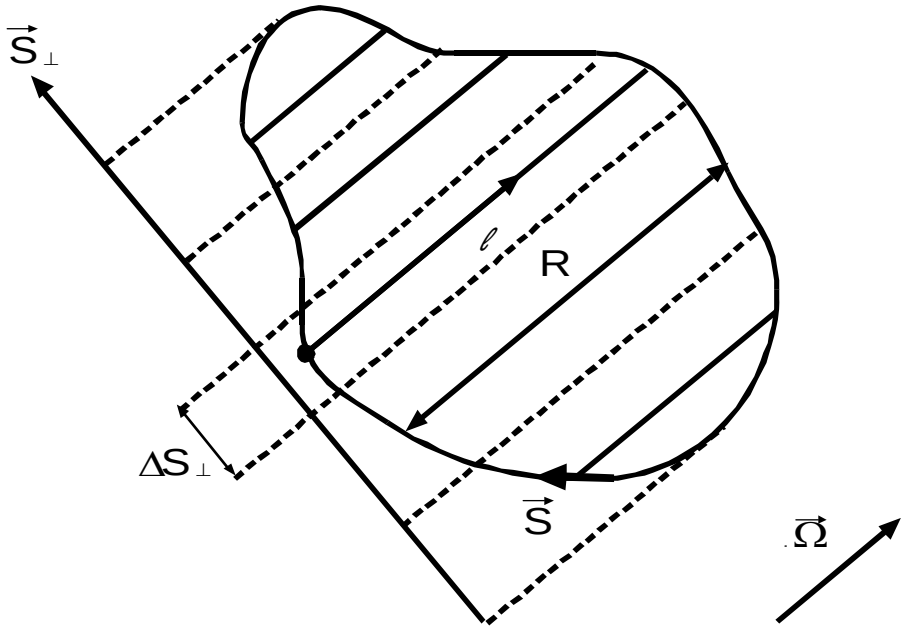
$$Q_j^{i+2} = \frac{1}{V_j} \int_{V_i} d\vec{r} Q^{i+2}(\vec{r}) = \Sigma_{s,0}^{j} \sum_{n'=1}^{N} \omega_{n'} \frac{1}{V_j} \int_{V_i} d\vec{r} \psi_{n'}^{i+1}(\vec{r}) + \frac{1}{V_j} \int_{V_i} d\vec{r} S_{in}(\vec{r})$$

$$Q_j^{i+2} = \Sigma_{s,0}^{j} \sum_{n'=1}^{N} \omega_{n'} \frac{1}{V_j} \int_{V_i} d\vec{r} \psi_{n'}^{i+1}(\vec{r}) + S_{in}^{j}$$

The Balance Equation (1)

- Now we have to understand how to compute: $\int_{V_J} d\vec{r}\psi_{n'}^{i+1}(\vec{r})$
- This term in reality is nothing more than the average angular for each direction $\vec{\Omega}_{n'}$ within each cell V_j
- We perform our classical change of coordinate and so we can recast the integral as it follows:

$$\int_{V_J} d\vec{r} = \int_{\partial V_J \perp \vec{\Omega}_n} d\vec{s}_{\perp} \int_{R_{\vec{s}}^{j,in}}^{R_{\vec{s}}^{j,out}} d\ell$$



The Balance Equation (2)

- One step at the time, lets start applying $\int_{R_{\vec{S}}^{j,in}}^{R_{\vec{S}}^{j,out}} d\ell$ to the transport equation:

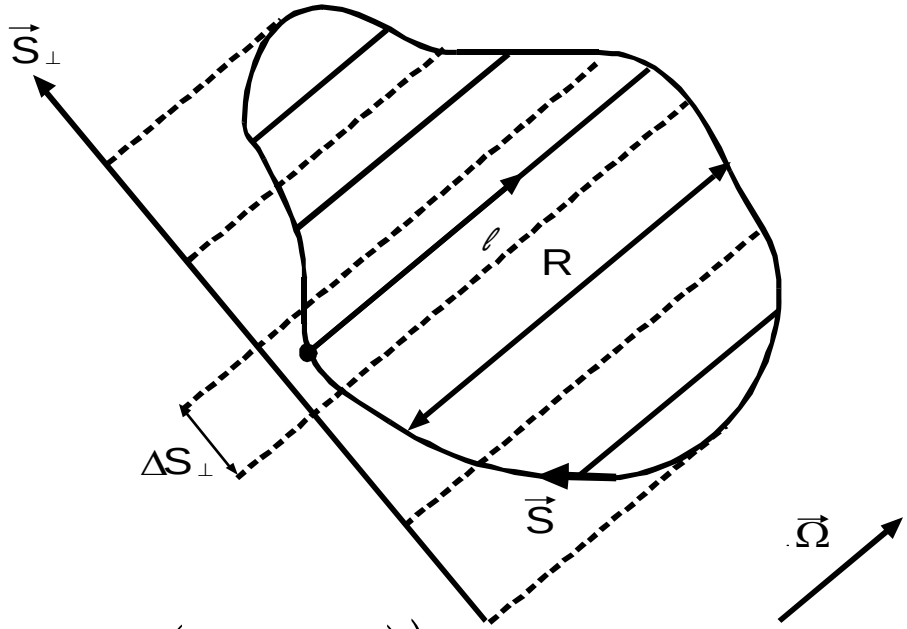
$$\int_{R_{\vec{S}}^{j,in}}^{R_{\vec{S}}^{j,out}} d\ell \left(\frac{\partial}{\partial \ell} + \Sigma_{T,j} \right) \psi_n^{i+1}\left(\ell, \vec{S}\right) = \int_{R_{\vec{S}}^{j,in}}^{R_{\vec{S}}^{j,out}} d\ell Q_j^{i+}$$

$$\psi_n^{i+1}\left(R_{\vec{S}}^{j,out}, \vec{S}\right) - \psi_n^{i+1}\left(R_{\vec{S}}^{j,in}, \vec{S}\right) + \Sigma_{T,j} \int_{R_{\vec{S}}^{j,in}}^{R_{\vec{S}}^{j,out}} d\ell \, \psi_n^{i+1}\left(\ell, \vec{S}\right) = R_{\vec{S}}^{j} Q_j^{i+1}$$

$$\int_{R_{\vec{S}}^{j,in}}^{R_{\vec{S}}^{j,out}} d\ell \, \psi_n^{i+1}\left(\ell, \vec{S}\right) = \frac{1}{\Sigma_{T,j}} \left(R_{\vec{S}}^{j} Q_j^{i+1} + \psi_n^{i+1}\left(R_{\vec{S}}^{j,in}, \vec{S}\right) - \psi_n^{i+1}\left(R_{\vec{S}}^{j,out}, \vec{S}\right) \right)$$

Now the Integral over the Perpendicular Surface

- We use a spatial 2D quadrature over $\vec{s}_\perp$



$$\int_{\partial V_J \perp \vec{\Omega}_n} d\vec{s}_\perp \int_{R_{\vec{S}}^{j,in}}^{R_{\vec{S}}^{j,out}} d\ell d\ell \, \psi_n^{i+1}\left(\ell, \vec{S}\right) =$$

$$= \frac{1}{\Sigma_{T,j}} \sum_{t_n \cap \partial V_J \perp \vec{\Omega}_n} \left(R_{\vec{S}}^{j} Q_j^{i+1} + \psi_n^{i+1}\left(R_{\vec{S}}^{j,in}, \vec{S}\right) - \psi_n^{i+1}\left(R_{\vec{S}}^{j,out}, \vec{S}\right) \right)$$

We made it!!

Better to Summarize…

- At iteration *i* we assume incoming flux known as the source within each element
- We propagate the neutron angular flux for all directions of the angular quadrature and all trajectories of the surface quadrature (a different one for each angle)

$$\psi_n^{i+1}\left(R_{\vec{S}}^{j,out},\vec{S}\right)=\psi_n^{i+1}\left(R_{\vec{S}}^{j,in},\vec{S}\right)e^{-\Sigma_T^j R_{\vec{S}}^j}+\frac{1-e^{-\Sigma_T^j R_{\vec{S}}^j}}{\Sigma_T^j}Q_j^{i+1}$$

- Once all the incoming and outgoing fluxes are known we can use the balance equation to compute the source for the next iteration

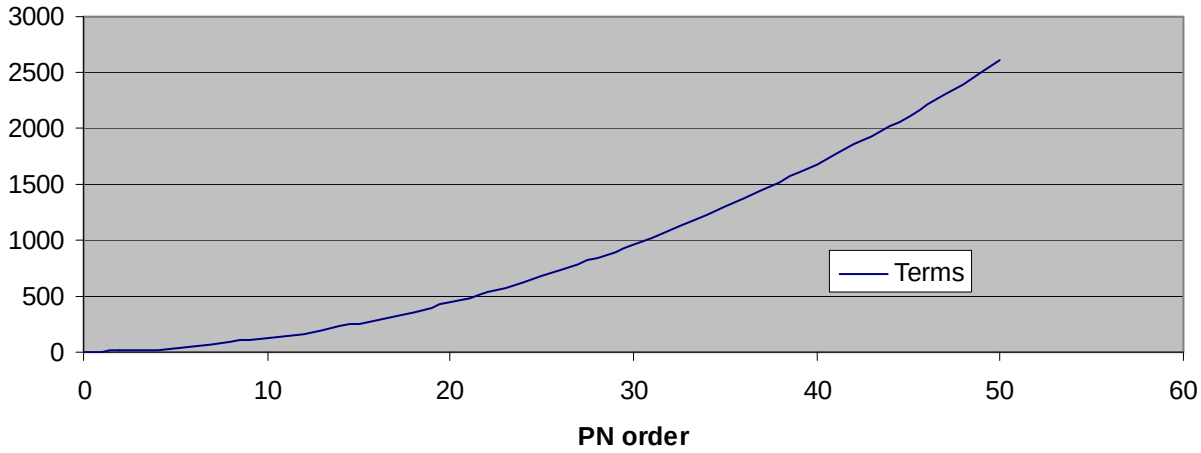
$$Q_j^{i+2}=\Sigma_{s,0}^j\sum_{n'=1}^{N}\omega_{n'}\frac{1}{V_j}\frac{1}{\Sigma_{T,j}}\sum_{t_n\cap\partial V_j\perp\vec{\Omega}_n}\left(R_{\vec{S}}^j Q_j^{i+1}+\psi_n^{i+1}\left(R_{\vec{S}}^{j,in},\vec{S}\right)-\psi_n^{i+1}\left(R_{\vec{S}}^{j,out},\vec{S}\right)\right)+S_{in}^j$$

Overview First Order PN Methods (1)

- It is a polynomial description of the angular dependence of the angular neutron flux
- Therefore it is suitable only for not too sharp angular gradients
- The angular structure of the matrix tends to become hill conditioned for high orders
- It is not widely used to lower overall performance with respect the second order form

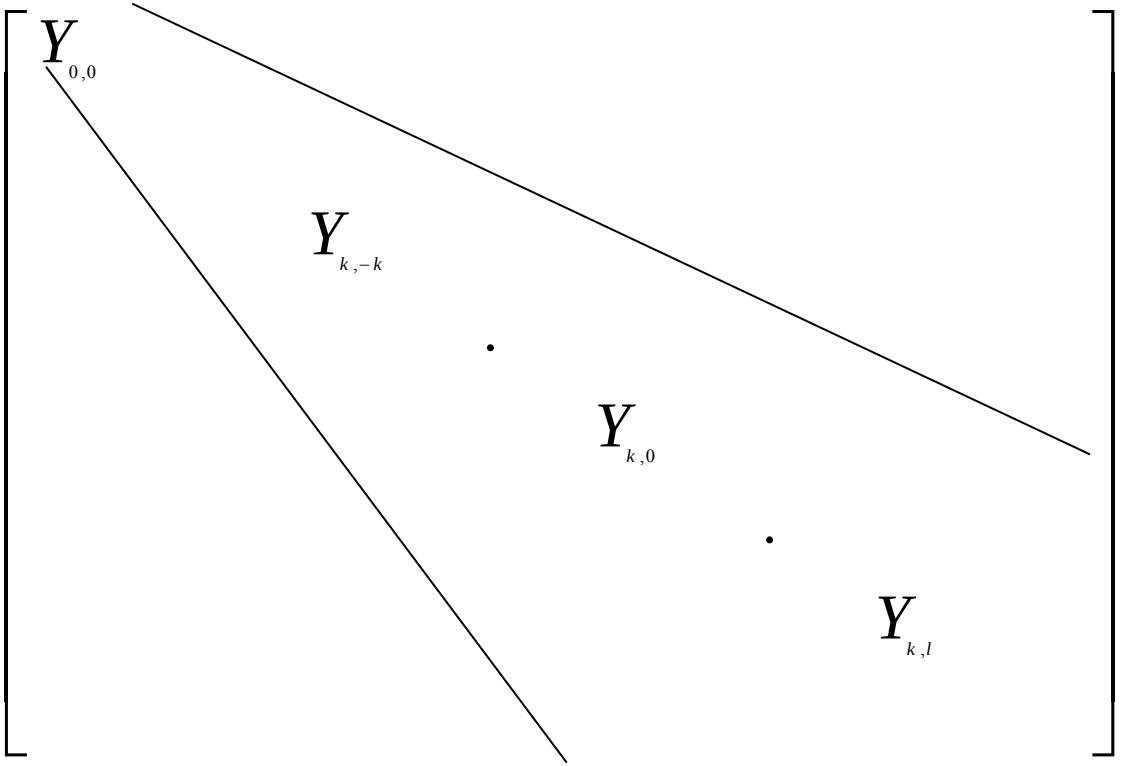
Overview First Order PN Methods (2)

- The number of angular unknown grows very fast as $(N+1)^2$



Overview First Order PN Methods (3)

- Scalability and preconditioning is limited by the growing bandwidth of the angular structure

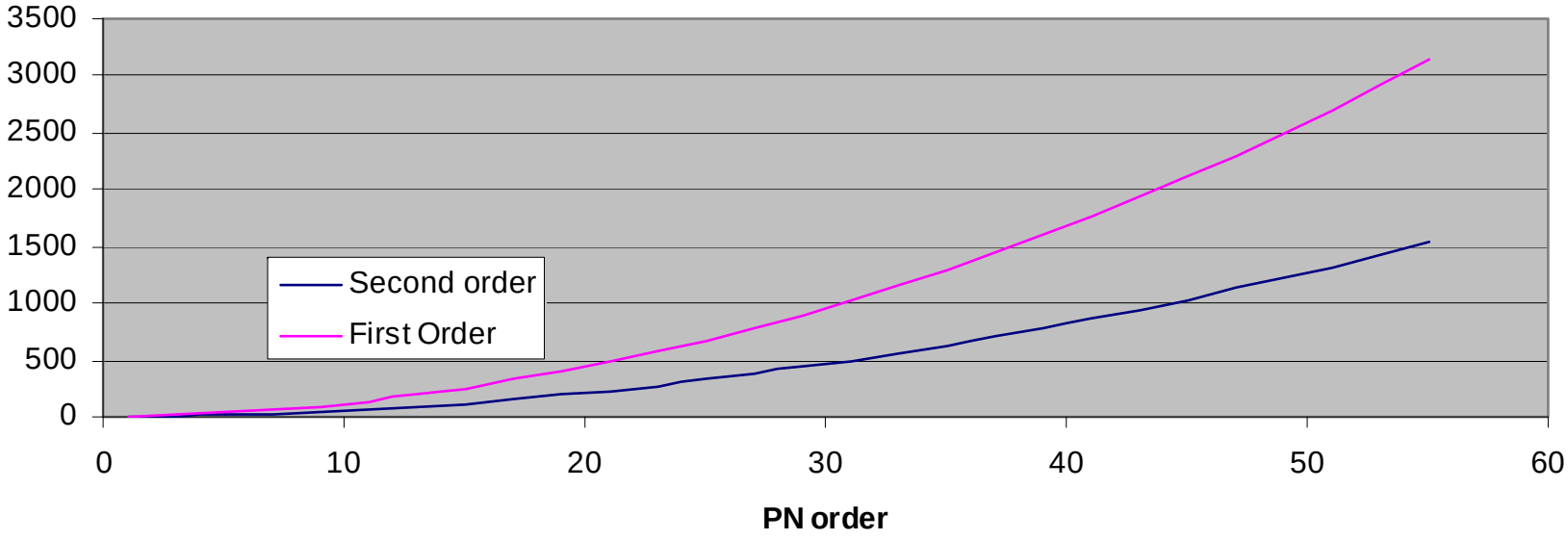


Overview Second Order PN Methods (2)

- It is a polynomial description of the angular dependence of the angular neutron flux
- Therefore it is suitable only for not too sharp angular gradients
- The lesser is the density of the medium the higher is the instability (undefined for void region)
- Its lower order form (diffusion!!) is the most used

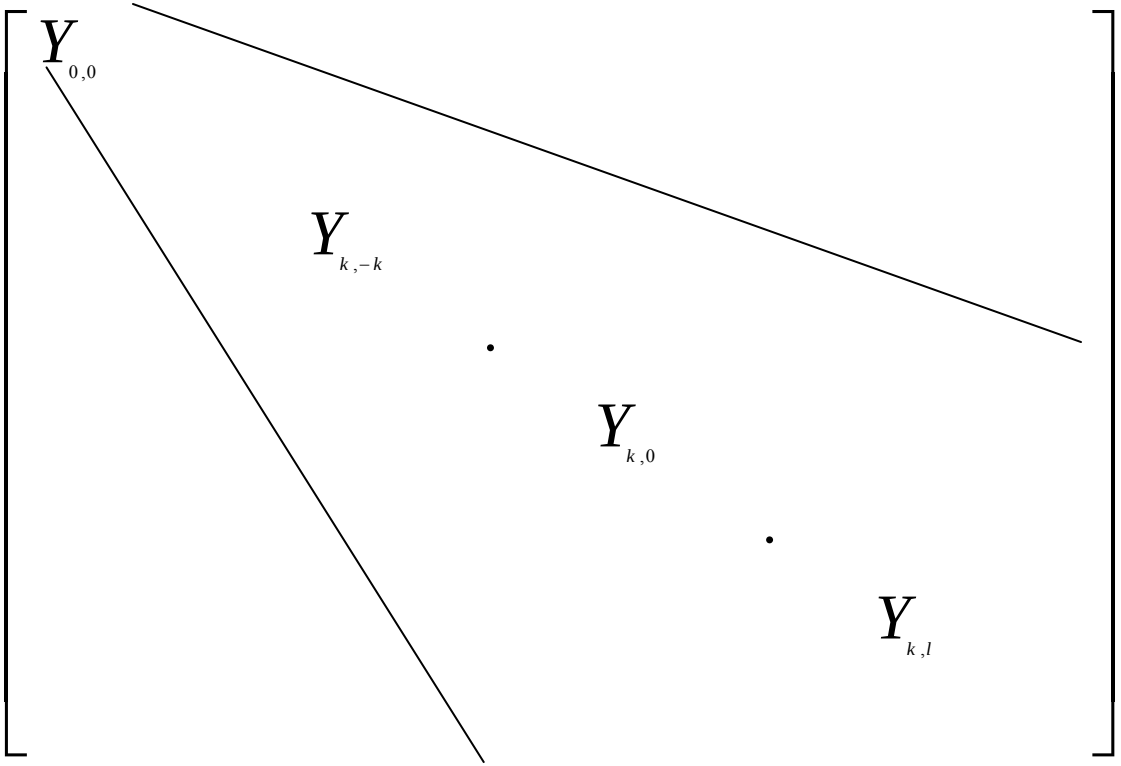
Overview Second Order PN Methods

- The number of unknown grows very fast as $(N+1)N/2$



Overview Second Order PN Methods (3)

- Scalability and preconditioning is limited by the growing bandwidth of the angular structure



Overview Second Order Sn Methods (1)

- It does not works in void
- Is a discontinuous representation in angle: deal well with discontinuity
- Neutrons tends to be propagated from the originating point along the direction of the angular quadrature originating what is called ray effect
- Even if scalability is difficult is achievable by angle due to the diffusion like structure

Overview First Order Sn Methods (1)

- Works in void
- Is a discontinuous representation in angle: deal well with discontinuity
- Neutrons tends to be propagated from the originating point along the direction of the angular quadrature originating what is called ray effect
- It is very difficult to achieve good scalability and so far, it has been only for structured meshes

Overview Quadrature

- Quadrature are still an ongoing research subject also because are needed in many other fields like quantum mechanics
- The most effective quadrature is the Lebedev-Laikov (number of point on the sphere / highest degree of polynomial exactly integrable) but number of points increases to fast
- We use other formulas that growth smoother but have negative weights for higher numbers of point leading to numerical instability

Questions??