A Modified Form of the SAAF Transport Equation with Fully Void-Compatible Feature

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Self-Adjoint Angular Flux (SAAF) Transport Equation

$$-\underline{\Omega}\cdot\underline{\nabla}\frac{1}{\sigma_t(\underline{r})}\left[\underline{\Omega}\cdot\underline{\nabla}\psi(\underline{r},\underline{\Omega})\right]+\sigma_t(\underline{r})\psi(\underline{r},\underline{\Omega})=Q(\underline{r})-\underline{\Omega}\cdot\underline{\nabla}\frac{Q(\underline{r})}{\sigma_t(\underline{r})}$$

where $Q(\underline{r})=\frac{1}{4\pi}\sigma_s(\underline{r})\phi(\underline{r})+\frac{1}{4\pi}S(\underline{r})$.

- **Advantages**
  - Second-order transport equation that is amenable to continuous finite element method (CFEM)
  - CFEM generally results in matrix equations that are symmetric positive-definite (SPD)
  - Boundary conditions are identical to those of the standard first-order transport equation (one-way coupling between incoming and outgoing fluxes)
- **Disadvantages**
  - The S_N source iteration equations cannot be solved with standard transport sweeping technique
  - Hard to deal with problems with void regions

Ref: Morel et al., “A Self-Adjoint Angular Flux Equation,” NSE, 1999.

Derivation of the SAAF Equation

1. Start with the standard 1st-order transport equation

$$\underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r}, \underline{\Omega}) + \sigma_t(\underline{r}) \psi(\underline{r}, \underline{\Omega}) = Q(\underline{r})$$

2. Write the equation in a form that formally represents $\psi(\underline{r}, \underline{\Omega})$

$$\psi(\underline{r}, \underline{\Omega}) = \boxed{\frac{1}{\sigma_t(\underline{r})}} [Q(\underline{r}) - \underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r}, \underline{\Omega})]$$

3. Substitute the $\psi(\underline{r}, \underline{\Omega})$ 'solution' back to the $\underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r}, \underline{\Omega})$ term in the original 1st-order equation

$$\underline{\Omega} \cdot \underline{\nabla} \left\{ \frac{1}{\sigma_t(\underline{r})} [Q(\underline{r}) - \underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r}, \underline{\Omega})] \right\} + \sigma_t(\underline{r}) \psi(\underline{r}, \underline{\Omega}) = Q(\underline{r})$$

4. After some manipulation

$$\boxed{-\underline{\Omega} \cdot \underline{\nabla} \left[\frac{1}{\sigma_t(\underline{r})} \underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r}, \underline{\Omega}) \right] + \sigma_t(\underline{r}) \psi(\underline{r}, \underline{\Omega}) = Q(\underline{r}) - \underline{\Omega} \cdot \underline{\nabla} \frac{Q(\underline{r})}{\sigma_t(\underline{r})}}$$

Derivation of the Modified SAAF Equation

1. Start with the standard 1st-order transport equation

$$\underline{\boldsymbol{\Omega}} \cdot \underline{\boldsymbol{\nabla}} \psi(\underline{r}, \underline{\Omega}) + \sigma_t(\underline{r}) \psi(\underline{r}, \underline{\Omega}) = Q(\underline{r})$$

2. Multiply the equation with $\sigma_t(\underline{r})$ and arrive at an equation

$$\sigma_t(\underline{r}) \underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r}, \underline{\Omega}) + \sigma_t^2(\underline{r}) \psi(\underline{r}, \underline{\Omega}) = \sigma_t(\underline{r}) Q(\underline{r})$$

3. Notice the following identity

$$\sigma_t(\underline{r}) \underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r}, \underline{\Omega}) = \underline{\Omega} \cdot \underline{\nabla} [\sigma_t(\underline{r}) \psi(\underline{r}, \underline{\Omega})] - \psi(\underline{r}, \underline{\Omega}) \underline{\Omega} \cdot \underline{\nabla} \sigma_t(\underline{r})$$

4. Re-write the equation in step 2

$$\underline{\Omega} \cdot \underline{\nabla} [\sigma_t(\underline{r}) \psi(\underline{r}, \underline{\Omega})] + \left[\sigma_t^2(\underline{r}) - \underline{\Omega} \cdot \underline{\nabla} \sigma_t(\underline{r})\right] \psi(\underline{r}, \underline{\Omega}) = \sigma_t(\underline{r}) Q(\underline{r})$$

5. Re-write the original 1st-order transport equation in the following form

$$\sigma_t(\underline{r}) \psi(\underline{r}, \underline{\Omega}) = Q(\underline{r}) - \underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r}, \underline{\Omega})$$

6. Substitute the $\sigma_t(\underline{r}) \psi(\underline{r}, \underline{\Omega})$ back to <u>the 'modified' steaming term</u> in the equation in step 4,

$$-\underline{\Omega} \cdot \underline{\nabla} [\underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r}, \underline{\Omega})] + \left[\sigma_t^2(\underline{r}) - \underline{\Omega} \cdot \underline{\nabla} \sigma_t(\underline{r})\right] \psi(\underline{r}, \underline{\Omega}) = \sigma_t(\underline{r}) Q(\underline{r}) - \underline{\Omega} \cdot \underline{\nabla} Q(\underline{r}).$$

The SAAF vs. Modified SAAF Equation

- **The standard SAAF equation**

$$-\underline{\boldsymbol{\Omega}} \cdot \underline{\boldsymbol{\nabla}} \frac{1}{\sigma_t(\underline{r})}\left[\underline{\boldsymbol{\Omega}} \cdot \underline{\boldsymbol{\nabla}} \psi(\underline{r}, \underline{\boldsymbol{\Omega}})\right] + \sigma_t(\underline{r})\psi(\underline{r}, \underline{\boldsymbol{\Omega}}) = Q(\underline{r}) - \underline{\boldsymbol{\Omega}} \cdot \underline{\boldsymbol{\nabla}} \frac{Q(\underline{r})}{\sigma_t(\underline{r})},$$

- **The modified SAAF equation**

$$-\underline{\boldsymbol{\Omega}} \cdot \underline{\boldsymbol{\nabla}}\left[\underline{\boldsymbol{\Omega}} \cdot \underline{\boldsymbol{\nabla}} \psi(\underline{r}, \underline{\boldsymbol{\Omega}})\right] + \left[\sigma_t^2(\underline{r}) - \boxed{\underline{\boldsymbol{\Omega}} \cdot \underline{\boldsymbol{\nabla}} \sigma_t(\underline{r})}\right]\psi(\underline{r}, \underline{\boldsymbol{\Omega}}) = \sigma_t(\underline{r})Q(\underline{r}) - \underline{\boldsymbol{\Omega}} \cdot \underline{\boldsymbol{\nabla}} Q(\underline{r}).$$

- **Features of the modified form:**
  - Self-Adjoint (?)
  - Conservative (?)

Numerical Methods (S_N)

- Consider the one-group one-dimension slab case

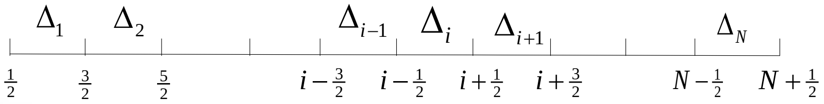
$$-\mu^2 \frac{\partial^2}{\partial x^2}\psi(x,\mu) + \left[\sigma_t^2(x) - \mu\frac{d}{dx}\sigma_t(x)\right]\psi(x,\mu) = \sigma_t(x)Q(x) - \mu\frac{d}{dx}Q(x)$$

- The discrete-ordinate form (i.e., S_N) of the equation

$$-\mu_m^2 \frac{\partial^2}{\partial x^2}\psi_m(x,\mu) + \left[\sigma_t^2(x) - \mu_m\frac{d}{dx}\sigma_t(x)\right]\psi_m(x,\mu) = \sigma_t(x)Q(x) - \mu_m\frac{d}{dx}Q(x)$$

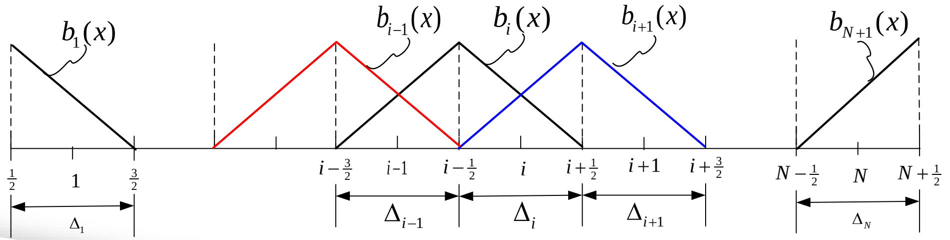
- Boundary conditions

$$\psi_{m,L}(x_{1/2}) = \begin{cases} f_{mL} & \mu_m > 0 \\ \psi_m(x_{1/2}) & \mu_m < 0 \end{cases}, \qquad \psi_{m,R} = \begin{cases} \psi_m(x_{N+1/2}) & \mu_m > 0 \\ f_{mR} & \mu_m < 0 \end{cases}.$$



Numerical Methods (CFEM)

- Start with the weak form of the modified SAAF equation
- Approximate the solution of the equation by a linear combination of trial functions
- Multiply the equation with weight functions, and apply the weighted residual method to get the desired numerical schemes
- Choose the weight function as the same function space of the trial functions (*Standard Galerkin Method*)



Numerical Schemes of the Standard LCFEM

- The equation for the **cell-edge angular flux** in the internal cells

$$A_{i,i-1}\psi_{i-\frac{1}{2}} + A_{i,i}\psi_{m,i+\frac{1}{2}} + A_{i,i+1}\psi_{m,i+\frac{3}{2}} = \sigma_{t,i+\frac{1}{2}}Q_{i+\frac{1}{2}}\Delta x_{i+\frac{1}{2}} - \mu_m(Q_{i+1} - Q_i)$$

where $A_{i,i-1} = -\frac{\mu_m^2}{\Delta x_i} + \frac{1}{6}\sigma_{t,i}^2\Delta x_i$, $A_{i,i} = \frac{\mu_m^2}{\Delta x_{i+1}} + \frac{\mu_m^2}{\Delta x_i} + \frac{1}{3}\left(\sigma_{t,i}^2\Delta x_i + \sigma_{t,i+1}^2\Delta x_{i+1}\right) - \mu_m\left(\sigma_{t,i+1} - \sigma_{t,i}\right)$, $A_{i,i+1} = -\frac{\mu_m^2}{\Delta x_{i+1}} + \frac{1}{6}\sigma_{t,i+1}^2\Delta x_{i+1}$.

- The equation for $\psi_{m,\frac{1}{2}}$ In the most left cell

$$A_{0,0}\psi_{m,\frac{1}{2}} + A_{0,1}\psi_{m,\frac{3}{2}} - \mu_m\sigma_{t,1}\psi_{m,L} = \sigma_{t,1}Q_1\frac{\Delta x_1}{2} - \mu_m Q_1$$

where $A_{0,0} = \frac{\mu_m^2}{\Delta x_1} + \frac{1}{2}\sigma_{t,1}^2\Delta x_1$, $A_{0,1} = -\frac{\mu_m^2}{\Delta x_1}$.

- The equation for $\psi_{m,I+\frac{1}{2}}$ In the most right cell

$$A_{I,I-1}\psi_{m,I-\frac{1}{2}} + A_{I,I}\psi_{m,I+\frac{1}{2}} + \mu_m\sigma_{t,I}\psi_{m,R} = \sigma_{t,I}Q_I\frac{\Delta x_I}{2} + \mu_m Q_I$$

where $A_{I,I-1} = -\frac{\mu_m^2}{\Delta x_I}$, $A_{I,I} = \frac{\mu_m^2}{\Delta x_I} + \frac{1}{2}\sigma_{t,I}^2\Delta x_I$

Nested Iterative Hierarchy for S_N Transport Solver

Start of program

*Begin of the **power iteration** (PI)*

Loop on the energy group g

*Begin of **source iteration** (SI)*

Transport sweep (loop on each direction and each spatial variable)

SAAF or modified SAAF calculations

DSA acceleration if needed

Check SI convergence to decide exit or update and continue

End of SI

End of the energy group loop

Check PI convergence to decide exit or update and continue

End of the PI

End of program

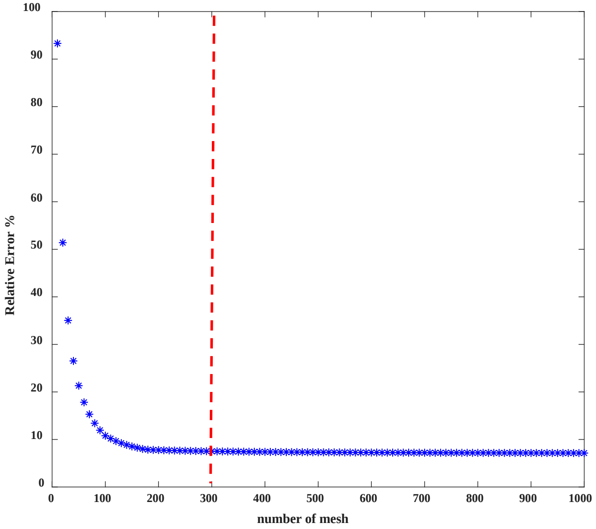
Numerical Example I

- **Problem one**: a three-region source problem.

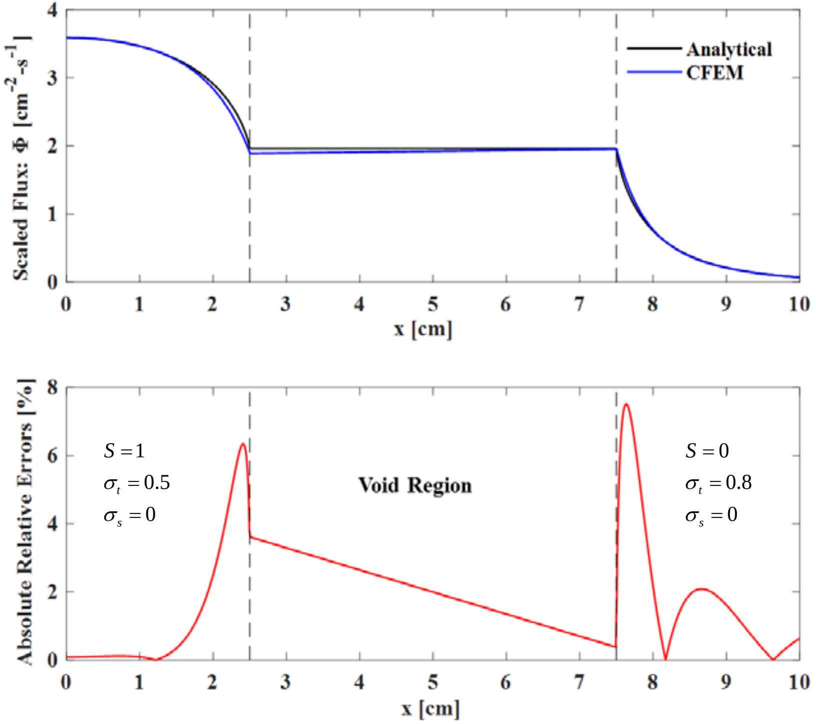
	Region 1	Region 2	Region 3
S **[cm^{-1}s^{-1}]**	1	0	0
σ_t **[cm^{-1}]**	0.5	0	0.8
σ_s **[cm^{-1}]**	0	0	0
x **[cm]**	$0 \leq x < 2.5$	$2.5 \leq x < 7.5$	$7.5 \leq x \leq 10$

- Reflecting B.C. on the left and Vacuum B.C. on the right side

Results of the Problem One



Error sensitivity w.r.t. mesh size.



Scalar flux distribution.

Numerical Examples II

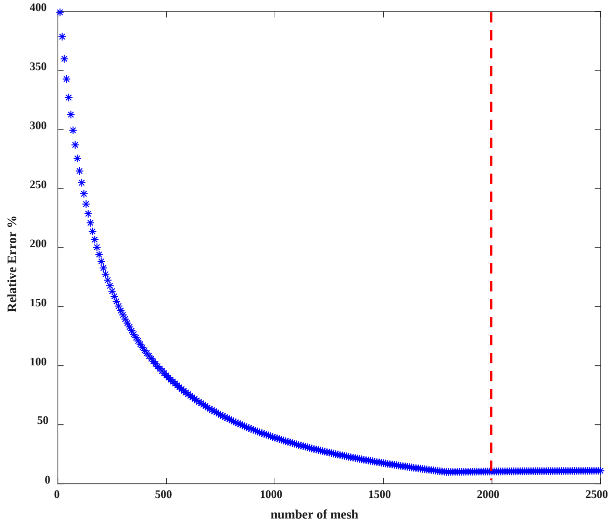
- **Problem Two**: a five-region source problem.

	Region 1	Region 2	Region 3	Region 4	Region 5
S [cm^{-1}s^{-1}]	100	0	0	0	1
σ_t [cm^{-1}]	100	0	1	5	1
σ_s [cm^{-1}]	0	0	0.9	0	0.9
x [cm]	$0 \leq x < 2$	$2 \leq x < 4$	$4 \leq x \leq 6$	$6 \leq x \leq 7$	$7 \leq x \leq 8$

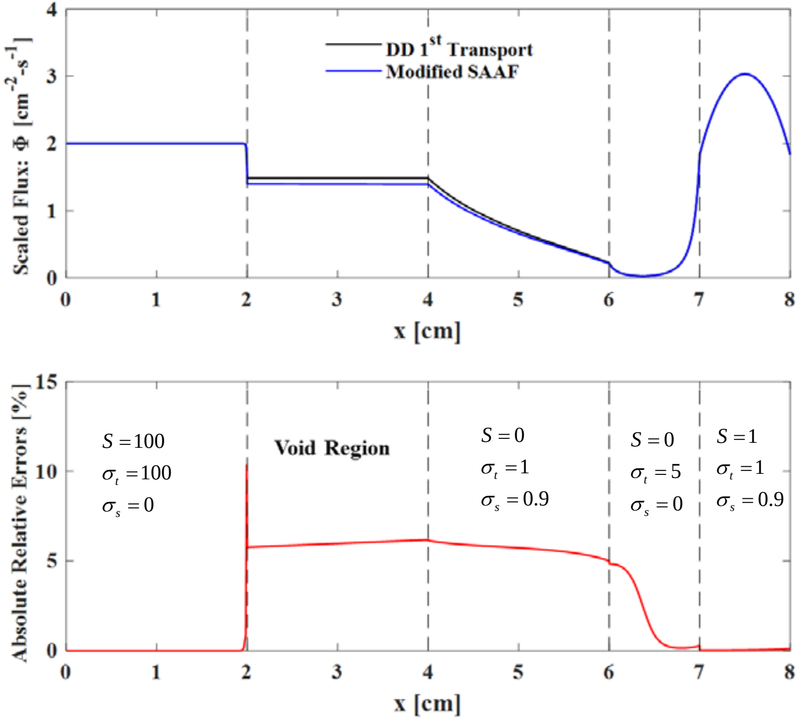
- Reflecting B.C. on the left and Vacuum B.C. on the right side

Ref.: Reed, "New Difference Schemes for the Neutron Transport Equation," NSE, 1971.

Results of the Problem Two



Error sensitivity w.r.t. mesh size.



Scalar flux distribution.

The Least-Squares form Transport Equation

- Start with the standard 1st-order transport equation
  $L\psi = \underline{\Omega} \cdot \underline{\nabla}\psi(\underline{r},\underline{\Omega}) + \sigma_t(\underline{r})\psi(\underline{r},\underline{\Omega}) = Q(\underline{r})$, where $L = \underline{\Omega} \cdot \underline{\nabla} + \sigma_t(\underline{r})$ is the *transport operator*.
- The *adjoint operator* of the transport operator is
  $$L^{+} = -\underline{\Omega} \cdot \underline{\nabla} + \sigma_t(\underline{r})$$
- Perform the adjoint operator on the 1st-order transport equation
  $$[-\underline{\Omega} \cdot \underline{\nabla} + \sigma_t(\underline{r})][\underline{\Omega} \cdot \underline{\nabla}\psi(\underline{r},\underline{\Omega}) + \sigma_t(\underline{r})\psi(\underline{r},\underline{\Omega})] = [-\underline{\Omega} \cdot \underline{\nabla} + \sigma_t(\underline{r})]Q(\underline{r})$$
- With some manipulation on the resulted equation, one will arrive at

$$-\underline{\Omega} \cdot \underline{\nabla}[\underline{\Omega} \cdot \underline{\nabla}\psi(\underline{r},\underline{\Omega})] + \left[\sigma_t^2(\underline{r}) - \underline{\Omega} \cdot \underline{\nabla}\sigma_t(\underline{r})\right]\psi(\underline{r},\underline{\Omega}) = \sigma_t(\underline{r})Q(\underline{r}) - \underline{\Omega} \cdot \underline{\nabla}Q(\underline{r}).$$

This is exactly identical to our modified form of the SAAF equation!

Ref.: Hansen et al, “A Least Squares Transport Equation Compatible with Voids,” JCTT, 2014.

How Least-Squares Transport Equation Come?

- Based on ***the variational principle***:

  Define a least squares form of ***functional*** as follows:

  $$f(\psi) = \langle L\psi - Q, L\psi - Q \rangle,$$

  Find a solution ψ that minimizes the functional. This solution is called a L-S solution.

  $$\begin{aligned} f(\psi) &= \langle L\psi - Q, L\psi - Q \rangle \\ &= \langle L\psi, L\psi \rangle - 2\langle L\psi, Q \rangle + \langle Q, Q \rangle \\ &= \langle L^{+} L\psi, \psi \rangle - 2\langle L^{+} Q, \psi \rangle + \langle Q, Q \rangle \end{aligned}$$

- To find a minimum value, it is required to $\frac{df(\psi)}{d\psi} = 0$.
- Performing the derivative will yield the least-squares transport equation

  $$L^{+} L\psi - L^{+} Q = 0.$$

- **Least-squares form transport is not unique, it is determined by the original functional.**

Distinction of Our Derivation

- Straightforward <u>goal-oriented</u> derivation procedure
- Purely <u>algebraic</u> derivation technique, no any *<u>fancy</u>* math involved
- Build a <u>bridge</u> connecting the SAAF equation and the Least-squares equation
- The ideas behind our derivation is easily <u>extended</u> to other equations with similar situations

Possibly Extension of Our Derivation Approach

- Diffusion equation can be derived from the P_1 equations

$$\begin{cases} \nabla \cdot \underline{J}(\underline{r}) + \sigma_a(\underline{r})\phi(\underline{r}) = Q(\underline{r}) \\ \frac{1}{3}\nabla\phi(\underline{r}) + \sigma_t(\underline{r})\underline{J}(\underline{r}) = 0 \end{cases}$$

- Standard diffusion equation

$$-\nabla \cdot \frac{1}{3\sigma_t(\underline{r})}\nabla\phi(\underline{r}) + \sigma_a(\underline{r})\phi(\underline{r}) = Q(\underline{r})$$

- Modified diffusion equation

$$\frac{1}{3}\nabla \cdot [\sigma_t(\underline{r})\nabla\phi(\underline{r})] - \frac{2}{3}\sigma_t(\underline{r})\nabla \cdot \nabla\phi(\underline{r}) + \sigma_t^2(\underline{r})\sigma_a(\underline{r})\phi(\underline{r}) = \sigma_t^2(\underline{r})Q(\underline{r})$$

Summary

- The SAAF equation is modified to be fully compatible with void problems.
- Advantages and disadvantages of the modified form of the SAAF equation are discussed
- Numerical results are presented to demonstrate the preliminary feasibility of the modified SAAF form applied in void problems
- Connection to the Least-squares form transport is introduced, some merits and future applications of our derivation are briefly discussed