# Multigrid for Sn Discretizations of the Boltzmann Transport Equation

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# The Boltzmann equation models the transport of a stream of particles in the presence of a source

- **The physical problem: a stream of particles collide with the nuclei of matter resulting in**
  - **scattering: incoming particles continue their flight but in altered directions**
  - **absorption: incoming particles are absorbed**
  - **streaming: incoming particles continue their flight in the same directions**

streaming-collision

scattering

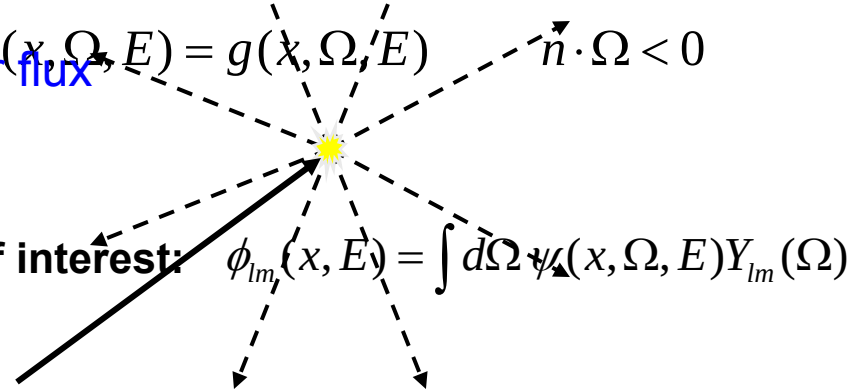
$$[\Omega \cdot \nabla + \sigma_t(x,E)]\psi(x,\Omega,E) = \int dE' \int d\Omega' \sigma_s(x,\Omega\cdot\Omega',E' \to E)\psi(x,\Omega',E') + q(x,\Omega,E)$$

streaming

angular flux

source

$$\psi(x,\Omega,E) = g(x,\Omega,E) \qquad n\cdot\Omega < 0$$



**Quantity of interest:** $\phi_{lm}(x,E) = \int d\Omega\, \psi(x,\Omega,E) Y_{lm}(\Omega)$



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# Discretization must be performed in energy, angle, and space dimensions

**Energy discretization: piecewise constant finite element**

$$\begin{bmatrix} (\Omega\bullet\nabla+\sigma_t^0-\int d\Omega\sigma_s^{00}) & -\int d\Omega\sigma_s^{01} & \cdots & -\int d\Omega\sigma_s^{0,G-1} & -\int d\Omega\sigma_s^{0G} \\ -\int d\Omega\sigma_s^{10} & \boxed{(\Omega\bullet\nabla+\sigma_t^1-\int d\Omega\sigma_s^{11})} & -\int d\Omega\sigma_s^{12} & \cdots & -\int d\Omega\sigma_s^{1G} \\ \vdots & & & \vdots & \vdots \\ \vdots & & & \vdots & \vdots \\ \vdots & & & \vdots & \vdots \end{bmatrix}\begin{bmatrix}\psi^0\\ \psi^1\\ \vdots\\ \psi^{G-1}\\ \psi^G\end{bmatrix}=\begin{bmatrix}f^0\\ f^1\\ \vdots\\ f^{G-1}\\ f^G\end{bmatrix}$$

**Angle & space discretization:**

**Sn: collocation in angle & finite difference/element/volume-like in space**

$$\begin{bmatrix} H_1 & & & & B_1 \\ & H_2 & & & B_2 \\ & & \ddots & & \vdots \\ & & & H_{nd} & B_{nd} \\ 0 & 0 & \cdots & 0 & [I-\sum C_i H_i^{-1} B_i] \\ C_1 & C_2 & \cdots & C_{nd} & I \end{bmatrix}\begin{bmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_{nd}\\ [\phi_{lm}]\end{bmatrix}=\begin{bmatrix}q_1\\ q_2\\ \vdots\\ q_{nd}\\ 0\end{bmatrix}=\begin{bmatrix}q_1\\ q_2\\ \vdots\\ q_{nd}\\ -\sum C_i H_i^{-1} q_i\end{bmatrix}\quad [\phi_{lm}]=\begin{bmatrix}\phi_{00}\\ \phi_{1,-1}\\ \phi_{1,0}\\ \vdots\\ \phi_{MM}\end{bmatrix}$$



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# The full discretization leads to a coupled system of integral equations

$$\left[\begin{array}{cccc:cccc} H^0 & & & & -\sigma_s^{00} & -\sigma_s^{01} & \cdots & -\sigma_s^{0G} \\ & H^1 & & & -\sigma_s^{10} & -\sigma_s^{11} & \cdots & -\sigma_s^{1G} \\ & & \ddots & & \vdots & \vdots & \ddots & \vdots \\ & & & H^G & -\sigma_s^{G0} & -\sigma_s^{G1} & \cdots & -\sigma_s^{GG} \\ \hdashline -W^0 & & & & I^0 & & & \\ & -W^1 & & & & I^1 & & \\ & & \ddots & & & & \ddots & \\ & & & -W^G & & & & I^G \end{array}\right] \left[\begin{array}{c} \psi^0 \\ \psi^1 \\ \vdots \\ \psi^G \\ \hdashline \varphi^0 \\ \varphi^1 \\ \vdots \\ \varphi^G \end{array}\right] = \left[\begin{array}{c} f^0 \\ f^1 \\ \vdots \\ f^G \\ \hdashline 0^0 \\ 0^1 \\ \vdots \\ 0^G \end{array}\right]$$

**integral equation** $\left[\vec{\mathbf{I}} - \vec{\mathbf{W}}\vec{\mathbf{H}}^{-1}\vec{\boldsymbol{\sigma}}_{\mathbf{s}}\right]\vec{\boldsymbol{\varphi}} = \vec{\mathbf{b}}$



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# The source/Picard/Richardson iteration is the basic approach for solving the mono-energetic equation

- **The scalar moments satisfy the integral equation**

$$[I - \sum C_i H_i^{-1} B_i][\phi_{lm}] = -\sum C_i H_i^{-1} q_i$$

- **To solve for the moments, iterate**

$$\phi_{lm}^{j} = \sum C_i H_i^{-1} B_i \, \phi_{lm}^{j-1} - \sum C_i H_i^{-1} q_i$$

  - **convergence rate depends on the ratio**

$$(\sigma_s / \sigma_t)$$

    - **acceleration techniques are needed**



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# There are several multigrid/multilevel approaches for solving the Boltzmann transport equation

- **DSA for Sn (Alcouffe, Brown, Larsen, Manteuffel, Morel, etc)**
  - **can be viewed as a two-level *multilevel* in angle**
  - **apply multigrid in the DSA preconditioner (spatial multigrid)**
  - **limited to isotropic scattering (Brown)**

**mono-energetic**

- **PN (Austin, Chang, Lee, Manteuffel)**
  - **requires solving large, strongly coupled systems of PDEs**
  - **many terms of the spherical harmonic expansion are needed for forward peak problems (Gibb's phenomena)**

**multi-energetic, anisotropic**

- **TSA for Sn (Adams, Nowak, Ramone)**
  - ***multilevel* in angle**

**mono-energetic**

- **Integral equation approaches fo Sn (Kelley, Klar, Lee, Seaid)**
  - **multigrid applied to the integral source iteration equation**
  - **multigrid in space *(+ angle and energy)***
    - **can be viewed as multigrid/Gauss elimination applied to the Sn system**

**multi-energetic, anisotropic**



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# There is an important distinction between multigrid and general multilevel methods

- A multilevel method solves a system using multiple levels, not necessarily taking advantage of the spectral properties of the system
  - e.g., DSA & TSA are multilevel methods that attempt to resolve the smallest spectral component (diffusion limit). They do not resolve the full spectrum.
  - DSA & TSA use different equations on the different levels
    - approximating this spectral component requires consistent DSA
- A multigrid method is a multilevel method that solves a system using a hierarchal decomposition of the spectrum
  - implies that the same base continuum equation must be used on each level
  - coarsens and removes spectral components at a conservative rate (gives the so-called good approximation property)
  - e.g., energy-space-angle multigrid applied to the integral equation



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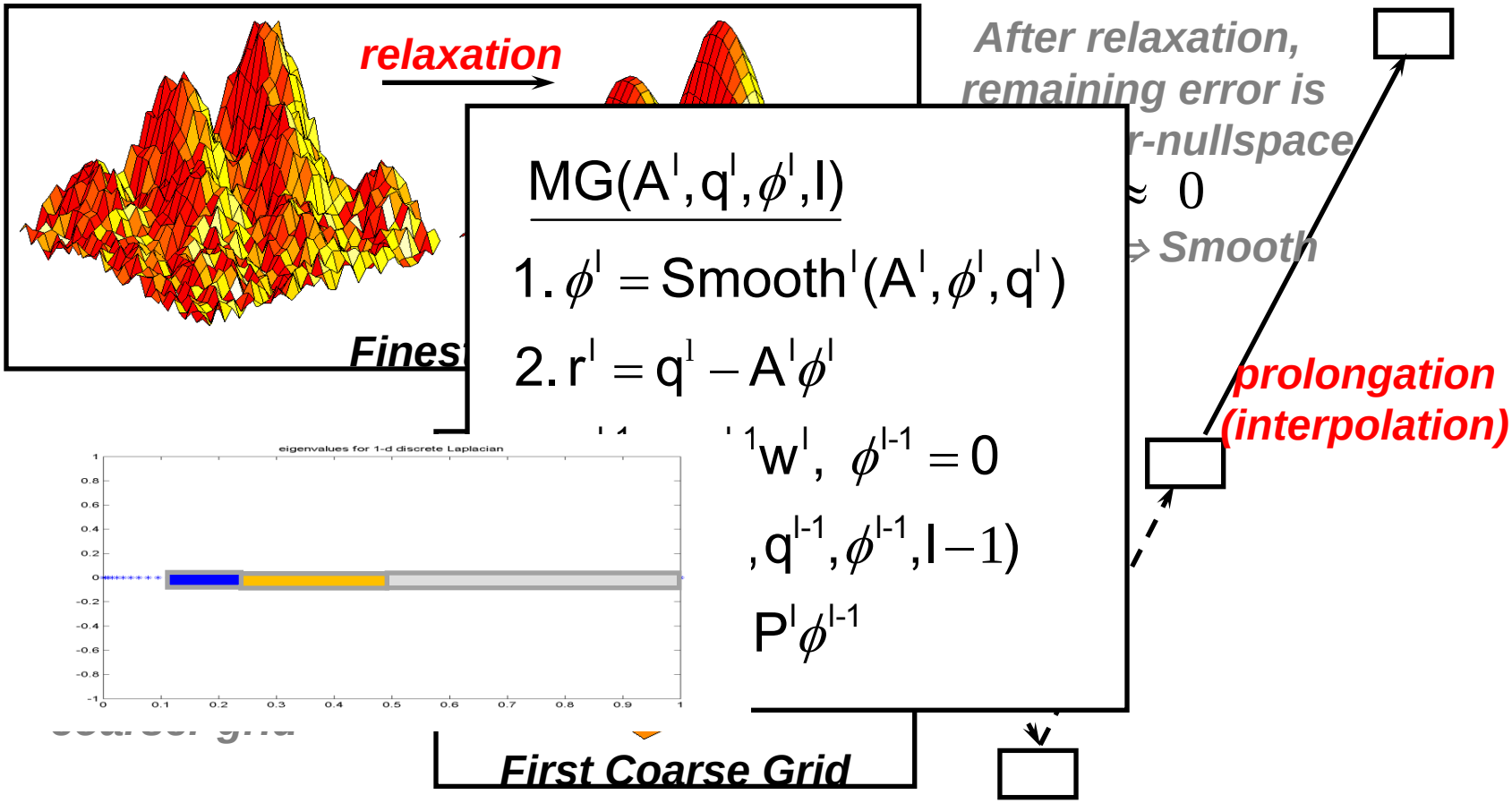
# Multigrid achieves its efficiency by handling the spectral components in hierarchal manner



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# Multigrid achieves its efficiency by handling the spectral components in hierarchal manner

$$\sum C_i H_i^{-1} B_i$$

$$A^{LR}\phi^{LR} := [I^{LR} - K^{LR}]\,\phi^{LR} = q^{LR}$$

$$\underline{SKMG(A^{IR}, q^{IR}, \phi^{IR}, IR)}$$

1. $\phi^{IR} = SrcIt^{IR}(A^{IR}, \phi^{IR}, q^{IR})$
2. $r^{IR} = q^{IR} - A^{IR}\phi^{IR}$
3. $w^{IR} = K^{IR} r^{IR}$
4. $q^{IR-1} = R^{IR-1} w^{IR}, \ \phi^{IR-1} = 0$ spatial coarsening
5. $SKMG(A^{IR-1}, q^{IR-1}, \phi^{IR-1}, IR-1)$
6. $\phi^{IR} = \phi^{IR} + P^{IR}\phi^{IR-1}$



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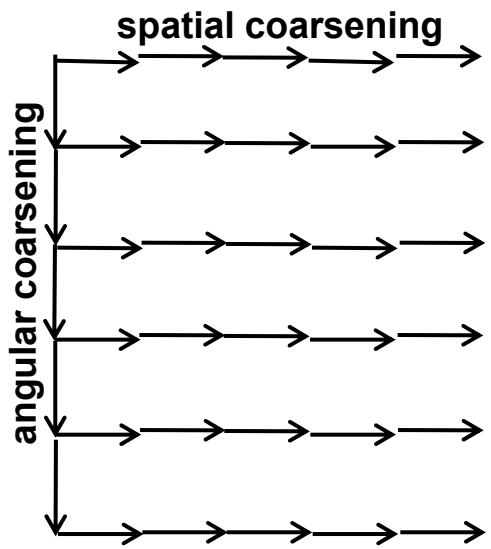
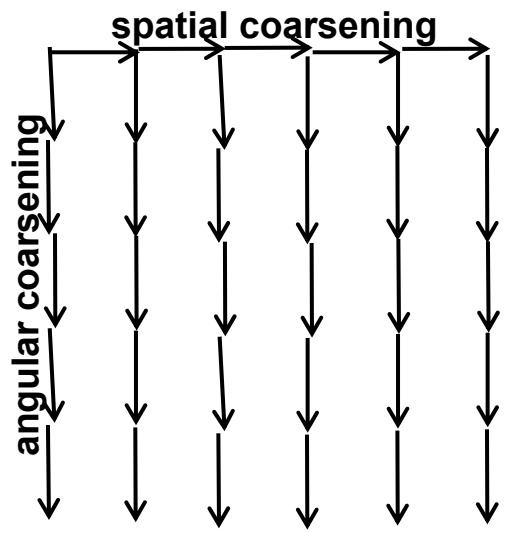
# The original space-angle multigrid method conservatively removes the spectral components




multiple/angle semi-coarsening tree

- each angle branch coarsens in space
- angle coarsening captures the near null-space; spatial coarsening captures the spatial variations of these angular near null-space components. Spectral analysis shows that this is needed.
- cost per multiple-coarsening cycle depends on the number of smoothing steps




multiple/spatial semi-coarsening tree

# Space-Angle Multigrid Cycle

**coarsening in angle**

$\mathrm{MGAngle}(A^{IE,I\Omega,LR}, q^{IE,I\Omega,LR}, \phi^{IE,I\Omega,LR}, I\Omega)$

1. $\phi^{IE,I\Omega,LR} = S^{IE,I\Omega,LR}(A^{IE,I\Omega,LR}, q^{IE,I\Omega,LR}, \phi^{IE,I\Omega,LR}, LR)$
2. $r^{IE,I\Omega,LR} = q^{IE,I\Omega,LR} - A^{IE,I\Omega,LR}\phi^{IE,I\Omega,LR}$
3. $q^{IE,I\Omega-1,LR} = R^{I\Omega-1} r^{IE,I\Omega,LR}, \ \phi^{IE,I\Omega-1,LR} = 0$
4. $\mathrm{MGAngle}(A^{IE,I\Omega-1,LR}, q^{IE,I\Omega-1,LR}, \phi^{IE,I\Omega-1,LR}, I\Omega-1)$
5. $\phi^{IE,I\Omega,LR} = \phi^{IE,I\Omega,LR} + P^{I\Omega}\phi^{IE,I\Omega-1,LR}$

**coarsening in space**

$S^{IE,I\Omega,IR}(A^{IE,I\Omega,IR}, q^{IE,I\Omega,IR}, \phi^{IE,I\Omega,IR}, IR)$

1. $\phi^{IE,I\Omega,IR} = \mathrm{GMRES}^{IE,I\Omega,IR}(A^{IE,I\Omega,IR}, \phi^{IE,I\Omega,IR}, q^{IE,I\Omega,IR})$
2. $r^{IE,I\Omega,IR} = q^{IE,I\Omega,IR} - A^{IE,I\Omega,IR}\phi^{IE,I\Omega,IR}$
3. $q^{IE,I\Omega,IR\text{-}1} = R^{IR-1} r^{IE,I\Omega,IR}, \ \phi^{IE,I\Omega,IR\text{-}1} = 0$
4. $S^{IE,I\Omega,IR}(A^{IE,I\Omega,IR\text{-}1} q^{IE,I\Omega,IR\text{-}1}, \phi^{IE,I\Omega,IR\text{-}1}, IR-1)$
5. $\phi^{IE,I\Omega,IR} = \phi^{IE,I\Omega,IR} + P^{IR}\phi^{IE,I\Omega,IR\text{-}1}$



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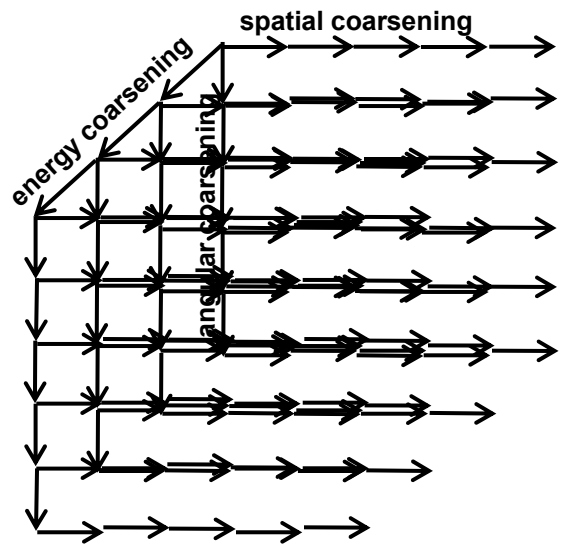
# Energy-Angle-Space Multigrid Cycle

## coarsening in energy

$\text{MGEnergy}(A^{IE,L\Omega,LR}, q^{IE,L\Omega,LR}, \phi^{IE,L\Omega,LR}, IE)$

1. $\phi^{IE,L\Omega,LR} = \text{MGAngle}(A^{IE,L\Omega,LR}, q^{IE,L\Omega,LR}, \phi^{IE,L\Omega,LR}, L\Omega)$
2. $r^{IE,L\Omega,LR} = q^{IE,L\Omega,LR} - A^{IE,L\Omega,LR}\phi^{IE,L\Omega,LR}$
3. $q^{IE-1,L\Omega,LR} = R^{IE-1} r^{IE,L\Omega,LR}, \ \phi^{IE-1,L\Omega,LR} = 0$
4. $\text{MGEnergy}(A^{IE-1,L\Omega,LR}, q^{IE-1,L\Omega,LR}, \phi^{IE-1,L\Omega,LR}, IE-1)$
5. $\phi^{IE,L\Omega,LR} = \phi^{IE,L\Omega,LR} + P^{IE}\phi^{IE-1,L\Omega,LR}$




## coarsening in angle

$\text{MGAngle}(A^{IE,I\Omega,LR}, q^{IE,I\Omega,LR}, \phi^{IE,I\Omega,LR}, I\Omega)$

1. $\phi^{IE,I\Omega,LR} = S^{IE,I\Omega,LR}(A^{IE,I\Omega,LR}, q^{IE,I\Omega,LR}, \phi^{IE,I\Omega,LR}, LR)$
2. $r^{IE,I\Omega,LR} = q^{IE,I\Omega,LR} - A^{IE,I\Omega,LR}\phi^{IE,I\Omega,LR}$
3. $q^{IE,I\Omega-1,LR} = R^{I\Omega-1} r^{IE,I\Omega,LR}, \ \phi^{IE,I\Omega-1,LR} = 0$
4. $\text{MGAngle}(A^{IE,I\Omega-1,LR}, q^{IE,I\Omega-1,LR}, \phi^{IE,I\Omega-1,LR}, I\Omega-1)$
5. $\phi^{IE,I\Omega,LR} = \phi^{IE,I\Omega,LR} + P^{I\Omega}\phi^{IE,I\Omega-1,LR}$

## coarsening in space

$S^{IE,I\Omega,IR}(A^{IE,I\Omega,IR}, q^{IE,I\Omega,IR}, \phi^{IE,I\Omega,IR}, IR)$

1. $\phi^{IE,I\Omega,IR} = \text{GMRES}^{IE,I\Omega,IR}(A^{IE,I\Omega,IR}, \phi^{IE,I\Omega,IR}, q^{IE,I\Omega,IR})$
2. $r^{IE,I\Omega,IR} = q^{IE,I\Omega,IR} - A^{IE,I\Omega,IR}\phi^{IE,I\Omega,IR}$
3. $q^{IE,I\Omega,IR-1} = R^{IR-1} r^{IE,I\Omega,IR}, \ \phi^{IE,I\Omega,IR-1} = 0$
4. $S^{IE,I\Omega,IR}(A^{IE,I\Omega,IR-1} q^{IE,I\Omega,IR-1}, \phi^{IE,I\Omega,IR-1}, IR-1)$
5. $\phi^{IE,I\Omega,IR} = \phi^{IE,I\Omega,IR} + P^{IR}\phi^{IE,I\Omega,IR-1}$



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# Why it works: captures the space-angle features of the near null-space components

- **Coarsening in space and angle effectively reduces the near null-space components, which have space-angle features**
  - **<u>angle features of near null-space:</u>**

$$(I-K)\phi \approx 0 \implies \phi \approx K\phi = \int H^{-1}(\sigma_s \phi)\, d\Omega = \int w(x,\Omega)\, d\Omega = P_{00} w$$

$$\begin{aligned} \|w(x,\Omega)\|_{x,\Omega} &= \|P_{00} w\|_x + \|(I-P_{00})w\|_{x,\Omega} \\ &\approx \|\phi\|_x + \|(I-P_{00})w\|_{x,\Omega} \end{aligned}$$

**But by regularity**

$$[\Omega \bullet \nabla + \sigma_t]w = \sigma_s \phi \quad \Rightarrow \quad \|w\|_{x,\Omega} \le \frac{\sigma_s}{\sigma_t}\|\phi\|_x \le \|\phi\|_x$$



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# Why it works: captures the space-angle features of the near null-space components

- **Coarsening in space and angle effectively reduces the near null-space components, which have space-angle features**
  - **<u>angle features of near null-space:</u>**

$$\|\phi\|_x + \|(I - P_{00})w\|_{x,\Omega} \approx \|w\|_{x,\Omega} \le \frac{\sigma_s}{\sigma_t}\|\phi\|_x \le \|\phi\|_x$$

- **near null-space exists if** $\frac{\sigma_s}{\sigma_t} \approx 1$
- **angular flux** $w(x,\Omega)$ **is essentially isotropic on "average" since the integration is over the spatial domain**
  - **can be locally anisotropic, especially for anisotropic scattering**
  - **isotropic** $\Rightarrow$ **coarsen in angle**



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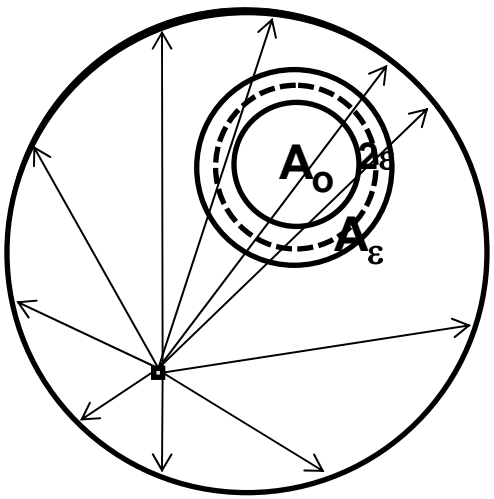
# Why it works: captures the space-angle features of the near null-space components

- **Coarsening in space and angle effectively reduces the near null-space components, which have space-angle features**
  - **<u>spatial features of near null-space:</u>**
    - **use the isotropic characteristics of the angular flux to determine the spatial smoothness**




$$w(x,\Omega) = \int_0^{d_R} e^{-\int_0^s \sigma_t(x-t\Omega)\,dt} \sigma_s(x-s\Omega)\phi(x-s\Omega)\,ds$$

**strongly anisotropic if spatially oscillatory**

**near null-space:** $$\phi(x) = \begin{cases} 1 & x \in A_o \\ 0 & x \in R/(A_\varepsilon \cup A_o) \\ 0^+ & x \in A_\varepsilon \end{cases}$$

**near null-space locally spatially smooth**



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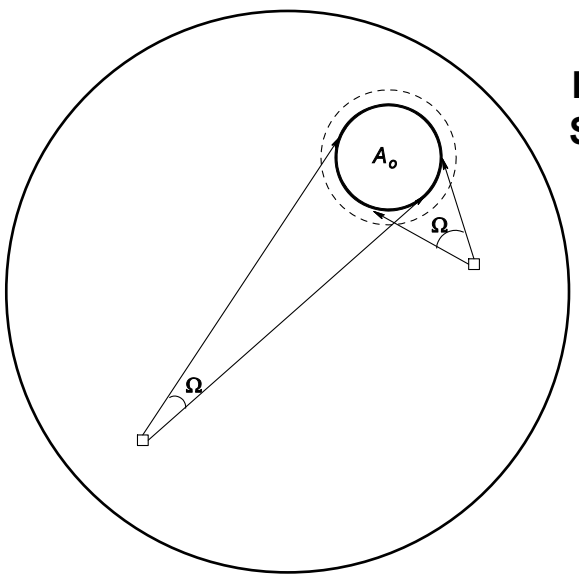
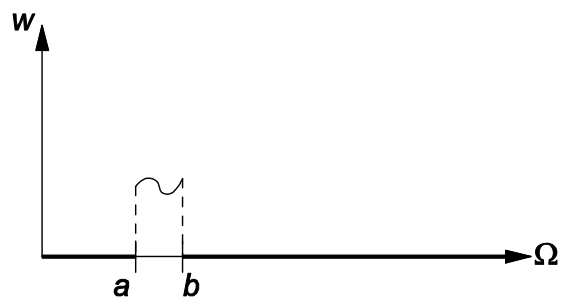
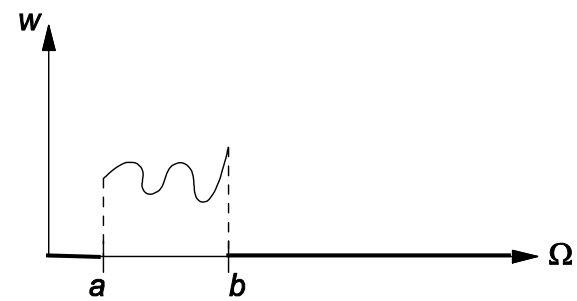
# This technique exposes the *subtle* necessity of angle coarsening

- **Near null-space is a scalar flux (independent of angle), so why coarsen in angle?**
  - **wrt the solver, cannot view the near null-space of the integral equation itself; must consider the angular flux generated by this scalar flux.**
  - **can be viewed as coarsening the integral kernel $H^{-1}\sigma_s$**
    - **angle coarsening must be performed to capture the angle variations of the "near null-space" angular flux**




**Isotropic in optically thick region and anisotropic away from region. Stronger (absolute) isotropic component near optically thick region.**



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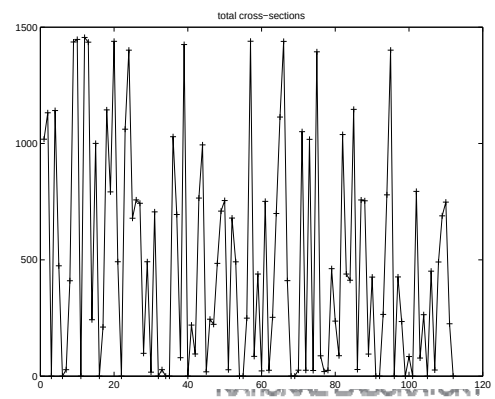
# This technique can be used on more general Boltzmann equations

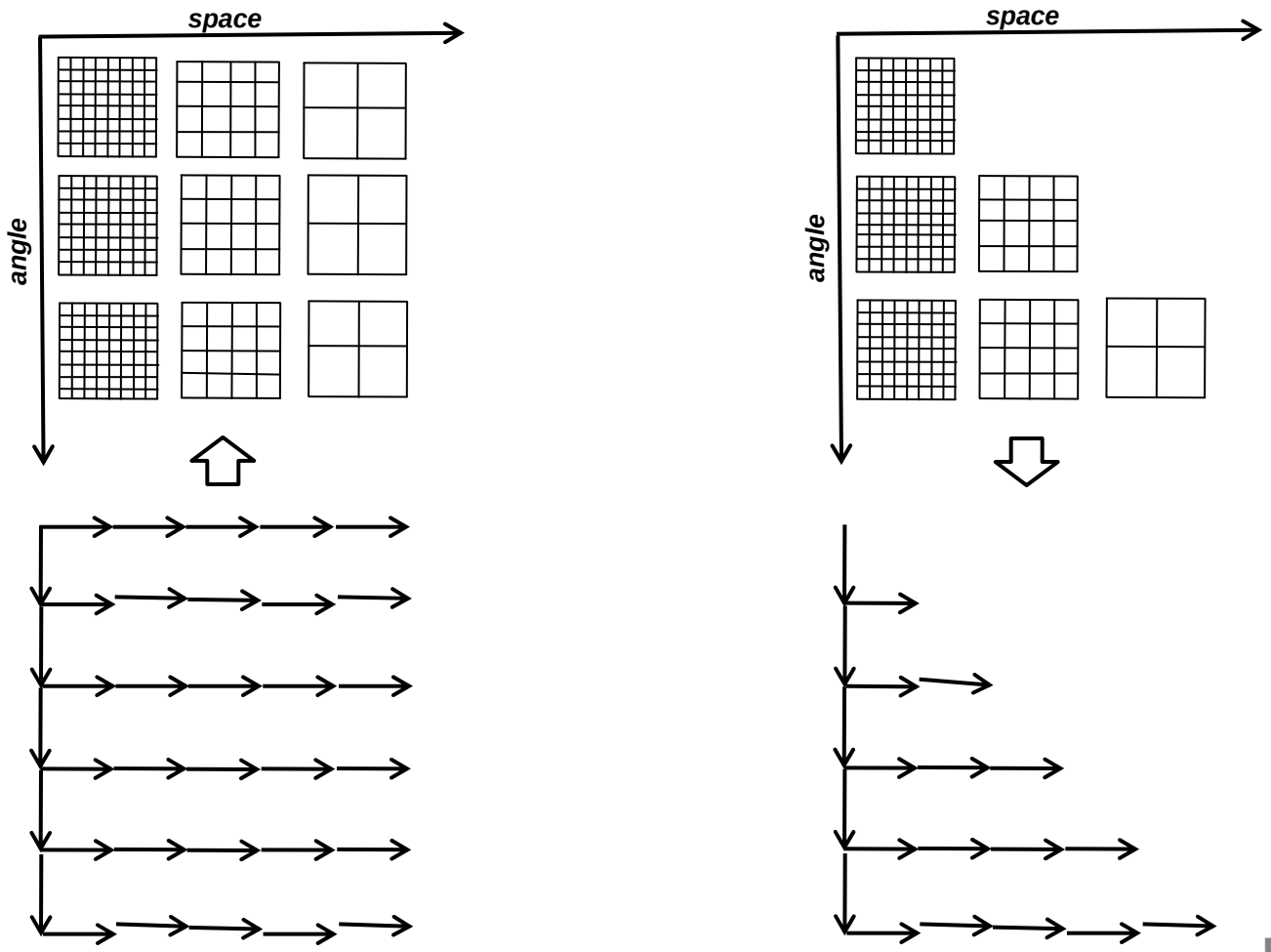
- **Anisotropic scattering: a similar set of near null-space can be determined**
  - **components couple more strongly in angle (Wigner 3j-symbol coupling)**
  - **form of near null-space indicates that spatial semi-coarsening multigrid cycle trees are more appropriate**

- **Multi-energetic equation: near null-space exists only if algebraic relations involving the scattering and total cross-sections hold**
  - **space-angle structure similar to the mono-energetic case**
  - **algebraic relations reveal how energy coarsening should be performed**
    - **generally should not coarsen by re-discretizing the energy integral**
    - **energy coarsening guided by the algebraic relations**
    - ***appropriate for even for highly oscillatory cross-sections***



# Energy, space, and angle descriptions of the near null-space lead to sparse coarsening strategies

## Space-Angle Multigrid



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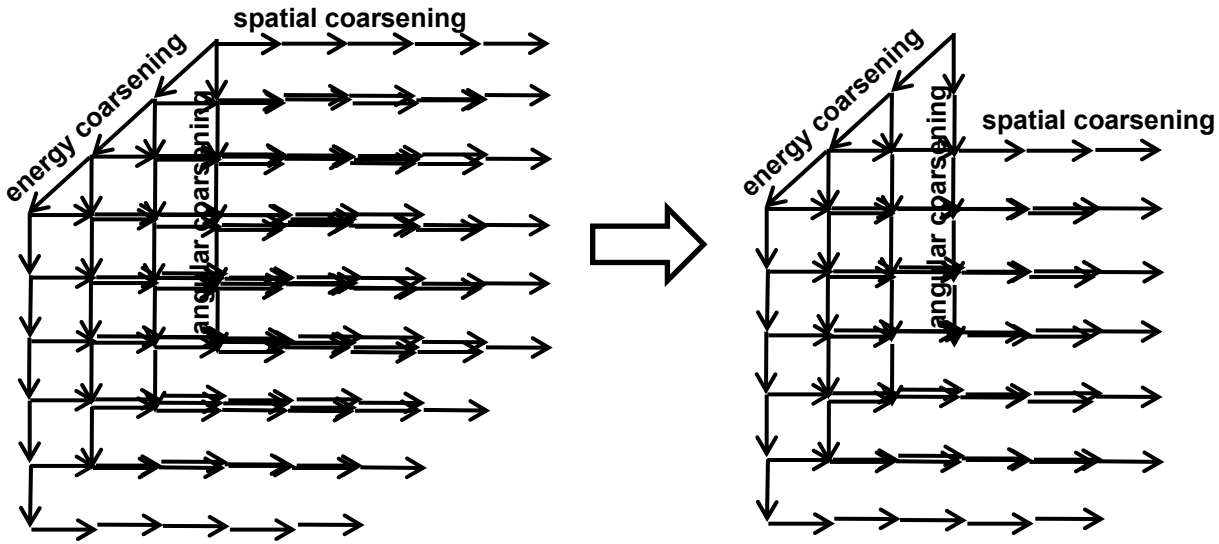
# Energy, space, and angle descriptions of the near null-space lead to sparse coarsening strategies

## Energy-Space-Angle Multigrid



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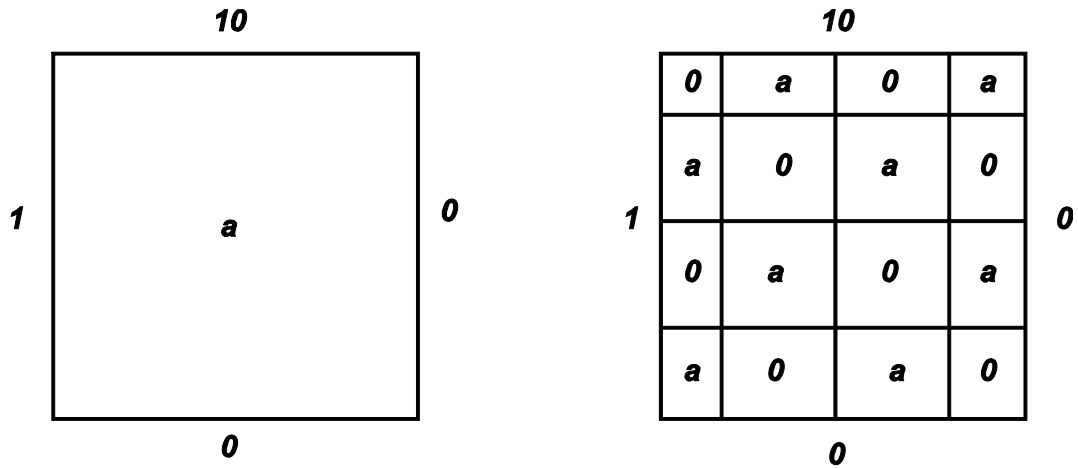
# Numerical Examples: Mono-energetic

- **Continuous & discontinuous cross-sections and isotropic & anisotropic scattering**




**a= 64, 640**

$$\sigma_{s,0} / \sigma_t = 0.9999$$

$$\sigma_{s,i} / \sigma_t = 0.9^i * (0.9999) \quad 0 < i \le L$$

PG, $h = 1/128$, 64 angles

$5+5*(L_\Omega - l_\Omega)$ Gmres sweeps

$V(1,0)$ tree cycles



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# Numerical Examples: Mono-energetic

| Problem | a | Semi-coarsening | Tree | L | | | |
|---|---|---|---|---|---|---|---|
| | | | | 0 | 1 | 2 | 3 |
| continuous σ | 64 | spatial | full | 3 | 3 | 4 | 4 |
| | | | sparse | 3 | 3 | 4 | 4 |
| | | angular | full | 5 | 6 | 5 | 5 |
| | | | sparse | 6 | 10 | 10 | 9 |
| | 640 | spatial | full | 5 | 6 | 6 | 10 |
| | | | sparse | 6 | 7 | 6 | 12 |
| | | angular | full | 6 | 9 | 9 | 10 |
| | | | sparse | 6 | 10 | 10 | 12 |
| discontinuous σ | 64 | spatial | full | 4 | 5 | 5 | 5 |
| | | | sparse | 4 | 5 | 5 | 5 |
| | | angular | full | 5 | 6 | 6 | 5 |
| | | | sparse | 7 | 11 | 11 | 10 |
| | 640 | spatial | full | 10 | 8 | 9 | 9 |
| | | | sparse | 12 | 10 | 9 | 11 |
| | | angular | full | 10 | 13 | 15 | 13 |
| | | | sparse | 14 | 17 | 21 | 17 |

# Numerical Examples: Multi-energetic

- **Assumption:**

$$\sigma_t(x,E) - \int dE' \sigma_s(x,E' \to E) \geq \alpha \qquad \sigma_t(x,E) - \int dE' \sigma_s(x,E \to E') \geq \alpha$$

$$\Rightarrow \quad \sigma_t^i(x) - \sum_{j=0}^{G} \sigma_s^{ij}(x) \geq \alpha \qquad \sigma_t^i(x) - \sum_{j=0}^{G} \sigma_s^{ji}(x) \geq \alpha$$

**Existence & uniqueness of solution (Dautray and Lions, 1993)**

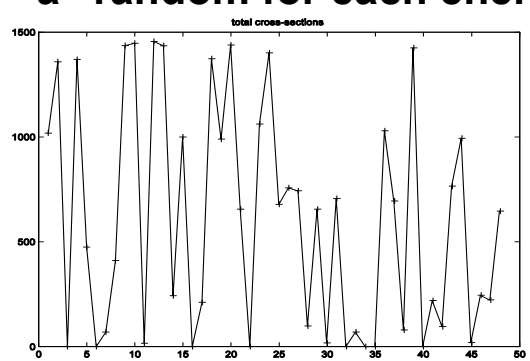
- **"Algebraic" coarsening of energy based on cross-section relations and space-angle coarsening on each energy level**

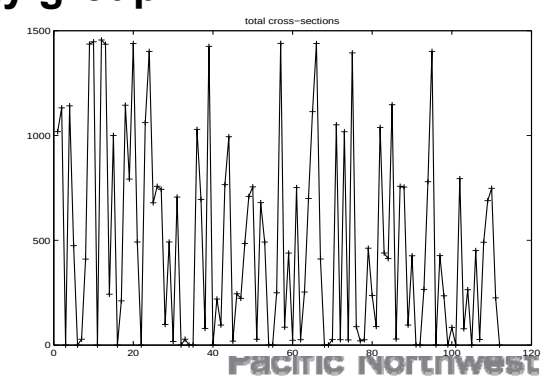
- **Discontinuous cross-sections and isotropic & anisotropic scattering**

| | | | |
|---|---|---|---|
| ε*a* | *a* | ε*a* | *a* |
| *a* | ε*a* | *a* | ε*a* |
| ε*a* | *a* | ε*a* | *a* |
| *a* | ε*a* | *a* | ε*a* |

**ε= 0.000001**

**"a" random for each energy group**



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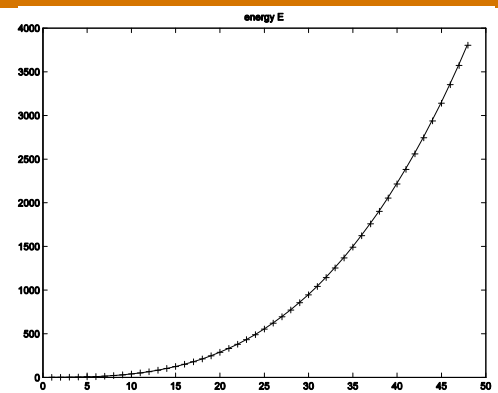
# Numerical Examples: Multi-energetic

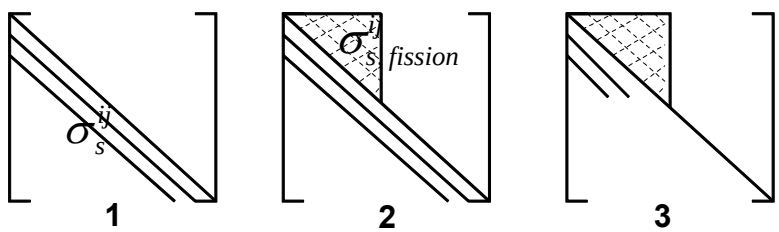
- **Cross-group scattering:**

$$\sigma_s^{ij} = \frac{\sigma_s^{ii}}{\left(E_i - E_j\right)^{1.25}} \qquad j < i$$

$$\sigma_{s,\,fission}^{ij} = \frac{\sigma_s^{ii}}{\left(j - i + 1\right)} \qquad j > i$$




  - **patterned coupling:**




- **Scattering-to-total cross-section ratios: as strong as**

$$\frac{\sigma_{s,00}^{ii}}{\sigma_t^i} = 0.999999 \qquad \frac{\sigma_{s,lm}^{ii}}{\sigma_t^i} \approx 0.9^l, \qquad l > 0$$



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# Numerical Examples: Multi-energetic

- **Petrov-Galerkin spatial discretization**
  - **Isotropic scattering, h= 1/64, 64 angles, 48 energy groups**

| Method | Problem | | |
|---|---|---|---|
| | 1 | 2 | 3 |
| Space-Angle MG | 36 | 5 | 47 |
| Energy-Space-Angle MG | 15 | 5 | 21 |
| Mono-Energetic Jacobi | 35 (8e-8) | 100 (4e-2) | diverge |



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# Numerical Examples: Multi-energetic

- **Petrov-Galerkin spatial discretization**
  - **anisotropic scattering, h= 1/32, 64 angles, 48 energy groups**

| L | Method | Problem | | |
|---|---|---|---|---|
| | | 1 | 2 | 3 |
| 0 | Space-Angle MG | 15 | 6 | 25 |
| | Energy-Space-Angle MG | 12 | 6 | 14 |
| 1 | Space-Angle MG | 11 | 9 | 14 |
| | Energy-Space-Angle MG | 8 | 9 | 5 |
| 2 | Space-Angle MG | 12 | 10 | 20 |
| | Energy-Space-Angle MG | 9 | 10 | 6 |
| 3 | Space-Angle MG | 16 | 9 | 32 |
| | Energy-Space-Angle MG | 8 | 9 | 10 |



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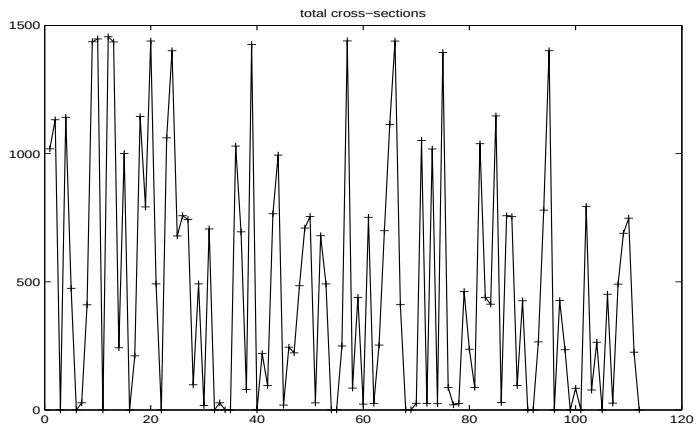
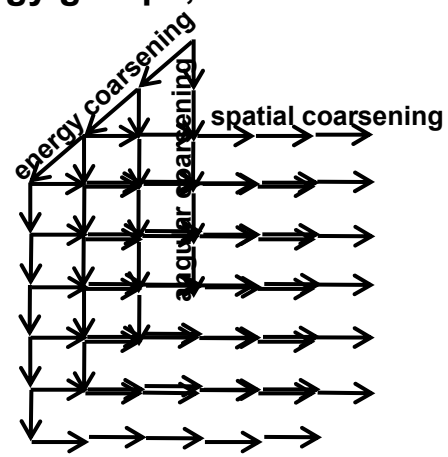
# Numerical Examples: Multi-energetic

- **Petrov-Galerkin spatial discretization**
  - **isotropic scattering, h= 1/32, 64 angles, 112 energy groups, Problem 3**




| Method | Iterations |
|---|---|
| “Sparse” Energy-Space-Angle | 12 |
| “Full” Energy-Space-Angle | 12 |



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# Conclusions

- **A multigrid approach for Sn discretizations of the Boltzmann equation must resolve the spectral components in hierarchal fashion**
  - **spectral components have energetic, spatial, and angular features**
    - **coarsening must be done in all of these dimensions**
    - **energy, space, and angle descriptions of the near null-space components guide the coarsening strategy**



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