Title of Qualification Exam Talk

J. S. Rehak

Qualification Exam
September 4^{th}, 2019

2019-08-22

Qualification Exam

Title of Qualification Exam Talk
J. S. Rehak
Qualification Exam
September 4^{th}, 2019

Outline

Qualification Exam

2019-08-22

└Outline

Outline

1. Motivation
2. Transport Equation
3. Acceleration Methods
4. BART

Motivation

Motivation

Transport Equation

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],

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

with a given boundary condition,

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

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],

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

with a given boundary condition,

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

The multigroup S_N equations

Apply the following discretizations:

- Apply a Petrov-Galerkin scheme in energy (multigroup method), splitting into G coupled equations.

The multigroup S_N equations
Apply the following discretizations:
- Apply a Petrov-Galerkin scheme in energy (multigroup method), splitting into G coupled equations.

- Multigroup method splits the equations into G coupled equations
- Collocation scheme in angle uses points for a quadrature rule for integrating angular flux to get flux moments
- Expand in Legendre polynomials, use polynomial addition theorem,

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 $\hat{\Omega}_a$.

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 $\hat{\Omega}_a$.

- Multigroup method splits the equations into G coupled equations
- Collocation scheme in angle uses points for a quadrature rule for integrating angular flux to get flux moments
- Expand in Legendre polynomials, use polynomial addition theorem,

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.

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

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

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 method splits the equations into G coupled equations
- Collocation scheme in angle uses points for a quadrature rule for integrating angular flux to get flux moments
- Expand in Legendre polynomials, use polynomial addition theorem,

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.

Multigroup S_N equations

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

- Multigroup method splits the equations into G coupled equations
- Collocation scheme in angle uses points for a quadrature rule for integrating angular flux to get flux moments
- Expand in Legendre polynomials, use polynomial addition theorem,

Iterative Solving Methods

Expressed in operator form, this is

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

Iterative Solving Methods
Expressed in operator form, this is
$$\mathbf{L}_g \mathbf{\Psi}_g = \mathbf{M} \sum_{g'=0}^{G} \mathbf{S}_{g'g} \mathbf{\Phi}_{g'} + \mathbf{Q}_g, \quad \mathbf{\Phi}_g = \mathbf{D} \mathbf{\Psi}_g \ .$$

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

Iterative Solving Methods

Expressed in operator form, this is

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

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

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

Iterative Solving Methods
Expressed in operator form, this is
$$\mathbf{L}_g\boldsymbol{\Psi}_g = \mathbf{M}\sum_{g'=0}^{G}\mathbf{S}_{g'g}\boldsymbol{\Phi}_{g'} + \mathbf{Q}_g, \quad \boldsymbol{\Phi}_g = \mathbf{D}\boldsymbol{\Psi}_g\ .$$
Splitting the scattering source into down-scattering and up-scattering terms,
$$\mathbf{L}_g\boldsymbol{\Psi}_g = \mathbf{M}\sum_{g'=0}^{g}\mathbf{S}_{g'g}\boldsymbol{\Phi}_{g'} + \mathbf{M}\sum_{g'=g+1}^{G}\mathbf{S}_{g'g}\boldsymbol{\Phi}_{g'} + \mathbf{Q}_g\ ,$$

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

Iterative Solving Methods

Expressed in operator form, this is

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

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

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

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

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

Iterative Solving Methods
Expressed in operator form, this is
$$\mathbf{L}_g \boldsymbol{\Psi}_g = \mathbf{M} \sum_{g'=0}^{G} \mathbf{S}_{g'g} \boldsymbol{\Phi}_{g'} + \mathbf{Q}_g, \quad \boldsymbol{\Phi}_g = \mathbf{D} \boldsymbol{\Psi}_g \; .$$
Splitting the scattering source into down-scattering and up-scattering terms,
$$\mathbf{L}_g \boldsymbol{\Psi}_g = \mathbf{M} \sum_{g'=0}^{g} \mathbf{S}_{g'g} \boldsymbol{\Phi}_{g'} + \mathbf{M} \sum_{g'=g+1}^{G} \mathbf{S}_{g'g} \boldsymbol{\Phi}_{g'} + \mathbf{Q}_g \; ,$$
And holding the source $\mathbf{Q}$ fixed leads to a Gauss-Seidel (scattering) source iteration,
$$\mathbf{L}_g \boldsymbol{\Psi}_g^{k+1} = \mathbf{M} \sum_{g'=0}^{g} \mathbf{S}_{g'g} \boldsymbol{\Phi}_{g'}^{k+1} + \mathbf{M} \sum_{g'=g+1}^{G} \mathbf{S}_{g'g} \boldsymbol{\Phi}_{g'}^{k} + \mathbf{Q}_g \; .$$

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

Iterative Solving Methods

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

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

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

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

Iterative Solving Methods

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

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

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

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

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.

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.

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.

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

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

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.

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

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

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.

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

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

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.

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

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

Acceleration Methods

Acceleration Methods

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,

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

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.
We define the source iteration scheme as discussed above,
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,

- 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.

Fourier Analysis

To perform an inverse Fourier transform, we need to choose a measure of spatial variation, an error "wavelength."

Fourier Analysis
To perform an inverse Fourier transform, we need to choose a measure of spatial variation, an error "wavelength."

- We can examine the modes of the spatial error by using an inverse fourier transform. This will give us an idea of how the spatial frequencies of the error. We need to decide on an error wavelength, which gives us a linear error frequency. Higher n means higher error frequency, with $n = 0$ being infinite wavelength, completely non-coupled error.
- 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.

Fourier Analysis

To perform an inverse Fourier transform, we need to choose a measure of spatial variation, an error "wavelength."

$$\lambda = \frac{\ell}{n}, \quad \forall n \in \mathbb{R} \implies \tilde{\nu} = \frac{1}{\lambda} = \frac{n}{\ell} = n \cdot \Sigma_t$$

Fourier Analysis
To perform an inverse Fourier transform, we need to choose a measure of spatial variation, an error "wavelength."
$\lambda = \frac{\ell}{n}, \quad \forall n \in \mathbb{R} \implies \tilde{\nu} = \frac{1}{\lambda} = \frac{n}{\ell} = n \cdot \Sigma_t$

- We can examine the modes of the spatial error by using an inverse fourier transform. This will give us an idea of how the spatial frequencies of the error. We need to decide on an error wavelength, which gives us a linear error frequency. Higher n means higher error frequency, with $n = 0$ being infinite wavelength, completely non-coupled error.
- 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.

Fourier Analysis

To perform an inverse Fourier transform, we need to choose a measure of spatial variation, an error "wavelength."

$$\lambda = \frac{\ell}{n}, \quad \forall n \in \mathbb{R} \implies \tilde{\nu} = \frac{1}{\lambda} = \frac{n}{\ell} = n \cdot \Sigma_t$$

Perform an inverse Fourier transform,

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

Fourier Analysis
To perform an inverse Fourier transform, we need to choose a measure of spatial variation, an error "wavelength."
$$\lambda = \frac{\ell}{n}, \quad \forall n \in \mathbb{R} \implies \tilde{\nu} = \frac{1}{\lambda} = \frac{n}{\ell} = n \cdot \Sigma_t$$
Perform an inverse Fourier transform,
$$e^k(x, \mu) = \int_{-\infty}^{\infty} \hat{e}^k(n, \mu) e^{i\Sigma_t n x} dn \; .$$

- We can examine the modes of the spatial error by using an inverse fourier transform. This will give us an idea of how the spatial frequencies of the error. We need to decide on an error wavelength, which gives us a linear error frequency. Higher n means higher error frequency, with $n = 0$ being infinite wavelength, completely non-coupled error.
- 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.

Fourier Analysis

To perform an inverse Fourier transform, we need to choose a measure of spatial variation, an error "wavelength."

$$\lambda = \frac{\ell}{n}, \quad \forall n \in \mathbb{R} \implies \tilde{\nu} = \frac{1}{\lambda} = \frac{n}{\ell} = n \cdot \Sigma_t$$

Perform an inverse Fourier transform,

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

After plugging into our equation for error and some rearranging,

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

Where

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

Fourier Analysis
To perform an inverse Fourier transform, we need to choose a measure of spatial variation, an error "wavelength."
$$\lambda = \frac{\ell}{n}, \quad \forall n \in \mathbb{R} \implies \tilde{\nu} = \frac{1}{\lambda} = \frac{n}{\ell} = n \cdot \Sigma_t$$
Perform an inverse Fourier transform,
$$e^k(x,\mu) = \int_{-\infty}^{\infty} \hat{e}^k(n,\mu) e^{i\Sigma_t n x} dn \ .$$
After plugging into our equation for error and some rearranging,
$$\int_{-1}^{1} \hat{e}^{k+1}(n,\mu) d\mu = \Lambda(n) \int_{-1}^{1} \hat{e}^k(n,\mu') d\mu' \ ,$$
Where
$$\Lambda(n) = \frac{\Sigma_s}{\Sigma_t} \cdot \frac{\tan^{-1}(n)}{n} \ .$$

- We can examine the modes of the spatial error by using an inverse fourier transform. This will give us an idea of how the spatial frequencies of the error. We need to decide on an error wavelength, which gives us a linear error frequency. Higher n means higher error frequency, with $n = 0$ being infinite wavelength, completely non-coupled error.
- 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.

Problem

Problem Statement

In the presence of up-scattering and a substantial scattering cross-section, Gauss-Seidel 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.

Problem

Problem Statement
In the presence of up-scattering and a substantial scattering cross-section, Gauss-Seidel 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.

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

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.

- This should speed up the solve by giving an addition reduction in those diffuse persistent error modes.

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

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

- This should speed up the solve by giving an addition reduction in those diffuse persistent error modes.

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

Two-grid Acceleration

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

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

Two-grid Acceleration

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

- This should speed up the solve by giving an addition reduction in those diffuse persistent error modes.

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 1: Solve the angular S_N source-iteration equation,
Step 2: Calculate the isotropic component of the residual,
Step 3: Calculate the error.

Two-grid acceleration

Step 3a: Calculate error using diffusion approximation.

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

Step 4: Correct the flux

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

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

Two-grid acceleration

Step 3a: Calculate error using diffusion approximation.

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

Step 4: Correct the flux

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

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

Two-grid Acceleration

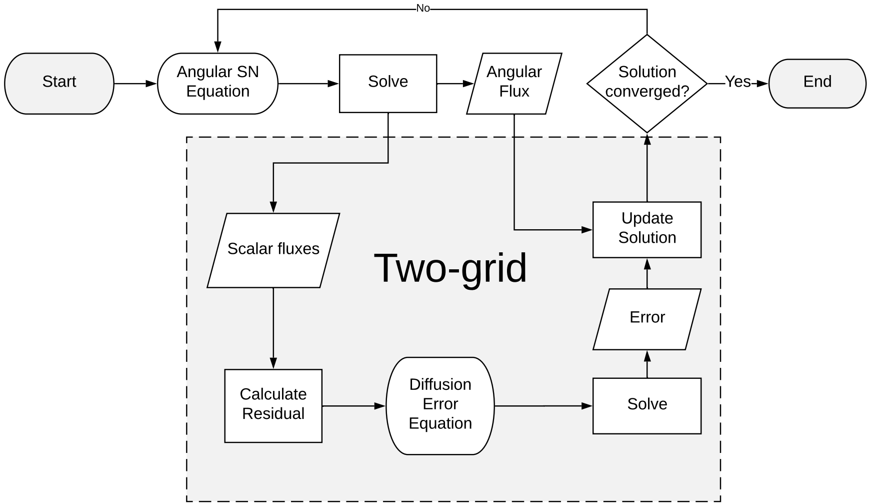
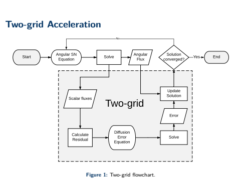


Figure 1: Two-grid flowchart

2019-08-22

Qualification Exam
└Acceleration Methods
└Two-grid Acceleration



Nonlinear Diffusion Acceleration (NDA)

Start, with the single-group first-order transport equation [4], 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:

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

Nonlinear Diffusion Acceleration (NDA)
Start, with the single-group first-order transport equation [4], 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:
$J_g = -D\nabla\phi_g + J_g^{\text{ang}} - J_g^{\text{ang}} = -D\nabla\phi_g + \int_{4\pi} d\hat{\Omega}\hat{\Omega}\psi_g + D\nabla\phi_g$

- 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),

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

Nonlinear Diffusion Acceleration (NDA)

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

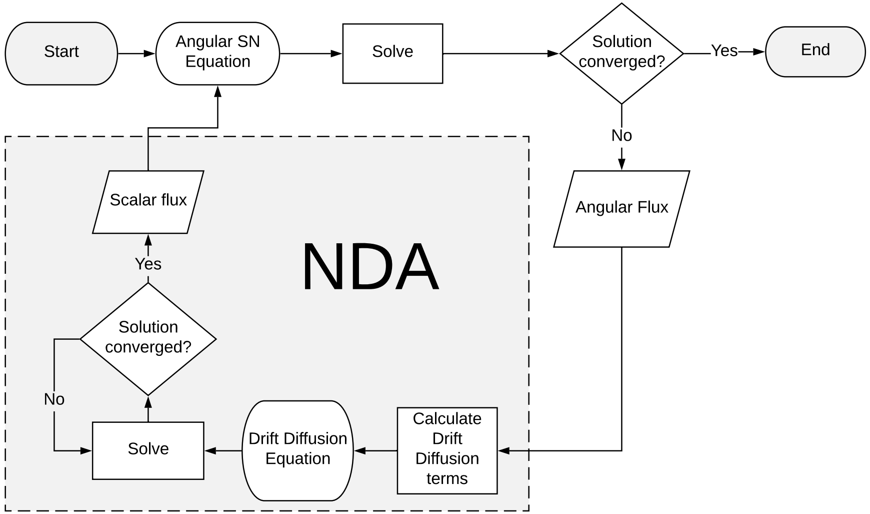
$$\begin{aligned} J_g &= -D\nabla\phi_g + \int_{4\pi} d\hat{\Omega}\hat{\Omega}\psi_g + D\nabla\phi_g \\ &= -D\nabla\phi_g + \left[\frac{\int_{4\pi} d\hat{\Omega}\hat{\Omega}\psi_g + D\nabla\phi_g}{\phi_g}\right]\phi_g \\ &= -D\nabla\phi_g + \hat{D}_g\phi_g\ . \end{aligned}$$

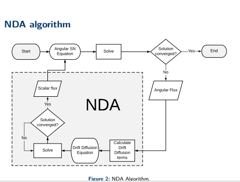
Plugging this into our integrated transport equation gives the low-order non-linear diffusion acceleration equation (LONDA).

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

- 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.

BART

BART

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

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 $\hat{\Omega} \cdot \nabla$.

- 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.

Second-order forms of the Transport Equation

Disadvantages include:

- CFEM methods result in a general sparse matrix, not a block lower-triangular.

Second-order forms of the Transport Equation

Disadvantages include:

- CFEM methods result in a general sparse matrix, not a block lower-triangular.

- Block lower-triangular would have allowed us to sweep.
- In pure scattering, there is a singularity in the scattering matrix for OP and SAAF in the spherical-harmonic basis. This is because it is diagonal and the first entry is $1/(\Sigma_t - \Sigma_{s0})$ which is $1/0$

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.

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.

- Block lower-triangular would have allowed us to sweep.
- In pure scattering, there is a singularity in the scattering matrix for OP and SAAF in the spherical-harmonic basis. This is because it is diagonal and the first entry is $1/(\Sigma_t - \Sigma_{s0})$ which is $1/0$

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.

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.

- Block lower-triangular would have allowed us to sweep.
- In pure scattering, there is a singularity in the scattering matrix for OP and SAAF in the spherical-harmonic basis. This is because it is diagonal and the first entry is $1/(\Sigma_t - \Sigma_{s0})$ which is $1/0$

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).

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).

- Block lower-triangular would have allowed us to sweep.
- In pure scattering, there is a singularity in the scattering matrix for OP and SAAF in the spherical-harmonic basis. This is because it is diagonal and the first entry is $1/(\Sigma_t - \Sigma_{s0})$ which is $1/0$

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.

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.

- Block lower-triangular would have allowed us to sweep.
- In pure scattering, there is a singularity in the scattering matrix for OP and SAAF in the spherical-harmonic basis. This is because it is diagonal and the first entry is $1/(\Sigma_t - \Sigma_{s0})$ which is $1/0$

Self-adjoint angular flux equation (SAAF)

Start with the single-group first-order transport equation [5]:

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

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 $\mathbf{r}\in\partial D$:

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

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

Self-adjoint angular flux equation (SAAF)
Start with the single-group first-order transport equation [5]:
$$\hat{\Omega}\cdot\nabla\psi + \Sigma_t\psi = S\psi + q\,. \tag{1}$$
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 $\mathbf{r}\in\partial D$:
$$\psi = f, \quad \hat{\Omega}\cdot\hat{n} < 0$$
$$\hat{\Omega}\cdot\nabla\psi + \Sigma_t\psi = S\psi + q, \quad \hat{\Omega}\cdot\hat{n} > 0$$

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

References

[1] B. T. Adams and Jim E. Morel.
A Two-Grid Acceleration Scheme for the Multigroup Sn Equations with Neutron Upscattering.
Nuclear Science and Engineering, 115(May):253–264, 1993.

[2] Marvin L. Adams and Edward W. Larsen.
Fast iterative methods for discrete-ordinates particle transport calculations.
Progress in Nuclear Energy, 2002.

[3] E. E. Lewis and W.F. Miller, Jr.
Computational Methods of Neutron Transport.
American Nuclear Society, 1993.

[4] Hans R Hammer, Jim E. Morel, and Yaqi Wang.
Nonlinear Diffusion Acceleration in Voids for the Weighted Least-Square Transport Equation.
In *Mathematics and Computation2*, 2017.

[5] J E Morel and J M Mcghee.
A Self-Adjoint Angular Flux Equation.
Nuclear Science and Engineering, 132:312–325, 1999.

Backup Slides

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,

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

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

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