

Title of Qualification Exam Talk

J. S. Rehak



Qualification Exam
September 4th, 2019

2019-08-20

Qualification Exam

Title of Qualification Exam Talk

J. S. Rehak



Qualification Exam
September 4th, 2019

Qualification Exam

Outline

① Motivation

Background

Acceleration Methods

Outline

2019-08-20

└ 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]

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

with a given boundary condition,

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

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

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

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

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

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

2019-08-20

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

2019-08-20

└ Self-adjoint angular flux equation (SAAF)

Self-adjoint angular flux equation (SAAF)

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

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

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

Self-adjoint angular flux equation (SAAF)

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

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

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.

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

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.

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

Self-adjoint angular flux equation (SAAF)

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

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

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

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

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

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

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 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

2019-08-20

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:

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

- 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)

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

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

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

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

Qualification Exam

Acceleration Methods

Nonlinear Diffusion Acceleration (NDA)

Nonlinear Diffusion Acceleration (NDA)

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

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

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

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

- 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.

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

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:

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

Nonlinear Diffusion Acceleration (NDA)

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

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

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.

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

Nonlinear Diffusion Acceleration (NDA)

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

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

- 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.

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

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

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),

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

- 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.

2019-08-20

Qualification Exam

Acceleration Methods

NDA algorithm

NDA algorithm

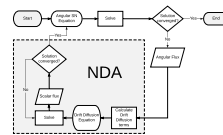
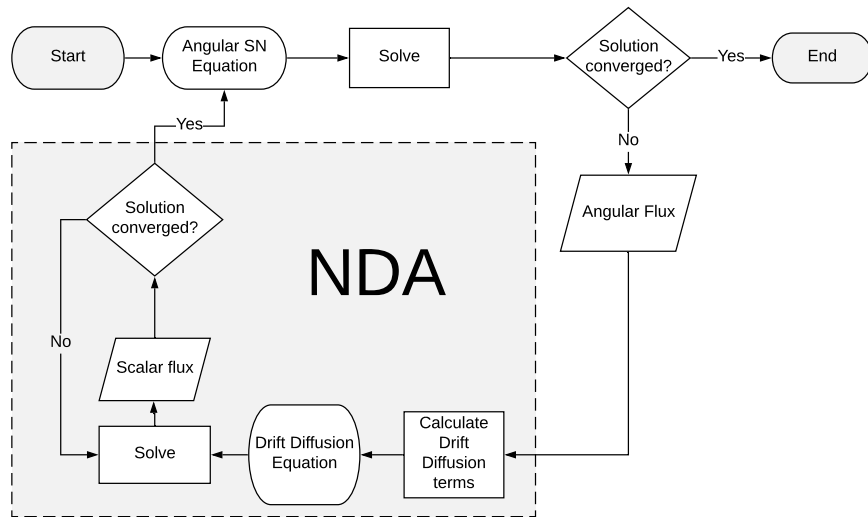


Figure 1: NDA algorithm



- 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,

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

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

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

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,

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

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

Acknowledgments



This work was prepared by Joshua Rehak under award number NRC-HQ-84-14-G-0042 from the Nuclear Regulatory Commission. The statements, findings, conclusions, and recommendations are those of the authors and do not necessarily reflect the view of the US Nuclear Regulatory Commission.

2019-08-20

Qualification Exam

└ Acceleration Methods

└ Acknowledgments

Acknowledgments



This work was prepared by Joshua Rehak under award number NRC-HQ-84-14-G-0042 from the Nuclear Regulatory Commission. The statements, findings, conclusions, and recommendations are those of the author and do not necessarily reflect the view of the US Nuclear Regulatory Commission.

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.

References

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.