Purpose

- The purpose is to reduce the computational time for multigroup (MG) transport simulations
- The scatter and fission transfer matrices are mapped onto a coarse energy grid, the sourced-particle flux is then mapped back onto the fine MG energy grid

Introduction: neutron transport equation

The neutron transport equation is

$$\frac{1}{v(E)}\frac{\partial \psi}{\partial t} + \hat{\Omega}\cdot\nabla\psi + \Sigma_t(\vec{r},E,t)\psi(\vec{r},\hat{\Omega},E,t) =$$

$$q(\vec{r},\hat{\Omega},E,t) + \sum_{i=1}^{I}\frac{\chi_{d,i}(E)}{4\pi}\lambda_i C_i(t) + \frac{1}{4\pi}\int_0^\infty dE'\,\Sigma_{pf}(\vec{r},E'\to E)\phi(\vec{r},E',t) +$$

$$\sum_{\ell=0}^{L}\sum_{m=-\ell}^{\ell}\frac{2\ell+1}{4\pi}Y_\ell^m(\hat{\Omega})\int_0^\infty dE'\,\Sigma_{s,\ell}(\vec{r},E'\to E)\phi_\ell^m(\vec{r},E',t).$$

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The multigroup (MG) method discretizes energy into groups

$$\Sigma_g\phi_g = \int_{E_g}^{E_{g-1}} dE\,\Sigma(E)\phi(E).$$

Background: the multigroup method

MG tries to also preserve the scattering reaction rates, as well as the energy and angular distribution of scattered neutrons

$$\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{2\ell+1}{4\pi} Y_\ell^m(\hat{\Omega}) \sum_{g'}^{G} \Sigma_{s,\ell,g'\to g} \phi_{\ell,g'}^m = \int_0^\infty dE' \, \Sigma_s(\hat{\Omega}' \cdot \hat{\Omega}, E' \to E) \psi(\hat{\Omega}', E')$$

Note:

- Energy is only 1 of the 7 dimensions in neutron transport, so energy is typically discretized into a few hundred groups
- Computing the scattering source requires $O(G^2)$ operations

The coarse scattering method

In the coarse scattering (CS) method, we make the following substitution to the MG transport equation to reduce the size of the scattering matrices

$$\sum_{g'} \Sigma_{s,\ell,g' \to g} \phi_{\ell,g'} \quad \to \quad S_{\ell,e \to g} \sum_{e'} \Sigma_{s,\ell,e' \to e} \phi_{\ell,e'}$$

where each fine-group g is a subset of a coarse-element e and

$$S_{\ell,e \to g} = \frac{\sum_{g'} \Sigma_{s,\ell,g' \to g} \phi_{\ell,g'}}{\sum_{e'} \Sigma_{s,\ell,e' \to e} \phi_{\ell,e'}}$$

$$\phi_{\ell,e} = \sum_{g \in e} \phi_{\ell,g}$$

The CS method can also be applied to the fission matrix

For fission, we make the following substitution

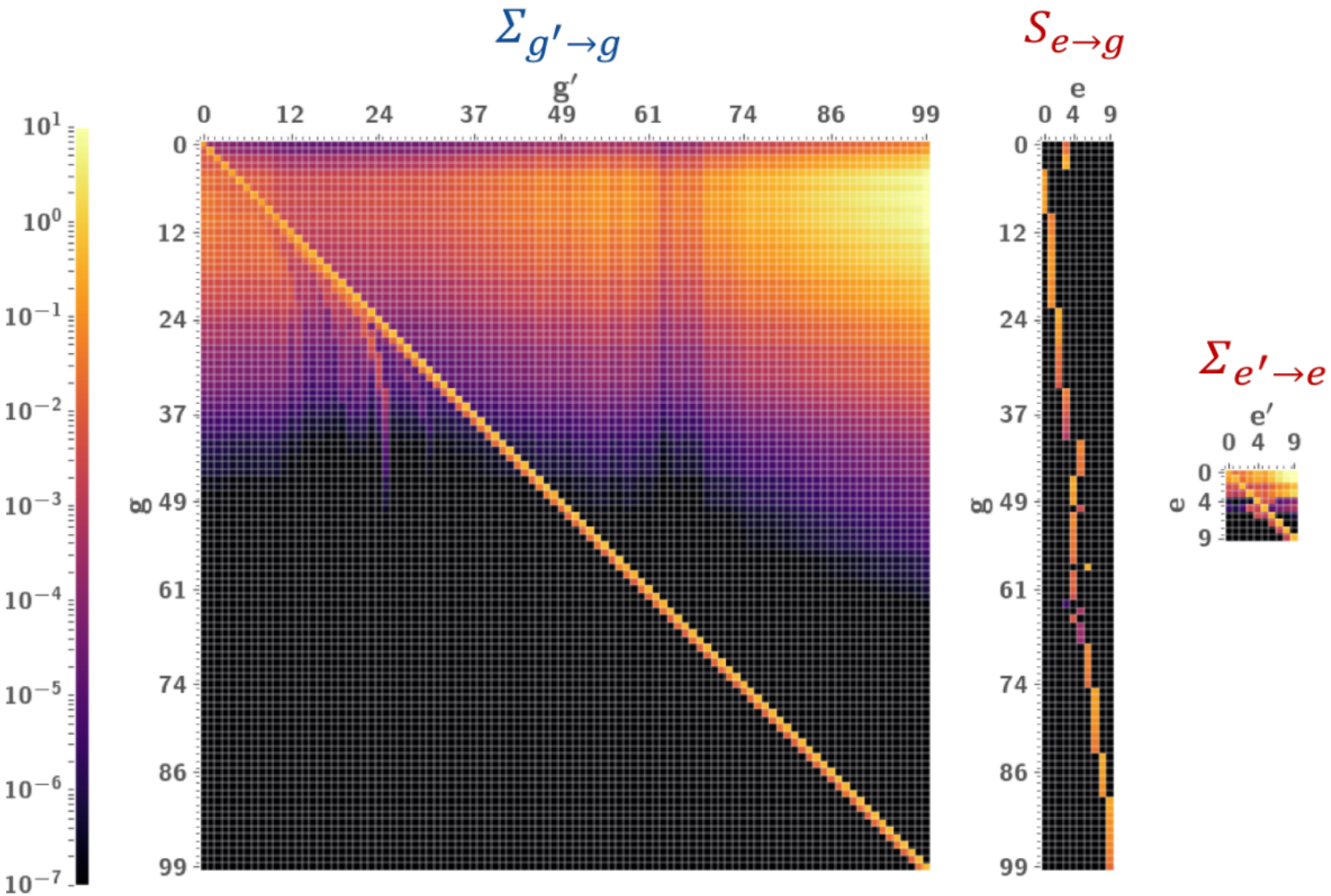
$$\sum_{g'} \Sigma_{f,g'\to g}\phi_{g'} \quad \to \quad F_{e\to g}\sum_{e'} \Sigma_{f,e'\to e}\phi_{e'}$$

where

$$F_{e\to g} = \frac{\sum_{g'} \Sigma_{f,g'\to g}\phi_{g'}}{\sum_{e'} \Sigma_{f,e'\to e}\phi_{e'}}$$

$$\phi_e = \sum_{g\in e} \phi_g$$

Example of fine transfer matrix being decomposed into a coarse transfer matrix and mapping operator



The standard source iteration method for MG

$$\left[\frac{1}{v_g}\frac{\partial}{\partial t} + \mu\frac{\partial}{\partial x} + \Sigma_{t,g}(\vec{r},t)\right]\psi_g^{(i+1)}(\vec{r},\mu,t) = q_g(\vec{r},\hat{\Omega},t) +$$
$$\sum_{\ell=0}^{L}\frac{2\ell+1}{2}P_\ell(\mu)\sum_{g'}^{G}\Sigma_{s,\ell,g'\to g}(\vec{r},t)\phi_{\ell,g'}^{(i)}(\vec{r},t) +$$
$$\frac{1}{2}\sum_{g'}^{G}\Sigma_{f,g'\to g}(\vec{r},t)\phi_{g'}^{(i)}(\vec{r},t)$$

Recall, the asymptotic computational cost of solving the MG transport equation is order G^2

The source iteration method is modified for CS

$$\left[\frac{1}{v_g}\frac{\partial}{\partial t}+\mu\frac{\partial}{\partial x}+\Sigma_{t,g}(\vec{r},t)\right]\psi_g^{(i+1)}(\vec{r},\mu,t)=q_g(\vec{r},\hat{\Omega},t)+$$
$$\sum_{\ell=0}^{L}\frac{2\ell+1}{2}P_\ell(\mu)S_{\ell,e\to g}^{(i-s)}\sum_{e'}^{E}\Sigma_{s,\ell,e'\to e}(\vec{r},t)\phi_{\ell,e'}^{(i)}(\vec{r},t)+$$
$$\frac{F_{e\to g}^{(i-f)}}{2}\sum_{e'}^{E}\Sigma_{f,e'\to e}(\vec{r},t)\phi_{e'}^{(i)}(\vec{r},t)$$

Note:

- It's not necessary to recompute both $S_{\ell,e\to g}$ and $F_{e\to g}$ every iteration
- Asymptotic computational cost of the CS method is order G in iterations when $S_{\ell,e\to g}$ and $F_{e\to g}$ are not recomputed and order G^2 only in iterations where $S_{\ell,e\to g}$ and $F_{e\to g}$ are recomputed

Particle balance is maintained

Particle balance is maintained if the following residual ρ is less than some specified tolerance in the last iteration

$$\rho = \sum_{g}^{G} \sum_{i}^{I} \Big[\Big(\sum_{g'}^{G} \Sigma_{s,0,g' \to g,i} \phi_{g',i} + \sum_{g'}^{G} \Sigma_{f,g' \to g,i} \phi_{g',i} \Big) - \Big(S_{0,e \to g,i} \sum_{e'}^{E} \Sigma_{s,0,e' \to e,i} \phi_{e',i} + F_{e \to g,i} \sum_{e'}^{E} \Sigma_{f,e' \to e,i} \phi_{e',i} \Big) \Big]$$

Alternatively, the MG method can be used in the last iteration

Test problem 1: description

Determine k-eigenvalue for an 8cm thick slab of uranium (20% enriched)

A S_N code was written in Python to simulate neutron transport and compare MG to CS:

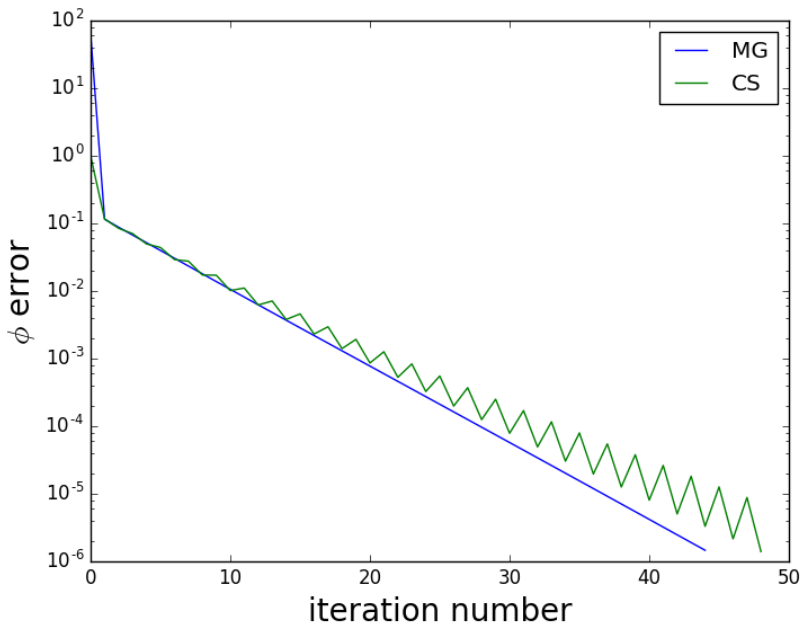
- 200 energy groups for MG
- 200 fine groups / 25 coarse-groups for CS
- 20 spatial cells (diamond-difference discretization)
- 8 polar angles
- isotropic scattering

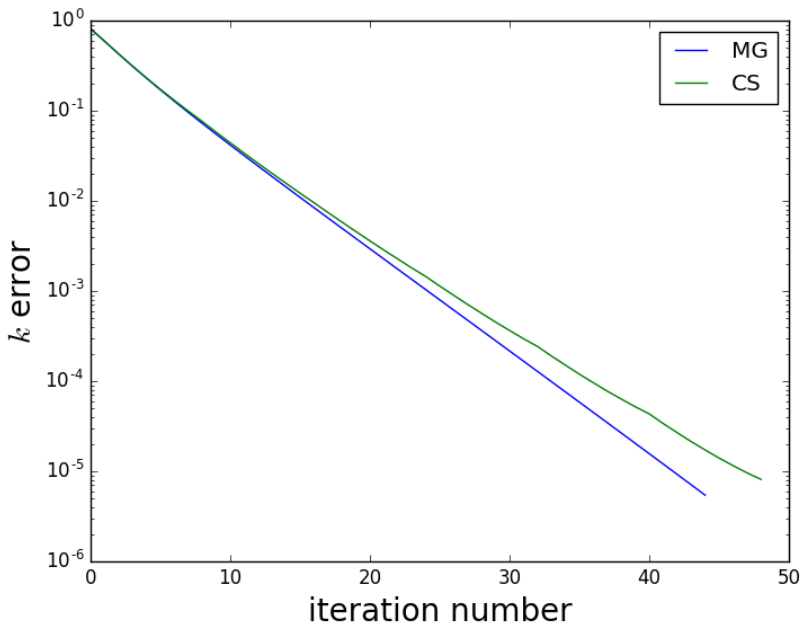
Test problem 1: how often the fission and scattering spectra were recomputed

- $F_{e \to g}$ recomputed every 8 iterations
- $S_{0,e \to g}$ recomputed every 2 iterations

Test problem 1: results for flux and k-eigenvalue

- Both MG and CS simulations resulted in a $k = 1.18173$
- The MG simulation converged in 45 iterations and the CS simulation converged in 49 iterations
- The MG simulation took 60s and the CS simulation took 31s





Test problem 2: description

Determine k-eigenvalue for an 8cm thick slab of uranium (20% enriched)

A S_N code was written in Python to simulate neutron transport and compare MG to CS:

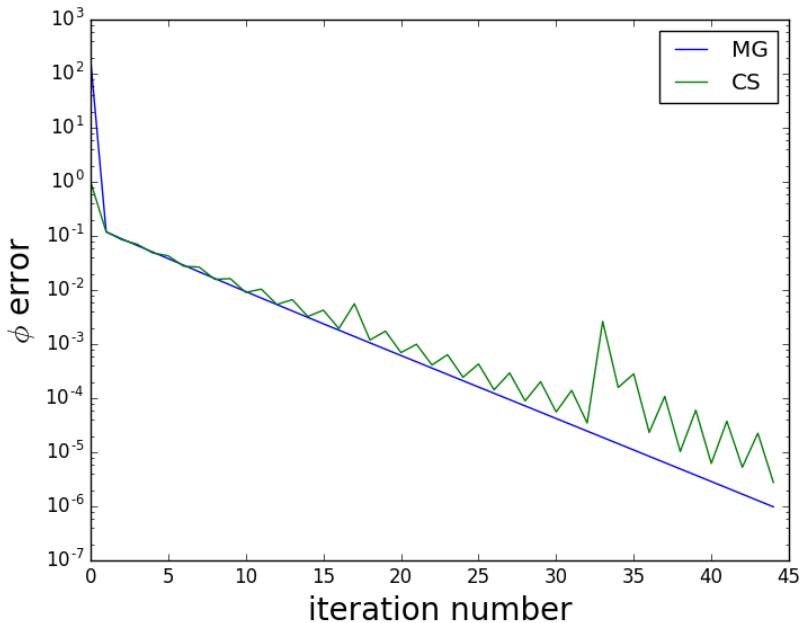
- 200 energy groups for MG
- 200 fine groups / 25 coarse-groups for CS
- 20 spatial cells (diamond-difference discretization)
- 32 polar angles
- P_7 scattering

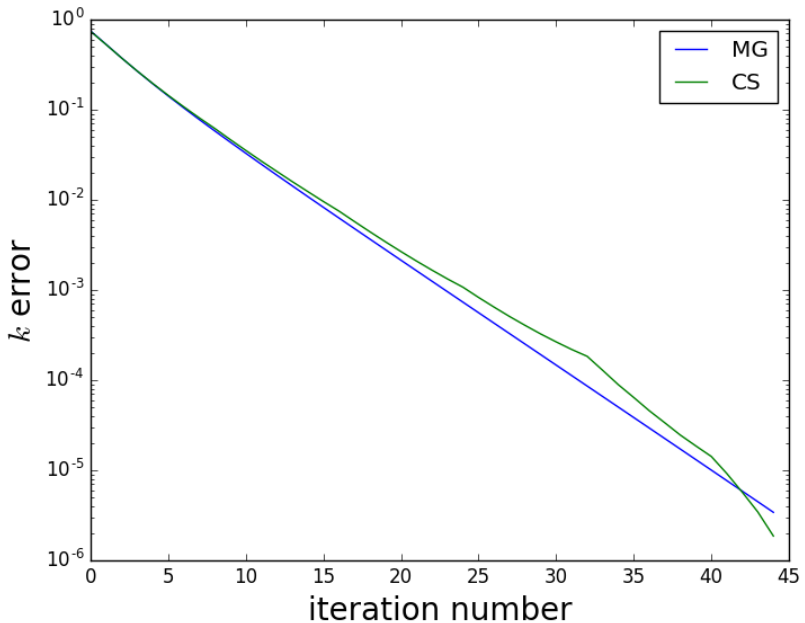
Test problem 2: how often the fission and scattering spectra were recomputed

- $F_{e \to g}$ recomputed every 8 iterations
- $S_{0,e \to g}$ recomputed every 2 iterations
- $S_{1,e \to g}$ recomputed every 16 iterations
- $S_{2,e \to g}$ recomputed every 16 iterations
- $S_{3,e \to g}$ recomputed every 32 iterations
- $S_{4,e \to g}$ recomputed every 32 iterations
- $S_{5,e \to g}$ recomputed every 32 iterations
- $S_{6,e \to g}$ recomputed every 32 iterations
- $S_{7,e \to g}$ recomputed every 32 iterations

Test problem 2: results for flux and k-eigenvalue

- Both MG and CS simulations resulted in a $k = 1.11677$
- Both MG and CS simulations converged in 45 iterations
- The MG simulation took 231s and the CS simulation took 131s





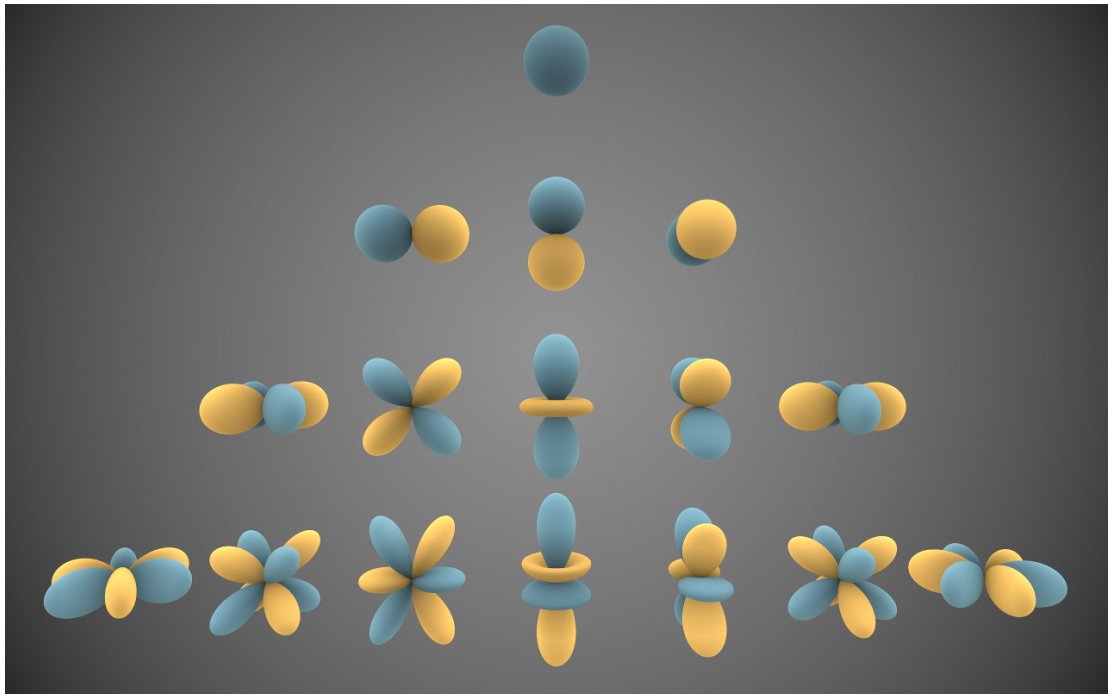
Conclusion

- CS maps scattering and fission onto a coarse grid, and then maps the sourced-particle flux back onto the fine grid
- CS converges to same solution as MG
- CS converged almost twice as fast as MG for test problems

Future work

- Explore possibility of maintaing particle balance in every iteration
- Develop critera for when $S_{\ell,e\to g}$ and $F_{e\to g}$ should be recomputed
- Try to combine CS with DSA

Future work: leverage properties of spherical harmonics



$$\int_{4\pi} d\Omega \, \frac{2\ell+1}{4\pi} Y_\ell^m(\hat{\Omega}) Y_{\ell'}^{m'}(\hat{\Omega}) = \delta_{\ell\ell'}\delta_{mm'}$$

$$\int_{4\pi} d\Omega \sum_{\ell=0}^{L} \sum_{m=-\ell}^{\ell} \frac{2\ell+1}{4\pi} Y_\ell^m(\hat{\Omega}) Y_0^0(\hat{\Omega}) = 1$$

Future work: particle balance might be maintained in every iteration if CS is only used for higher moments

$$\int_{4\pi} d\Omega\, Y_0^0(\hat{\Omega}) \sum_{\ell=0}^{L} \sum_{m=-\ell}^{\ell} \frac{2\ell+1}{4\pi} Y_\ell^m(\hat{\Omega}) \sum_{g'}^{G} \Sigma_{s,\ell,g'\to g} \phi_{\ell,g'}^m = \Sigma_{s,0,g'\to g} \phi_{0,g'}$$

$$\int_{4\pi} d\Omega\, Y_0^0(\hat{\Omega}) \Big\{ \frac{1}{4\pi} Y_0^0(\hat{\Omega}) \sum_{g'}^{G} \Sigma_{s,0,g'\to g} \phi_{0,g'} + \sum_{\ell=1}^{L} \sum_{m=-\ell}^{\ell} \frac{2\ell+1}{4\pi} Y_\ell^m(\hat{\Omega}) S_{e\to g} \sum_{e'}^{E} \Sigma_{s,\ell,e'\to e} \phi_{\ell,e'}^m \Big\} = \Sigma_{s,0,g'\to g} \phi_{0,g'}$$

Thank you

Questions?