Multigrid discontinuous Galerkin method for multigroup particle transport

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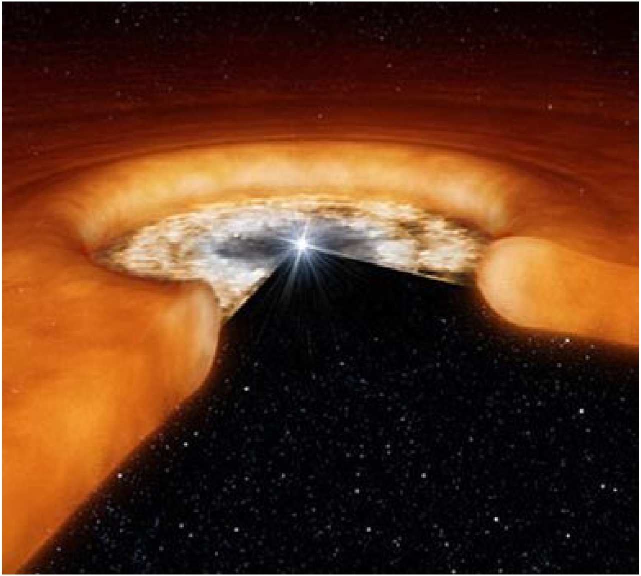
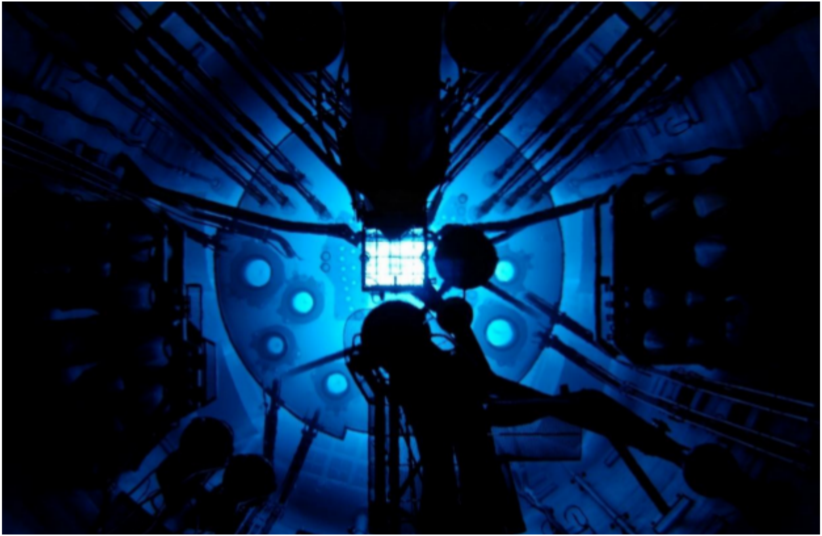
Radiative transfer in astrophysics

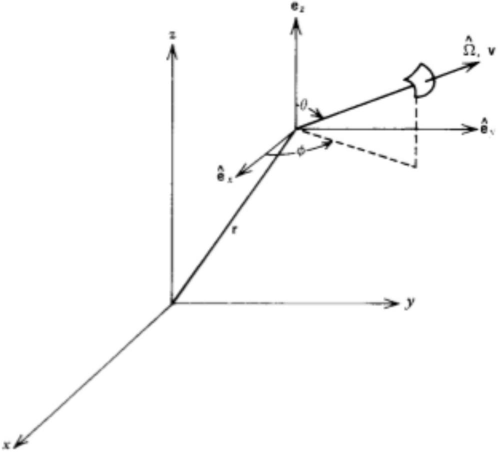


Radiative transfer in climatology

Radiative transfer in neutron and gamma transport



Particle density description



Transport equation

$$\boldsymbol{\Omega} = (\psi, \phi) \qquad \Psi = \Psi(\boldsymbol{\Omega}, E, \boldsymbol{x}) \qquad \Psi' = \Psi(\boldsymbol{\Omega}', E', \boldsymbol{x})$$

$$\sigma_T = \sigma_T(E, \boldsymbol{x}) \quad \sigma_{s(\boldsymbol{\Omega}', E')} = \sigma_s(\boldsymbol{\Omega}' \to \boldsymbol{\Omega}, E' \to E, \boldsymbol{x}) \quad q = q(\boldsymbol{\Omega}, E, \boldsymbol{x})$$

Transport equation

$$\boxed{\boldsymbol{\Omega} \cdot \nabla \Psi + \sigma_T \Psi - \int_0^{E_{max}} \int_S \sigma_{s(\boldsymbol{\Omega}', E')} \Psi' d\boldsymbol{\Omega}' dE' = q,}$$

$$\forall (\boldsymbol{\Omega}, E, \boldsymbol{x}) \in S \times (0, E_{max}] \times \mathcal{D}$$

Boundary condition

$$\boxed{\Psi(\boldsymbol{\Omega}, E) = 0 \qquad \forall (\boldsymbol{\Omega}, E) \in S \times (0, E_{max}] \times \partial \mathcal{D}, \boldsymbol{\Omega} \cdot \mathbf{n} < 0}$$

Transport equation with fission

$$\nu\sigma_f' = \nu\sigma_f(E') \qquad \chi = \chi(E)$$

Transport equation

$$\boxed{\mathbf{\Omega}\cdot\nabla\Psi + \sigma_T\Psi - \int_0^{E_{max}}\int_S \sigma_{s(\mathbf{\Omega}',E')}\Psi' d\mathbf{\Omega}' dE' - \chi\int_0^{E_{max}} \nu\sigma_f'\Psi' dE' = q}$$

Eigenvalue problem

$$\boxed{\mathbf{\Omega}\cdot\nabla\Psi + \sigma_T\Psi - \int_0^{E_{max}}\int_S \sigma_{s(\mathbf{\Omega}',E')}\Psi' d\mathbf{\Omega}' dE' = \frac{1}{k_{eff}}\chi\int_0^{E_{max}} \nu\sigma_f'\Psi' dE'}$$

Diffusion approximation

$$\boldsymbol{J} = \boldsymbol{J}(E, \boldsymbol{x}) = \int_S \boldsymbol{\Omega} \Psi d\boldsymbol{\Omega} \qquad \Phi = \Phi(E, \boldsymbol{x}) = \int_S \Psi d\boldsymbol{\Omega}$$

$$\boldsymbol{\Omega} \cdot \nabla \Psi = \nabla \cdot (\boldsymbol{\Omega} \Psi) = \nabla \cdot \boldsymbol{J} \qquad \boldsymbol{J} \approx -D(E, \boldsymbol{x}) \nabla \Phi$$

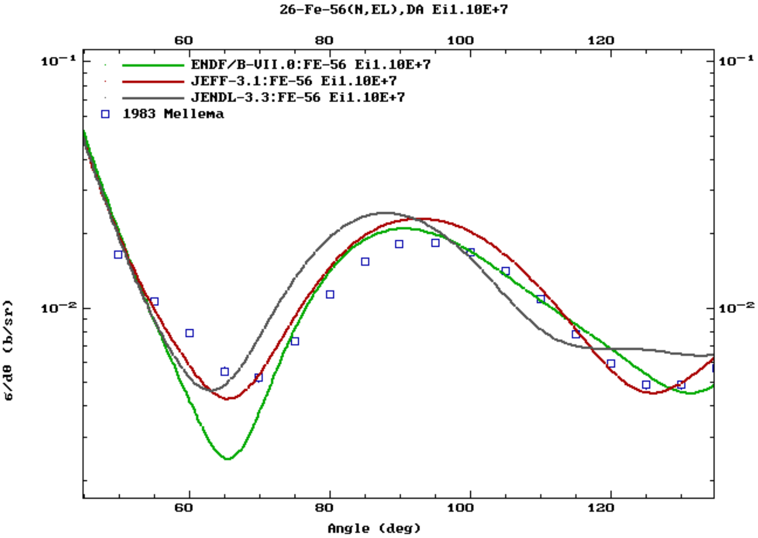
Diffusion equation

$$\boxed{-\nabla \cdot (D \nabla \Phi) + \sigma_T \Phi - \int_0^{E_{max}} \sigma_{s(E')} \Phi' dE' = q}$$

$$\boxed{-\nabla \cdot (D \nabla \Phi) + \sigma_T \Phi - \int_0^{E_{max}} \sigma_{s(E')} \Phi' dE' - \chi \int_0^{E_{max}} \nu \sigma_f' \Phi' dE' = q}$$

$$\boxed{-\nabla \cdot (D \nabla \Phi) + \sigma_T \Phi - \int_0^{E_{max}} \sigma_{s(E')} \Phi' dE' = \frac{1}{k_{eff}} \chi \int_0^{E_{max}} \nu \sigma_f' \Phi' dE'}$$

Angle description



Angle collocation S_n

$$\boxed{\boldsymbol{\Omega}\cdot\nabla\Psi+\sigma_T\Psi-\int_0^{E_{max}}\int_S\sigma_{s(\boldsymbol{\Omega}',E')}\Psi' d\boldsymbol{\Omega}' dE' = q,}$$

$$\Psi_i = \Psi(\boldsymbol{\Omega}_i, E, \boldsymbol{x}) \qquad \Psi_{i'} = \Psi(\boldsymbol{\Omega}_{i'}, E', \boldsymbol{x})$$

$$\sigma_{s(E')}^{i'i} = \sigma_s(\boldsymbol{\Omega}_{i'} \to \boldsymbol{\Omega}_i, E' \to E, \boldsymbol{x}) \qquad q_i = q(\boldsymbol{\Omega}_i, E, \boldsymbol{x})$$

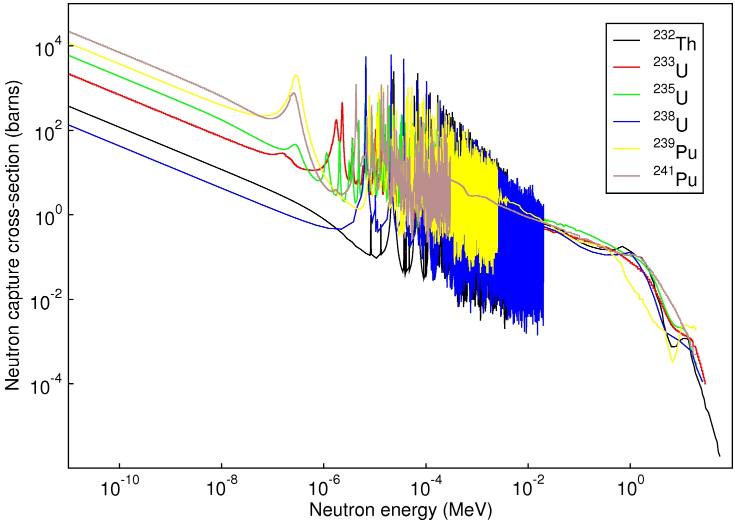
$$\int_0^{E_{max}}\int_S\sigma_{s(\boldsymbol{\Omega}',E')}\Psi' d\boldsymbol{\Omega}' dE' \approx \int_0^{E_{max}}\sum_{i'=1}^{n}\omega_{i'}\sigma_{s(E')}^{i'i}\Psi_{i'} dE'$$

Angle collocation S_n

$$\boxed{\boldsymbol{\Omega} \cdot \nabla\Psi + \sigma_T \Psi - \int_0^{E_{max}} \int_S \sigma_{s(\boldsymbol{\Omega}',E')} \Psi' d\boldsymbol{\Omega}' dE' = q,}$$

$$\begin{cases}
\boldsymbol{\Omega}_1 \cdot \nabla\Psi_1 + \sigma_T \Psi_1 - \int_0^{E_{max}} \sum_{i'=1}^{n} \omega_{i'} \sigma_{s(E')}^{i'1} \Psi_{i'} dE' = q_1 \\
\dots \\
\boldsymbol{\Omega}_i \cdot \nabla\Psi_i + \sigma_T \Psi_i - \int_0^{E_{max}} \sum_{i'=1}^{n} \omega_{i'} \sigma_{s(E')}^{i'i} \Psi_{i'} dE' = q_i \\
\dots \\
\boldsymbol{\Omega}_n \cdot \nabla\Psi_n + \sigma_T \Psi_n - \int_0^{E_{max}} \sum_{i'=1}^{n} \omega_{i'} \sigma_{s(E')}^{i'n} \Psi_{i'} dE' = q_n
\end{cases}$$

Multigroup



Neutron capture cross-section (barns)
Neutron energy (MeV)
10^{4}
10^{2}
10^{0}
10^{-2}
10^{-4}
10^{-10}
10^{-8}
10^{-6}
10^{-4}
10^{-2}
10^{0}
^{232}Th
^{233}U
^{235}U
^{238}U
^{239}Pu
^{241}Pu

Multigroup

$$\boxed{\boldsymbol{\Omega}_i \cdot \nabla \Psi_i + \sigma_T \Psi_i - \int_0^{E_{max}} \sum_{i'=1}^{n} \omega_{i'} \sigma_{s(E')}^{i'i} \Psi_{i'} dE' = q_i,}$$

$$(0, E_{max}] = (0, E_1] \cup \ldots \cup (E_{g-1}, E_g] \cup \ldots \cup (E_{G-1}, E_{max}]$$

$$\Psi_{i,g} = \int_{E_{g-1}}^{E_g} \Psi(\boldsymbol{\Omega}_i, E, \boldsymbol{x}) dE \qquad \sigma_T^{i,g} = \frac{\int_{E_{g-1}}^{E_g} \sigma_T(E, \boldsymbol{x}) dE}{\Psi_{i,g}}$$

$$\sigma_s^{i'i,g'g} = \frac{\int_{E_{g-1}}^{E_g} \int_0^{E_{max}} \sum_{i'=1}^{n} \omega_{i'} \sigma_{s(E')}^{i'i} \Psi_{i'} dE' dE}{\Psi_{i,g'}}$$

Multigroup

$$\boxed{\mathbf{\Omega}_i \cdot \nabla \Psi_i + \sigma_T \Psi_i - \int_0^{E_{max}} \sum_{i'=1}^{n} \omega_{i'} \sigma_{s(E')}^{i' i} \Psi_{i',g'} dE' = q_i,}$$

$$\begin{cases} \mathbf{\Omega}_i \cdot \nabla \Psi_{i,1} + \sigma_{T,1} \Psi_{i,1} - \sum_{g'=1}^{G} \sum_{i'=1}^{n} \omega_{i'} \sigma_s^{i' i, g' 1} \Psi_{i',g'} = q_{i,1} \\ \dots \\ \mathbf{\Omega}_i \cdot \nabla \Psi_{i,g} + \sigma_{T,g} \Psi_{i,g} - \sum_{g'=1}^{G} \sum_{i'=1}^{n} \omega_{i'} \sigma_s^{i' i, g' g} \Psi_{i',g'} = q_{i,g} \\ \dots \\ \mathbf{\Omega}_i \cdot \nabla \Psi_{i,G} + \sigma_{T,G} \Psi_{i,G} - \sum_{g'=1}^{G} \sum_{i'=1}^{n} \omega_{i'} \sigma_s^{i' i, g' G} \Psi_{i',g'} = q_{i,G} \end{cases}$$

Discrete angle and energy system

$$
\begin{bmatrix}
\begin{bmatrix} 1,1 & \dots & i',1 & \dots & n,1 \\ \dots & \dots & i',1 & \dots & \dots \\ 1,i & \dots & i',i & \dots & n,i \\ \dots & \dots & i',1 & \dots & \dots \\ 1,n & \dots & i',1 & \dots & n,n \end{bmatrix}_{1,1} & \dots & \begin{bmatrix} 1,1 & \dots & i',1 & \dots & n,1 \\ \dots & \dots & i',1 & \dots & \dots \\ 1,i & \dots & i',i & \dots & n,i \\ \dots & \dots & i',1 & \dots & \dots \\ 1,n & \dots & i',1 & \dots & n,n \end{bmatrix}_{g',1} & \dots & \begin{bmatrix} 1,1 & \dots & i',1 & \dots & n,1 \\ \dots & \dots & i',1 & \dots & \dots \\ 1,i & \dots & i',i & \dots & n,i \\ \dots & \dots & i',1 & \dots & \dots \\ 1,n & \dots & i',1 & \dots & n,n \end{bmatrix}_{G,1} \\
\dots & \dots & \dots & \dots & \dots \\
\begin{bmatrix} 1,1 & \dots & i',1 & \dots & n,1 \\ \dots & \dots & i',1 & \dots & \dots \\ 1,i & \dots & i',i & \dots & n,i \\ \dots & \dots & i',1 & \dots & \dots \\ 1,n & \dots & i',1 & \dots & n,n \end{bmatrix}_{1,g} & \dots & \begin{bmatrix} 1,1 & \dots & i',1 & \dots & n,1 \\ \dots & \dots & i',1 & \dots & \dots \\ 1,i & \dots & i',i & \dots & n,i \\ \dots & \dots & i',1 & \dots & \dots \\ 1,n & \dots & i',1 & \dots & n,n \end{bmatrix}_{g',g} & \dots & \begin{bmatrix} 1,1 & \dots & i',1 & \dots & n,1 \\ \dots & \dots & i',1 & \dots & \dots \\ 1,i & \dots & i',i & \dots & n,i \\ \dots & \dots & i',1 & \dots & \dots \\ 1,n & \dots & i',1 & \dots & n,n \end{bmatrix}_{G,g} \\
\dots & \dots & \dots & \dots & \dots \\
\begin{bmatrix} 1,1 & \dots & i',1 & \dots & n,1 \\ \dots & \dots & i',1 & \dots & \dots \\ 1,i & \dots & i',i & \dots & n,i \\ \dots & \dots & i',1 & \dots & \dots \\ 1,n & \dots & i',1 & \dots & n,n \end{bmatrix}_{1,G} & \dots & \begin{bmatrix} 1,1 & \dots & i',1 & \dots & n,1 \\ \dots & \dots & i',1 & \dots & \dots \\ 1,i & \dots & i',i & \dots & n,i \\ \dots & \dots & i',1 & \dots & \dots \\ 1,n & \dots & i',1 & \dots & n,n \end{bmatrix}_{g',G} & \dots & \begin{bmatrix} 1,1 & \dots & i',1 & \dots & n,1 \\ \dots & \dots & i',1 & \dots & \dots \\ 1,i & \dots & i',i & \dots & n,i \\ \dots & \dots & i',1 & \dots & \dots \\ 1,n & \dots & i',1 & \dots & n,n \end{bmatrix}_{G,G}
\end{bmatrix}
$$

Discontinuous Galerkin finite elements

$$\boxed{\boldsymbol{\Omega}_i \cdot \nabla \Psi_{i,g}(\boldsymbol{x}) + \sigma_{T,g}(\boldsymbol{x})\Psi_{i,g}(\boldsymbol{x}) - \sum_{g'=1}^{G}\sum_{i'=1}^{n} \omega_{i'}\sigma_s^{i'i,g'g}(\boldsymbol{x})\Psi_{i',g'}(\boldsymbol{x}) = q_{i,g}(\boldsymbol{x})}$$

$$V_h = \left\{ v \in L^2(\mathcal{D}) \,\middle|\, v_{|K} \in P_K \right\}$$

$$\{\!\{v\}\!\} := \frac{v_1 + v_2}{2} \qquad \{\!\{v\boldsymbol{n}\}\!\} := \frac{v_1\boldsymbol{n}_1 + v_2\boldsymbol{n}_2}{2}$$

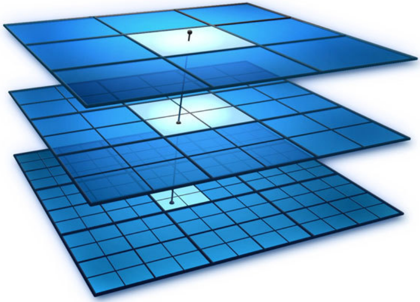
Discontinuous Galerkin finite elements

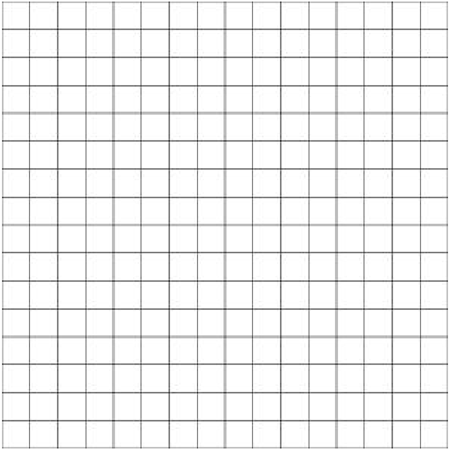
$$a_h(\psi, v) = \sum_{K\in\mathbb{T}_h} \sum_{g=1}^{G} \sum_{i=1}^{n} \omega_i \int_K \left(\boldsymbol{\Omega}_i \cdot \nabla \psi_{i,g} + \sigma_{T,g}\psi_{i,g} - \sum_{g'=1}^{G} \sum_{i'=1}^{n} \omega_{i'} \sigma_s^{i'i,g'g} \psi_{i',g'} \right) v_{i,g} d\boldsymbol{x}$$

$$+ \sum_{F\in\mathbb{F}_h^b} \sum_{g=1}^{G} \sum_{\boldsymbol{\Omega}_i\cdot\boldsymbol{n}\leq 0} \omega_i \int_F \left|\boldsymbol{\Omega}_i \cdot \boldsymbol{n}\right| \psi_i v_i d\boldsymbol{x} + b_h(\psi, v)$$

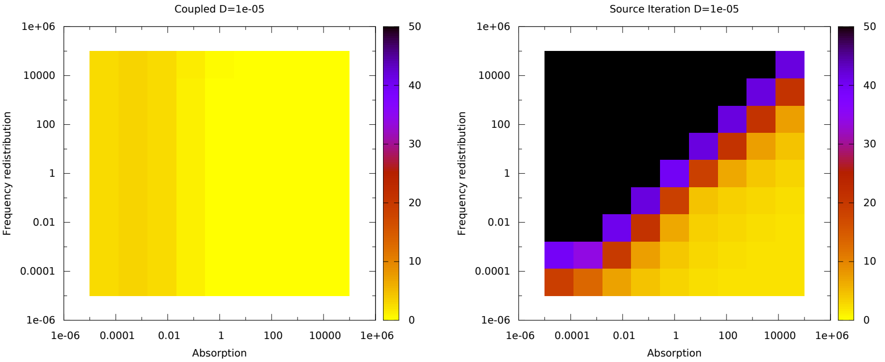
$$b_h(\psi, v) = \sum_{F\in\mathbb{F}_h^j} \sum_{g=1}^{G} \sum_{i=1}^{n} \omega_i \int_F \left(\frac{4}{max\{4, \sigma_s h\}} \left|\boldsymbol{\Omega}_i \cdot \boldsymbol{n}\right| \{\!\{\psi_{i,g}\boldsymbol{n}\}\!\} \{\!\{v_{i,g}\boldsymbol{n}\}\!\} - 2\boldsymbol{\Omega}_i \cdot \{\!\{\psi_{i,g}\boldsymbol{n}\}\!\} \{\!\{v_{i,g}\}\!\} \right) d\boldsymbol{x}$$

Multigrid preconditioner with Schwarz smoothers





Source iteration?



Diffusion with $\sigma_a = 1$

$$-\nabla \cdot (\epsilon D \nabla \Phi) + \frac{1}{\epsilon}\left(\sigma_T \Phi - \int_0^{E_{max}} \sigma_{s(E')} \Phi' dE'\right) = q$$

lev|eps	0	-1	-2	-3	-4	-5	-6
4	5	5	4	2	1	1	1
5	6	5	5	3	2	1	1
6	6	6	5	4	2	1	1
7	6	6	5	5	3	2	1
8	6	6	6	5	4	2	1
9	6	6	6	6	5	3	2

Diffusion with $\sigma_a = 0$ 2G

$$-\nabla \cdot (\epsilon D \nabla \Phi) + \frac{1}{\epsilon}\left(\sigma_T \Phi - \int_0^{E_{max}} \sigma_{s(E')} \Phi' dE'\right) = q$$

lev|eps	0	-1	-2	-3	-4	-5	-6
4	5	5	4	2	1	1	1
5	6	6	6	6	6	6	6
6	6	6	6	6	6	6	6
7	6	6	6	6	6	6	6
8	6	6	6	6	6	6	6
9	6	6	6	6	6	6	6

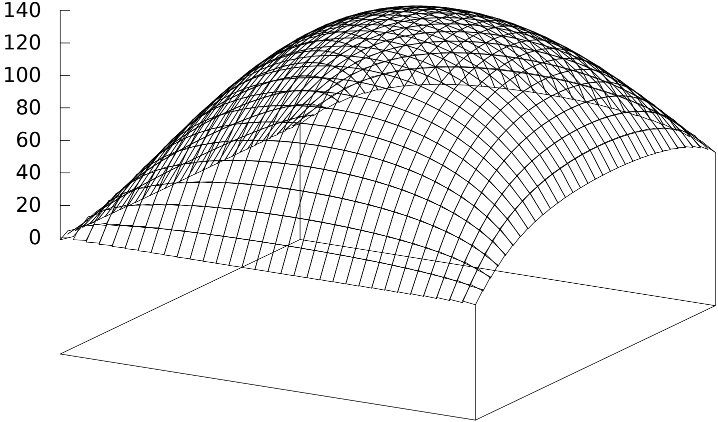
Diffusion with $\sigma_a = 0$ 5G

$$-\nabla \cdot (\epsilon D \nabla \Phi) + \frac{1}{\epsilon}\left(\sigma_T \Phi - \int_0^{E_{max}} \sigma_{s(E')} \Phi' dE'\right) = q$$

lev|eps	0	-1	-2	-3	-4	-5	-6
4	5	5	5	5	5	5	5
5	6	6	6	6	6	6	6
6	6	6	6	6	6	6	6
7	6	6	6	6	6	6	6
8	6	6	6	6	6	6	6
9	6	6	6	6	6	6	6

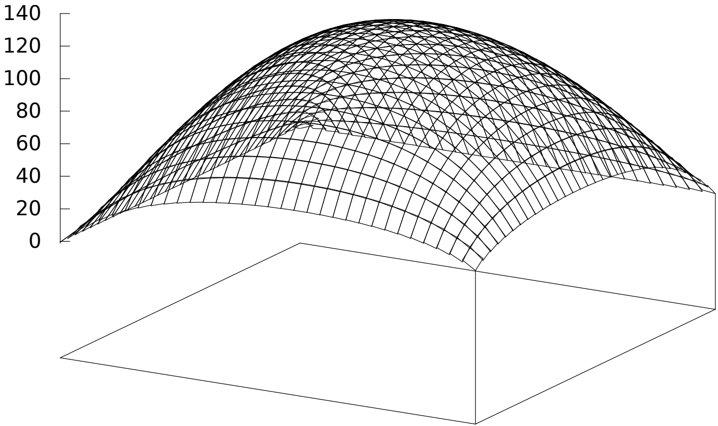
3 group transport

$$\Psi_1(\boldsymbol{\Omega}_1, \boldsymbol{x})$$



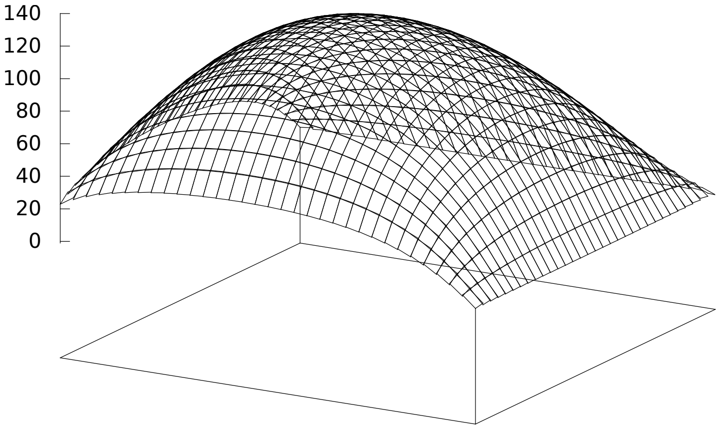
3 group transport

$\Psi_1(\boldsymbol{\Omega}_2, \boldsymbol{x})$

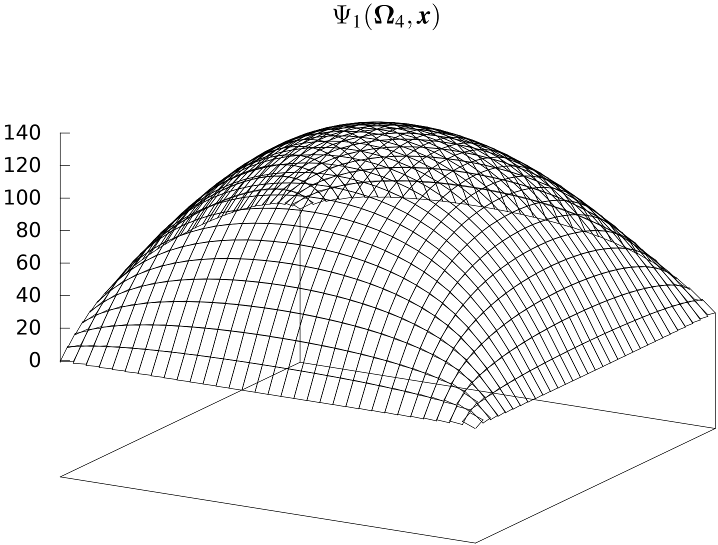


3 group transport

$$\Psi_1(\boldsymbol{\Omega}_3, \boldsymbol{x})$$

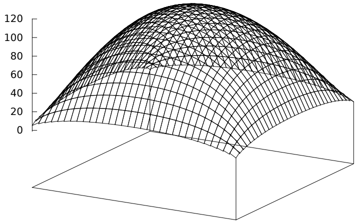


3 group transport

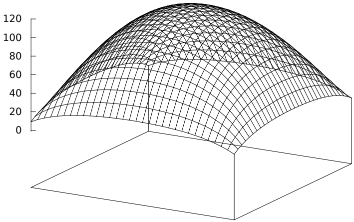


3 group transport

$$\Phi_1(\boldsymbol{x})$$



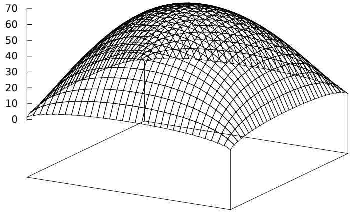
Result



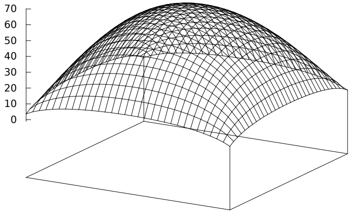
Reference

3 group transport

$$\Phi_2(\boldsymbol{x})$$



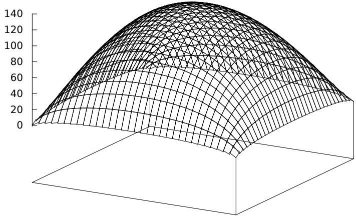
Result



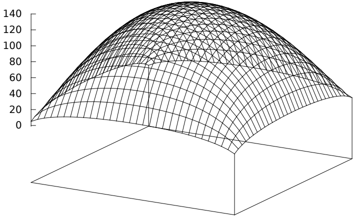
Reference

3 group transport

$$\Phi_3(\boldsymbol{x})$$



Result



Reference

3 group k_{eff}

$$\mathbf{\Omega}\cdot\nabla\Psi+\sigma_T\Psi-\int_0^{E_{max}}\int_S \sigma_{s(\mathbf{\Omega}',E')}\Psi' d\mathbf{\Omega}' dE' = \frac{1}{k_{eff}}\chi\int_0^{E_{max}}\nu\sigma_f'\Psi' dE'$$

#elem	Result	Reference	diff [pcm]
16	0.9017874	0.9016819	12
32	0.9019407	0.9018984	5
64	0.9019622	0.9019520	2
128	0.9019651	0.9019654	< 1

1 group convergence

$$\boldsymbol{\Omega} \cdot \nabla \Psi + \frac{1}{\epsilon} \left(\sigma_T \Psi - \int_0^{E_{max}} \int_S \sigma_{s(\boldsymbol{\Omega}', E')} \Psi' d\boldsymbol{\Omega}' dE' \right) = q,$$

lev|eps	0	-1	-2	-3	-4	-5	-6
4	3	5	7	7	8	8	9
5	3	5	8	9	9	10	11
6	3	5	9	10	10	11	12
7	3	4	8	10	11	11	12
8	3	4	8	10	11	11	12
9	3	4	8	9	10	11	12

2 group convergence

$$\boxed{\mathbf{\Omega} \cdot \nabla\Psi + \frac{1}{\epsilon}\left(\sigma_T\Psi - \int_0^{E_{max}}\int_S \sigma_{s(\mathbf{\Omega}',E')}\Psi' d\mathbf{\Omega}' dE'\right) = q,}$$

lev|eps	0	-1	-2	-3	-4	-5	-6
4	3	5	10	10	11	12	13
5	3	5	10	11	12	13	14
6	3	5	10	12	13	14	15
7	3	4	10	12	13	14	15
8	3	4	10	12	13	14	15
9	3	4	9	11	12	13	15

3 group convergence

$$\boxed{\boldsymbol{\Omega}\cdot\nabla\Psi+\frac{1}{\epsilon}\left(\sigma_T\Psi-\int_0^{E_{max}}\int_S\sigma_{s(\boldsymbol{\Omega}',E')}\Psi' d\boldsymbol{\Omega}' dE'\right)=q,}$$

lev|eps	0	-1	-2	-3	-4	-5	-6
4	3	5	12	12	13	14	15
5	3	5	12	14	15	16	17
6	3	5	12	14	15	17	18
7	3	4	12	14	15	17	18
8	3	4	11	14	15	16	18
9	3	4	11	13	15	16	17

4 group convergence

$$\boxed{\Omega \cdot \nabla\Psi + \frac{1}{\epsilon}\left(\sigma_T\Psi - \int_0^{E_{max}}\int_S \sigma_{s(\Omega',E')}\Psi' d\Omega' dE'\right) = q,}$$

lev|eps	0	-1	-2	-3	-4	-5	-6
4	3	5	12	14	15	16	17
5	3	5	13	15	17	18	20
6	3	5	13	16	17	19	20
7	3	4	12	16	17	19	20
8	3	4	12	15	17	18	20
9	3	4	11	15	17	18	19

5 group convergence

$$\boldsymbol{\Omega} \cdot \nabla \Psi + \frac{1}{\epsilon} \left(\sigma_T \Psi - \int_0^{E_{max}} \int_S \sigma_{s(\boldsymbol{\Omega}', E')} \Psi' d\boldsymbol{\Omega}' dE' \right) = q,$$

lev|eps	0	−1	−2	−3	−4	−5	−6
4	3	5	13	15	16	18	19
5	3	5	14	17	19	20	22
6	3	5	14	18	19	21	22
7	3	4	13	17	19	21	22
8	3	4	12	17	19	20	22
9	3	4	12	16	18	20	21

6 group convergence

$$\boxed{\mathbf{\Omega}\cdot\nabla\Psi+\frac{1}{\epsilon}\left(\sigma_T\Psi-\int_0^{E_{max}}\int_S\sigma_{s(\mathbf{\Omega}',E')}\Psi' d\mathbf{\Omega}' dE'\right)=q,}$$

lev|eps	0	−1	−2	−3	−4	−5	−6
4	3	5	14	16	18	19	20
5	3	5	15	19	20	22	24
6	3	5	14	19	21	23	24
7	3	4	14	19	21	22	24
8	3	4	13	18	20	22	24
9	3	4	12	17	20	21	23

7 group convergence

$$\boxed{\Omega \cdot \nabla \Psi + \frac{1}{\epsilon}\left(\sigma_T \Psi - \int_0^{E_{max}} \int_S \sigma_{s(\Omega', E')} \Psi' d\Omega' dE'\right) = q,}$$

lev|eps	0	-1	-2	-3	-4	-5	-6
4	3	5	14	17	19	20	21
5	3	5	15	20	22	23	25
6	3	5	14	21	22	24	26
7	3	4	14	20	22	24	26
8	3	4	13	19	21	23	25
9	3	4	13	18	21	23	25

8 group convergence

$$\boldsymbol{\Omega} \cdot \nabla \Psi + \frac{1}{\epsilon} \left(\sigma_T \Psi - \int_0^{E_{max}} \int_S \sigma_{s(\boldsymbol{\Omega}', E')} \Psi' d\boldsymbol{\Omega}' dE' \right) = q,$$

lev|eps	0	-1	-2	-3	-4	-5	-6
4	3	5	14	18	19	21	22
5	3	5	15	21	23	25	27
6	3	5	15	22	23	26	28
7	3	4	14	21	23	25	28
8	3	4	13	20	23	25	27
9	–	–	13	20	22	24	26

Conclusions

- Energy iteration solver in each cell.
- Diffusion scales well in space, energy and parameter-wise.
- Transport does well in space and fair parameter-wise but does not scale well in energy $\Longrightarrow$ multigrid in energy.
- ARPACK allows easy implementation of the eigenvalue problem with good performance.

To do

- Prove the behavior of the diffusion solver, get insights for transport.
- Implement multigrid in energy (maybe multigrid in angle?)
- Use Schwarz-preconditioned Inexact Newton to include local thermodynamic equilibrium for astrophysics applications.
- Once a scalable algorithm is ready, implement the method matrix-free in parallel.

Thank you.