A Semi-Analytic Solution on the 1D S_N Transport Equation by Decoupling the In-Scattering Operator

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MG Discrete Ordinates (S_N) 1D Transport Equation

$$\mu_m \frac{\partial \psi_{mg}(x)}{\partial x} + \Sigma_{tg}(x)\psi_{mg}(x) = \sum_{l=0}^{L} \frac{2l+1}{2} \Sigma_{sl,g\to g}(x) P_l(\mu_m)\phi_{lg}(x)$$
$$+ \sum_{\substack{g'=1 \\ g'\neq g}}^{G} \sum_{l=0}^{L} \frac{2l+1}{2} \Sigma_{sl,g'\to g}(x) P_l(\mu_m)\phi_{lg'}(x) + \frac{1}{k}\frac{\chi_g}{2} \sum_{g'=1}^{G} \nu\Sigma_{fg'}(x)\phi_{0g'}(x)$$

- **Advantages**
  - *k*-eigenvalue transport problem can be solved using power iteration
  - Demonstrates convergent behavior with small mesh sizes
  - Various boundary conditions require simple treatments
- **Disadvantages**
  - The **source iteration** with standard **transport sweeping** technique to solve for the flux is **time-inefficient**
  - Matrix **instabilities** with highly diffusive media (negative eigenvalues, high condition number)

Adapting to One-Group S_N Equations (1/2)

1. **Define the angular flux moment coupled to the first equation**

$$\phi_{lg}(x) = \sum_{m'=1}^{N} w_{m'} P_l(\mu_{m'}) \psi_{m'g}(x)$$

2. **Write the equation in terms of a known source**

$$S_g(x) = \sum_{\substack{g'=1 \\ g'\neq g}}^{G} \sum_{l=0}^{L} \frac{2l+1}{2} \Sigma_{sl,g'\to g}(x) P_l(\mu_m) \phi_{lg'}(x) + \frac{1}{k} \frac{\chi_g}{2} \sum_{g'=1}^{G} \nu\Sigma_{fg'}(x) \phi_{0g'}(x)$$

3. **Reduce the first equation using substitution**

$$\mu_m \frac{\partial \psi_{mg}(x)}{\partial x} + \Sigma_{tg}(x)\psi_{mg}(x) = \sum_{l=0}^{L} \frac{2l+1}{2} \Sigma_{sl,g\to g}(x) P_l(\mu_m) \phi_{lg}(x) + S_g(x)$$

4. **Consider the equation with angular flux moment order *l*=1**

$$\mu_m \frac{\partial \psi_{mg}(x)}{\partial x} + \Sigma_{tg}(x)\psi_{mg}(x) = \frac{1}{2} \Sigma_{s0,g\to g}(x) \phi_{0g}(x) + \frac{3}{2} \Sigma_{s1,g\to g}(x) \mu_m \phi_{1g}(x) + S_g(x)$$

Adapting to One-Group S_N Equations (2/2)

4. Define the scalar flux in terms of Gauss-Legendre components

$$\phi_{0g}(x) = \sum_{m'=1}^{N} w_{m'}\psi_{m'g}(x), \quad \phi_{1g}(x) = \sum_{m'=1}^{N} w_{m'}\mu_{m'}\psi_{m'g}(x)$$

5. Reduce to one-group by dropping ***g*** subscripts, where ***N*** is the quadrature order

$$\mu_m \frac{\partial \psi_m(x)}{\partial x} + \Sigma_t(x)\psi_m(x) = \frac{1}{2}\Sigma_{s0}(x)\sum_{m'=1}^{N} w_{m'}\psi_{m'}(x) + \frac{3}{2}\Sigma_{s1}(x)\mu_m \sum_{m'=1}^{N} w_{m'}\mu_{m'}\psi_{m'}(x) + S(x), m = 1,\ldots,N$$

6. Assume homogenous materials and a simple domain $x_{i-1/2} < x < x_{i+1/2}$

$$\mu_m \frac{\partial \psi_m(x)}{\partial x} + \Sigma_t^i \psi_m(x) = \frac{1}{2}\Sigma_{s0}^i \sum_{m'=1}^{N} w_{m'}\psi_{m'}(x) + \frac{3}{2}\Sigma_{s1}^i \mu_m \sum_{m'=1}^{N} w_{m'}\mu_{m'}\psi_{m'}(x) + S(x), \quad m = 1,\ldots,N$$

7. Combine scattering terms to complete the transformation

$$\frac{\partial \psi_m(x)}{\partial x} + \frac{\Sigma_t^i}{\mu_m}\psi_m(x) = \frac{1}{\mu_m}\left[\frac{1}{2}\Sigma_{s0}^i \sum_{m'=1}^{N} w_{m'}\psi_{m'}(x) + \frac{3}{2}\Sigma_{s1}^i \mu_m \sum_{m'=1}^{N} w_{m'}\mu_{m'}\psi_{m'}(x)\right] + \frac{1}{\mu_m}S(x), \quad m = 1,\ldots,N$$

Forming the Coefficient Matrix (1/2)

1. Write the One-Group S_N Equation in a **vector-matrix** form as follows

$$\frac{\partial \boldsymbol{\psi}(x)}{\partial x} + \mathbf{A}^{i}\boldsymbol{\psi}(x) = S(x)\mathbf{b}$$

2. Where the vectors $\boldsymbol{\psi}(x)$ and ***b*** are respectively

$$\boldsymbol{\psi}(x) = \begin{bmatrix} \psi_1(x) \\ \psi_2(x) \\ \vdots \\ \psi_N(x) \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 1/\mu_1 \\ 1/\mu_2 \\ \vdots \\ 1/\mu_N \end{bmatrix}$$

3. Lastly, we form the **Coefficient Matrix** by combining righthand components in the modified One-Group S_N Equations

Forming the Coefficient Matrix (2/2)

- The Coefficient Matrix is as follows:

$$\mathbf{A}^i = \begin{bmatrix} \frac{1}{\mu_1}\left(\Sigma_t^i - \frac{1}{2}\Sigma_{s0}^i w_1 - \frac{3}{2}\Sigma_{s1}^i w_1 \mu_1^{\,2}\right) & -\frac{1}{\mu_1}\left(\frac{1}{2}\Sigma_{s0}^i w_2 + \frac{3}{2}\Sigma_{s1}^i \mu_1 w_2 \mu_2\right) & \cdots & -\frac{1}{\mu_1}\left(\frac{1}{2}\Sigma_{s0}^i w_N + \frac{3}{2}\Sigma_{s1}^i \mu_1 w_N \mu_N\right) \\ -\frac{1}{\mu_2}\left(\frac{1}{2}\Sigma_{s0}^i w_1 + \frac{3}{2}\Sigma_{s1}^i \mu_2 w_1 \mu_1\right) & \frac{1}{\mu_2}\left(\Sigma_t^i - \frac{1}{2}\Sigma_{s0}^i w_2 - \frac{3}{2}\Sigma_{s1}^i w_2 \mu_2^{\,2}\right) & \cdots & -\frac{1}{\mu_2}\left(\frac{1}{2}\Sigma_{s0}^i w_N + \frac{3}{2}\Sigma_{s1}^i \mu_2 w_N \mu_N\right) \\ \vdots & \vdots & \ddots & \vdots \\ -\frac{1}{\mu_N}\left(\frac{1}{2}\Sigma_{s0}^i w_1 + \frac{3}{2}\Sigma_{s1}^i \mu_N w_1 \mu_1\right) & -\frac{1}{\mu_N}\left(\frac{1}{2}\Sigma_{s0}^i w_2 + \frac{3}{2}\Sigma_{s1}^i \mu_N w_2 \mu_2\right) & \cdots & \frac{1}{\mu_N}\left(\Sigma_t^i - \frac{1}{2}\Sigma_{s0}^i w_N - \frac{3}{2}\Sigma_{s1}^i w_N \mu_N^{\,2}\right) \end{bmatrix}$$

- If only isotropic scattering considered, it becomes

$$\mathbf{A}^i = \begin{bmatrix} \frac{1}{\mu_1}\left(\Sigma_t^i - \frac{1}{2}\Sigma_{s0}^i w_1\right) & -\frac{1}{\mu_1}\left(\frac{1}{2}\Sigma_{s0}^i w_2\right) & \cdots & -\frac{1}{\mu_1}\left(\frac{1}{2}\Sigma_{s0}^i w_N\right) \\ -\frac{1}{\mu_2}\left(\frac{1}{2}\Sigma_{s0}^i w_1\right) & \frac{1}{\mu_2}\left(\Sigma_t^i - \frac{1}{2}\Sigma_{s0}^i w_2\right) & \cdots & -\frac{1}{\mu_2}\left(\frac{1}{2}\Sigma_{s0}^i w_N\right) \\ \vdots & \vdots & \ddots & \vdots \\ -\frac{1}{\mu_N}\left(\frac{1}{2}\Sigma_{s0}^i w_1\right) & -\frac{1}{\mu_N}\left(\frac{1}{2}\Sigma_{s0}^i w_2\right) & \cdots & \frac{1}{\mu_N}\left(\Sigma_t^i - \frac{1}{2}\Sigma_{s0}^i w_N\right) \end{bmatrix}$$

Semi-Analytic Solution (1/2)

- By decoupling the scattering terms from the angular flux vector, we can linearly transform the flux vector into the eigenspace of the matrix ***A***

$$\mathbf{A}^{i}\mathbf{u}_m = \lambda_m \mathbf{u}_m \quad (m = 1,\ldots,N)$$

- The vectors $\boldsymbol{\psi}(x)$ and ***b*** can be written in terms of the basis-vector **u**

$$\psi(x) = \sum_{m=1}^{N} \varphi_m(x)\mathbf{u}_m \qquad\qquad \mathbf{b} = \sum_{m=1}^{N} b_m \mathbf{u}_m$$

- The coefficients $\varphi_m(x)$ are to be determined. Substitution yields

$$\sum_{m=1}^{N} \frac{\partial \varphi_m(x)}{\partial x}\mathbf{u}_m + \sum_{m=1}^{N} \varphi_m(x)\mathbf{A}^{i}\mathbf{u}_m = S(x)\sum_{m=1}^{N} b_m \mathbf{u}_m$$

Semi-Analytic Solution (2/2)

- Rearrangement leaves a set of **First-Order** ODE's

$$\sum_{m=1}^{N} \mathbf{u}_m \left[\frac{\partial \varphi_m(x)}{\partial x} + \lambda_m \varphi_m(x) - b_m S(x) \right] = 0$$

- Because $\mathbf{u}_m$ are independent basis vectors of the eigen-space of **A**, the equations hold iff

$$\frac{\partial \varphi_m(x)}{\partial x} + \lambda_m \varphi_m(x) - b_m S(x) = 0 \quad \text{for} \quad m = 1,\ldots,N$$

- These decoupled equations are linked to only one respective ordinate or angular flux component, and can be individually solved with analytical techniques.

ODE Solution and Boundaries

- In **1D Slab-Geometry**, boundary conditions require known incident flux components at slab edges -> Also directionally dependent **(±μ)**

$$\varphi_m(x) = e^{-\lambda_m x}\left(\varphi_{mL} - \frac{S_0 b_m}{\lambda_m}\right) + \frac{S_0 b_m}{\lambda_m}$$

$$\mu_m > 0$$

$$\varphi_m(x) = e^{\lambda_m (L-x)}\left(\varphi_{mR} - \frac{S_0 b_m}{\lambda_m}\right) + \frac{S_0 b_m}{\lambda_m}$$

$$\mu_m < 0$$

- The subscripts ***R*** and ***L*** denote the Right and Left boundary components

- **"Semi-Analytic"** refers to the discrete directional components, but analytical solution in space ***(x)***

Formation of the Scalar Flux

- The ***real*** angular flux is a linear combination of abscissa weights and the ***fake*** angular flux components

$$\psi(x) = \sum_{m=1}^{N} \varphi_m(x)\mathbf{u}_m$$

- Substituting this into the definition of the scalar flux

$$\phi(x) = \sum_{i=1}^{N} w_i \psi_i = \sum_{i=1}^{N} w_i \left(\sum_{m=1}^{N} \varphi_m(x) u_{im} \right)$$

- Defining a dummy variable for simplicity

$$w'_m = \sum_{i=1}^{N} w_i \mathbf{u}_{im}$$

- The scalar flux becomes a simple summation of components

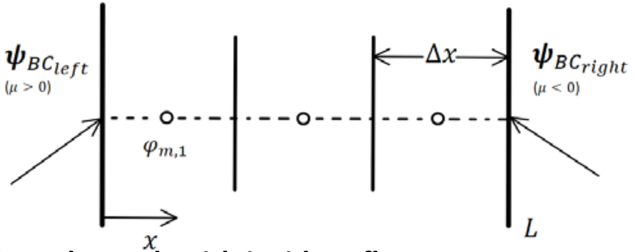
$$\phi(x) = \sum_{m=1}^{N} \varphi_m(x) w'_m$$

Incident Flux and 'Boundary Iteration'

- The solution requires solving for N/2 unknown components of $\psi(x)$ at boundaries and region interfaces. The simple inverse transformation allows for conversion between φ and ψ

$$\varphi_m = \mathbf{u}_m^{-1}\psi$$

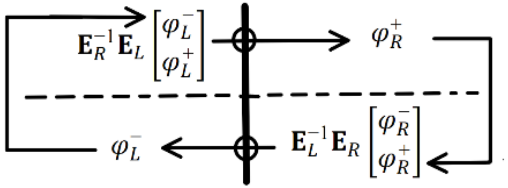
- Using this, we can guess the half unknown components of the incident flux and iterate by replacing the guesses with values of φ found analytically



Sample mesh with incident flux components

Boundary Iteration vs Source Iteration

- **Power Iteration** methods with DD schemes, for instance, require a standard **Transport Sweep** to converge on a solution
- The **Semi-Analytical** method proposed only requires iteration on boundaries and region interfaces, meaning there is a dramatic reduction in CPU time, despite the large number of equations being solved
- After converging on boundary values, the analytical solutions can be calculated simultaneously.
- With ***E*** denoting the eigenvector matrix of a given region (Left and Right), the simple interface scheme converges naturally with the boundary iteration



Program Hierarchy for the SA Solver

Start of program

Allocate Matrix Storage and Solve for Region Constants

*Beginning of **Semi-Analytic Iteration (SA)***

Loop on boundaries

Calculate scalar flux at boundary meshes

Check Boundary convergence, update values of $\boldsymbol{\varphi}$

End boundary Loop

Calculate all desired values of scalar flux using converged solutions

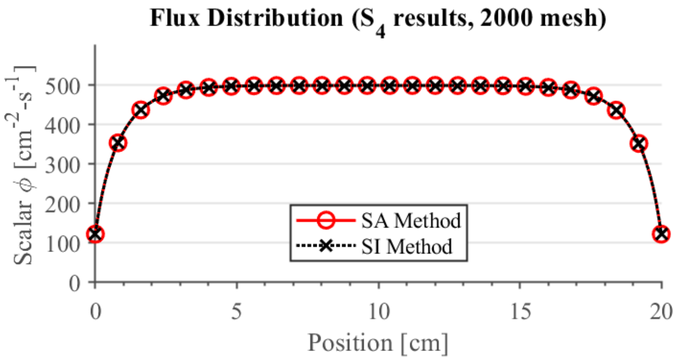
*End of **SA***

End of program

Numerical Analysis (1/2)

- A one-region source problem

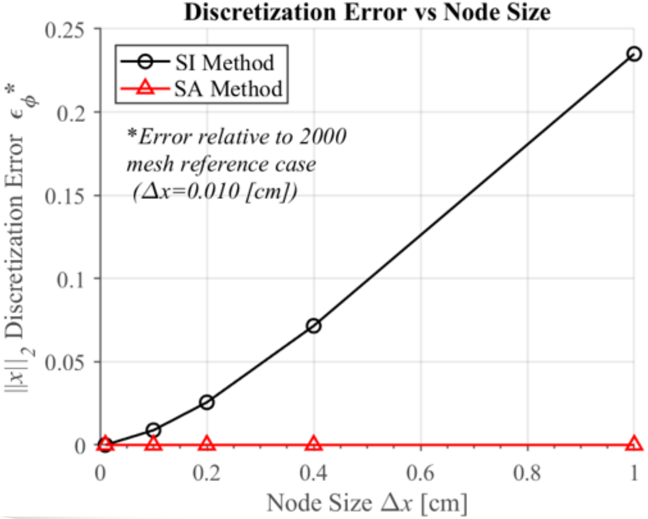
	Region 1
S [cm^{-1}s^{-1}]	100
σ_t [cm^{-1}]	2.0
σ_s [cm^{-1}]	1.8
x [cm]	$0 \leq x < 20$

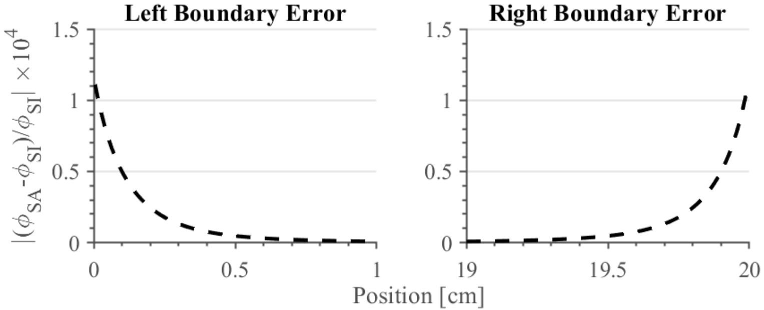


- Vacuum B.C. is applied on both sides

Numerical Analysis (2/2)

- Benchmarked to SI method with same mesh size and quadrature order
- Large edge-error typical of SI





Scattering Ratio c	SA Number	SA Time† [s]	SI Number	SI Time† [s]	Relative Error*
0.1	3	0.048	9	0.050	8.07E-04
0.5	6	0.067	26	0.095	6.69E-04
0.9	15	0.155	143	0.381	4.04E-04
0.95	32	0.223	275	0.616	3.27E-04
0.99			463	1.005	

† Computations on an Intel i7 7700K w/ 32GB DDR5 RAM

*** Relative 2-normalized error between SI and SA flux**

Heterogeneous Case Solution (1/2)

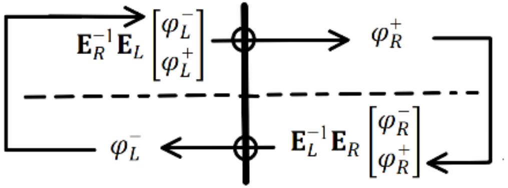
- A multi-region source problem w/ anisotropic scattering

	Region 1	Region 2	Region 3
S [cm^{-1}s^{-1}]	0	1.0	2.0
σ_t [cm^{-1}]	1.0	1.0	2.0
σ_{s0} [cm^{-1}]	0.9	0.6	0.8
σ_{s1} [cm^{-1}]	0.8	0.3	0.8
x [cm]	$0 \leq x < 10$	$10 \leq x < 17$	$17 \leq x \leq 20$

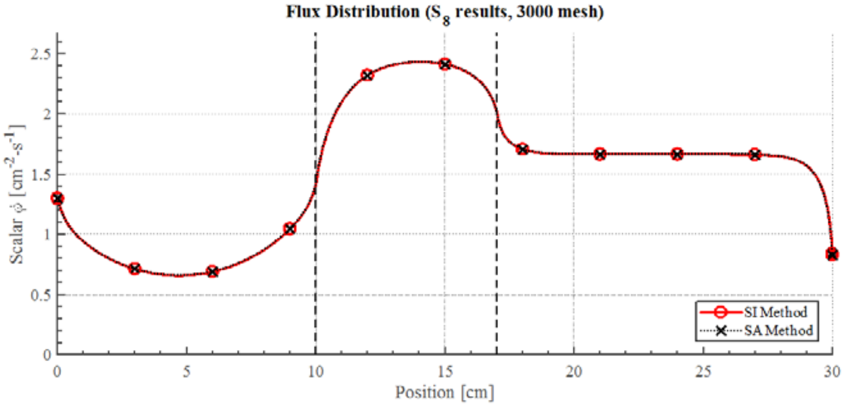
- Vacuum B.C. is applied on R.H.S, Incident Flux on L.H.S. so that $\psi(L)=1.0$ for $\mu>0$

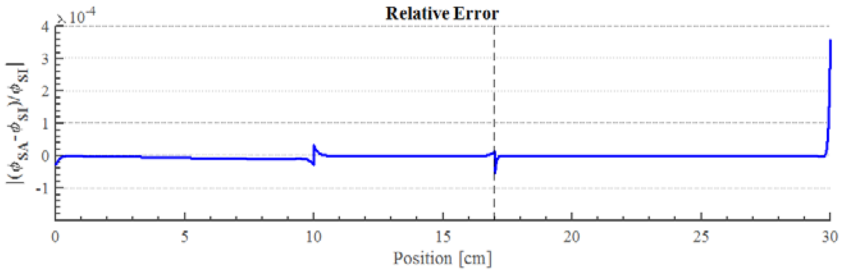
Heterogeneous Case Solution (2/2)

- Benchmarked to SI method with same mesh size and quadrature order
- Convergence Tolerance $\varepsilon = 10^{-7}$



- Natural convergence at interfaces
- Some error at region interfaces
- In this case, SA is ~10x faster than SI





Distinctions of Our Method

- Analytic characteristic removes spacial discretization errors
- Simple implementation in 1D case with various conditions
- Uses linear algebra (eigenvalues) and standard 1^{st} ODE solutions
- Bypass time-inefficient transport sweeps and source iteration
- Apply to *k*-eigenvalue problems
- Straightforwardly expands to multigroup and anisotropic scattering cases
- Potentially expanded to multi-dimensional cases

Future Work

- Currently comparing similar methods involving RTE's and BNTE's
- K-eigenvalue criticality and two-group case possible to implement
- Two Dimensional case is achievable using Gauss-Legendre discretization, for Cartesian and spherical/cylindrical geometries
- Benchmarking using published examples (*see Barros & Larsen, 1990)*
- Method requires use of basis-vectors of asymmetric ill-conditioned matrix, resulting in negative eigenvalues and divergent behavior with a scattering ratio $c > 0.97$
- Requires work on variable storage optimization to reduce total CPU time

Summary

- The **Semi-Analytical (SA)** method is a simple solution to the 1D S_N transport problem using **decoupled linear ODE's** through eigen-vector expansion of a scattering coefficient matrix
- Solution of the ODE's are found for the given boundary conditions
- Numerical results are presented to demonstrate the preliminary feasibility of the SA Method and subsequent modifications
- Problems and future additions to the project were discussed