Title of Qualification Exam Talk

J. S. Rehak

Qualification Exam
September 4th, 2019

2019-08-20

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Outline

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1. Motivation
2. Background
3. Acceleration Methods
4. BART

Motivation

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Background

Background

Steady-state Boltzman Transport Equation

Our problem of interest is the time-independent transport equation for a critical system on a domain of interest $\mathbf{r} \in V$ [1],

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

with a given boundary condition,

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

Steady-state Boltzman Transport Equation

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The multigroup S_N equations

To get the standard multigroup S_N equations, we 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 (the P_N method).

$$\left[\hat{\Omega}^a \cdot \nabla + \Sigma_t^g(\mathbf{r})\right] \psi^g(\mathbf{r}, \hat{\Omega}^a) = \sum_{g'=0}^{G} \sum_{\ell=0}^{N} \sum_{m=-\ell}^{\ell} \Sigma_{s,\ell}^{g' \to g} Y_{\ell,m}(\hat{\Omega}^a) \phi_{\ell,m}^{g'}(\mathbf{r}) + Q^g(\mathbf{r}, \hat{\Omega}^a)$$

In operator form:

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

The multigroup S_N equations
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Apply a collocation scheme in angle, solving at angles $\hat{\Omega}_a$.
Expanding scattering cross-section in Legendre Polynomials with a maximum degree N (the P_N method).
In operator form:

- 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,

Acceleration Methods

Acceleration Methods

Nonlinear Diffusion Acceleration (NDA)

Start, with the single-group first-order transport equation [2], 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:

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

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

Nonlinear Diffusion Acceleration (NDA)

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

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

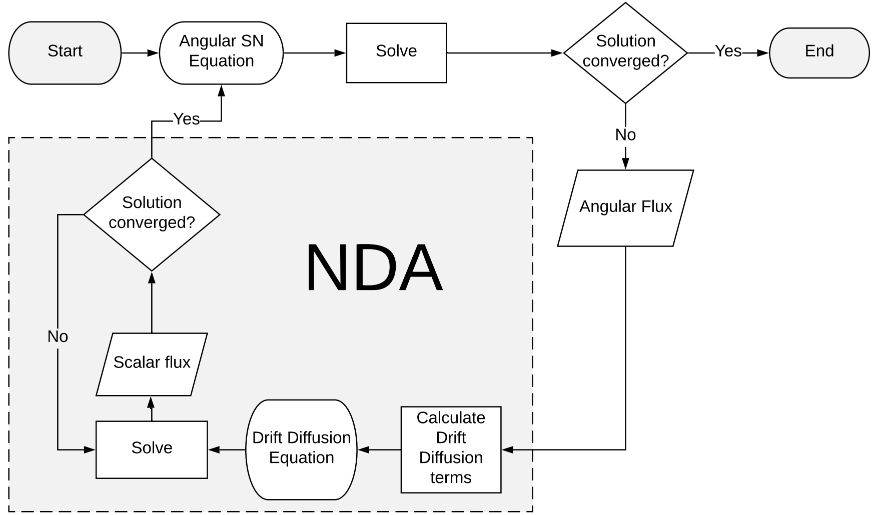
Plugging this into our integrated transport equation gives the low-order non-linear diffusion acceleration equation (LONDA),

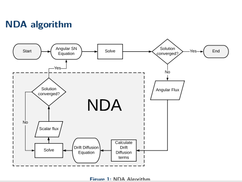
$$
\nabla\cdot\left[-D\nabla + \hat{D}_g\right]\phi_g + \left(\Sigma_{t,g} - \Sigma_s^{g\to g}\right)\phi_g = \sum_{g'\neq g}\Sigma_s^{g'\to g}\phi_{g'} + q_g
$$

Nonlinear Diffusion Acceleration (NDA)
Fold the additive correction into a *drift-diffusion vector*:
Plugging this into our integrated transport equation gives the low-order non-linear diffusion acceleration equation (LONDA).

- 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

Transport equation second-order forms

Consider the mono-energetic form of the transport equation, using the scattering operator $S\psi(\mathbf{r},\hat{\Omega}) = \int_{4\pi} d\hat{\Omega}'\Sigma_s(\mathbf{r},\hat{\Omega}' \rightarrow \hat{\Omega})\psi(\mathbf{r},\hat{\Omega}')$:

$$\left[\hat{\Omega}\cdot\nabla + \Sigma_t(\mathbf{r})\right]\psi(\mathbf{r},\hat{\Omega}) = S\psi(\mathbf{r},\hat{\Omega}) + Q \qquad (1)$$

Substitute $-\hat{\Omega}$ for $\hat{\Omega}$, add to Eq. (1), and divide by two to get a function of even- and odd-parity angular fluxes.

$$\hat{\Omega}\cdot\nabla\psi^- + \Sigma_t\psi^+ = S^+\psi^+ + Q^+$$

where,

$$\psi^+ = \frac{1}{2}\left(\psi(\hat{\Omega}) + \psi(-\hat{\Omega})\right)$$
$$\psi^- = \frac{1}{2}\left(\psi(\hat{\Omega}) - \psi(-\hat{\Omega})\right)$$

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Self-adjoint angular flux equation (SAAF)

Start with the single-group first-order transport equation [3]:

$$\hat{\Omega}\cdot\nabla\psi + \Sigma_t\psi = S\psi + q\ . \qquad (2)$$

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.2.

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

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

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

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

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

[2] 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.

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

References

[1] E. E. Lewis and W.F. Miller, Jr.
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Backup Slides

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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,

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

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