Title of Qualification Exam Talk

J. S. Rehak

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Outline

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Steady-state Boltzman Transport Equation

Our problem of interest is the time-independent transport equation for a critical system on a domain of interest $\mathbf{r} \in V$ [2],

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

with a given boundary condition,

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

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- Expanding scattering cross-section in Legendre Polynomials with a maximum degree N (the P_N method).

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

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

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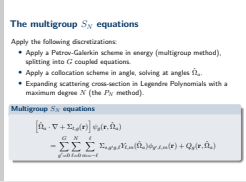
Multigroup S_N equations

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



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Expressed in operator form, this is

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

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

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

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

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

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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),

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Fourier analysis

To see how the error in our iterative schemes evolves, we can use Fourier analysis [1]. 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,

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

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

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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

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

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Acceleration Methods

Two-grid acceleration

Back to the operator form of the multi-group S_N equation,

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

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- Go back to the operator form of the multi-group S_N equation.
- Like in our Fourier analysis, we can subtract the GS iteration scheme from the equation it is trying to solve, giving us an equation for the error.

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Subtract the two to get an equation for the error in our iterative method,

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

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

where,

$$\epsilon_g^{k+1} = \mathbf{\Psi}_g - \mathbf{\Psi}_g^{k+1}, \quad \varepsilon_g^{k+1} = \mathbf{D} \epsilon_g^{k+1},$$
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Nonlinear Diffusion Acceleration (NDA)

Start, with the single-group first-order transport equation [3], and integrate over angle:

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

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),

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

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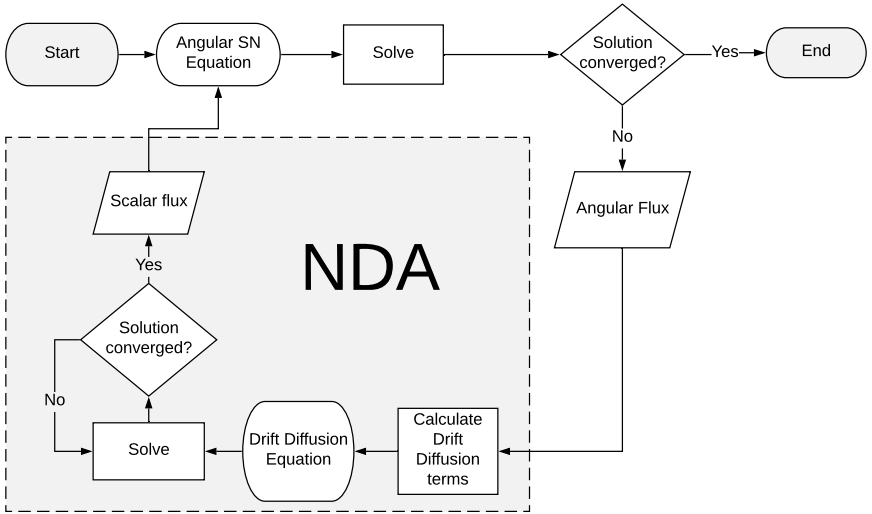
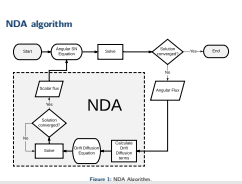
Fold the additive correction into a drift-diffusion vector:
$$\begin{aligned} J_g &= -D\nabla\phi_g + \int_{4\pi} d\hat{\Omega}\hat{\Omega}\psi_g + D\nabla\phi_g \\ &= -D\nabla\phi_g + \left[\frac{\int_{4\pi} d\hat{\Omega}\hat{\Omega}\psi_g + D\nabla\phi_g}{\phi_g}\right]\phi_g \\ &= -D\nabla\phi_g + \hat{D}_g\phi_g \ . \end{aligned}$$
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

Second-order forms of the Transport Equation

There are various second-order forms of the transport equation, that have a second-order derivative of the flux.

- Even/Odd-parity equations.
- Weighted least-squared formulation.
- Self-adjoint angular flux (SAAF).

Benefits of second-order forms:

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Second-order forms of the Transport Equation

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- Self-adjoint angular flux (SAAF).

Benefits of second-order forms:
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Self-adjoint angular flux equation (SAAF)

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

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

Solve for ψ,

$$\psi = \frac{1}{\Sigma_t} \left[S\psi + q - \hat{\Omega} \cdot \nabla \psi \right] \; ,$$

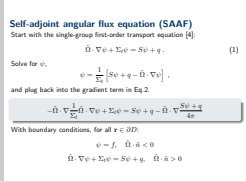
and plug back into the gradient term in Eq.2.

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

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

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

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



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

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Computational Methods of Neutron Transport.
American Nuclear Society, 1993.

[3] Hans R Hammer, Jim E. Morel, and Yaqi Wang.
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In *Mathematics and Computation2*, 2017.

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A Self-Adjoint Angular Flux Equation.
Nuclear Science and Engineering, 132:312–325, 1999.

References

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,

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

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