



# ANS Winter Meeting & Expo

2018

Joining Forces to Advance Nuclear



## The Coarse Scattering Method



**ENGINEERING**  
TEXAS A&M UNIVERSITY

# 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

$$\begin{aligned} \frac{1}{v(E)} \frac{\partial \psi}{\partial t} + \hat{\Omega} \cdot \nabla \psi + \Sigma_t(\vec{r}, E, t) \psi(\vec{r}, \hat{\Omega}, E, t) = \\ q(\vec{r}, \hat{\Omega}, E, t) + \sum_{i=1}^I \frac{\chi_{d,i}(E)}{4\pi} \lambda_i C_i(t) + \frac{1}{4\pi} \int_0^\infty dE' \Sigma_{pf}(\vec{r}, E' \rightarrow E) \phi(\vec{r}, E', t) + \\ \sum_{\ell=0}^L \sum_{m=-\ell}^{\ell} \frac{2\ell+1}{4\pi} Y_\ell^m(\hat{\Omega}) \int_0^\infty dE' \Sigma_{s,\ell}(\vec{r}, E' \rightarrow E) \phi_\ell^m(\vec{r}, E', t). \end{aligned}$$

## Introduction: neutron transport equation

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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

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

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

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

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

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

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

## The CS method can also be applied to the fission matrix

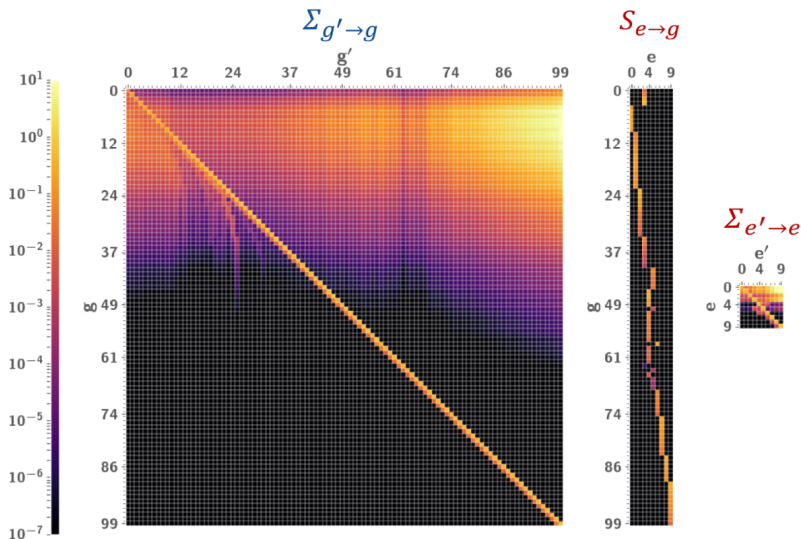
For fission, we make the following substitution

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

where

$$F_{e \rightarrow g} = \frac{\sum_{g'} \Sigma_{f,g' \rightarrow g} \phi_{g'}}{\sum_{e'} \Sigma_{f,e' \rightarrow e} \phi_{e'}}$$
$$\phi_e = \sum_{g \in e} \phi_g$$

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





## The standard source iteration method for MG

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

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

## The source iteration method is modified for CS

$$\left[ \frac{1}{v_g} \frac{\partial}{\partial t} + \mu \frac{\partial}{\partial x} + \Sigma_{t,g}(\vec{r}, t) \right] \psi_g^{(i+1)}(\vec{r}, \mu, t) = q_g(\vec{r}, \hat{\Omega}, t) +$$

$$\sum_{\ell=0}^L \frac{2\ell+1}{2} P_\ell(\mu) S_{\ell, e \rightarrow g}^{(i-s)} \sum_{e'}^E \Sigma_{s, \ell, e' \rightarrow e}(\vec{r}, t) \phi_{\ell, e'}^{(i)}(\vec{r}, t) +$$

$$\frac{F_{e \rightarrow g}^{(i-f)}}{2} \sum_{e'}^E \Sigma_{f, e' \rightarrow e}(\vec{r}, t) \phi_{e'}^{(i)}(\vec{r}, t)$$

Note:

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

## Particle balance is maintained

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

$$\rho = \sum_g^G \sum_i^I \left[ \left( \sum_{g'}^G \Sigma_{s,0,g' \rightarrow g,i} \phi_{g',i} + \sum_{g'}^G \Sigma_{f,g' \rightarrow g,i} \phi_{g',i} \right) - \right. \\ \left. \left( S_{0,e \rightarrow g,i} \sum_{e'}^E \Sigma_{s,0,e' \rightarrow e,i} \phi_{e',i} + F_{e \rightarrow g,i} \sum_{e'}^E \Sigma_{f,e' \rightarrow e,i} \phi_{e',i} \right) \right]$$

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:

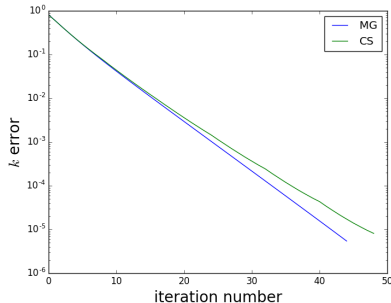
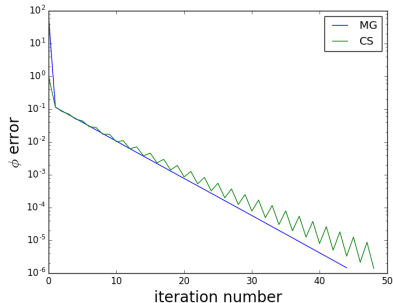
- 200 energy groups for MG
- 200 fine groups / 25 coarse-groups for CS
- 20 spatial cells (diamond-difference discretization)
- 8 polar angles
- isotropic scattering

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

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

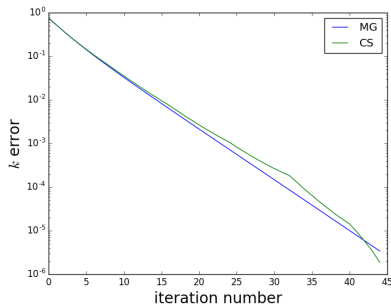
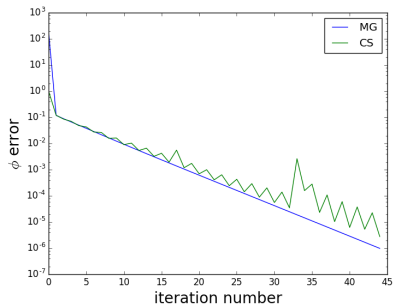
## Test problem 2: how often the fission and scattering spectra were recomputed

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



## Test problem 2: results for flux and $k$ -eigenvalue

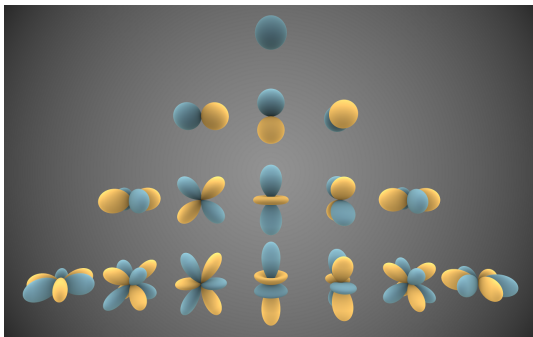
- Both MG and CS simulations resulted in a  $k = 1.11677$
- Both MG and CS simulations converged in 45 iterations
- The MG simulation took 231s and the CS simulation took 131s



- 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

- Explore possibility of maintaining particle balance in every iteration
- Develop criteria for when  $S_{\ell, e \rightarrow g}$  and  $F_{e \rightarrow g}$  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

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

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

Thank you

Questions?