

DE LA RECHERCHE À L'INDUSTRIE

cea



www.cea.fr

HIGHER ORDER ACCELERATED MOC METHOD

by

Laurent Graziano & Simone Santandrea

METHOD OF CHARACTERISTICS (MOC)

- ▣ *source iterative solution*

$$(\Omega \cdot \nabla + \Sigma)\psi^{(n+1)} = q^{(n)}$$

$$\psi_{in}^{(n+1)} = \beta\psi_{out}^{(n)} + \psi_0$$

(one-group problem)

$$\downarrow$$

$$\psi(\mathbf{r}, \Omega)$$

$$q^{(n)} = H\psi^{(n)} + S$$

$$\text{albedo operator } \beta : \psi_{out} \rightarrow \psi_{in}$$

- ▣ *angular approximation*

$$S_N = \{w_n, \Omega_n, n = 1, N\} \rightarrow \frac{1}{4\pi} \int_{(4\pi)} d\Omega f(\Omega) \sim \sum_n w_n f(\Omega_n)$$

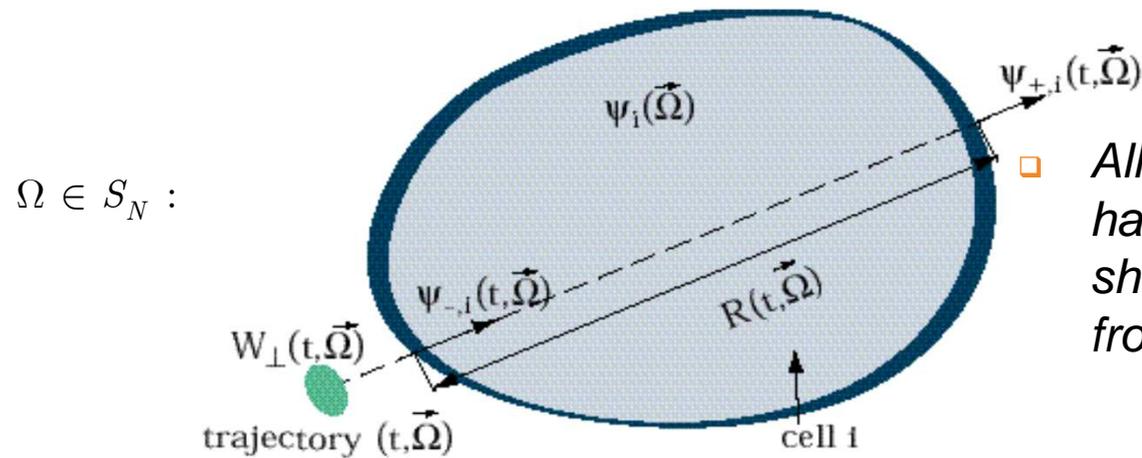
- ▣ *flat flux approximation over homogeneous regions*

$$D = \cup_i D_i, \quad D_i \text{ of homogeneous support}$$

$$\psi(\mathbf{r}, \Omega) \sim \sum_i \psi_i(\Omega) \theta_i(\mathbf{r})$$

MOC 1 : DISCRETIZATION SCHEME

- numerical implementation based on trajectories
(in 2D XY 'planar' trajectories are lifted to polar directions)

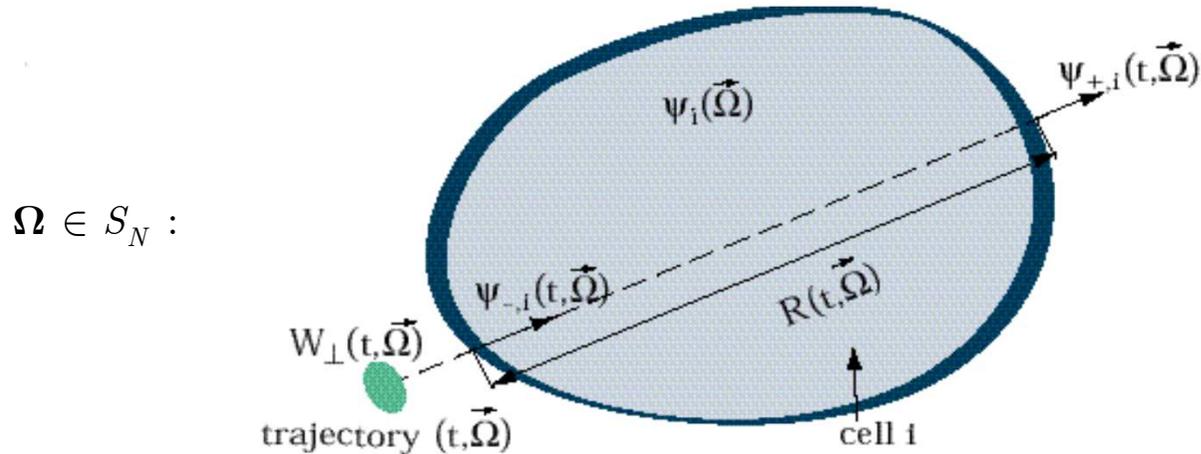


- balance equation along a trajectory

$$\psi_{+,i}(t, \Omega) - \psi_{-,i}(t, \Omega) + \sum_i R_i(t, \Omega) \psi_i(t, \Omega) = R_i(t, \Omega) q_i^{(n)}(\Omega)$$

↓

$$V_i \psi_i(\Omega) = \int_{(i)} dr \psi(r, \Omega) \sim \sum_{t \parallel \Omega} \omega_{\perp}(t, \Omega) R_i(t, \Omega) \psi_i(t, \Omega)$$



- *propagation equation across a region (flat source approximation)*

$$\underbrace{\psi_+(\mathbf{r}, \Omega) = e^{-\tau(r, r_m)} \psi_-(\mathbf{r}_{in}, \Omega) + \int_0^{R(t, \Omega)} dR' e^{-\tau(\mathbf{r}, \mathbf{r}')} q(\mathbf{r}', \Omega)}_{\downarrow} \quad (\mathbf{r}' = \mathbf{r} - R' \Omega)$$

$$\psi_{+,i}(t, \Omega) = T_i(t, \Omega) \times \psi_{-,i}(t, \Omega) + E_i(t, \Omega) \times q_i^{(n)}(\Omega)$$

transmission & escape coefficients : $T_i(t, \Omega) = e^{-\Sigma_i R_i(t, \Omega)}$, $E_i(t, \Omega) = \frac{1 - T_i(t, \Omega)}{\Sigma_i}$

HIGHER ORDER BALANCE EQUATION: A CONSISTENCY PROBLEM

Defining a scalar product on a chord

$$\langle f, g \rangle_L = \int_0^L dt f(t)g(t),$$

the following generalized average balance per chord can be written

$$\Sigma_r \langle \vec{P}, \Psi_r \rangle_L = \langle \vec{P}, \vec{P} \rangle_L \vec{q}_r + \vec{P}(0)\Psi_r(0) - \vec{P}(L)\Psi_r(L) + \left\langle \frac{\partial \vec{P}}{\partial t}, \Psi_r \right\rangle_L, \text{ (Sanchez 2012)}$$

so that defining the polynomial coupling region matrix

$$\bar{P}P(\vec{\Omega}) = \frac{1}{V_r} \int_r d\vec{r} \vec{P}(\vec{z}) \otimes \vec{P}(\vec{z}) \simeq \frac{1}{V_r(\vec{\Omega})} \sum_{\substack{t \parallel \vec{\Omega} \\ t \cap r}} \langle \vec{P}, \vec{P} \rangle_{L_t},$$

the « polynomial angular » balance equation is:

$$\bar{C} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ \frac{1}{\Delta z/2} & 0 & 0 & 0 \\ 0 & \frac{2}{\Delta z/2} & 0 & 0 \\ 0 & 0 & \frac{3}{\Delta z/2} & 0 \\ 0 & 0 & \ddots & \ddots \end{bmatrix}.$$

$$\Sigma_r {}' \vec{\Psi}_r(\vec{\Omega}) = \bar{P}P(\vec{\Omega}) \cdot \vec{q}_r(\vec{\Omega}) - \Delta \vec{J}_r(\vec{\Omega}) + \mu \bar{C} {}' \vec{\Psi}_r(\vec{\Omega}).$$

BALANCE FROM ANGLE TO MOMENTS

The collision/fission operators use angular moments in the place of angular fluxes:

$$\vec{\Phi}_r^n = \oint \frac{d\vec{\Omega}}{4\pi} A_n(\vec{\Omega}) \vec{\Psi}_r(\vec{\Omega}).$$

Recall also that a « correspondence » exists between spatial moment and coefficients

$$\vec{\Psi}_r(\vec{\Omega}) = P\bar{P}^{-1} \cdot {}'\vec{\Psi}_r(\vec{\Omega})$$

If you define then the suite of angular-polynomial function base

$$\vec{\mathcal{Z}}(\vec{z}, \vec{\Omega}) = \{A^0(\vec{\Omega})P_0(\vec{z}), A^1(\vec{\Omega})P_0(\vec{z}), \dots, A^0(\vec{\Omega})P_1(\vec{z}), A^1(\vec{\Omega})P_1(\vec{z}), \dots\}$$

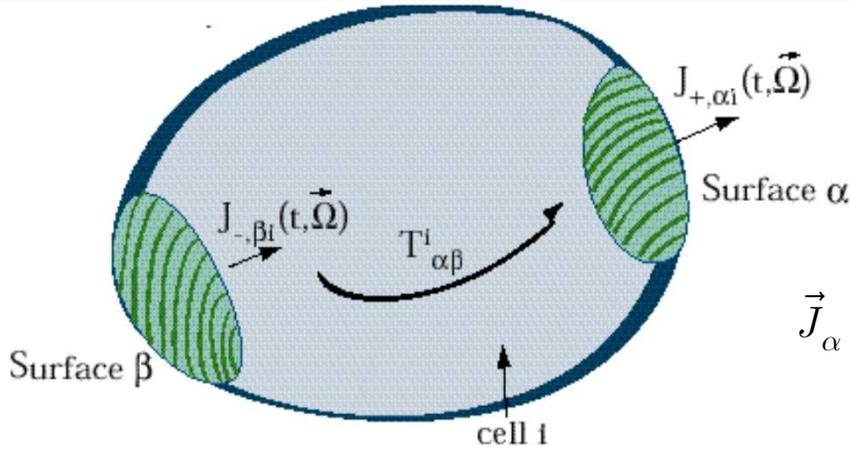
and project with over this in angle-space you get

$$\Sigma_r {}'\vec{\Phi}_r = \mathcal{Z}\mathcal{Z} \cdot \vec{q}_r - \oint \frac{d\vec{\Omega}}{4\pi} \vec{A}(\vec{\Omega}) \otimes \Delta \vec{J}_r(\vec{\Omega}) + \mathcal{D} \cdot {}'\vec{\Phi}_r. \quad \mathcal{Z}\mathcal{Z} = \oint \frac{d\vec{\Omega}}{4\pi} \left(\vec{A}(\vec{\Omega}) \otimes \vec{A}(\vec{\Omega}) \right) \otimes P\bar{P}(\vec{\Omega})$$

which in the typical “free” iteration scheme (index “i”) takes an easy to solve lower triangular form:

$$\Sigma_r {}'\vec{\Phi}_{r,p}^i = \left(\mathcal{Z}\mathcal{Z} \cdot \vec{q}_r^{i-1} \right)_p - \frac{1}{4\pi} \oint d\vec{\Omega} \vec{A}(\vec{\Omega}) \otimes \left(\Delta \vec{J}_r(\vec{\Omega}) \right)_p^i + \frac{p}{\Delta z/2} \cdot \bar{\alpha}_p \cdot {}'\vec{\Phi}_{r,p-1}^i \quad 6$$

DP_N : SYNTHETIC ACCELERATION



$$\psi_{\pm}(\mathbf{r}, \Omega) \sim \vec{A}_S(\Omega) \cdot \sum_{\alpha \in \partial i} \vec{\psi}_{\pm, \alpha} \theta_{\alpha}(\mathbf{r})$$

$$\vec{J}_{\alpha} = \frac{1}{4\pi S_{\alpha}} \int_{\alpha} dS \int_{(4\pi)} d\Omega |\Omega n| \vec{Z} \psi \underset{DP_n}{\sim} A_{\alpha,+} \vec{\psi}_{\alpha,+}$$

$$A_{\alpha,+} = \frac{1}{4\pi S_{\alpha}} \int_{\alpha} dS \int_{(2\pi+)} d\Omega \vec{Z} \otimes \vec{Z} = ppA_{\alpha,-}$$

- *propagation & balance equations :*

$$\begin{bmatrix} \vec{J}_{\alpha_v}^+ \\ \vec{J}_{\alpha_h}^+ \end{bmatrix} = \sum_{\beta \in r} \begin{bmatrix} \mathcal{T}_{\alpha_v^+ \beta_v^-} & \mathcal{T}_{\alpha_v^+ \beta_h^-} \\ \mathcal{T}_{\alpha_h^+ \beta_v^-} & \mathcal{T}_{\alpha_h^+ \beta_h^-} \end{bmatrix} \cdot \begin{bmatrix} \vec{\Phi}_{\beta_v}^- \\ \vec{\Phi}_{\beta_h}^- \end{bmatrix} + \begin{bmatrix} \mathcal{E}_{\alpha_v^+} \\ \mathcal{E}_{\alpha_h^+} \end{bmatrix} \cdot \vec{q}_r,$$

$$(\Sigma_r - \mathcal{D}) \cdot \vec{\Phi}_r = \mathcal{Z} \mathcal{Z}_D \cdot \vec{q}_r - \frac{1}{V_r} \sum_{\alpha \in r} (\vec{J}_{\alpha}^+ - \vec{J}_{\alpha}^-),$$

- *After “some” algebra a multi-collisional version of the DP_N operator is used to solve:*

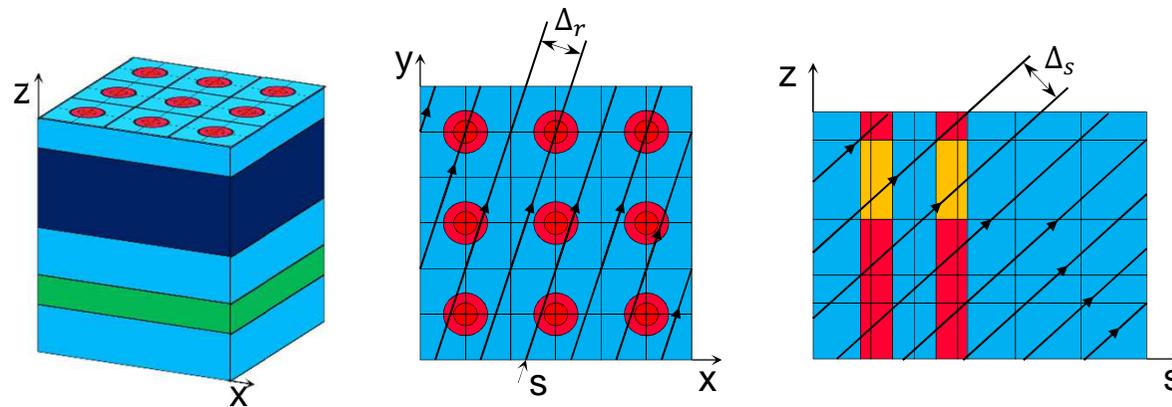
$$\vec{J}^+ = \dagger \mathcal{T} \cdot \vec{J}^- + \dagger \mathcal{E} \cdot \vec{q}_r^{ext},$$

$$\dagger \mathcal{T} = \left(\tilde{\mathcal{T}} + \vec{\mathcal{E}}^+ \Sigma_{s,r}^g \cdot \dagger \mathcal{I} \right),$$

$$\dagger \mathcal{E} = \vec{\mathcal{E}}^+ \left(\mathcal{I}_d + \Sigma_{r,s}^g \cdot \dagger \mathcal{C} \right)$$

GOING TO AXIAL 3D GEOMETRIES

The basic difficulty for 3D MOC calculation is that we cannot store realistic 3D tracking data. To avoid this we consider only (at the beginning!) 3D axial geometries:



For these geometries the 3D tracking can be decomposed into 2 phases:

1. Tracking a general 2D geometry on the x-y plane
2. Tracking a cartesian geometry on the s-z plane

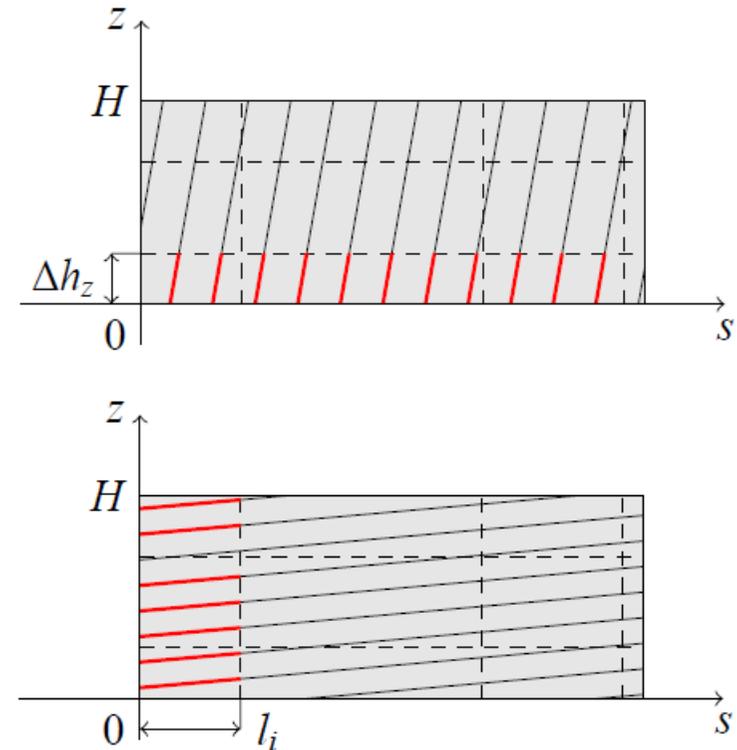
Only 1 need to be stored but reconstruct 2 can be too expensive!

Thanks to axial regularity the set of 3D chords can be decomposed into a low number of classes that not only allow to reduce memory but also to decrease computational cost.

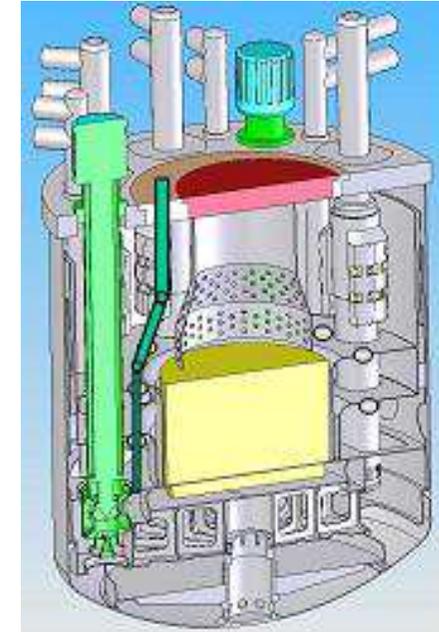
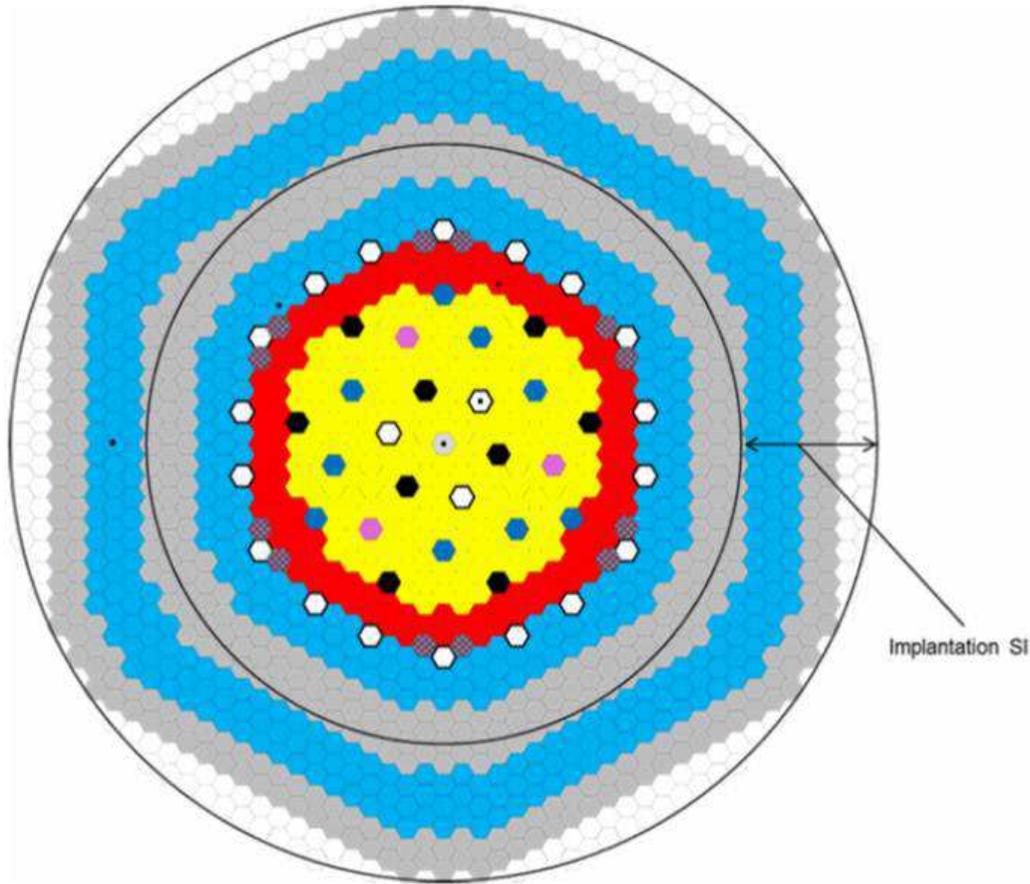
Thus, transmission coefficients,

$$T_i(t, \Omega) = e^{-\Sigma_i R_i(t, \Omega)}$$

are computed only per class and medium.

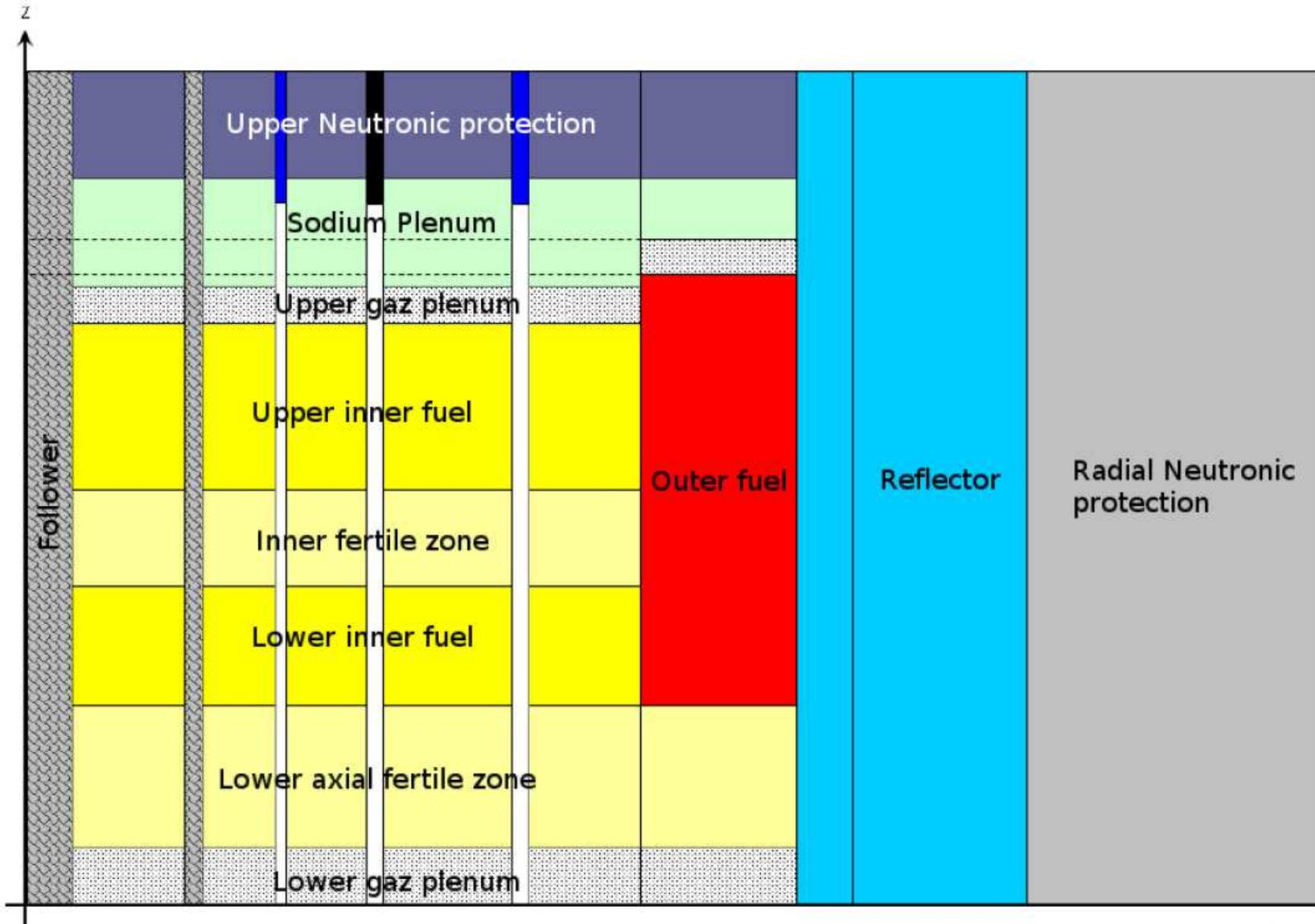


ASTRID REACTOR EXAMPLE: 2D SECTION

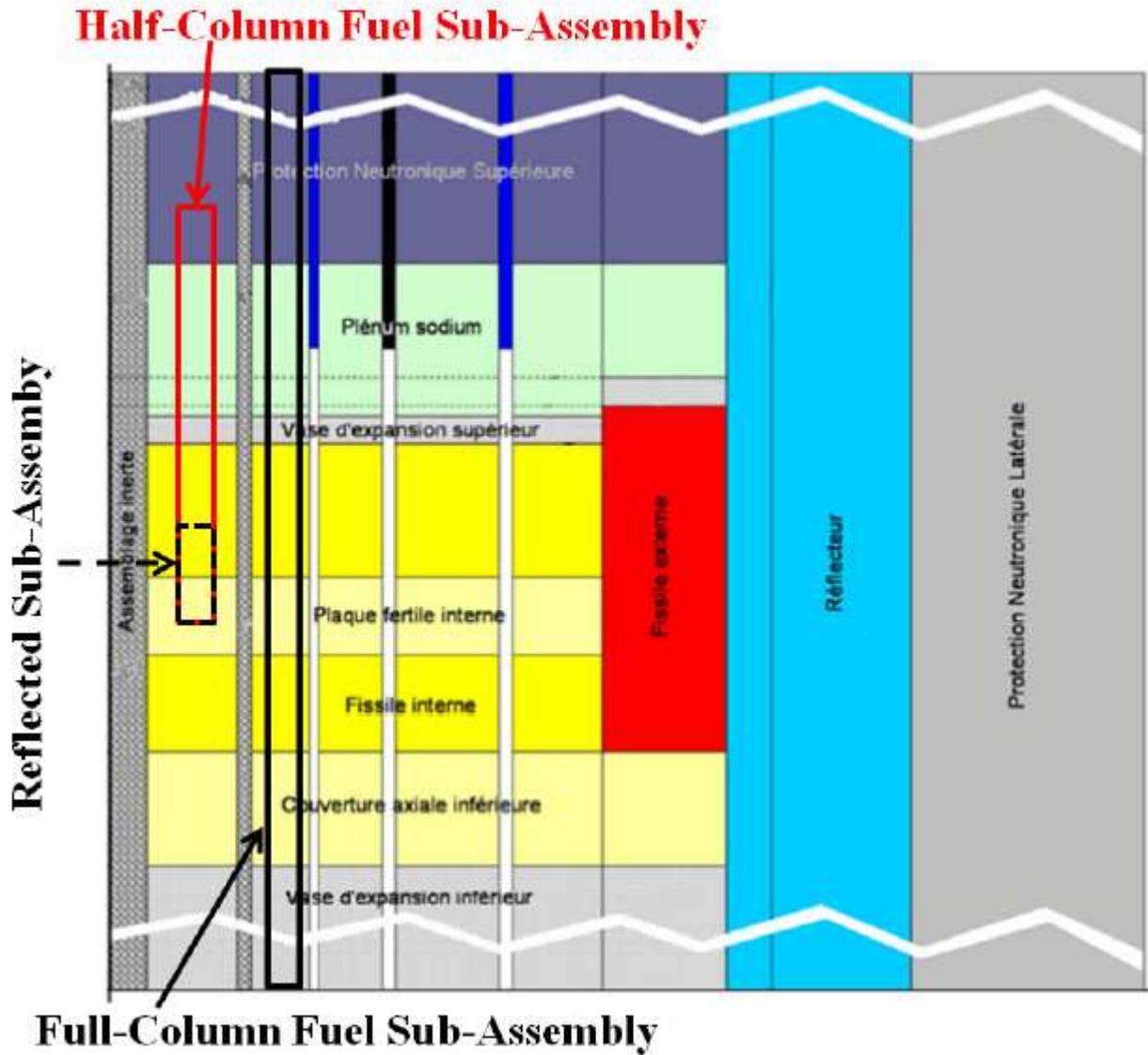


- | | |
|--|---|
| <ul style="list-style-type: none"> ○ Assemblage inerte (position pouvant être occupée par un assemblage absorbant) ● Assemblages combustibles cœur interne ● Assemblages combustibles cœur externe ● Assemblages RBC ● Assemblages RBD ● DIMEP B | <ul style="list-style-type: none"> ● Assemblages Réflecteurs ● Assemblages PNL ● Assemblages (DCS-P)-H ● Assemblages (DCS-M)-TT ○ Positions pouvant être utilisées ● Positions Réflecteurs pouvant être occupées par des assemblages combustibles |
|--|---|

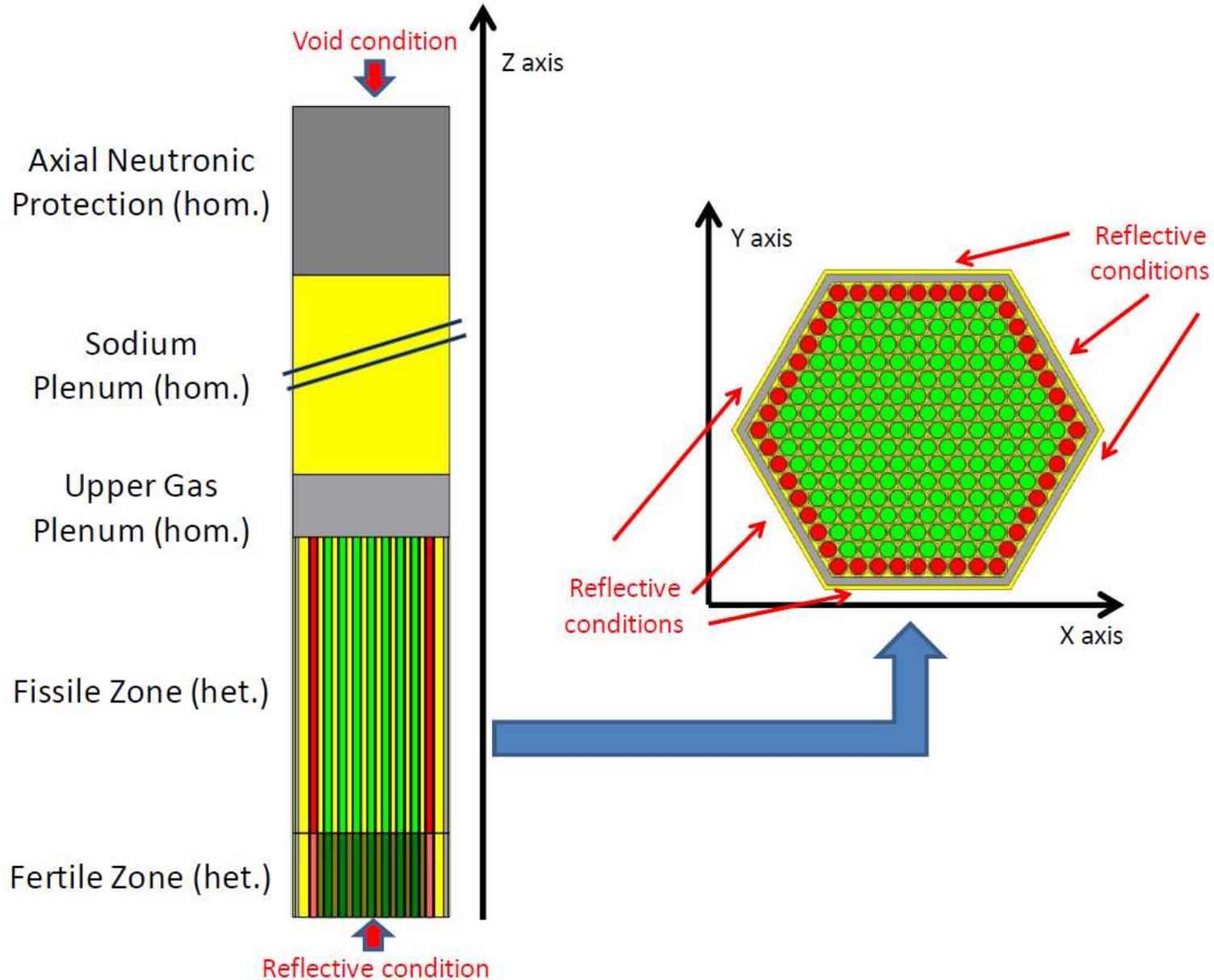
ASTRID REACTOR: AXIAL VIEW



ASTRID REACTOR CALCULATIONS

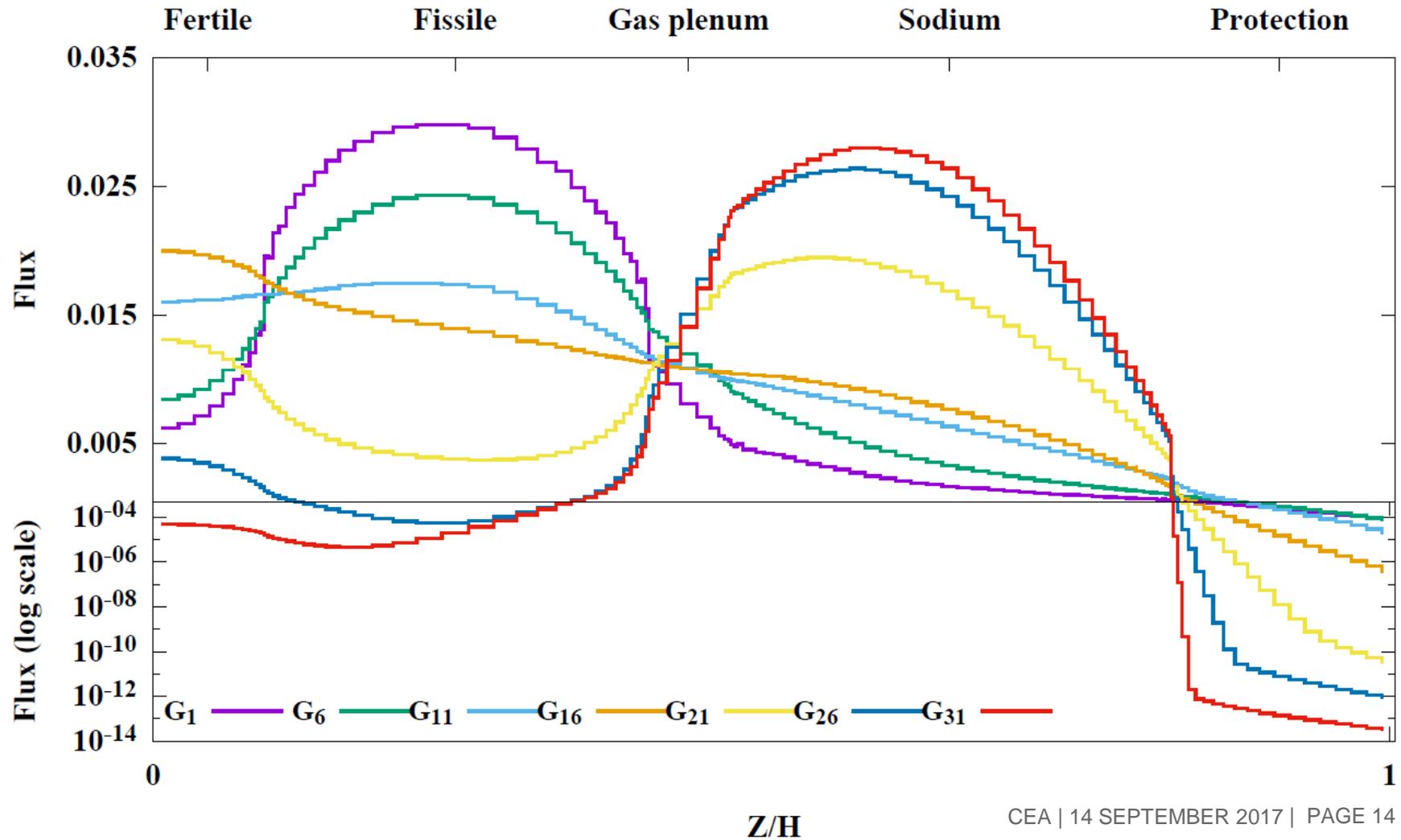


ASTRID REACTOR: SECOND CALCULATION



ASTRID REACTOR: SECOND CALCULATION

Sub-assembly axial flux profile Step



POLYNOMIAL BASIS DEFINITION

Polynomial basis to express fluxes and sources moments:

$$\vec{P}(\tilde{z}_r) = \{\tilde{z}_r^p = \left(\frac{z_r - \bar{z}_r}{\Delta z_r/2}\right)^p, \quad 0 \leq p \leq N_p\} \quad \tilde{z}_r \in [-1, 1]$$

POLYNOMIAL BASIS DEFINITION

Polynomial basis to express fluxes and sources moments:

$$\vec{P}(\tilde{z}_r) = \{\tilde{z}_r^p = \left(\frac{z_r - \bar{z}_r}{\Delta z_r/2}\right)^p, \quad 0 \leq p \leq N_p\} \quad \tilde{z}_r \in [-1, 1]$$

$$q(\vec{r}, \vec{\Omega}) = \sum_{n=1}^{N_m} A_n(\vec{\Omega}) \cdot q^n(\vec{r})$$

Polynomial basis to express fluxes and sources moments:

$$\vec{P}(\tilde{z}_r) = \{\tilde{z}_r^p = \left(\frac{z_r - \bar{z}_r}{\Delta z_r/2}\right)^p, \quad 0 \leq p \leq N_p\} \quad \tilde{z}_r \in [-1, 1]$$

$$q(\vec{r}, \vec{\Omega}) = \sum_{n=1}^{N_m} A_n(\vec{\Omega}) \cdot q^n(\vec{r})$$

Step approximation \longrightarrow $q^n(\vec{r}) \simeq q_r^n$

Polynomial basis to express fluxes and sources moments:

$$\vec{P}(\tilde{z}_r) = \{ \tilde{z}_r^p = \left(\frac{z_r - \bar{z}_r}{\Delta z_r / 2} \right)^p, \quad 0 \leq p \leq N_p \} \quad \tilde{z}_r \in [-1, 1]$$

$$q(\vec{r}, \vec{\Omega}) = \sum_{n=1}^{N_m} A_n(\vec{\Omega}) \cdot q^n(\vec{r})$$

Step approximation \longrightarrow $q^n(\vec{r}) \simeq q_r^n$

Polynomial approximation \longrightarrow $q^n(\vec{r}) = \sum_p^{N_p} P_p(\tilde{z}_r) \cdot q_{r,pol,p}^n$

POLYNOMIAL BASIS DEFINITION

Polynomial basis to express fluxes and sources moments:

$$\vec{P}(\tilde{z}_r) = \{ \tilde{z}_r^p = \left(\frac{z_r - \bar{z}_r}{\Delta z_r / 2} \right)^p, \quad 0 \leq p \leq N_p \} \quad \tilde{z}_r \in [-1, 1]$$

$$q(\vec{r}, \vec{\Omega}) = \sum_{n=1}^{N_m} A_n(\vec{\Omega}) \cdot q^n(\vec{r})$$

Step approximation \longrightarrow $q^n(\vec{r}) \simeq q_r^n$

Polynomial approximation \longrightarrow $q^n(\vec{r}) = \sum_p^{N_p} P_p(\tilde{z}_r) \cdot q_{r,pol,p}^n$

$$q(\vec{r}, \vec{\Omega}) = \vec{P}(\tilde{z}_r) \cdot \vec{q}_{r,pol}(\vec{\Omega})$$

$$q_{r,pol,p}(\vec{\Omega}) = \sum_n^{N_m} A_n(\vec{\Omega}) \cdot q_{r,pol,p}^n$$

POLYNOMIAL TRANSMISSION EQUATION

- Polynomial transmission equation:

$$q(\vec{r}, \vec{\Omega}) = \vec{P}(\vec{z}_r) \cdot \vec{q}_{r,pol}(\vec{\Omega})$$

$$\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \int_{t^{in}}^{t^{out}} dt' q(\vec{r}(t'), \vec{\Omega}) e^{-\Sigma_r(t^{out}-t')}$$
A black arrow points from the $q(\vec{r}, \vec{\Omega})$ term in the equation above to the $q(\vec{r}(t'), \vec{\Omega})$ term in the integrand of the equation below.

- Polynomial transmission equation:

$$q(\vec{r}, \vec{\Omega}) = \vec{P}(\vec{z}_r) \cdot \vec{q}_{r,pol}(\vec{\Omega})$$

$$\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \int_{t^{in}}^{t^{out}} dt' q(\vec{r}(t'), \vec{\Omega}) e^{-\Sigma_r(t^{out}-t')}$$

- Numerical polynomial transmission equation:

$$\begin{aligned} \Psi_r(t^{out}, \vec{\Omega}) = & \Psi_r(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \\ & + \sum_{k=0}^{N_p} P_k(z^{in}) \cdot \sum_{p=k}^{N_p} c_{pk} \mu^{p-k} \left(\frac{2}{\Delta z} \right)^{p-k} E_{p-k}(\tau) \frac{\left(\vec{q}_{r,pol}(\vec{\Omega}) \right)_p}{\Sigma_r} \end{aligned}$$

- Polynomial transmission equation:

$$q(\vec{r}, \vec{\Omega}) = \vec{P}(\tilde{z}_r) \cdot \vec{q}_{r,pol}(\vec{\Omega})$$

$$\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \int_{t^{in}}^{t^{out}} dt' q(\vec{r}(t'), \vec{\Omega}) e^{-\Sigma_r(t^{out}-t')}$$

- Numerical polynomial transmission equation:

$$\Psi_r(t^{out}, \vec{\Omega}) = \Psi_r(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \sum_{k=0}^{N_p} P_k(z^{in}) \cdot \sum_{p=k}^{N_p} C_{pk} \mu^{p-k} \left(\frac{2}{\Delta z}\right)^{p-k} E_{p-k}(\tau) \frac{\left(\vec{q}_{r,pol}(\vec{\Omega})\right)_p}{\Sigma_r}$$

Axial coordinate at the trajectory entering point in the r region

Binomial coefficient

POLYNOMIAL TRANSMISSION EQUATION

- Polynomial transmission equation:

$$q(\vec{r}, \vec{\Omega}) = \vec{P}(\vec{z}_r) \cdot \vec{q}_{r,pol}(\vec{\Omega})$$

$$\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \int_{t^{in}}^{t^{out}} dt' q(\vec{r}(t'), \vec{\Omega}) e^{-\Sigma_r(t^{out}-t')}$$

- Numerical polynomial transmission equation:

$$\Psi_r(t^{out}, \vec{\Omega}) = \Psi_r(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \sum_{k=0}^{N_p} P_k(z^{in}) \cdot \sum_{p=k}^{N_p} c_{pk} \mu^{p-k} \left(\frac{2}{\Delta z}\right)^{p-k} E_{p-k}(\tau) \frac{\left(\vec{q}_{r,pol}(\vec{\Omega})\right)_p}{\Sigma_r}$$

Geometrical coefficients

Source term

- Polynomial transmission equation:

$$q(\vec{r}, \vec{\Omega}) = \vec{P}(\vec{z}_r) \cdot \vec{q}_{r,pol}(\vec{\Omega})$$

$$\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \int_{t^{in}}^{t^{out}} dt' q(\vec{r}(t'), \vec{\Omega}) e^{-\Sigma_r(t^{out}-t')}$$

- Numerical polynomial transmission equation:

$$\Psi_r(t^{out}, \vec{\Omega}) = \Psi_r(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} +$$

$$+ \sum_{k=0}^{N_p} P_k(z^{in}) \cdot \sum_{p=k}^{N_p} c_{pk} \mu^{p-k} \left(\frac{2}{\Delta z} \right)^{p-k} \frac{E_{p-k}(\tau) \left(\vec{q}_{r,pol}(\vec{\Omega}) \right)_p}{\Sigma_r}$$

Escape coefficient:

$$E_{p-k}(\tau) = \frac{1}{\Sigma_r^{(p-k)}} \int_{\tau(t^{in})}^{\tau(t^{out})} d\tau' \tau'^{p-k} e^{(\tau'-\tau(t^{in}))}$$

where $\tau = \Sigma_r t$

STEP VS POLYNOMIAL TRANSMISSION

- Step transmission:

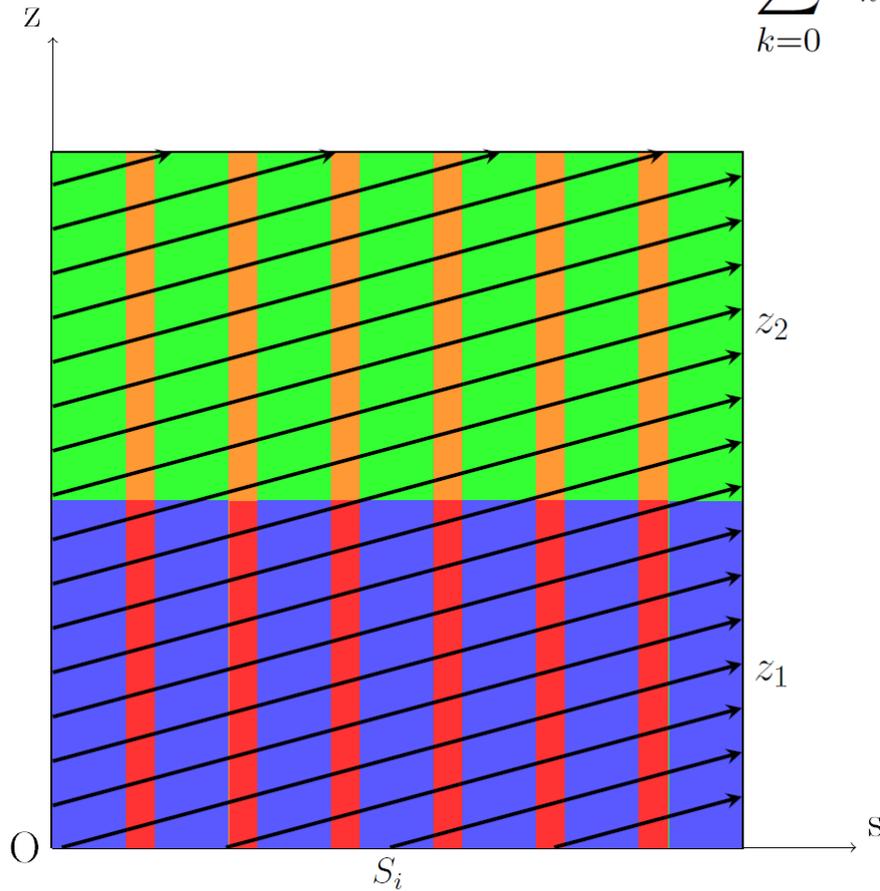
$$\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \left(1 - e^{-\Sigma_r l}\right) \cdot \frac{q_r(\vec{\Omega})}{\Sigma_r}$$

- Polynomial transmission:

$$\begin{aligned} \Psi_r(t^{out}, \vec{\Omega}) = & \Psi_r(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \\ & + \sum_{k=0}^{N_p} P_k(z^{in}) \cdot \sum_{p=k}^{N_p} c_{pk} \mu^{p-k} \left(\frac{2}{\Delta z}\right)^{p-k} E_{p-k}(\tau) \frac{\left(\vec{q}_{r,pol}(\vec{\Omega})\right)_p}{\Sigma_r} \end{aligned}$$

CHORDS CLASSIFICATION

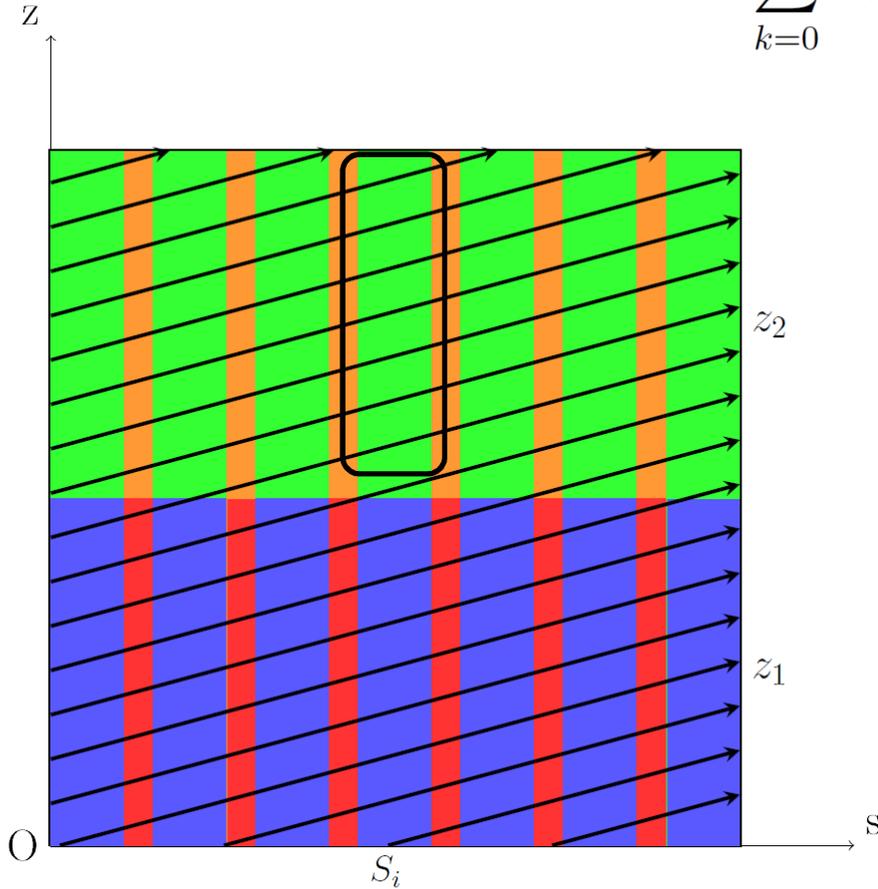
$$\Psi_r(t^{out}, \vec{\Omega}) = \Psi_r(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \sum_{k=0}^{N_p} P_k(z^{in}) \cdot \sum_{p=k}^{N_p} c_{pk} \mu^{p-k} \left(\frac{2}{\Delta z}\right)^{p-k} E_{p-k}(\tau) \frac{\left(\vec{q}_{r,pol}(\vec{\Omega})\right)_p}{\Sigma_r}$$



CHORDS CLASSIFICATION

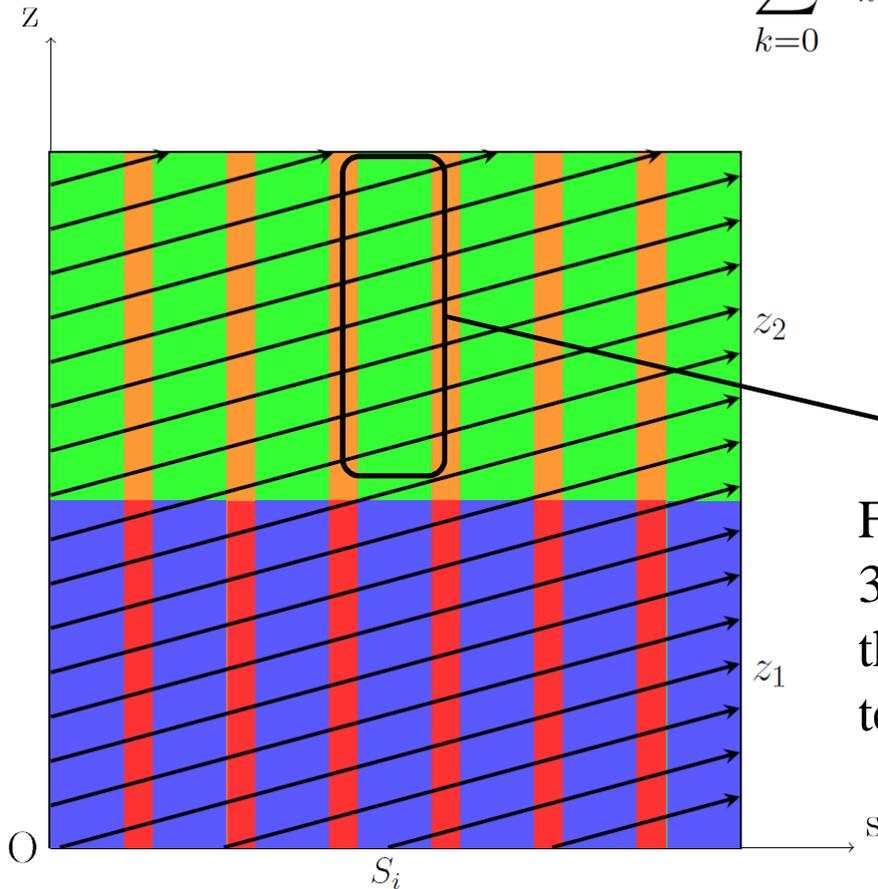
Thanks to chords classification...

$$\Psi_r(t^{out}, \vec{\Omega}) = \Psi_r(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \sum_{k=0}^{N_p} P_k(z^{in}) \cdot \sum_{p=k}^{N_p} c_{pk} \mu^{p-k} \left(\frac{2}{\Delta z}\right)^{p-k} E_{p-k}(\tau) \frac{\left(\vec{q}_{r,pol}(\vec{\Omega})\right)_p}{\Sigma_r}$$



Thanks to chords classification...

$$\Psi_r(t^{out}, \vec{\Omega}) = \Psi_r(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \sum_{k=0}^{N_p} P_k(z^{in}) \cdot \underbrace{\sum_{p=k}^{N_p} c_{pk} \mu^{p-k} \left(\frac{2}{\Delta z}\right)^{p-k} E_{p-k}(\tau) \frac{(\vec{q}_{r,pol}(\vec{\Omega}))_p}{\Sigma_r}}_{}$$



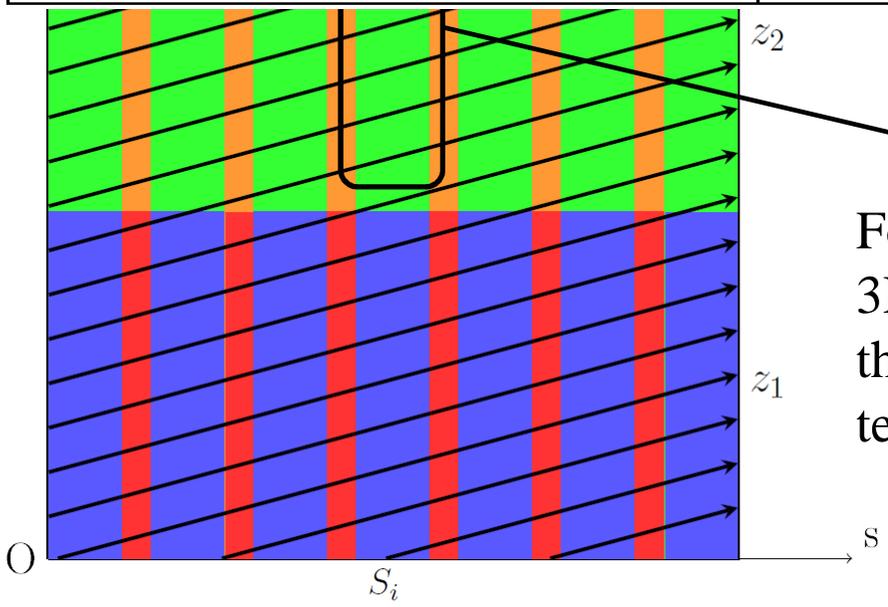
For a given angle, z-plane and 2D-chord, each 3D chords with the same length, belongs to the same class and has the same values of this term

CHORDS CLASSIFICATION

Thanks to chords classification...

$$\Psi_r(t^{out}, \vec{\Omega}) = \Psi_r(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \sum_{k=0}^{N_p} P_k(z^{in}) \cdot \underbrace{\sum_{p=k}^{N_p} c_{pk} \mu^{p-k} \left(\frac{2}{\Delta z}\right)^{p-k} E_{p-k}(\tau) \frac{(\vec{q}_{r,pol}(\vec{\Omega}))_p}{\Sigma_r}}_{\text{Term from table}}$$

● Total number of chords	10.39 M
● Number of classes	0.814 M



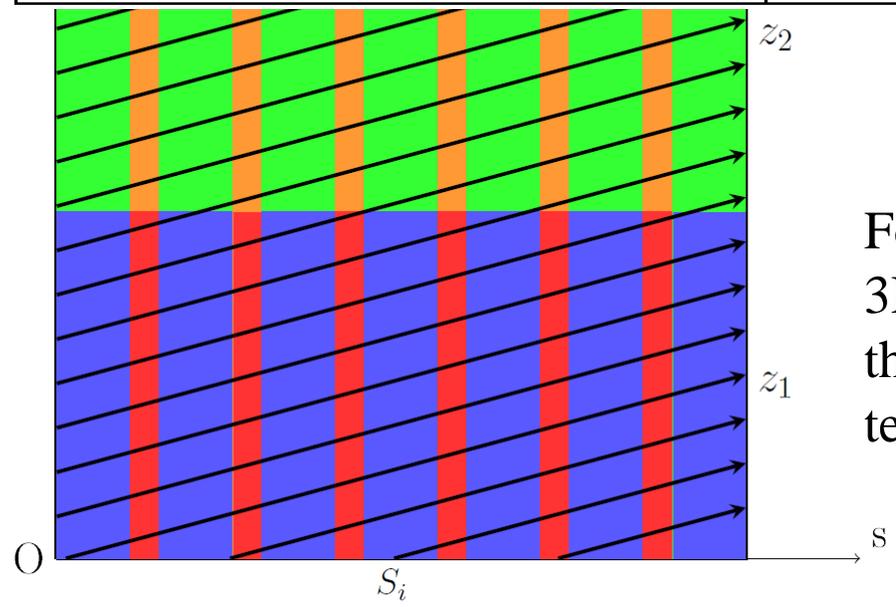
For a given angle, z-plane and 2D-chord, each 3D chords with the same length, belongs to the same class and has the same values of this term

Thanks to chords classification...

This is only computed for the ~ 8 % of chords

$$\Psi_r(t^{out}, \vec{\Omega}) = \Psi_r(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r t} + \sum_{k=0}^{N_p} P_k(z^{in}) \cdot \sum_{p=k}^{N_p} c_{pk} \mu^{p-k} \left(\frac{2}{\Delta z}\right)^{p-k} E_{p-k}(\tau) \frac{\left(\vec{q}_{r,pol}(\vec{\Omega})\right)_p}{\Sigma_r}$$

● Total number of chords	10.39 M
● Number of classes	0.814 M



For a given angle, z-plane and 2D-chord, each 3D chords with the same length, belongs to the same class and has the same values of this term

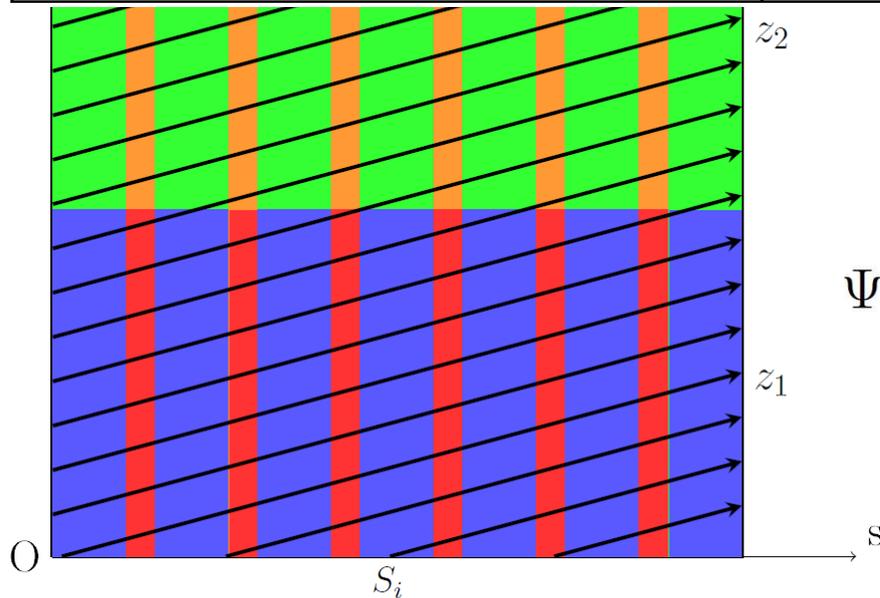
Thanks to chords classification...

This is only computed for the ~ 8 % of chords

$$\Psi_r(t^{out}, \vec{\Omega}) = \Psi_r(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \sum_{k=0}^{N_p} P_k(z^{in}) \cdot \sum_{p=k}^{N_p} c_{pk} \mu^{p-k} \left(\frac{2}{\Delta z}\right)^{p-k} E_{p-k}(\tau) \frac{(\vec{q}_{r,pol}(\vec{\Omega}))_p}{\Sigma_r}$$

z

● Total number of chords	10.39 M
● Number of classes	0.814 M



$$\Psi_r(t^{out}, \vec{\Omega}) = \Psi_r(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \vec{P}(\vec{z}^{in}) \cdot \vec{T}$$

STEP VS POLYNOMIAL

- For a fair comparison:

Step
$$\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \left(1 - e^{-\Sigma_r l}\right) \cdot \frac{q_r(\vec{\Omega})}{\Sigma_r}$$

Polynomial
$$\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \vec{P}(\vec{z}^{in}) \cdot \vec{T}$$

STEP VS POLYNOMIAL

- For a fair comparison:

Step	$\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + (1 - e^{-\Sigma_r l}) \cdot \frac{q_r(\vec{\Omega})}{\Sigma_r}$
Polynomial	$\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \vec{P}(\vec{z}^{in}) \cdot \vec{T}$

1 floating point operation

STEP VS POLYNOMIAL

- For a fair comparison:

Step $\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + (1 - e^{-\Sigma_r l}) \cdot \frac{q_r(\vec{\Omega})}{\Sigma_r}$

Polynomial

$$\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \vec{P}(\vec{z}^{in}) \cdot \vec{T}$$

N_p floating point operations

1 floating point operation

STEP VS POLYNOMIAL

- For a fair comparison:

Step $\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + (1 - e^{-\Sigma_r l}) \cdot \frac{q_r(\vec{\Omega})}{\Sigma_r}$

Polynomial $\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \vec{P}(\vec{z}^{in}) \cdot \vec{T}$

N_p floating point operations

1 floating point operation

Plus the information needed for the **balance equation**:

Step $\Psi_r(\vec{\Omega}) = \frac{1}{\Sigma_r} \left[q_r(\vec{\Omega}) - \frac{S_{\perp}}{V_r} \sum_{\substack{t \parallel \vec{\Omega} \\ t \cap r}} (\Psi(t^{out}, \vec{\Omega}) - \Psi(t^{in}, \vec{\Omega})) \right]$

STEP VS POLYNOMIAL

- For a fair comparison:

Step $\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + (1 - e^{-\Sigma_r l}) \cdot \frac{q_r(\vec{\Omega})}{\Sigma_r}$

Polynomial $\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \vec{P}(\vec{z}^{in}) \cdot \vec{T}$

N_p floating point operations

1 floating point operation

Plus the information needed for the **balance equation**:

Step $\Psi_r(\vec{\Omega}) = \frac{1}{\Sigma_r} \left[q_r(\vec{\Omega}) - \frac{S_{\perp}}{V_r} \sum_{\substack{t \parallel \vec{\Omega} \\ t \cap r}} (\Psi(t^{out}, \vec{\Omega}) - \Psi(t^{in}, \vec{\Omega})) \right]$

STEP VS POLYNOMIAL

- For a fair comparison:

Step $\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + (1 - e^{-\Sigma_r l}) \cdot \frac{q_r(\vec{\Omega})}{\Sigma_r}$

Polynomial

$$\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \vec{P}(\vec{z}^{in}) \cdot \vec{I}$$

1 floating point operation

N_p floating point operations

Plus the information needed for the **balance equation**:

Step $\Psi_r(\vec{\Omega}) = \frac{1}{\Sigma_r} \left[q_r(\vec{\Omega}) - \frac{S_{\perp}}{V_r} \sum_{\substack{t \parallel \vec{\Omega} \\ t \cap r}} (\Psi(t^{out}, \vec{\Omega}) - \Psi(t^{in}, \vec{\Omega})) \right]$

Polynomial $\tilde{\delta}_{r,p}(\vec{\Omega}) = \sum_{\substack{t \parallel \vec{\Omega} \\ t \cap r}} [P_p(\vec{z}^{out}) \cdot \Psi(t^{out}) - P_p(\vec{z}^{in}) \cdot \Psi(t^{in})]$

STEP VS POLYNOMIAL

- For a fair comparison:

Step $\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + (1 - e^{-\Sigma_r l}) \cdot \frac{q_r(\vec{\Omega})}{\Sigma_r}$

Polynomial $\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \vec{P}(\vec{z}^{in}) \cdot \vec{T}$

N_p floating point operations

1 floating point operation

Plus the information needed for the **balance equation**:

Step $\Psi_r(\vec{\Omega}) = \frac{1}{\Sigma_r} \left[q_r(\vec{\Omega}) - \frac{S_{\perp}}{V_r} \sum_{\substack{t \parallel \vec{\Omega} \\ t \cap r}} (\Psi(t^{out}, \vec{\Omega}) - \Psi(t^{in}, \vec{\Omega})) \right]$

N_p floating point operations

Polynomial $\tilde{\delta}_{r,p}(\vec{\Omega}) = \sum_{\substack{t \parallel \vec{\Omega} \\ t \cap r}} [P_p(\vec{z}^{out}) \cdot \Psi(t^{out}) - P_p(\vec{z}^{in}) \cdot \Psi(t^{in})]$

STEP VS POLYNOMIAL

- For a fair comparison:

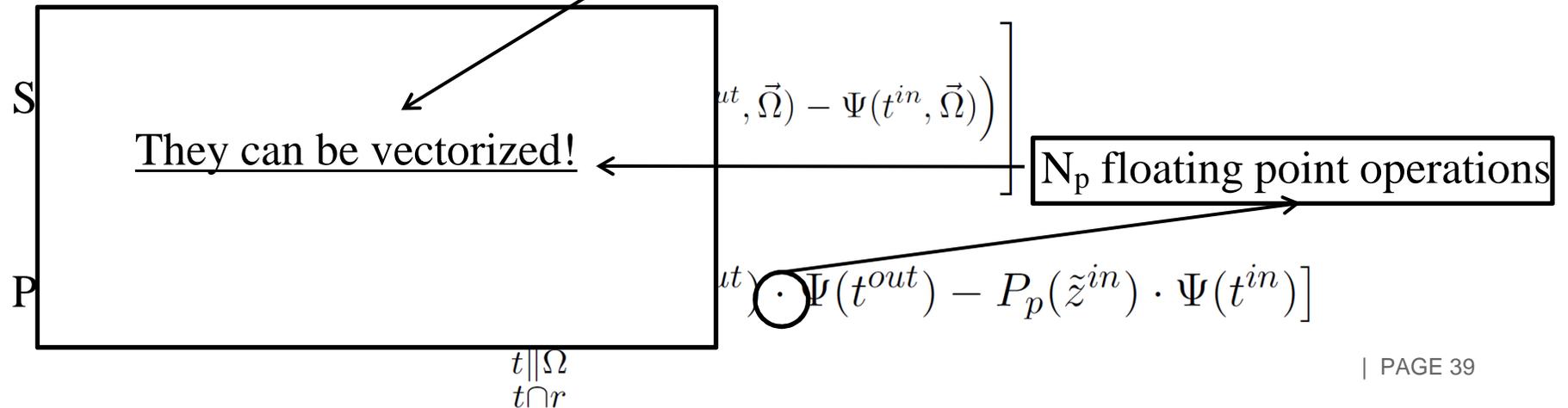
Step $\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + (1 - e^{-\Sigma_r l}) \odot \frac{q_r(\vec{\Omega})}{\Sigma_r}$

Polynomial $\Psi(t^{out}, \vec{\Omega}) = \Psi(t^{in}, \vec{\Omega}) \cdot e^{-\Sigma_r l} + \vec{P}(\vec{z}^{in}) \odot \vec{T}$

1 floating point operation

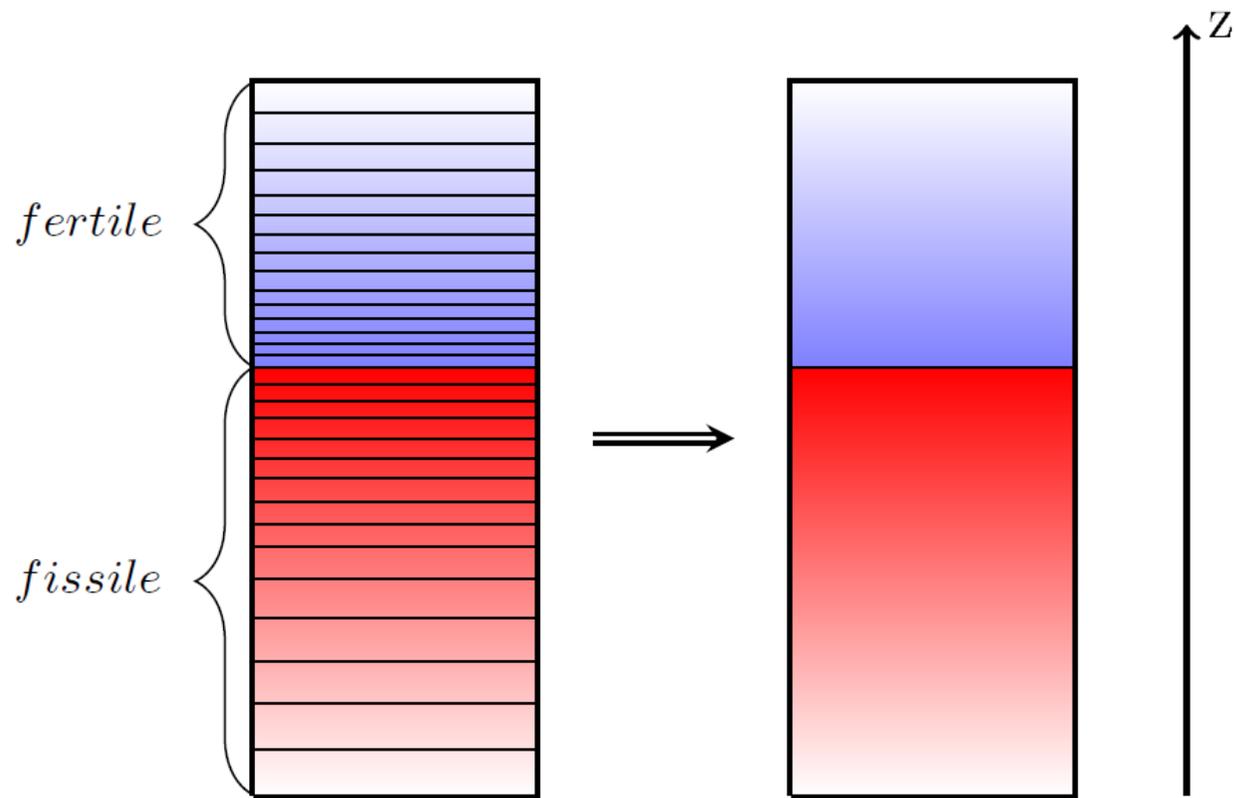
N_p floating point operations

Plus the information needed for the **balance equation**:



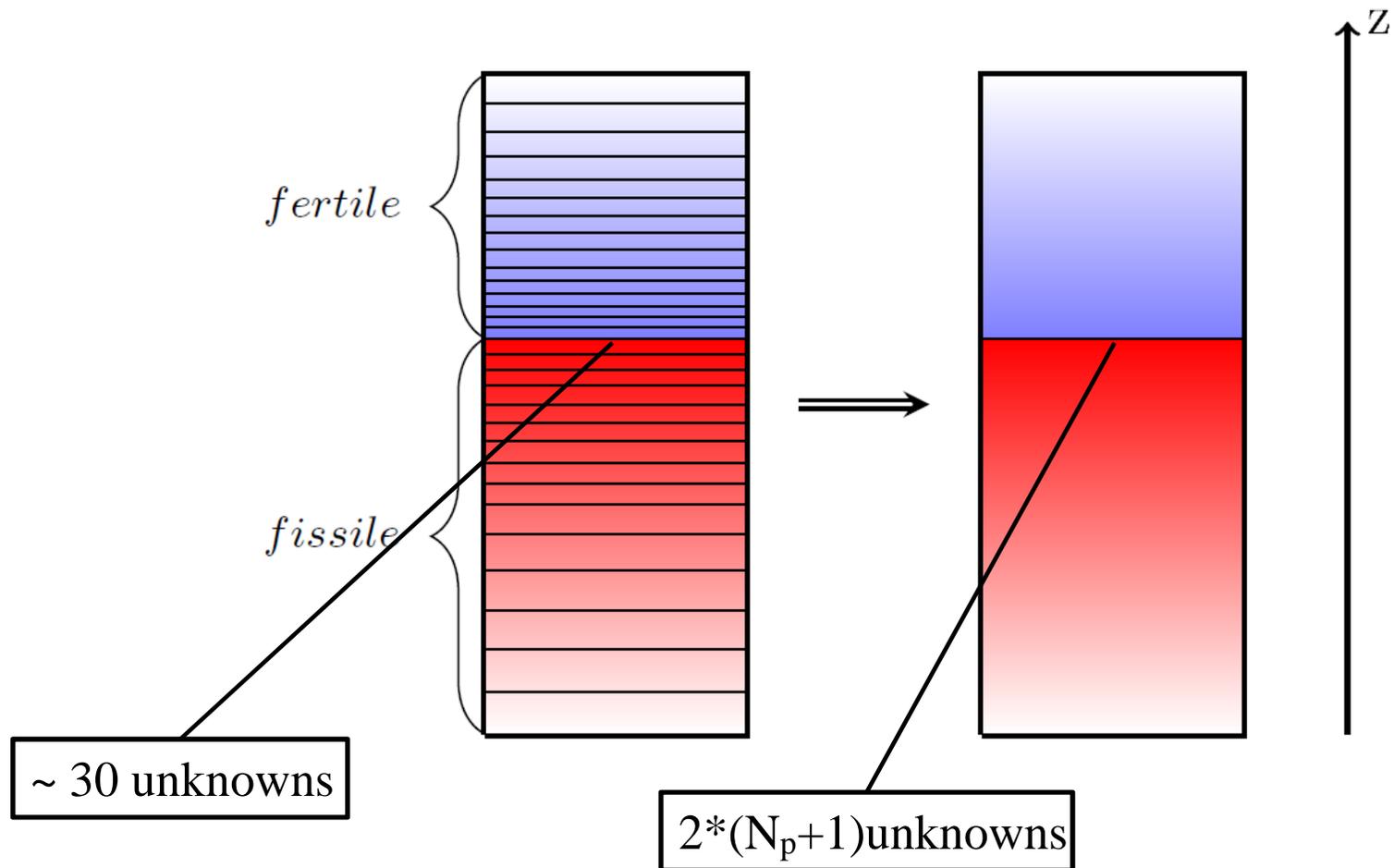
AXIAL DISCRETIZATION

Difference between the axial discretization needed in the Step Constant and in the Polynomial case:



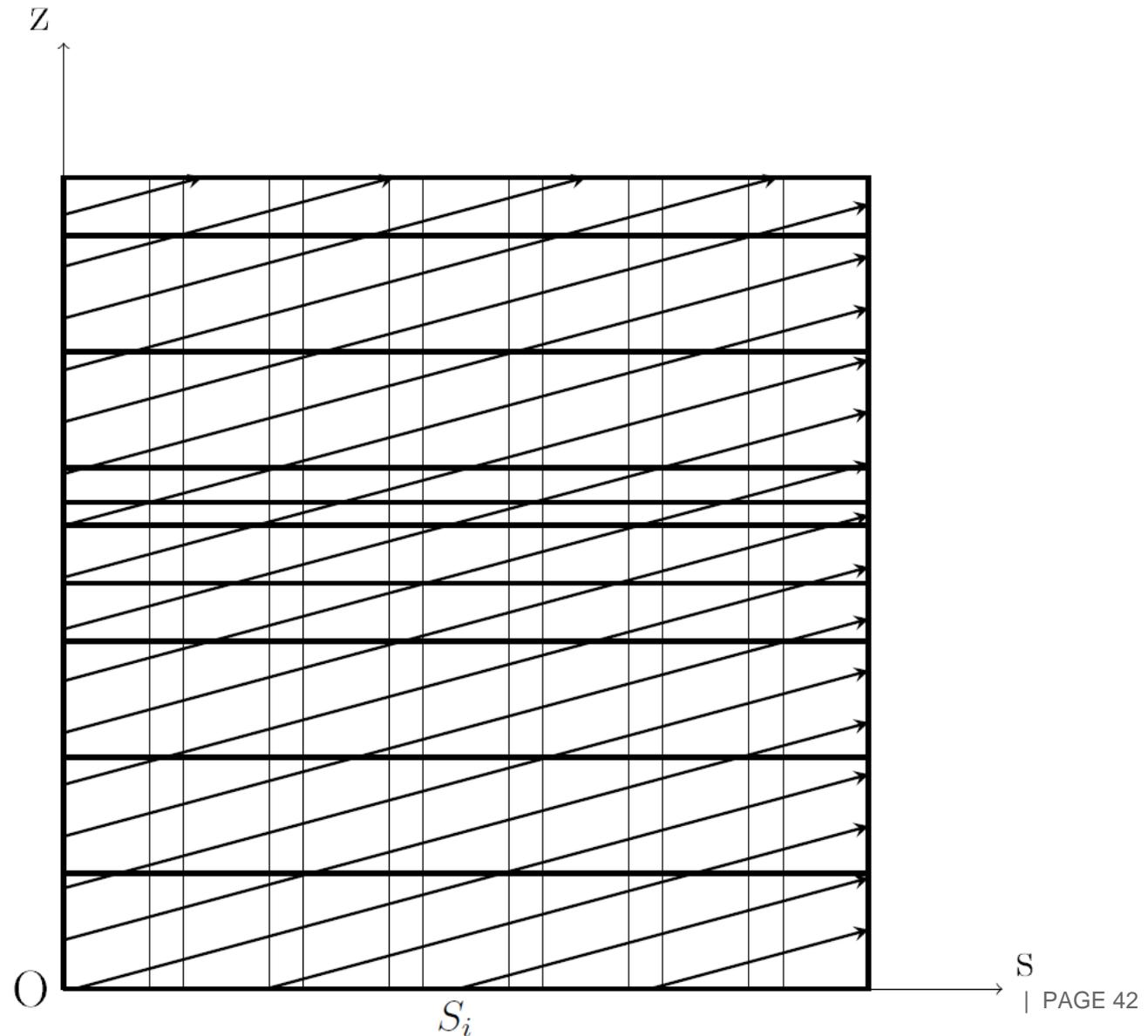
AXIAL DISCRETIZATION

Difference between the axial discretization needed in the Step Constant and in the Polynomial case:



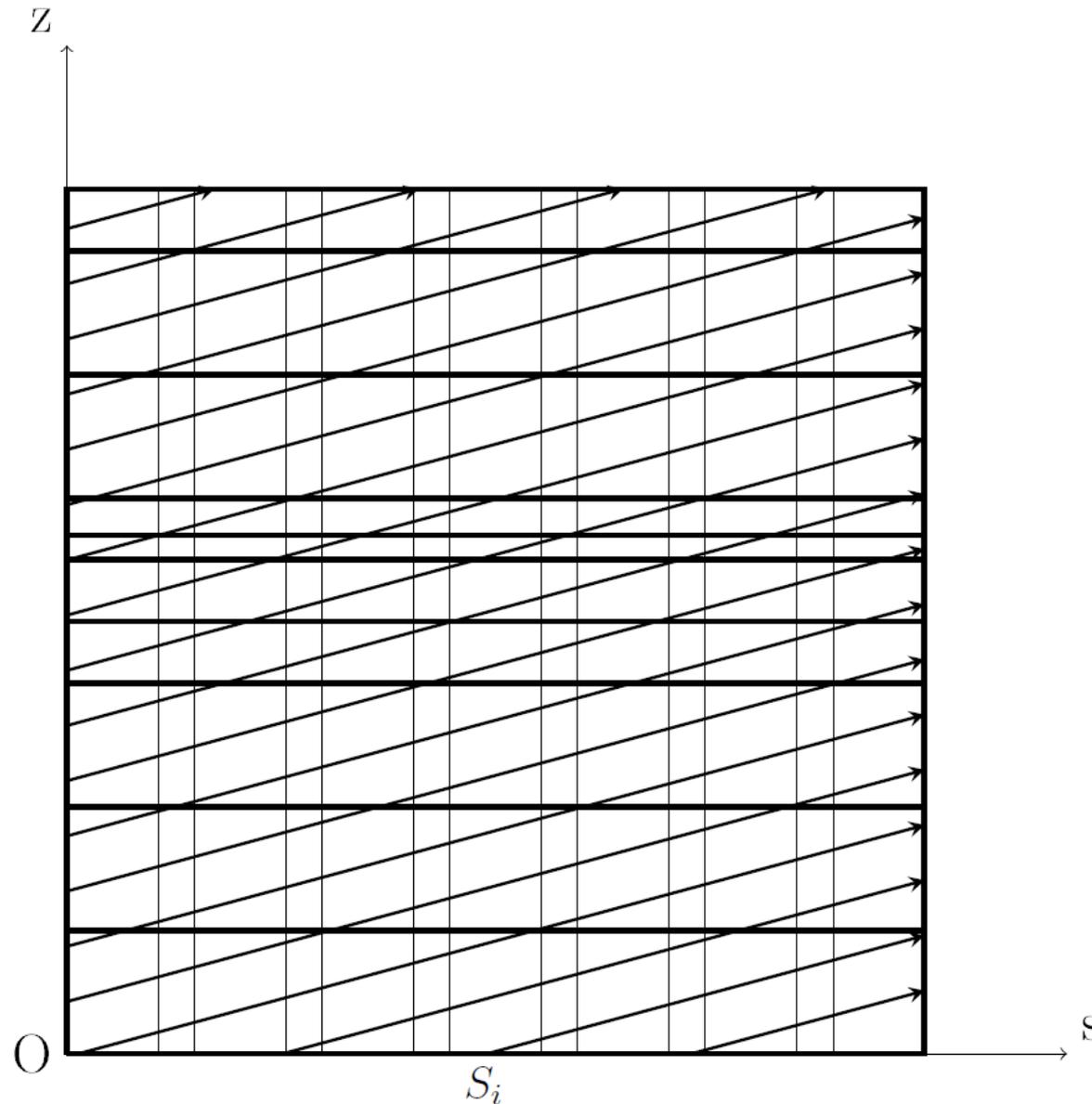
FINAL CONSIDERATIONS

- Higher numbers of floating point operations per chord



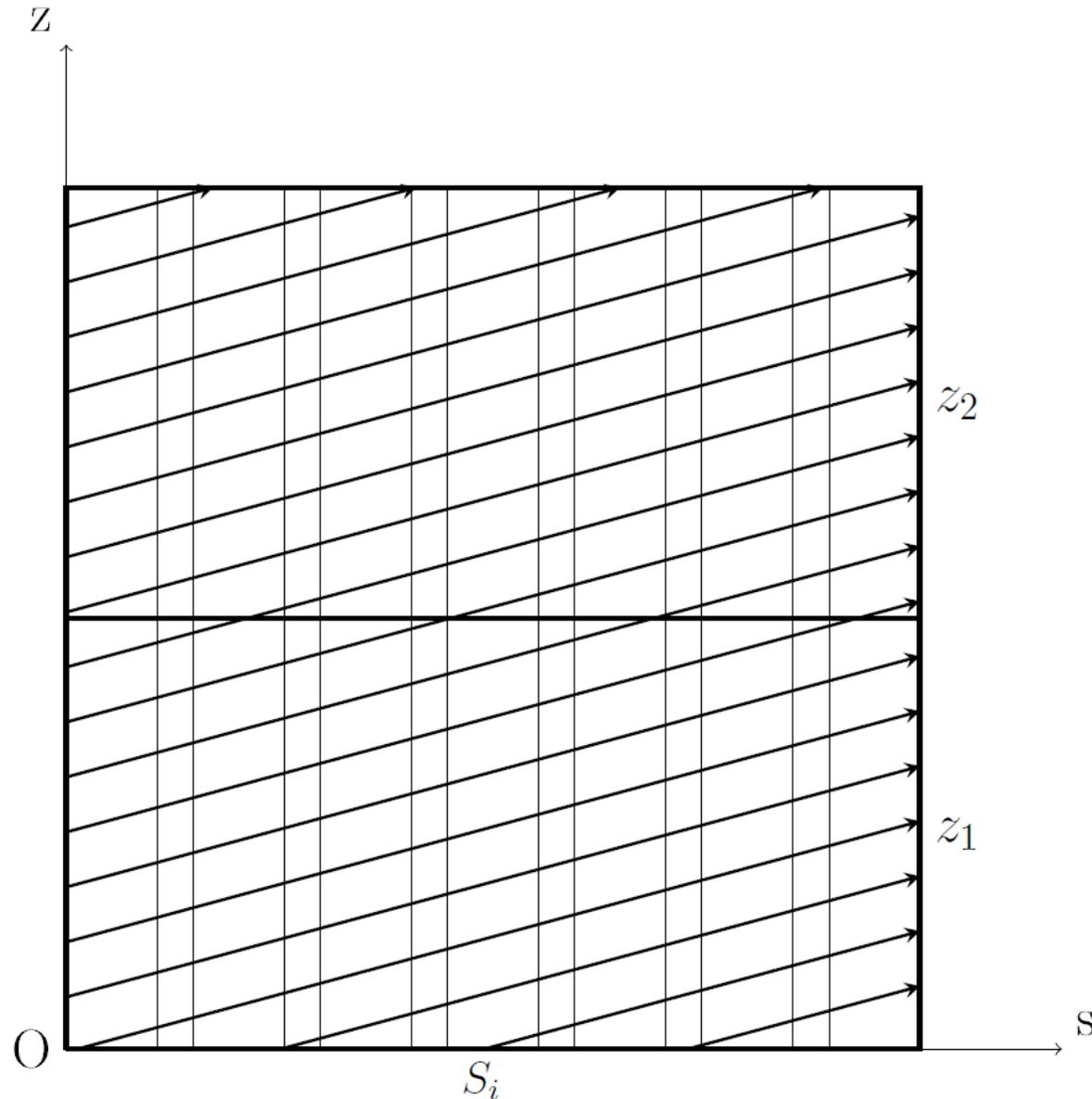
FINAL CONSIDERATIONS

- Higher numbers of floating point operations per chord
- Some of them can be vectorized



FINAL CONSIDERATIONS

- Higher numbers of floating point operations per chord
- Some of them can be vectorized
- Less axial planes also means less chords ($\sim -15\%$)
- Less memory needed



POLYNOMIAL VS STEP: RESULTS 2

Method	Step					Polynomial ($N_p=2$)		
Δr (cm)	0.05					0.05		
Δs (cm)	1.0					1.0	0.5	
Axial meshes	57	110	180	257	600	5	6	12
# chords	29.57 M	31.88 M	34.93 M	38.29 M	53.24 M	27.31 M	27.35 M	55.24 M
# classes	17.07 M	21.12 M	21.80 M	20.33 M	18.16 M	1.90 M	2.28 M	4.57 M
Classification	83.82 %	74.67 %	66.68 %	59.56 %	52.39 %	98.4 %	98.09 %	96.21 %
Self-shielding	Tone:							
k_{eff}	1.163761	1.165075	1.165412	1.165672	1.165744	1.165584	1.165805	1.165801
ρ err/T4 (PCM)	-96.45	+0.44	+25.43	+44.66	+49.72	+37.76	+54.00	+53.92
Time	12 210 s	22 719 s	37 785 s	55 472 s	127 809 s	15 384 s	16 326 s	34 775 s
Self-shielding	Sub-Groups:							
k_{eff}	1.164114	1.16543	1.165767	1.166027	1.166094	1.165927	1.166147	1.166154
ρ err/T4 (PCM)	-70.54	+26.38	+ 51.22	+70.28	+75.42	+ 63.01	+ 79.27	+79.72
Time	12 575 s	24 031 s	38 454 s	56 500 s	124 470 s	16 174 s	17 316 s	50 620 s

- An impressive gain in computational meshes is obtained

Self-shielding effect		
	k_{eff}	δk_{eff}
NO self-shielding	1.093190	-2932 PCM
Sub-Groups method	1.127149	+84 PCM
Tone method	1.126910	+62 PCM

Table 5: Self-shielding effect for the full-column case in nominal conditions. δk_{eff} refers to the relative error (in PCM) with respect to the reference Tripoli4 calculation. Nominal conditions.

Acceleration effectiveness			
Acc./Free	DP_1 polynomial order		
	0	1	2
Time	0.16	–	0.06
Outers	0.66	–	0.11
Inners	0.11	–	0.02
Memory	1.96	–	10.06

Table 6: Ratios of times, number of iterations and memory footprint between accelerated calculations and free iterations for varying order of the spatial polynomial order of the DP_1 operator. The case considered is the full-column assembly in nominal conditions.

- A factor 20 of computational time reduction can be obtained but there is a memory price to pay. (Work on it is under way!)
- NOTE: All micro/macro-scopic reaction rate errors are below 1%

- Polynomial MOC is on the way
- Classifications of chords is of fundamental importance
- Dpn acceleration works but it is memory expensive
- Many ways are possible for memory reduction
- How about XS?

1. Sanchez, R. (2012), 'Prospects in deterministic three-dimensional whole-core transport calculations' Nuclear Engineering and Technology 44(5), 113-150.
2. W. Boyd, A. Siegel, S. He, B. Forget and K. Smith: "Parallel performance results for the OpenMOC method of characteristic code on multi-core platforms", <http://dx.doi.org/10.1177/1094342016630388> International Journal of High Performance Computing Applications, February 15, 2016.
3. D.Sciannandrone, , S. Santandrea, R.Sanchez: "Optimized tracking strategies for step MOC calculations in extruded 3D axial geometries", Ann. Nucl. Energy Vol.87 49-60 (2016) <http://dx.doi.org/10.1016/j.anucene.2015.05.014>.
4. Santandrea S., Sciannandrone D., Sanchez R., Mao L. and Graziano L.: " A neutron transport characteristics method for 3D axially extruded geometries coupled with a fine group self-shielded environment", published in NSE 2017
5. Santandrea S., Graziano L & Sciannandrone D.: "Accelerated Polynomial axial expansions for full 3D neutron transport MOC in the APOLLO3R code system as applied to the ASTRID fast breeder reactor » published ANE 2018

MOC 1 : BASIC ITERATIVE SCHEME

□ *scattering term expansion* $q(\mathbf{r}, \Omega) \sim \sum_i q_i(\Omega) \theta_i(\mathbf{r})$

$$q_i(\Omega) = \underbrace{\sum_{k=0}^K \Sigma_{sk,i} \sum_{l=-k}^k \phi_{k,i}^l A_k^l(\Omega)}_{\text{scattering}} + \underbrace{S_i(\Omega)}_{\text{external source}}$$

□ *cell averaged angular flux moments*

$$\phi_{k,i}^l = \frac{1}{4\pi} \int_{(4\pi)} d\Omega A_k^l(\Omega) \psi_i(\Omega) \sim \sum_n w_n A_k^l(\Omega_n) \psi_i(\Omega_n)$$

- *positive method*
- *no fix-up is necessary*
- *arbitrary anisotropy order*

□ Synthetic acceleration

- *perform a free iteration*

$$\begin{pmatrix} \Phi^{(n)} \\ J_+^{(n)} \end{pmatrix} \rightarrow \begin{pmatrix} \Phi_{free}^{(n+1)} \\ J_{+,free}^{(n+1)} \end{pmatrix}$$

- *solve synthetic acceleration for*

$$D \begin{pmatrix} \delta\Phi^{(n)} \\ \delta J_+^{(n)} \end{pmatrix} = H \begin{pmatrix} \Phi_{free}^{(n+1)} - \Phi_{free}^{(n)} \\ J_{+,free}^{(n+1)} - J_{+,free}^{(n)} \end{pmatrix}$$

- *correct free iteration values*

$$\Phi_{acce}^{(n+1)} = \Phi_{free}^{(n+1)} + \delta\Phi$$

$$J_{+,acce}^{(n+1)} = J_{+,free}^{(n+1)} + \delta J_+$$

- *this approach can be extended from inhomogeneous to eigenvalue problems*

- *transmission and escape first flight probabilities (symmetry and conservation preserved by numerical scheme) for SC method:*

$$T_{\alpha\beta}^{\rho\nu} = T_{\beta\alpha}^{\rho\nu} = \int_{\alpha} dS \int_{\beta \rightarrow \alpha} d\Omega A^{\rho}(\boldsymbol{\Omega}) A^{\nu}(\boldsymbol{\Omega}) |\mathbf{n} \cdot \boldsymbol{\Omega}| e^{-\Sigma_i R(\mathbf{r}, \boldsymbol{\Omega})} \quad (\text{symmetry})$$

$$E_{\alpha}^{\rho\nu} = \frac{1}{\sum_i V_i} \left(A_{\alpha}^{\rho\nu} - \sum_{\alpha \in \partial i} T_{\alpha\beta}^{\rho\nu} \right) \quad (\text{conservation})$$

- *similar formulas can be written for the Linear Surface method.*
- *numerical evaluation (coherence with transport)*

$$T_{\alpha\beta}^{\rho\nu} \sim \sum_{\Omega} w_{\Omega} A^{\rho}(\boldsymbol{\Omega}) A^{\nu}(\boldsymbol{\Omega}) \sum_{(t, \boldsymbol{\Omega}) \in \beta \rightarrow \alpha} w_{\perp}(t, \boldsymbol{\Omega}) e^{-\Sigma_i R(t, \boldsymbol{\Omega})}$$

- *after elimination of cell fluxes, the DP_N acceleration equations are solved iteratively for the currents*

$$\vec{J}_{+, \alpha} = \sum_{\beta \in \partial i} \hat{T} \vec{J}_{-, \beta} + \vec{J}_S$$

$$\hat{T}_{\alpha\beta}^{\rho\nu} = T_{\alpha\beta}^{\rho\nu} + E_{\alpha}^{\rho 0} \frac{\Sigma_i V_i \Sigma_{si}}{\Sigma_{ai} + E^{00} \Sigma_{si}} E_{\beta}^{0\nu} S^{\nu} \quad \text{generalized transmission}$$

related to multicollisional processes

- *solution with a Krilov iterator (BCGS or GMRES):* $M \vec{\psi} = \vec{S}$

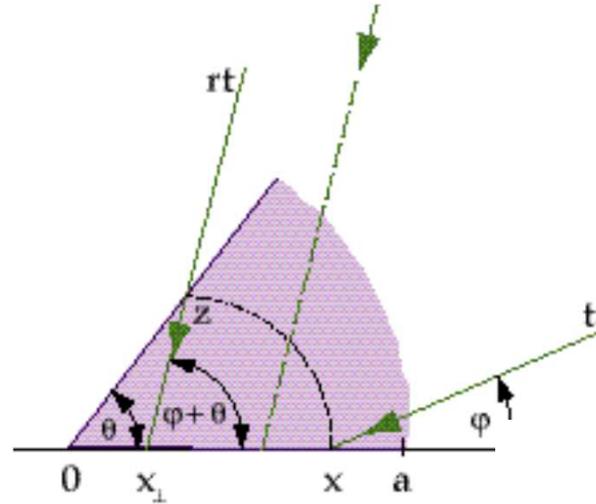
iterator : $M = 1 - \hat{T}$

with an adapted ILU0 and domain decomposition method.

MOC 3 : BOUNDARY CONDITIONS

Adapted tracking is done to exactly take into account symmetries and boundary conditions

$p / 2$ rotation



Cyclic tracking for infinite periodic systems

