BART

A new framework for developing and evaluating acceleration schemes for the neutron transport equation

J. S. Rehak

Qualification Exam

September 4$^{\text{th}}$, 2019

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Outline

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└Outline

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1. Transport Equation
2. Analyzing Acceleration
3. BART
4. The S_N equations
5. Acceleration Methods
6. Plan and Future Work

Steady-state Boltzman Transport Equation

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

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

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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Iterative Solving Method

Assuming the source Q is not a function of ψ, we define the source-iteration iterative scheme for iteration i,

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Error Analysis

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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.

Error Analysis

Start with the single-energy, one dimension, infinite homogeneous medium with isotropic scattering.

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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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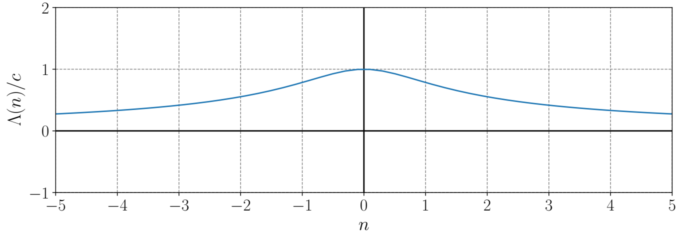
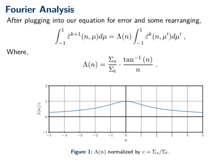


Figure 1: $\Lambda(n)$ normalized by $c = \Sigma_s/\Sigma_t$.



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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, and reactors with a large amount of scattering
You'll notice these use diffusion, because the diffusion equation will be good at calculating these large diffuse errors that are not coupled to space.

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What is Acceleration?

What is Acceleration?

The problem with this is that it's unclear how much actual work is being done in each step. You could form an acceleration scheme that solves in a single outer iteration, but is doing so *actually* accelerating removing more error in less work, or just moving work around?

We can use Fourier analysis like before, but things get complicated when we move into multidimensional problems, and start combining accelerating schemes. We need more insight into the acceleration process.

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For an method to *accelerate* the solve, it must remove more error from the solution for less work. Defining *work* is challenging. In general, we use inversions of the transport matrix (or *sweeps*) as a unit of work.

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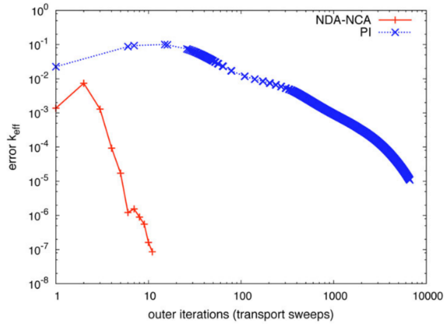

Figure 2: NDA convergence vs standard power iteration [7]

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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 3: Iteration results table. [4]

Analysis Challenges

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 acceleration schemes, but we need to dis-aggregate the computer science from the mathematics.

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- Use object oriented programming and polymorphism to make it easier to implement new methods, and to limit the code needed to do so.
- Include enough tools to allow researchers to analyze the effectiveness of acceleration schemes.
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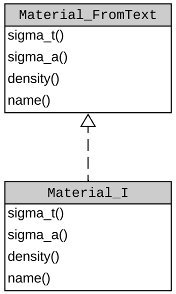
Polymorphism

Material_I
sigma_t()
sigma_a()
density()
name()

Polymorphism

Polymorphism



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Qualification Exam
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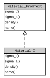

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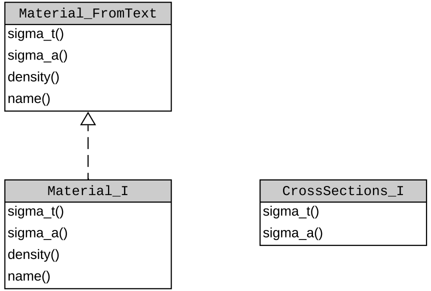

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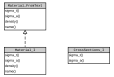

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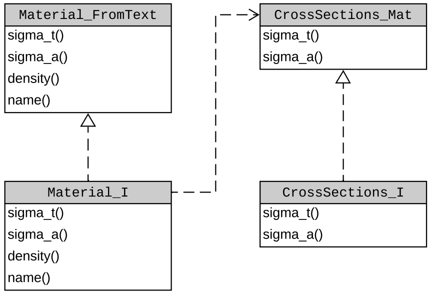

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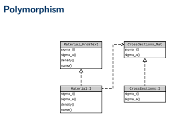

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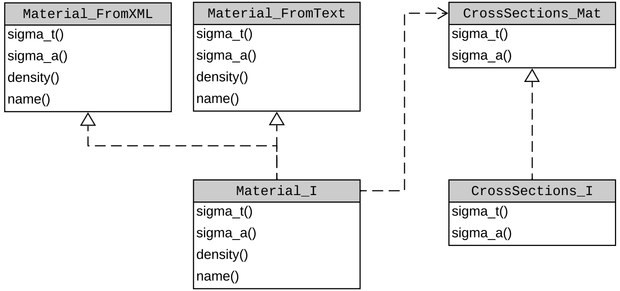

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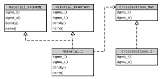

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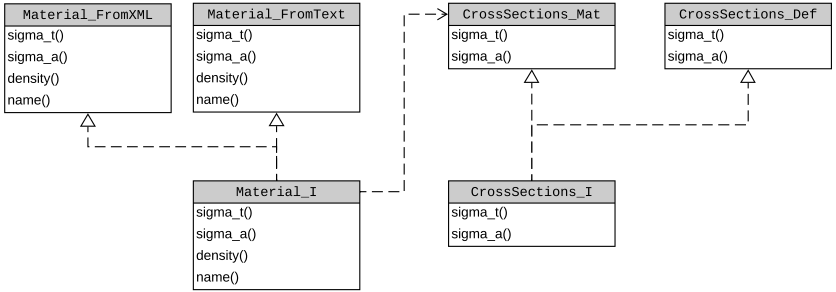

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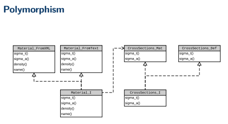

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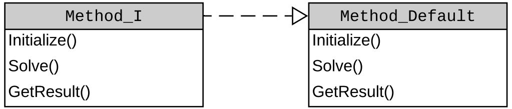

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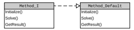

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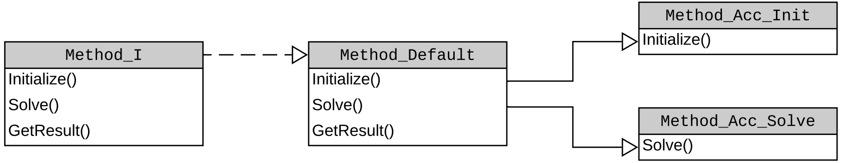

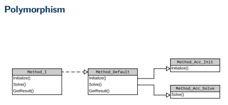

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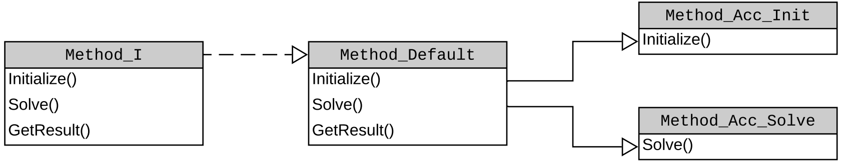

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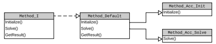

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Framework for experimentation

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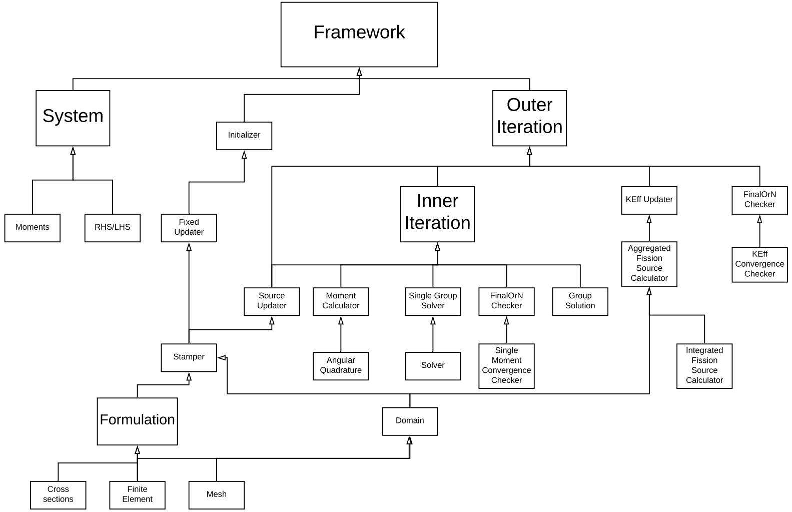

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Modern Coding Practices

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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Benefits:

- Structured data format.

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  string id = 3;

  uint32 number_of_groups = 4;
  uint32 thermal_groups = 5;
  bool   is_fissionable = 6;

  repeated ScalarProperty scalar_property = 7;
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Outline

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1 Transport Equation
2 Analyzing Acceleration
3 BART
4 The S_N equations
5 Acceleration Methods
6 Plan and Future Work

The multigroup S_N equations

Apply the following discretizations:

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Expressed in operator form, this is

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- M is the moment-to-discrete, D is the reverse
- Important to note that the G-th energy group is the lowest.

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- Important to note that the G-th energy group is the lowest.

Iterative Solving Methods

Expressed in operator form, this is

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

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

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And holding the source $\mathbf{Q}$ fixed leads to a Gauss-Seidel (scattering) source iteration,

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

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Nonlinear Diffusion Acceleration (NDA)

Big Idea

Accelerate power iteration by using a diffusion solve in place of the standard transport equation source iteration [7].

Couples an angular solve with a diffusion solve and,

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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.

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

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

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Nonlinear Diffusion Acceleration (NDA)

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

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

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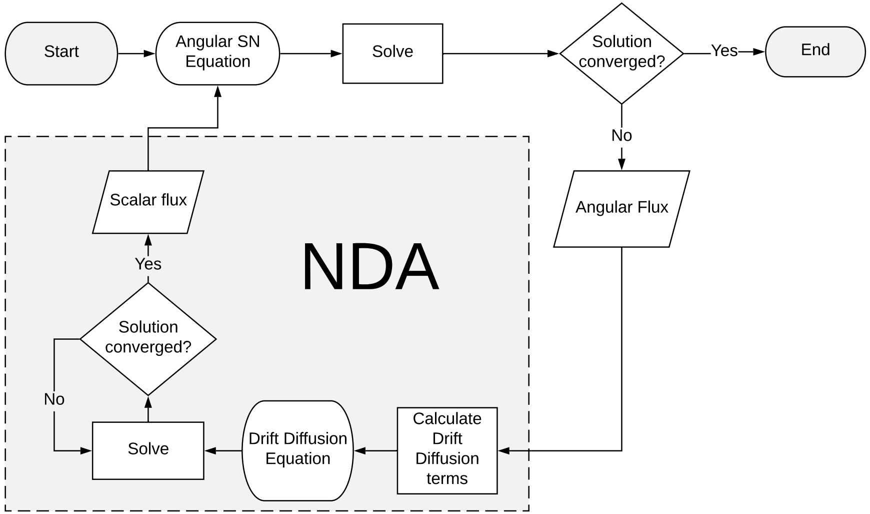
- We combine these corrections into a drift diffusion vector.
- This gives us the LONDA equation, which is just the same integrated transport equation with a corrected current term.
- Presumably, the "higher order" angular solve will have better current information, so we can use it to calculate the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

NDA algorithm



Qualification Exam
└Acceleration Methods
└NDA algorithm

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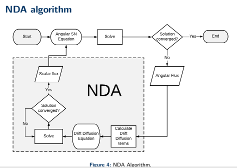

- NDA algorithm showing inner low order loop, and outer high order loop.
- In general, outer loop updates both scattering and fission source, checking for k convergence. Inner loop updates fission source, also checking k convergence.

Two-grid acceleration

To mitigate convergence issues in source-iteration Adams and Morel [1] developed the two-grid method which rests on two assumptions:

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Step 2: Calculate the isotropic component of the residual,

$$\mathbf{R}_{g,0}^{i+\frac{1}{2}} = \sum_{g'=g+1}^{G} \mathbf{S}_{g'g} \left(\mathbf{\Phi}_{g'}^{i+\frac{1}{2}} - \mathbf{\Phi}_{g'}^{i} \right)$$

Step 3: Calculate the error.

$$\mathbf{L}_g \epsilon_g^{i+\frac{1}{2}} = \mathbf{M} \sum_{g'=0}^{G} \mathbf{S}_{g'g} \varepsilon_{g'}^{i+\frac{1}{2}} + \mathbf{R}_g^{i+\frac{1}{2}}$$

Qualification Exam
└─Acceleration Methods
└─Two-grid acceleration

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Step 3a: Calculate error using integrated diffusion approximation.

$$\left(-\nabla \cdot \langle D_g \rangle \nabla + \Sigma_g\right) \tilde{\varepsilon}_g^{i+\frac{1}{2}} = \sum_{g'=0}^{G} \Sigma_{s,g'g,0} \tilde{\varepsilon}_{g'}^{i+\frac{1}{2}} + \mathbf{R}_{g,0}^{i+\frac{1}{2}}$$

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$$\mathbf{\Psi}_g^{i+1} = \mathbf{\Psi}_g^{i+\frac{1}{2}} + \mathbf{M}\tilde{\varepsilon}_g^{i+\frac{1}{2}}$$

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Qualification Exam
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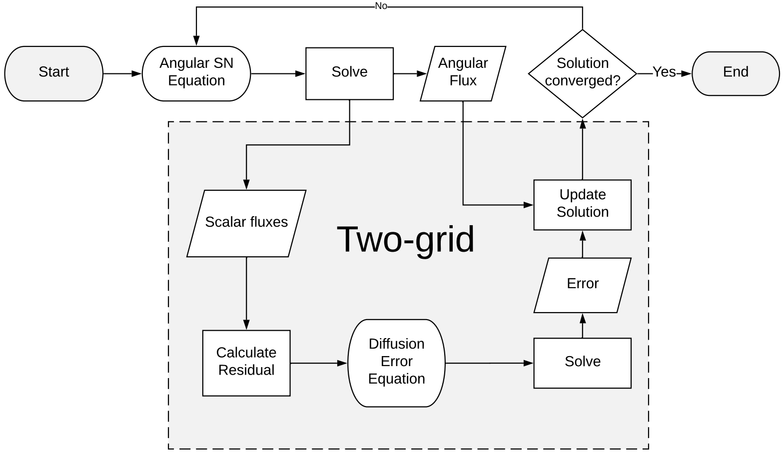

Figure 5: Two-grid flowchart.

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Qualification Exam
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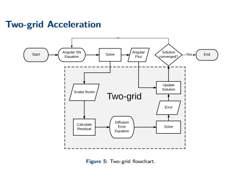

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Two acceleration methods:

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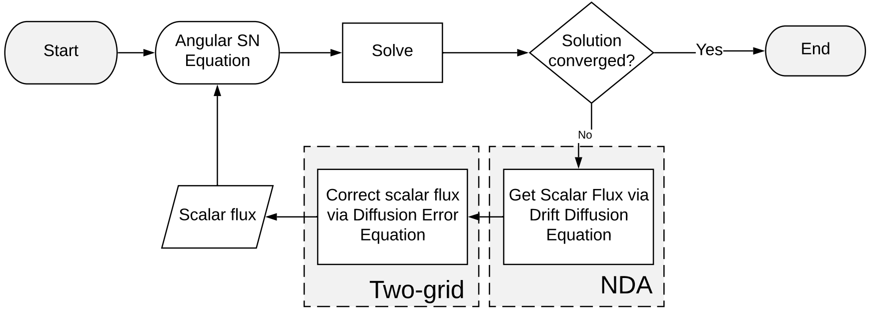

Figure 6: Two-grid flowchart.

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Qualification Exam
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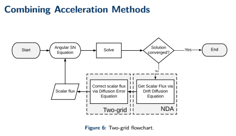

Outline

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2. Analyzing Acceleration
3. BART
4. The S_N equations
5. Acceleration Methods
6. Plan and Future Work

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Outline

❼ **Backup Slides**

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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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$E_h = \{E_1, E_2, \ldots, E_G\}\,, \quad \mathbb{E} = \bigcup_{g=1}^{G} E_g$
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,
$\left[\hat{\Omega} \cdot \nabla + \Sigma_{t,g}(\mathbf{r})\right] \psi_g(\mathbf{r}, \hat{\Omega}) = \sum_{g'=0}^{G} \Sigma_{s,g' \to g}(\mathbf{r}, \hat{\Omega}' \to \hat{\Omega}) \psi_{g'}(\mathbf{r}, \hat{\Omega}') + Q_g(\mathbf{r}, \hat{\Omega})\,.$

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

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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).
- CFEM methods result in symmetric positive-definite (SPD) matrices.
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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]:

$$\hat{\Omega} \cdot \nabla \psi + \Sigma_t \psi = S\psi + q \, . \tag{3}$$

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.3.

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

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