Title of Qualification Exam Talk

J. S. Rehak

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Outline

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Motivation
Transport Equation
Acceleration Methods
Analyzing Acceleration Schemes
BART
Plan and Future Work

Motivation

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Transport Equation

Steady-state Boltzman Transport Equation

Our problem of interest is the time-independent transport equation for a critical system on a domain of interest $\mathbf{r} \in V$ [3],

$$\begin{aligned}\left[\hat{\Omega}\cdot\nabla+\Sigma_t(\mathbf{r},E)\right]\psi(\mathbf{r},E,\hat{\Omega}) \\ =\int_0^\infty dE'\int_{4\pi}d\hat{\Omega}'\Sigma_s(\mathbf{r},E'\to E,\hat{\Omega}'\to\hat{\Omega})\psi(\mathbf{r},E',\hat{\Omega}') \\ +Q(\mathbf{r},E,\hat{\Omega})\ ,\end{aligned}$$

with a given boundary condition,

$$\psi(\mathbf{r},E,\hat{\Omega})=\Gamma(\mathbf{r},E,\hat{\Omega}),\quad \mathbf{r}\in\partial V,\quad \hat{\Omega}\cdot\hat{n}<0$$

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Apply the following discretizations:

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- Expanding scattering cross-section in Legendre Polynomials with a maximum degree N.

$$\Sigma_{s,g'g,\ell} = \int_{-1}^{1} \Sigma_{s,g'g}(\mathbf{r},\mu) P_\ell(\mu) d\mu, \quad \mu = \hat{\Omega}' \cdot \hat{\Omega}$$

$$\phi_{g,\ell,m} = \int_{4\pi} \phi_g(\mathbf{r},\hat{\Omega}') Y_{\ell,m}(\hat{\Omega}') d\hat{\Omega}'$$

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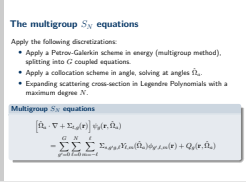
Multigroup S_N equations

$$\left[\hat{\Omega}_a \cdot \nabla + \Sigma_{t,g}(\mathbf{r})\right] \psi_g(\mathbf{r}, \hat{\Omega}_a) = \sum_{g'=0}^{G} \sum_{\ell=0}^{N} \sum_{m=-\ell}^{\ell} \Sigma_{s,g'g,\ell} Y_{\ell,m}(\hat{\Omega}_a) \phi_{g',\ell,m}(\mathbf{r}) + Q_g(\mathbf{r}, \hat{\Omega}_a)$$



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Iterative Solving Methods

Expressed in operator form, this is

$$\mathbf{L}_g \mathbf{\Psi}_g = \mathbf{M} \sum_{g'=0}^{G} \mathbf{S}_{g'g} \mathbf{\Phi}_{g'} + \mathbf{Q}_g, \quad \mathbf{\Phi}_g = \mathbf{D}\mathbf{\Psi}_g \ .$$

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Splitting the scattering source into down-scattering and up-scattering terms,

$$\mathbf{L}_g\mathbf{\Psi}_g = \mathbf{M}\sum_{g'=0}^{g}\mathbf{S}_{g'g}\mathbf{\Phi}_{g'} + \mathbf{M}\sum_{g'=g+1}^{G}\mathbf{S}_{g'g}\mathbf{\Phi}_{g'} + \mathbf{Q}_g \ ,$$

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For a multiplying-medium problem, the fixed source $\mathbf{Q}$ is replaced with the fission source,

$$\mathbf{L}_g \mathbf{\Psi}_g = \mathbf{M} \sum_{g'=0}^{G} \left[\mathbf{S}_{g'g} \mathbf{\Phi}_{g'} + \frac{1}{k} \mathbf{F}_{g'} \mathbf{\Phi}_{g'} \right] .$$

Holding the scattering source fixed leads to power iteration (fission source iteration),

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Acceleration Methods

Nonlinear Diffusion Acceleration (NDA)

Start, with the single-group first-order transport equation [7, 5], and integrate over angle:

$$\nabla \cdot J_g + (\Sigma_{t,g} - \Sigma_s^{g\to g})\,\phi_g = \sum_{g'\neq g} \Sigma_s^{g'\to g}\phi_{g'} + q_g, \quad J_g \equiv \int d\hat{\Omega}\hat{\Omega}\psi_g(\hat{\Omega})\ .$$

As a closure to this problem, it is common to define current using *Fick's law*,

$$J_g = -D\nabla\phi_g\ .$$

Construct an additive correction to the current using information from an angular solve:

$$\begin{aligned} J_g &= -D\nabla\phi_g + J_g^{\text{ang}} - J_g^{\text{ang}} \\ &= -D\nabla\phi_g + \int_{4\pi} d\hat{\Omega}\hat{\Omega}\psi_g + D\nabla\phi_g \end{aligned}$$

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- Uses a lower order diffusion solve to accelerate a higher order solve.
- Start with the same single-group first-order transport equation, multiply by and integrate over angle, giving the "neutron continuity equation."
- We need closure for this problem, so often we use Fick's law, we will introduce a correction onto Fick's Law based on a higher order solve.
- We will introduce an additive correction based on our two definitions of the current.

Nonlinear Diffusion Acceleration (NDA)

Fold the additive correction into a *drift-diffusion vector*:

$$\begin{aligned} J_g &= -D\nabla\phi_g + \int_{4\pi} d\hat{\Omega}\hat{\Omega}\psi_g + D\nabla\phi_g \\ &= -D\nabla\phi_g + \left[\frac{\int_{4\pi} d\hat{\Omega}\hat{\Omega}\psi_g + D\nabla\phi_g}{\phi_g}\right]\phi_g \\ &= -D\nabla\phi_g + \hat{D}_g\phi_g \ . \end{aligned}$$

Plugging this into our integrated transport equation gives the low-order non-linear diffusion acceleration equation (LONDA),

$$\nabla\cdot\left[-D\nabla + \hat{D}_g\right]\phi_g + \left(\Sigma_{t,g} - \Sigma_s^{g\to g}\right)\phi_g = \sum_{g'\neq g}\Sigma_s^{g'\to g}\phi_{g'} + q_g$$

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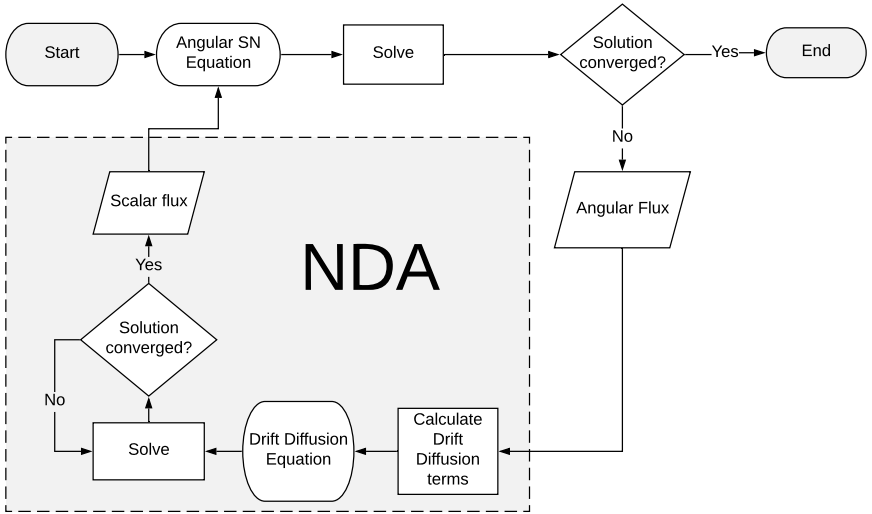
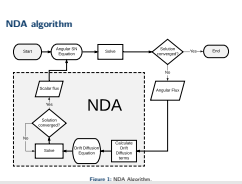
- We combine these corrections into a drift diffusion vector.
- This gives us the LONDA equation, which is just the same integrated transport equation with a corrected current term.
- Presumably, the "higher order" angular solve will have better current information, so we can use it to calculate the drift diffusion vector.

NDA algorithm





- NDA algorithm showing inner low order loop, and outer high order loop.
- In general, outer loop updates both scattering and fission source, checking for k convergence. Inner loop updates fission source, also checking k convergence.

Fourier analysis

To see how the error in our iterative schemes evolves, we can use Fourier analysis [2]. To do so, we use a one-group, one dimension, infinite homogeneous medium with isotropic scattering.

$$\mu\frac{\partial}{\partial x}\psi(x,\mu)+\Sigma_t\psi(x,\mu)=\frac{\Sigma_s}{2}\int_{-1}^{1}\psi(x,\mu')d\mu'+\frac{Q}{2}\ .$$

We define the source iteration scheme as discussed above,

$$\mu\frac{\partial}{\partial x}\psi^{k+1}(x,\mu)+\Sigma_t\psi^{k+1}(x,\mu)=\frac{\Sigma_s}{2}\int_{-1}^{1}\psi^{k}(x,\mu')d\mu'+\frac{Q}{2}\ .$$

and subtract the two to get an equation for the error in iteration k, giving us a similar equation for the error in iteration $k+1$ as it relates to the error in iteration k,

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- How can we be sure that source iteration will converge? What controls the convergence rate? To determine this we can use a Fourier analysis.
- We need to start with a lot of assumptions to get a very simplified version of our transport equation.
- We define what we mean by error, and get an equation that relates the error in each step to the previous step. Unsurprisingly it looks like our original equation, because the evolution of the solution and the evolution of the error are related.

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- If we plug this back into our previous equation and do a large amount of manipulation, we get a fairly simple relationship between the integrated error in one step to the integrated error in the previous step.
- This lambda function is maximized when $n = 0$. The lowest frequency error converges the slowest, and at a rate proportional to Σ_s/Σ_t.

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After plugging into our equation for error and some rearranging,

$$\int_{-1}^{1} \hat{e}^{k+1}(n, \mu) d\mu = \Lambda(n) \int_{-1}^{1} \hat{e}^k(n, \mu') d\mu' \ ,$$

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This motivates the development of acceleration schemes to speed up this convergence. This is especially applicable to shielding problems where scattering is dominant

Two-grid acceleration

To mitigate this issue Adams and Morel [1] developed the two-grid method which rests on two assumptions:

- The persistent error modes can be accurately determined by a course-grid approximation.

Two-grid acceleration

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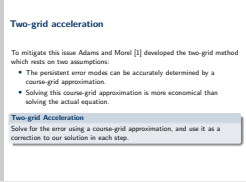
Solve for the error using a course-grid approximation, and use it as a correction to our solution in each step.



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Step 1: Solve the angular S_N source-iteration equation,

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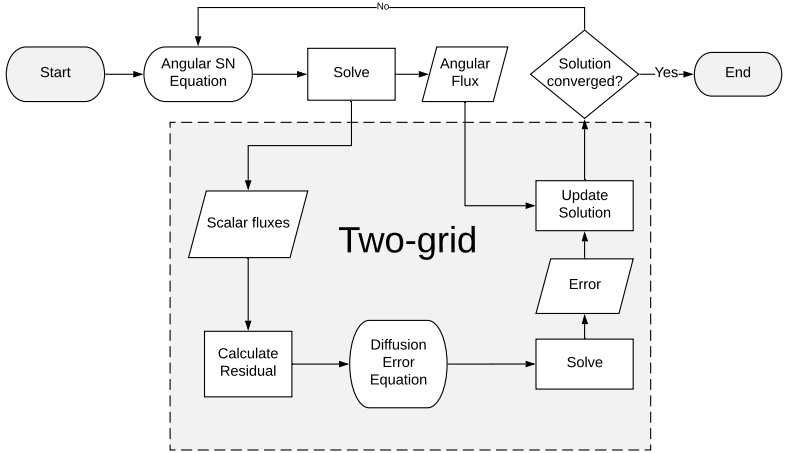
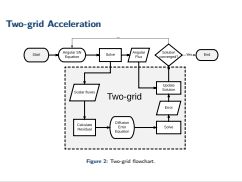


Figure 2: Two-grid flowchart.



Acceleration Methods

Two acceleration methods:

- **Nonlinear Diffusion Acceleration**: improves the convergence of the multi-group Gauss-Seidel iteration, but suffers from convergence issues with a large amount of upscattering.
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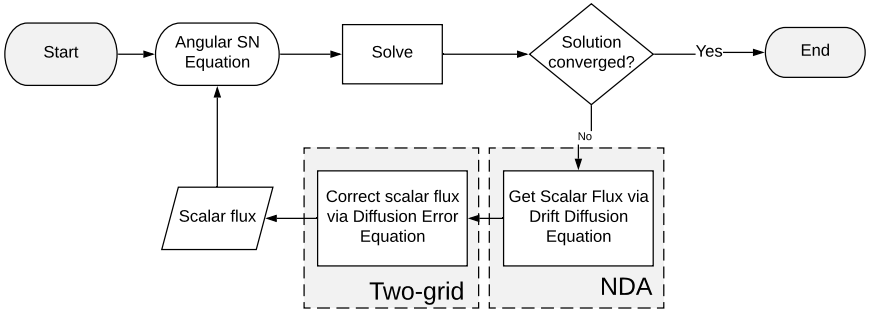

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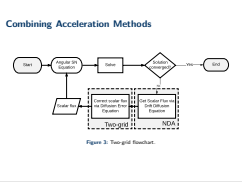

Analyzing Acceleration Schemes

State of the art

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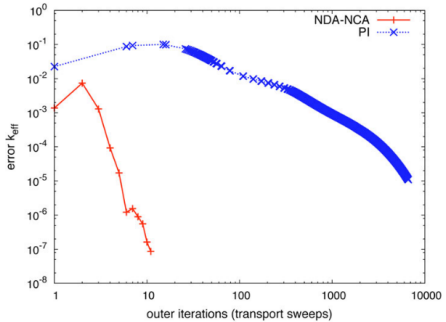
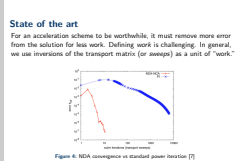


Figure 4: NDA convergence vs standard power iteration [7]



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Analysis Challenges

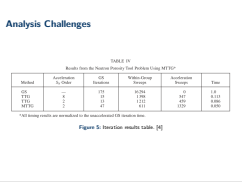
TABLE IV

Results from the Neutron Porosity Tool Problem Using MTTG*

Method	Acceleration S_N Order	GS Iterations	Within-Group Sweeps	Acceleration Sweeps	Time
GS	—	175	16 294	0	1.0
TTG	8	15	1 398	547	0.113
TTG	2	13	1 212	459	0.086
MTTG	2	47	611	1329	0.050

*All timing results are normalized to the unaccelerated GS iteration time.

Figure 5: Iteration results table. [4]



Here is an example of an iteration table from a paper analyzing the two-grid method. It shows both Gauss-Seidel iterations, within group sweeps and acceleration sweeps, but we don't have a clear idea of what parts of the problem are doing all the work. We don't know where the error is being removed, and if this method is doing it more economically or just shifting it around. The *time* is a good indication, but not ideal. Is it proper to use clock time? CPU Time? How do we know that it's not faster because of better computer science. We not only need insight into the inner workings of acelleration schemes, but we need to disaggregate the computer science from the mathematics.

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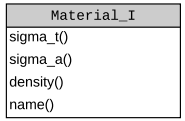

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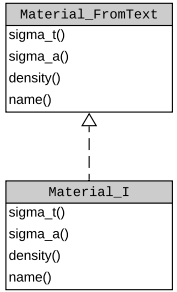

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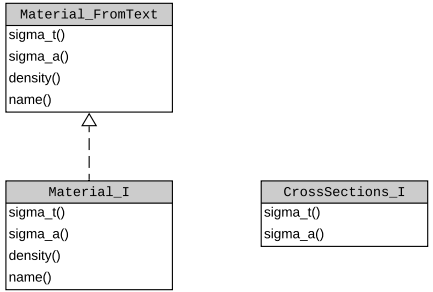

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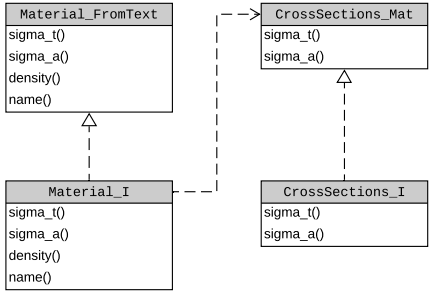

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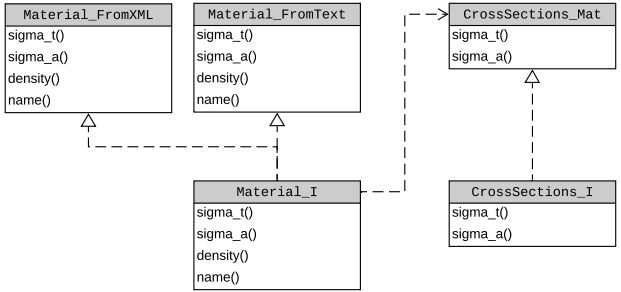

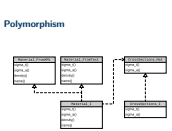

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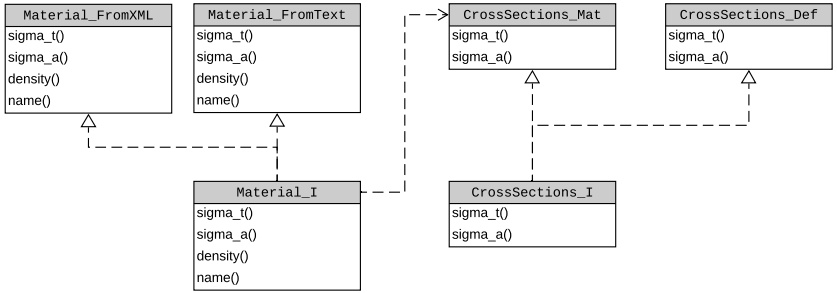
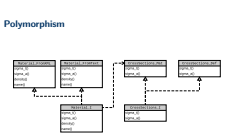


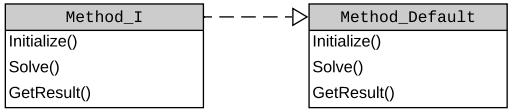


Polymorphism

Method_I
Initialize()
Solve()
GetResult()

Polymorphism

Polymorphism



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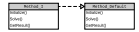

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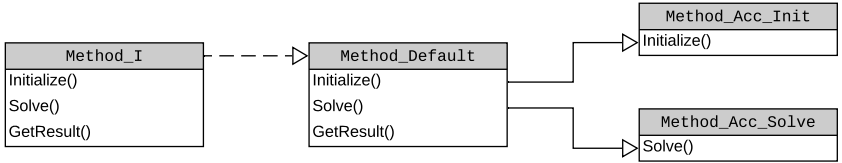

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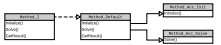

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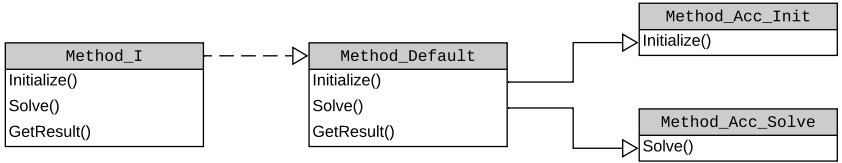

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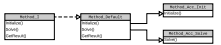

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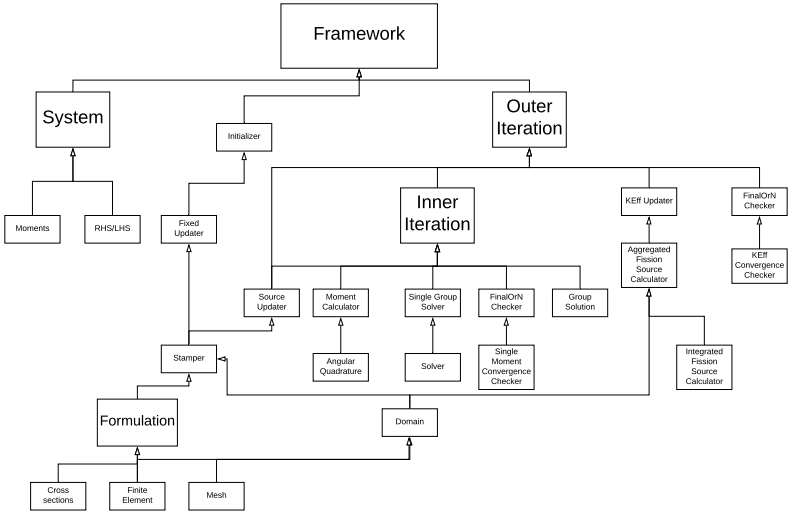

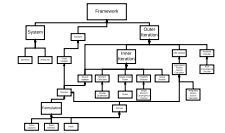

Modern C++

Goal 4

Utilize modern coding and tests practices to make it easier for users to develop and have confidence in their solutions.

- Build using the methods of modern `C++-14`.
- BART uses the `googletest` and `googlemock` libraries for unit testing. Unit testing coverage via `codecov`
- All dependencies for BART are built in an available Docker container.
- Continuous integration via `travis.ci`.

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References

Backup Slides

Energy discretization

Introduce a discretization of the energy domain $\mathbb{E}$ into G non-overlapping elements, such that

$$E_h = \{E_1, E_2, \ldots, E_G\}, \quad \mathbb{E} = \bigcup_{g=1}^{G} E_g$$

Assume that the energy-dependent angular flux can be separated into a group angular flux and a energy function within each of these groups

$$\psi(\mathbf{r}, E, \hat{\Omega}) \approx \psi_g(\mathbf{r}, \hat{\Omega}) f_g(E), \quad E \in E_g$$

This gives us G coupled equations for each energy group, converting the integral scattering term into a summation,

$$\left[\hat{\Omega} \cdot \nabla + \Sigma_{t,g}(\mathbf{r})\right] \psi_g(\mathbf{r}, \hat{\Omega}) = \sum_{g'=0}^{G} \Sigma_{s,g' \to g}(\mathbf{r}, \hat{\Omega}' \to \hat{\Omega}) \psi_{g'}(\mathbf{r}, \hat{\Omega}') + Q_g(\mathbf{r}, \hat{\Omega}) \, .$$

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- Say that the function f_g is zero inside element, and 0 outside, Petrov-Galerkin scheme.

Second-order forms of the Transport Equation

There are various second-order, self-adjoint forms of the transport equation.

- Even/Odd-parity equations (EP).
- Weighted least-squared formulation (WLS).
- Self-adjoint angular flux (SAAF).

With advantages and disadvantages compared to the standard first-order forms. Advantages include:

- They can be solved on multidimensional finite element meshes using standard continuous finite element methods (CFEM).
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- First-order forms of the TE form block lower-triangular that can be swept. But on many meshes, there are slightly re-entrant cells that will break this pattern.
- Solution methods for SPD matrices are better, CG vs. GMRES.

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Self-adjoint angular flux equation (SAAF)

Start with the single-group first-order transport equation [6]:

$$\hat{\Omega} \cdot \nabla \psi + \Sigma_t \psi = S\psi + q \; . \tag{1}$$

Solve for ψ,

$$\psi = \frac{1}{\Sigma_t} \left[S\psi + q - \hat{\Omega} \cdot \nabla \psi \right] \; ,$$

and plug back into the gradient term in Eq.1.

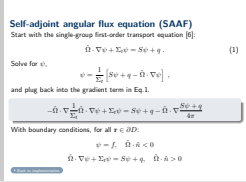
$$-\hat{\Omega} \cdot \nabla \frac{1}{\Sigma_t} \hat{\Omega} \cdot \nabla \psi + \Sigma_t \psi = S\psi + q - \hat{\Omega} \cdot \nabla \frac{S\psi + q}{4\pi}$$

With boundary conditions, for all $\mathbf{r} \in \partial D$:

$$\psi = f, \quad \hat{\Omega} \cdot \hat{n} < 0$$

$$\hat{\Omega} \cdot \nabla \psi + \Sigma_t \psi = S\psi + q, \quad \hat{\Omega} \cdot \hat{n} > 0$$

Back to implementation



The Self-adjoint angular flux equation (SAAF) is a second-order from of the transport equation introduced by Morel and McGhee in 1999. To derive, consider scattering term part of tte source. Properties of SAAF

- +Can solve using standard CFEM methods, which give SPD matrices (can use CG instead of GMRES)
- +Full angular flux is obtained by solve (unlike Even/Odd parity)
- +BCs only coupled in one direction when reflective
- -General sparse matrix, not block lower-triangular (no sweeping)
- -Pure scattering causes issues like odd-parity