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

J. S. Rehak

Qualification Exam
September 4th, 2019

2019-09-04

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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],

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

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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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.

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

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

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After plugging into our equation for error and some rearranging,

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

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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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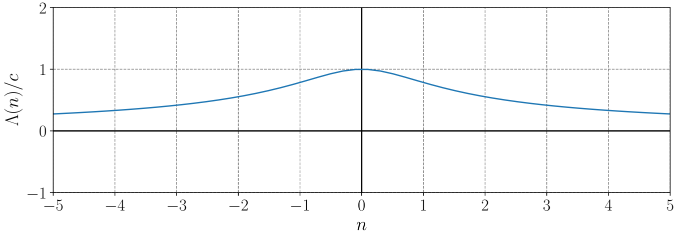
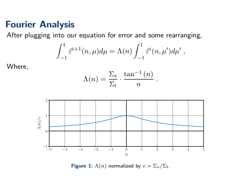


Figure 1: $\Lambda(n)$ normalized by $c = \Sigma_s/\Sigma_t$.



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In the presence of a substantial scattering cross-section, source-iteration can converge arbitrarily slow because the error in diffuse, persistent modes after each iteration reduces by a factor of Σ_s/Σ_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

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What is Acceleration?

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.

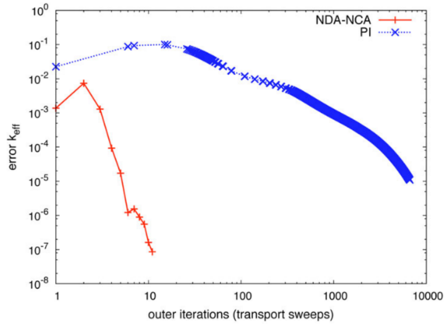
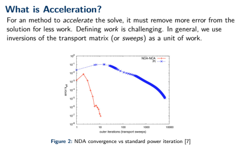


Figure 2: NDA convergence vs standard power iteration [7]



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.

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
Figure 3: 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 acceleration schemes, but we need to dis-aggregate the computer science from the mathematics.

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- Our definition of work is based on assumptions about algorithmic efficiency of the entire transport solve.
- Combining or using complex acceleration schemes may invalidate these assumptions.
- Implementing new schemes can be complicated, making it difficult to dis-aggregate implementation from theory.
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To create a novel tool that addresses these challenges, and acts as a laboratory for researchers to develop, test, and analyze acceleration schemes.

This tool will provide a laboratory for researchers that:

- Provides a controlled environment to run experiments.
- Provides analysis tools to make informed decisions about the results.
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- Enables a controlled environment to test methods.
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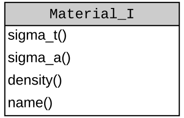
4. Utilize modern coding and testing practices.

- 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.
- Provide an framework for users to experiment with novel combinations of and modifications to existing acceleration schemes.
- Utilize modern coding and test practices to make it easier for users to develop and have confidence in their solutions.

Polymorphism



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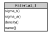

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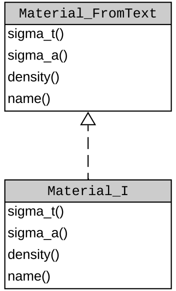

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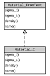

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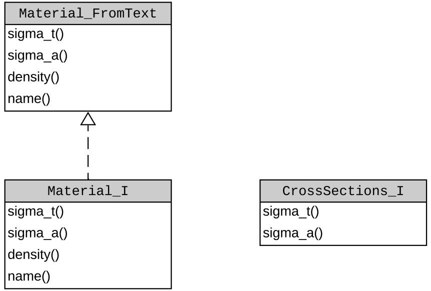

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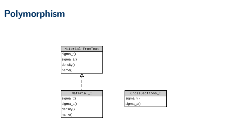

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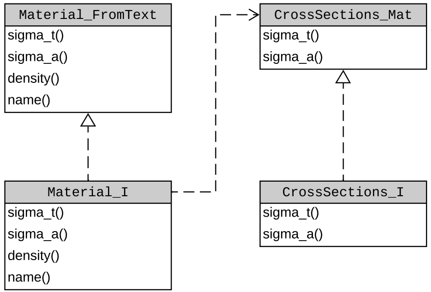

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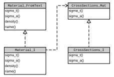

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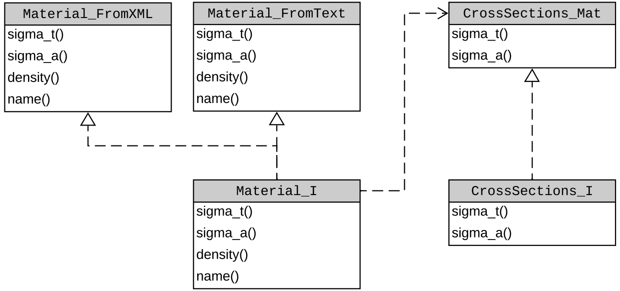

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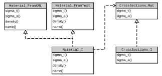

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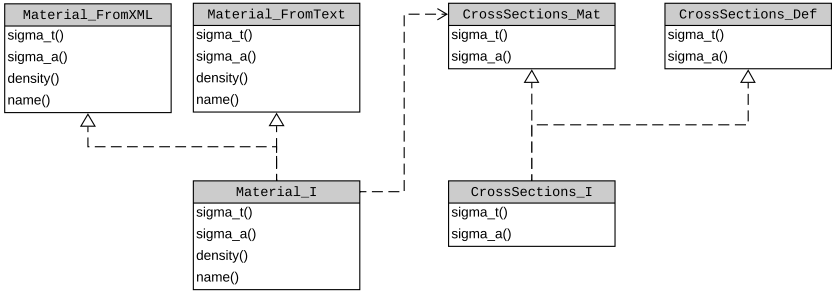

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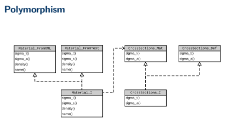

Polymorphism

Method_I
Initialize()
Solve()
GetResult()

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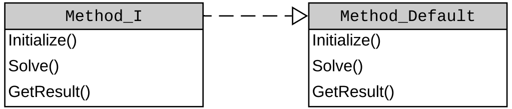

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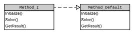

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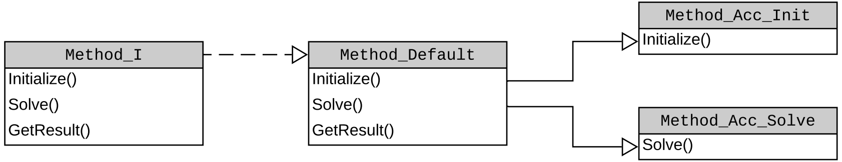

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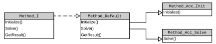

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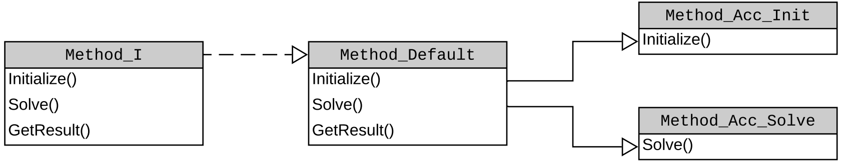

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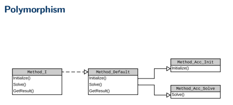

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Instrumentation

Goal 2

Include tools to analyze the effectiveness of acceleration schemes.

BART will include the ability to *instrument* a solve to gather enough data to draw useful conclusions about the effectiveness of acceleration schemes.

- Storage of solve parameters (eigenvalues, fluxes).
- Storage of hierarchy of iterations.
- Calculation and storage of error or residual.
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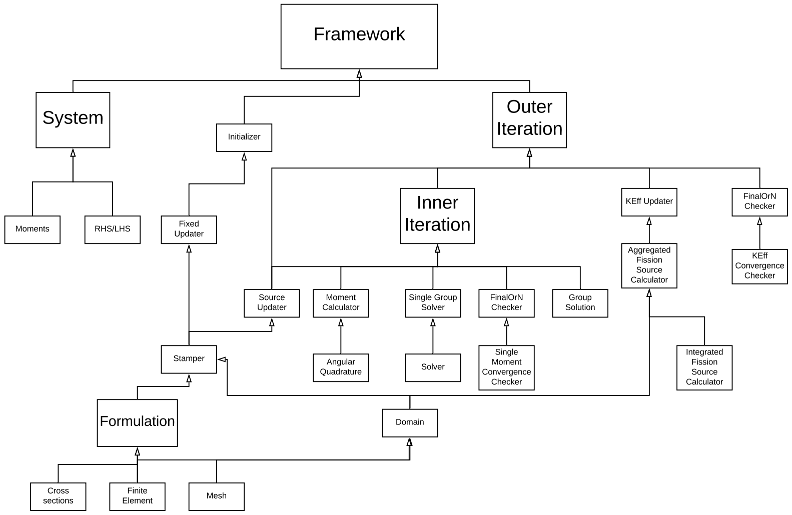

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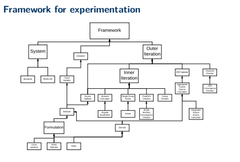

Modern Coding Practices

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.
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Protocol Buffers

Cross-sections can be stored in a novel protocol buffer format.

Benefits:

- Structured data format.
- Automatic generation of parsing code.
- Very fast parsing and small file size.

```
syntax = "proto3";

message Material {
  string full_name = 1;
  string abbreviation = 2;
  string id = 3;

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

  repeated ScalarProperty scalar_property = 7;
  repeated VectorProperty vector_property = 8;
  repeated MatrixProperty matrix_property = 9;

  enum ScalarId {
    UNKNOWN_SCALAR = 0;
    DENSITY = 1;
  }

  enum VectorId {
    UNKNOWN_VECTOR = 0;
    ENERGY_GROUPS = 1; // edges of energy groups in eV
    CHI = 2;
    SIGMA_T = 3; // group homogenized cross sections in 1/cm
    SIGMA_A = 4;
    NU_SIG_F = 5;
    KAPPA_SIG_F = 6;
    Q = 7;
    DIFFUSION_COEFF = 8;
  }

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2019-09-04

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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
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Apply the following discretizations:

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

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Iterative Solving Methods

Expressed in operator form, this is

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2019-09-04

Qualification Exam
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Big Idea

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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)

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

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

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Fold the additive correction into a drift-diffusion vector:

- We combine these corrections 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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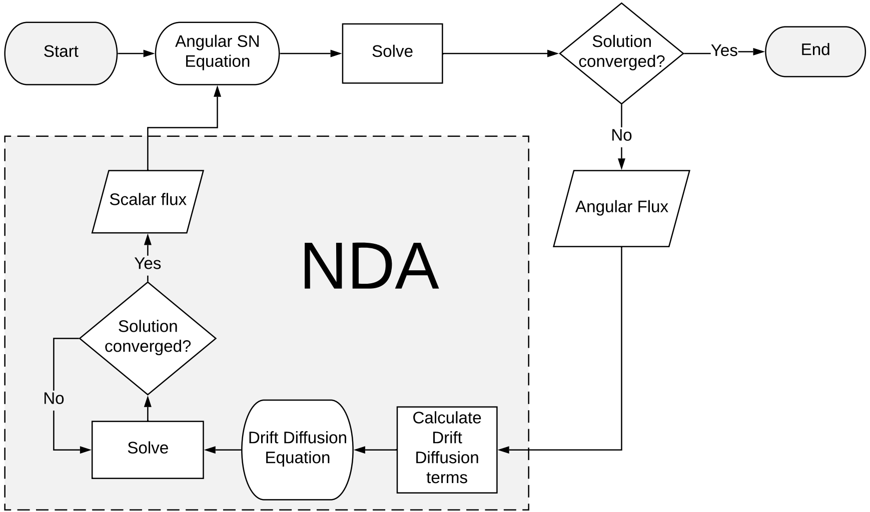
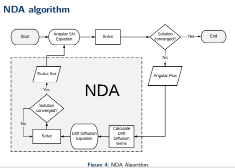
NDA algorithm





- 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.

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2019-09-04

Qualification Exam
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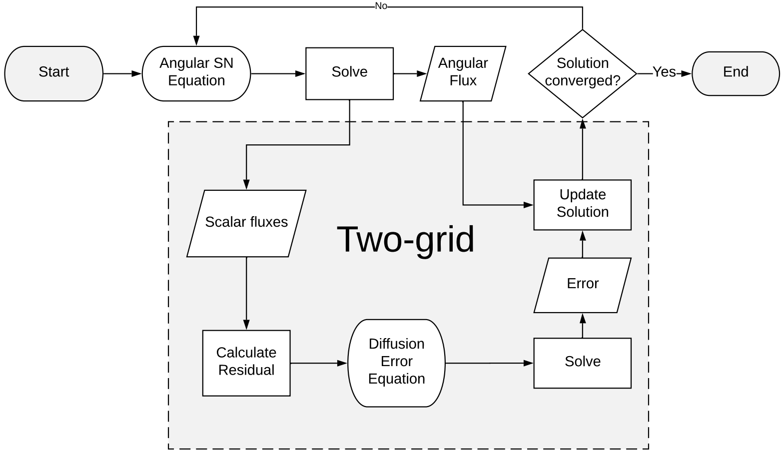

Figure 5: Two-grid flowchart.

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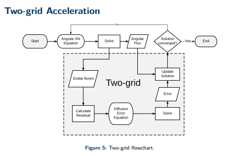
└Acceleration Methods
└Two-grid Acceleration



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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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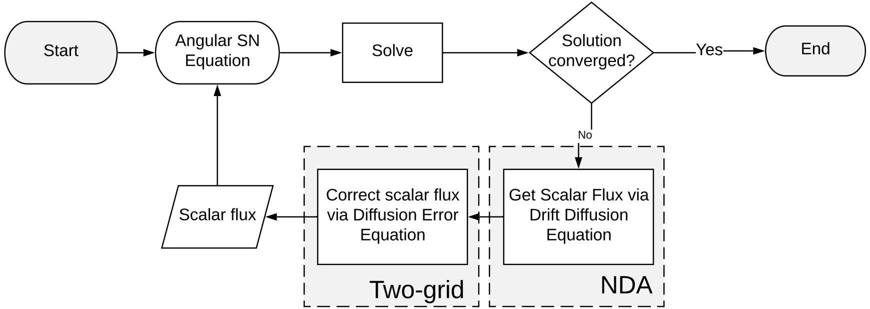

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└Acceleration Methods
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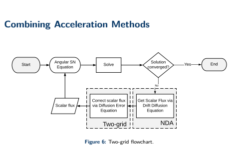

Outline

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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

BART Implementation Plan

Formulations:

- Interface for second-order transport equation formulations using continuous finite element methods.
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Outline

7 Backup Slides

Qualification Exam
└─Backup Slides
└─Outline

2019-09-04

Outline

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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,

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

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Qualification Exam
Backup Slides
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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).
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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