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

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Outline

Transport Equation

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],

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

with a given boundary condition,

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

Iterative Solving Method

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

$$\left[\hat{\Omega} \cdot \nabla + \Sigma_t(\mathbf{r}, E)\right] \boxed{\psi^{i+1}}(\mathbf{r}, E, \hat{\Omega}) \\ = \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}' \Sigma_s(\mathbf{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega}) \boxed{\psi^{i}}(\mathbf{r}, E', \hat{\Omega}') \\ + Q(\mathbf{r}, E, \hat{\Omega}) \ ,$$

with the same boundary condition and initial condition $\psi^0(\mathbf{r}, E, \hat{\Omega})$.

Question

How does the error in our iterative solution ψ^i evolve with time?

Error Analysis

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

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

$$\mu = \cos\theta$$

With source iteration scheme,

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

Subtracting Eq. (2) from Eq. (1) gives an equation for the iteration error,

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

Fourier Analysis

To see how the error evolves in space with each iteration, we can use Fourier analysis [2]. Let λ define a spatial wavelength,

$$\lambda = \frac{\ell}{n}, \quad \ell = \frac{1}{\Sigma_t}, \quad \forall n \in \mathbb{R} \, .$$

With associated linear wave number,

$$\tilde{\nu} = \frac{1}{\lambda} = \frac{n}{\ell} = n \cdot \Sigma_t \, .$$

Perform an inverse Fourier transform, expressing error in spatial frequency space,

$$\varepsilon^i(x, \mu) = \int_{-\infty}^{\infty} \hat{\varepsilon}^i(n, \mu) e^{i \Sigma_t n x} dn \, .$$

Fourier Analysis

After plugging into our equation for error and some rearranging,

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

Where,

$$\Lambda(n) = \frac{\Sigma_s}{\Sigma_t} \cdot \frac{\tan^{-1}(n)}{n} \ .$$

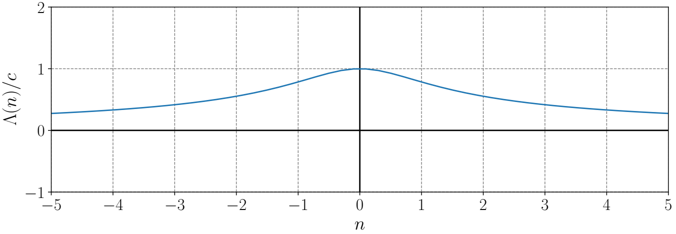


Figure 1: $\Lambda(n)$ normalized by $c = \Sigma_s/\Sigma_t$.

Conclusion

Conclusion

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.

Some acceleration schemes that have been developed:

- Diffusion synthetic acceleration (DSA).
- Nonlinear diffusion acceleration (NDA).
- Diffusion and transport two-grid methods (TG, TTG).

Analyzing Acceleration

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.

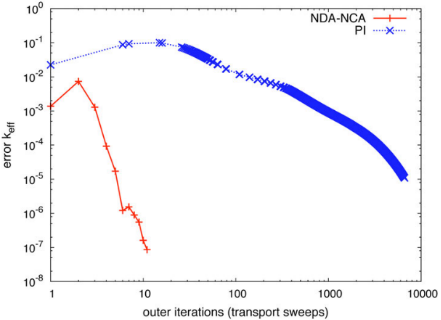


Figure 2: NDA convergence vs standard power iteration [7]

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

A few challenges when analyzing the effectiveness of acceleration schemes include:

- Work definition requires assumptions about algorithm efficiency.
- Combined or complex schemes may invalidate assumptions.
- Implementation and reproducibility can be difficult.

Project Motivation

Project

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.
- Acts as a testing ground for new methods.
- Produces code that is portable, reproducible, and testable.

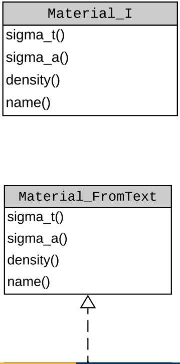
BART

Design Goals for BART

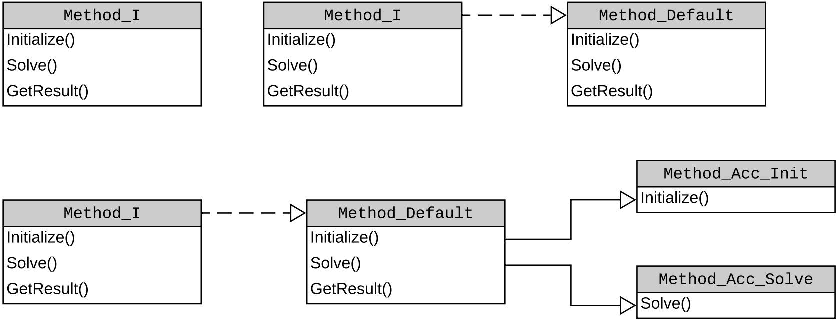
The Bay Area Radiation Transport (BART) is the new code in development with design goals to meet these needs. These goals include:

1. Leverage an object-oriented language and polymorphism.
2. Include analysis tools.
3. Provide a framework for experimentation.
4. Utilize modern coding and tests practices.

Polymorphism



Polymorphism



Polymorphism Benefits

The use of polymorphism in BART

- Minimizes code changes needed to implement new methods, making it faster and easier.
- Enables a true comparison of the accelerated solve to a control solve.
- Makes the modifications *portable*.
- Enables us to compare the implementation of the method to dis-aggregate the computer science from the method itself.

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.

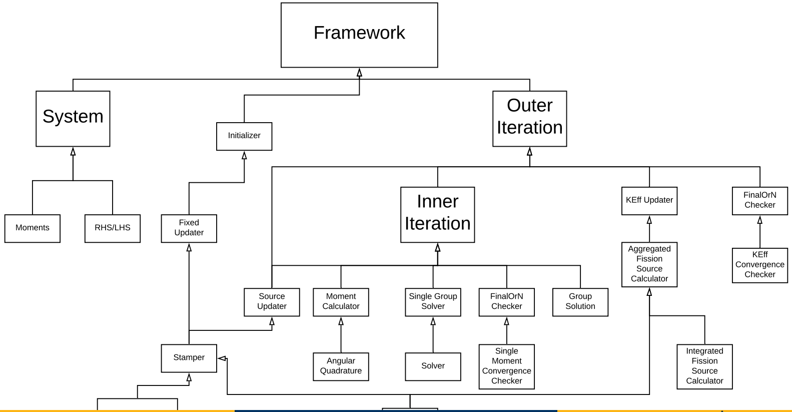
- Storage of solve parameters (eigenvalues, fluxes).
- Storage of hierarchy of iterations.
- Calculation and storage of error or residual.
- Analysis of Fourier error modes coefficients.

Adding new instrumentation must be easy!

Framework for experimentation

Goal 3

Provide a framework for users to experiment with novel combinations of and modifications to existing acceleration schemes.



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`.
- Cross-sections have the capability of being stored in Google Protocol Buffers.
- 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`.

Project Deliverable

1. A new `C++` code that solves the transport equation using continuous finite-element methods.
2. Implementation of a novel acceleration method.
3. An in-depth analysis of this acceleration methods using instrumentation implemented in the code.

The S_N equations

The multigroup S_N equations

Apply the following discretizations:

- Apply a Petrov-Galerkin scheme in energy (multigroup method), splitting into G coupled equations.
- Apply a collocation scheme in angle, solving at angles $\hat{\Omega}_a$.
- Expanding scattering cross-section in Legendre Polynomials with a maximum degree N.

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

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

Multigroup S_N equations

$$\left[\hat{\Omega}_a \cdot \nabla + \Sigma_{t,g}(\mathbf{r})\right] \psi_g(\mathbf{r}, \hat{\Omega}_a)$$

$G \quad N \quad \ell$

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,

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

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

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

Iterative Solving Methods

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),

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

In general, to converge both the fission and scattering sources, power iteration is paired with source iteration in an inner-outer convergence scheme.

Iterative Solve Error

Much of our analysis will require an examination of the error in each step of an iterative method. This is found by subtracting our method from the original equation.

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

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

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

$$\epsilon_g^{i+1} = \mathbf{\Psi}_g - \mathbf{\Psi}_g^{i+1}$$
$$\varepsilon_g^{i+1} = \mathbf{D} \epsilon_g^{i+1}$$

Conclusion (Reprise)

Conclusion

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.

To be implemented and analyzed:

- Nonlinear diffusion acceleration (NDA).
- Diffusion and transport two-grid methods (TG, TTG).
- A novel combination of NDA and TG.

Acceleration Methods

Nonlinear Diffusion Acceleration (NDA)

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

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

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:

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

Nonlinear Diffusion Acceleration (NDA)

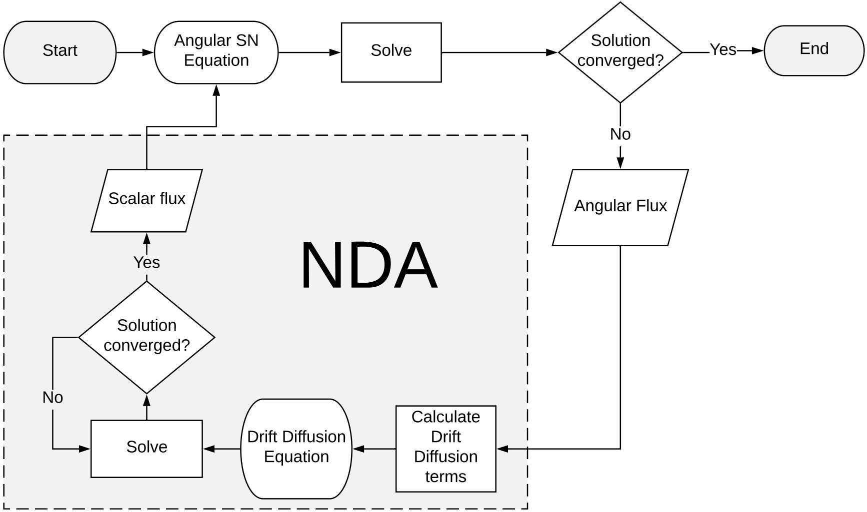
Fold the additive correction into a *drift-diffusion vector*:

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

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

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

NDA algorithm



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 coarse-grid approximation.
- Solving this coarse-grid approximation is more economical than solving the actual equation.

Two-grid Acceleration

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

Two-grid acceleration

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

$$\mathbf{L}_g \mathbf{\Psi}_g^{i+\frac{1}{2}} = \mathbf{M} \sum_{g'=0}^{g} \mathbf{S}_{g'g} \mathbf{\Phi}_{g'}^{i+\frac{1}{2}} + \mathbf{M} \sum_{g'=g+1}^{G} \mathbf{S}_{g'g} \mathbf{\Phi}_{g'}^{k} + \mathbf{Q}_g \ .$$

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.

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

Two-grid acceleration

Step 3a: Calculate error using integrated diffusion approximation.

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

Step 4: Correct the flux

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

This will accelerate our solution only if it removes more error with less work than our original method.

Two-grid Acceleration

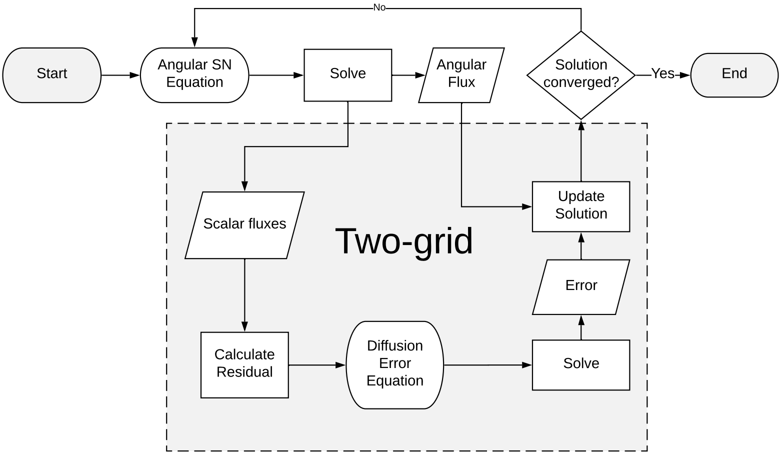


Figure 5: Two-grid flowchart.

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.
- **Two-grid Acceleration**: improves the convergence of multi-group problems with a large amount of upscattering.

Novel Combination

Use two-grid acceleration to improve the convergence rate of the low-order portion of the NDA solve.

Combining Acceleration Methods

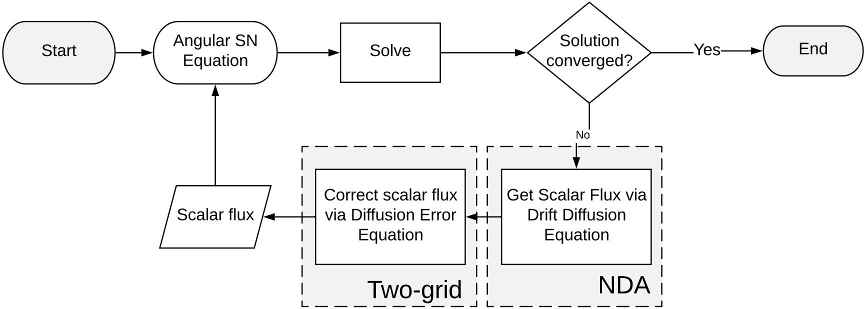


Figure 6: Two-grid flowchart.

Plan and Future Work

BART Implementation Plan

Formulations:

- Interface for second-order transport equation formulations using continuous finite element methods.
- Implementation of Diffusion.
- Implementation of Self-Adjoint angular flux equation.

Acceleration methods:

- Nonlinear diffusion acceleration.
- Two-grid acceleration.
- Nonlinear diffusion acceleration with two-grid acceleration.

Instrumentation:

- In-step Fourier-transform.
- Iteration hierarchy counting.
- Automated runs based on mesh refinement.

Future Work

- Addition of Discontinuous-Galerkin Finite Element Formulations support to BART.
- More acceleration methods implemented to test different combinations.
- Better or more complex *in situ* analysis of acceleration efficiency.
- Automated acceleration control (adaptive acceleration).

References

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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,

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

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.
- When using the P_N formulation, the flux moments are strongly coupled via $\hat{\Omega} \cdot \nabla$.

Second-order forms of the Transport Equation

Disadvantages include:

- CFEM methods result in a general sparse matrix, not a block lower-triangular.
- In some forms (EP), reflective boundary conditions have fully implicit coupling between incoming and outgoing flux. SAAF avoids this only coupling incoming to outgoing.
- Full angular flux can be hard to calculate for parity-forms.
- Difficulties with solving in voids (can be avoided using SAAF).
- Difficulties in a pure scattering media.

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