

# Title of Qualification Exam Talk

J. S. Rehak



Qualification Exam  
September 4<sup>th</sup>, 2019

2019-08-20

Qualification Exam

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# Outline

## ① Motivation

## ② Background

## ③ Acceleration Methods

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## Qualification Exam

└ Outline

Outline

- ① Motivation
- ② Background
- ③ Acceleration Methods

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

with a given boundary condition,

$$c_0 \psi(\mathbf{r}, \hat{\Omega}, E) + c_1 \frac{\partial \psi(\mathbf{r}, \hat{\Omega}, E)}{\partial \mathbf{r}} = f(\mathbf{r}, \hat{\Omega}, E), \quad \hat{n} \cdot \hat{\Omega} < 0, \mathbf{r} \in \partial \mathbb{D}$$

# Steady-state Boltzman Transport Equation

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

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

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# Energy discretization

Introduce a discretization of the energy domain  $\mathbb{E}$  into  $G$  non-overlapping elements, such that

$$E_h = \{E_1, E_2, \dots, E_G\}, \quad \mathbb{E} = \bigcup_{g=1}^G E_g$$

Assume that the energy-dependent angular flux can be separated into a group angular flux and a energy function within each of these groups

$$\psi(\mathbf{r}, E, \hat{\Omega}) \approx \psi_g(\mathbf{r}, \hat{\Omega}) f_g(E), \quad E \in E_g$$

Finally, assume that

$$\int_{E_{g'} \in E_h} f_g(E) dE = \delta_{g,g'}$$

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Qualification Exam  
└─ BACKGROUND

## └─ Self-adjoint angular flux equation (SAAF)

# Self-adjoint angular flux equation (SAAF)

The Self-adjoint angular flux equation (SAAF) is a second-order form of the transport equation introduced by Morel and McGhee in 1999. To derive, consider scattering term part of the 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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└ Self-adjoint angular flux equation (SAAF)

## Self-adjoint angular flux equation (SAAF)

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

$$\hat{\Omega} \cdot \nabla \psi + \Sigma_t \psi = S \psi + q. \quad (1)$$

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$$\hat{\Omega} \cdot \nabla \psi + \Sigma_t \psi = S\psi + q. \quad (1)$$

Solve for  $\psi$ ,

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

and plug back into the gradient term in Eq.1.

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

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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## Qualification Exam

## └ Acceleration Methods

## └ Nonlinear Diffusion Acceleration (NDA)

# Nonlinear Diffusion Acceleration (NDA)

- 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.

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

## Nonlinear Diffusion Acceleration (NDA)

Start, again, with the single-group first-order transport equation [2],  
integrated over angle:

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As a closure to this problem, it is common to define current using *Fick's law*,

$$J_g = -D \nabla \phi_g.$$

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Construct an additive correction to the current using information from an angular solve:

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

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

# Nonlinear Diffusion Acceleration (NDA)

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

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

- 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.

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

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

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

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# Qualification Exam

## Acceleration Methods

### NDA algorithm

NDA algorithm

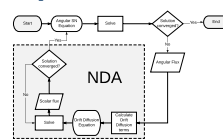
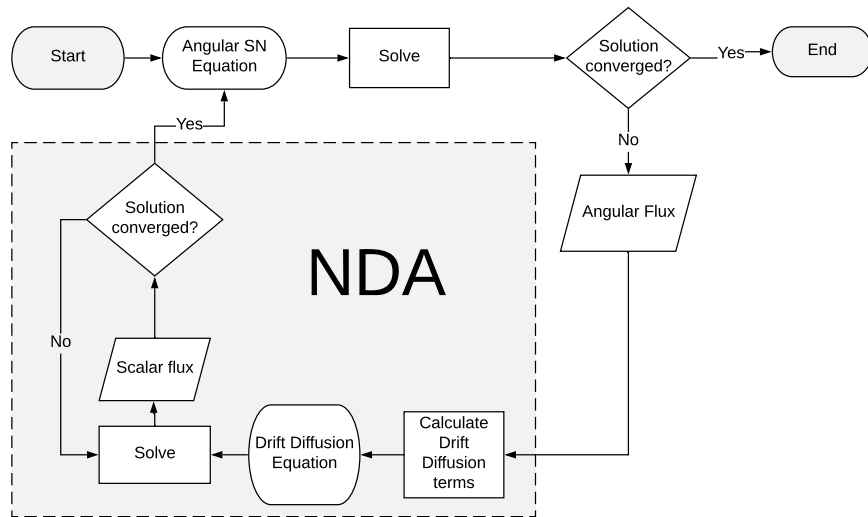


Figure 1: NDA algorithm



- 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.

$$\begin{aligned} & \left[ \hat{\Omega} \cdot \nabla + \Sigma_s(\mathbf{r}, E) \right] \psi_g(\mathbf{r}, \hat{\Omega}) \\ &= \sum_{g'=1}^G \int_{4\pi} d\hat{\Omega}' \Sigma_s(\mathbf{r}, E_{g'} \rightarrow E_g, \hat{\Omega}' \rightarrow \hat{\Omega}) \psi_{g'}(\mathbf{r}, \hat{\Omega}') + Q_g(\mathbf{r}, \hat{\Omega}) \end{aligned}$$

$$\begin{aligned} & \left[ \hat{\Omega} \cdot \nabla + \Sigma_t(\mathbf{r}, E) \right] \psi_g(\mathbf{r}, \hat{\Omega}) \\ &= \sum_{g'=1}^G \int_{4\pi} d\hat{\Omega}' \Sigma_s(\mathbf{r}, E_{g'} \rightarrow E_g, \hat{\Omega}' \rightarrow \hat{\Omega}) \psi_{g'}(\mathbf{r}, \hat{\Omega}') + Q_g(\mathbf{r}, \hat{\Omega}) \end{aligned}$$



# Transport equation second-order forms

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

$$\left[ \hat{\Omega} \cdot \nabla + \Sigma_t(\mathbf{r}) \right] \psi(\mathbf{r}, \hat{\Omega}) = S\psi(\mathbf{r}, \hat{\Omega}) + Q \quad (2)$$

Substitute  $-\hat{\Omega}$  for  $\hat{\Omega}$ , add to Eq. (2), 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,

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

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

$$\left[ \hat{\Omega} \cdot \nabla + \Sigma_t(\mathbf{r}) \right] \psi(\mathbf{r}, \hat{\Omega}) = S\psi(\mathbf{r}, \hat{\Omega}) + Q \quad (2)$$

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

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# 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 Computation*2, 2017.

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

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