A Semi-Analytic Solution to the 1D S_N Transport Equation for a Multi-Region Problem

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INTRODUCTION

The one-dimensional discrete ordinate (1D S_N) transport equation with even-order Gauss-Legendre quadrature sets are commonly used in large radiation transport problems. [1] The source iteration (SI) approach is a standard technique to solve the S_N equations because the in-scattering source term appeared in equation couples angular fluxes in all directions. While accurate, the SI method requires excessive flux solution convergence-time in problems with higher scattering ratios, higher quadrature order, and larger nodal mesh densities. In this summary, we develop a transport solution method with the objective to eliminate the conventional SI procedure in transport solvers. This is achieved by decoupling the transport operation terms and converting the original S_N transport equations to a number of decoupled equations. We end up achieving a semi-analytic solution for the S_N transport equation without no spatial truncation errors.

Many efforts on 1D analytic transport solutions for various computational purposes can be identified in literatures. In 1960s and early 1970s, neutron transport experts such as Siewert and Zweifel [2] developed a concert of full analytic solution forms for transport equation, providing excellent analytic computational benchmarks but limited to very simple applications. Barros and Larsen published an analytic transport solution using auxiliary Green's function to obtain homogeneous solutions [3]. This approach can achieve accurate analytic solutions for 1D transport equation with linear anisotropic scattering but may involve algebraic complexity in cases with higher degree of anisotropy. Warsa [4] developed an analytic S_N solution for transport equation in heterogeneous slabs with the assistant of symbolic algebra computer tools. Segattto et al. [5], and continued by Ganapol [6], solved the transport equation analytically using Heaviside expansion technique and directly yield the homogeneous solutions to the equation. Roberts [7] implemented a direct solution using a built-in MATLAB Krylov-solver with ILU preconditioning to bypass the SI procedure in transport solver, however, with Legendre quadrature orders over N = 8, the usefulness of the method diminishes due to matrix construction time. And most recently, Wang [8] developed an analytic transport solution through a matrix inversion process by constructing the transport equation in a matrix-vector form. The semi-analytic solution we developed in this summary more or less has differences from all the previous developments. Our approach appears to use a similar fundamental idea as the ones in Ref. 3, 5 and 6, but employ a rather different realization process and implementation procedure, making it more advantageous to handle high order of anisotropic scattering scenarios and more readily to be extended to multi-dimensional cases.

In this summary, we will present the recently developed semi-analytic (SA) method that is relatively faster with low quadratures ($N < 16$) and can be easily generalized. We will focus on the one-group transport model with isotropic scattering and a fixed source to demonstrate its efficacy. By linearly transforming the transport operator as demonstrated in our previous paper [9], we can bypass the standard source iteration that is usually required by the transport solver and isolate the iteration scheme to region boundaries only. This becomes possible because each angular component of the 'new' flux (we referred to it as 'fake' flux) yielded with the linear transform of the scattering operator is no longer coupled to other angular components. The computational benefits, as will soon be seen, are derived from needing to solve only one analytical equation per mesh, per quadrature direction.

METHODOLOGIES

In this section, we will briefly summarize the SA method and the extended efforts we have made from our earlier work [9]. Previously, we mainly analyze the approach in a simple one-region problem with the intension to verify the efficiency and accuracy of the approach by comparing it to the standard SI approach, this summary expands the scope to a multi-region problem.

Transport Operator Expansion

The center idea of the SA approach is to perform an eigenvalue expansion to the transport operator in the S_N transport equation. We start the journey with the 1D one-group S_N transport equations with a P_1 approximation to the scattering kernel, and assume the material of cell i within the domain $x_{i-1/2} < x < x_{i+1/2}$ is fixed. With standard notations, the transport equation in the cell is described as

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

where N is the quadrature order used in the S_N method. If the angular flux components are expressed in a vector as:

$$\boldsymbol{\psi}(x)=\begin{bmatrix}\psi_1(x)\\ \psi_2(x)\\ \vdots\\ \psi_N(x)\end{bmatrix}, \tag{2}$$

Eq. (1) can be rewritten as

$$\frac{\partial\boldsymbol{\psi}(x)}{\partial x}+\mathbf{A}^i\boldsymbol{\psi}(x)=S(x)\mathbf{b}\,, \tag{3}$$

where the vector **b** is given as

$$\mathbf{b}=\begin{bmatrix}1/\mu_1\\ 1/\mu_2\\ \vdots\\ 1/\mu_N\end{bmatrix}, \tag{4}$$

and the transport operator matrix $\mathbf{A}^{\mathrm{i}}$ must be (the P_1 scattering terms are omitted due to column space limit)

$$\mathbf{A}^i=\begin{bmatrix}\frac{1}{\mu_1}\left(\Sigma_t^i-\frac{1}{2}\Sigma_{s0}^i w_1\right) & -\frac{1}{\mu_1}\left(\frac{1}{2}\Sigma_{s0}^i w_2\right) & \cdots & -\frac{1}{\mu_1}\left(\frac{1}{2}\Sigma_{s0}^i w_N\right)\\ -\frac{1}{\mu_2}\left(\frac{1}{2}\Sigma_{s0}^i w_1\right) & \frac{1}{\mu_2}\left(\Sigma_t^i-\frac{1}{2}\Sigma_{s0}^i w_2\right) & \vdots & -\frac{1}{\mu_2}\left(\frac{1}{2}\Sigma_{s0}^i w_N\right)\\ \vdots & \vdots & \ddots & \vdots\\ -\frac{1}{\mu_N}\left(\frac{1}{2}\Sigma_{s0}^i w_1\right) & -\frac{1}{\mu_N}\left(\frac{1}{2}\Sigma_{s0}^i w_2\right) & \cdots & \frac{1}{\mu_N}\left(\Sigma_t^i-\frac{1}{2}\Sigma_{s0}^i w_N\right)\end{bmatrix}. \tag{5}$$

If we perform a linear transform on the angular flux in Eq.(1) into the eigenspace of $\mathbf{A}^{\mathrm{i}}$ using eigenvectors $\mathbf{u}_m$ in

$$\mathbf{A}^i\mathbf{u}_m=\lambda_m\mathbf{u}_m \quad (m=1,\cdots,N)\,, \tag{6}$$

we essentially express the angular flux vector $\boldsymbol{\psi}(x)$ as a linear combination of the above eigenvectors

$$\boldsymbol{\psi}(x)=\sum_{m=1}^{N}\varphi_m(x)\mathbf{u}_m\,, \tag{7}$$

where $\varphi_m(x)$ is the expansion coefficient associated with the eigenvector $\mathbf{u}_m$. Similarly, the vector **b** is expressed as

$$\mathbf{b}=\sum_{m=1}^{N}b_m\mathbf{u}_m\,. \tag{8}$$

where b_m is the expansion coefficient.

By substituting Eqs. (7) and (8) into Eq.(3), we get

$$\sum_{m=1}^{N}\frac{\partial\varphi_m(x)}{\partial x}\mathbf{u}_m+\sum_{m=1}^{N}\varphi_m(x)\mathbf{A}^i\mathbf{u}_m=S(x)\sum_{m=1}^{N}b_m\mathbf{u}_m\,, \tag{9}$$

which can easily be re-formed as

$$\sum_{m=1}^{N}\mathbf{u}_m\left[\frac{\partial\varphi_m(x)}{\partial x}+\lambda_m\varphi_m(x)-b_mS(x)\right]=0\,. \tag{10}$$

Because $\mathbf{u}_{\mathrm{m}}$ are independent basis vectors of the eigenspace of $\mathbf{A}^{\mathrm{i}}$, these equations hold if and only if

$$\frac{\partial\varphi_m(x)}{\partial x}+\lambda_m\varphi_m(x)-b_mS(x)=0 \quad \text{for} \quad m=1,\cdots,N\,. \tag{11}$$

To this point, we convert the original S_N transport equation Eq.**Error! Reference source not found.** to a new transport equation Eq.(11), which does not have the coupled scattering source term. And the coefficients $\{\lambda_m,\ b_m\}$ appeared in Eq.(11) can be pre-calculated following the derivation procedure, which essentially makes Eq.(11) be the first order ordinary differential equations (ODEs) with constant coefficients. The analytic solutions to the ODEs can be readily achieved without much difficulty.

Semi-Analytic Solution

It is clear now we first need solve for φ (lowercase phi) in Eq.(11), which we will call the 'fake phi' or 'fake flux' to indicate its lack of physical meaning. Solving Eq. (11) for φ requires basic ODE skill. Separating the non-homogenous source term and using an integrating factor, we arrive at an integrable equation

$$d\left[e^{\lambda_m x}\varphi_m(x)\right]=b_mS(x)e^{\lambda_m x}dx\,. \tag{12}$$

For the 1D S_N problem, implementing transport sweeps where our equations have directional dependencies means the analytical solution must accommodate different boundary conditions as shown in Fig. 1.

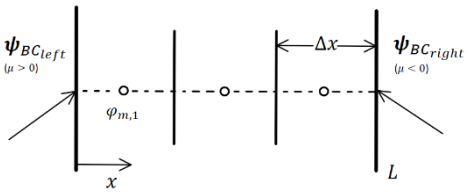

Fig.1. 1D transport mesh scheme with boundary conditions.

In the transport scheme in Fig. 1, we begin sweeps from the left where $\mu>0$ and $x=0$, working on node centers. The return sweep is from right to left, where $\mu<0$ and $x=L$. Integrating Eq. (12) for over these limits also including cases with and without a source term, we have

$$\varphi_m(x)=\varphi_{mL}e^{-\lambda_m x}+\frac{S_0b_m}{\lambda_m}\left(1-e^{-\lambda_m x}\right), \tag{13}$$

$$\varphi_m(x)=\frac{S_0b_m}{\lambda_m}\left(1-e^{\lambda_m(L-x)}\right)+\varphi_{mR}e^{\lambda_m(L-x)}. \tag{14}$$

For $\mu>0$ and $\mu<0$ respectively. These analytical solutions are trivial once the left and right boundary values, denoted by φ_{mL} and φ_{mR}, are known. However, their acquisition requires iteration, as the incident flux depicted in Fig.1 is unknown. Before discussing this further, we must derive how to find the real scalar flux using the fake flux in Eqs. (13) and (14).

Forming the Scalar Flux

The scalar flux is merely the sum of the product of the angular flux components and their corresponding quadrature weights w,

$$\phi(x) = \sum_{i=1}^{N} w_i \psi_i(x) \quad \text{for} \quad i = 1, \cdots, N \,. \tag{15}$$

We can combine this and Eq. (7), denoting the eigenvector components with i and m, the index corresponding to each quadrature value and the coupled vector to each eigenvalue respectively, we get

$$\phi(x) = \sum_{i=1}^{N} w_i \left(\sum_{m=1}^{N} \varphi_m(x) u_{im} \right). \tag{16}$$

We define a dummy variable to simplify the vector summation:

$$w'_m = \sum_{i=1}^{N} w_i \mathbf{u}_{im} \,. \tag{17}$$

Accordingly, the scalar flux becomes

$$\phi(x) = \sum_{m=1}^{N} \varphi_m(x) w'_m \,. \tag{18}$$

Transport Sweep with Boundary Flux Iteration

Applying Eqs. (6) and (8), we can pre-calculate and store the region-dependent constants necessary to find the fake flux and therefore the angular flux components and scalar flux. Conventional transport sweep using the nodal mesh in Fig.1 for all values of $\mu > 0$ and $\mu < 0$ require that the boundary values are known. We will discuss the similar problem of region interfaces later. For now, we describe the case of a one-region homogenous slab with vacuum boundaries. Eq.(7) implies the 'fake' angular flux has to be transformed by the whole spectrum of the real angular flux. Since the vacuum boundary condition only provides a half range of known angular flux at the boundaries, to use the analytic solutions for the 'fake' angular flux in Eqs. (13) and (14), we begin with an arbitrary but positive guess for the non-zero components of the boundary flux.

Using Eq. (7), we decompose the angular boundary flux into its components of the fake flux, and use these as the boundary values. A simple 'semi-analytical' iterative scheme can be implemented by finding the fake flux analytically using Eqs.(13) and (14), and updating the boundary fake flux values after each directional sweep. The real angular boundary flux is re-formed using Eq.(7), then the null components of the angular flux are replaced in the next iteration. Decomposing the updated angular flux again completes the scheme, and the subsequent return sweep can proceed, where the same procedure occurs. The convergence criterion for the boundary angular flux is as follows:

$$\varepsilon_{bc} = \left\| \frac{{\psi_{bc}}^{(n+1)} - {\psi_{bc}}^{(n)}}{{\psi_{bc}}^{(n+1)}} \right\|_2 . \tag{19}$$

In our practice, we used $\varepsilon \le 10^{-6}$ as the termination value for both SA and SI methods.

Multi-Region Interfaces

Since the 'fake' angular flux in each region are associated with the corresponding eigenspace at that region, extending the methodology to a multi-region case introduces a problem at the interfaces. However, the real angular flux at the interfaces must be continuous, so using Eq. (7) we equate the angular flux of two adjacent regions at the interface and assume the following equation holds

$$\sum_{m=1}^{N} \varphi_L \mathbf{u}_L = \sum_{m=1}^{N} \varphi_R \mathbf{u}_R \,. \tag{20}$$

where the subscripts L and R denote left and right arbitrary regions respectively. We denote the eigenspace of the region spanned by $\mathbf{u}$ with a matrix $\mathbf{E}$ to clarify the following steps. With this notation, Eq.(20) can be denoted as

$$\mathbf{E}_L \boldsymbol{\varphi}_L = \mathbf{E}_R \boldsymbol{\varphi}_R \tag{21}$$

Similar to the one region case, we proceed with transport sweep from left to right for $\mu > 0$, following the same boundary flux iteration procedure as before. Once at the interface, we decompose the 'fake' angular flux using Eq. (7) with the guessed values for the unknown components and the values acquired from the sweep for other components by applying

$$\mathbf{E}_R^{-1} \mathbf{E}_L \begin{bmatrix} \boldsymbol{\varphi}_L^- \\ \boldsymbol{\varphi}_L^+ \end{bmatrix} = \begin{bmatrix} \cancel{\boldsymbol{\varphi}_R^-} \\ \boldsymbol{\varphi}_R^+ \end{bmatrix} . \tag{22}$$

where the positive and negative signs indicate the set of φ for $\mu > 0$ and $\mu < 0$ respectively. For the $\mu > 0$ case, $\boldsymbol{\varphi}_L^-$ has to be guessed in the first iteration, and the unneeded values $\boldsymbol{\varphi}_R^-$ is marked out. Once we acquire $\boldsymbol{\varphi}_R^+$ by Eq.(22), we can proceed the sweep to the next region, and repeat the process until reach the opposing vacuum boundary. On the return sweep ($\mu < 0$), we will use a similar form as Eq.(22)

$$\mathbf{E}_L^{-1} \mathbf{E}_R \begin{bmatrix} \boldsymbol{\varphi}_R^- \\ \boldsymbol{\varphi}_R^+ \end{bmatrix} = \begin{bmatrix} \boldsymbol{\varphi}_L^- \\ \cancel{\boldsymbol{\varphi}_L^+} \end{bmatrix} . \tag{23}$$

With $\boldsymbol{\varphi}_L^-$ found, we have naturally taken care of the region-dependent 'fake' flux sets which ensures the convergence and continuity of the real angular flux at the interfaces when the boundary fluxes converge. After the first iteration, the scheme in Eq.(22) and (23) becomes

$$\begin{aligned} \mathbf{E}_R^{-1} \mathbf{E}_L \begin{bmatrix} {\varphi_L^-}^{(k-1)} \\ {\varphi_L^+}^{(k)} \end{bmatrix} &= \begin{bmatrix} \cancel{\varphi_R^-} \\ \varphi_R^+ \end{bmatrix} \qquad (\mu > 0) \\ \mathbf{E}_L^{-1} \mathbf{E}_R \begin{bmatrix} {\varphi_R^-}^{(k)} \\ {\varphi_R^+}^{(k-1)} \end{bmatrix} &= \begin{bmatrix} \varphi_L^- \\ \cancel{\varphi_L^+} \end{bmatrix} \qquad (\mu < 0) \end{aligned} \tag{24}$$

where the $(k)^{\text{th}}$ iteration values come from active transport sweep, and the $(k\text{-}1)^{\text{th}}$ iteration values come from the

eigenspace transformations in the previous iteration. Fig.2 illustrates the way in which this iteration is nested around the interfacial node following the conventions in Fig.1.

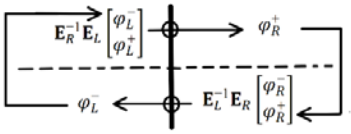

Fig. 2. Interface flux convergence scheme.

RESULTS

In our previous paper [9], we compared the computational speed of the SA method to the SI method in the one-region problem. In this work, we compare the relative error of the flux in an arbitrary three-region slab with varying material properties and extraneous sources. The problem configuration and results comparison are illustrated in Fig. 3.

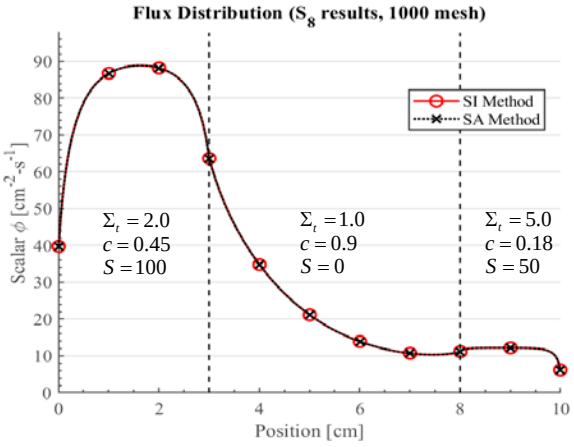

Fig. 3. Heterogenous slab flux distribution.

A crude benchmark was formed by spatially truncating a fine-mesh SI solution ($h = 0.000001\,cm$) with a convergence criterion of $\varepsilon \le 10^{-9}$. Results given by Barros [3] will be used in future analysis instead. Fig.4 reflects the known inaccuracy of SI solutions inside heterogenous regions.

Previously, an investigation into the highly diffusive case was made. In our previous study [9], we observed divergent behavior with $c > 0.97$. Also, in manipulating quadrature order, it appears that the SA method is much faster with low N values. Notably as well, as the mesh size decreases, the SI method slows significantly, while the SA method is hardly affected.

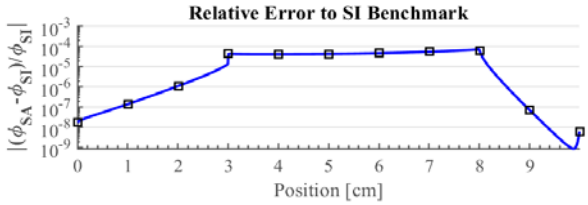

Fig. 4. Heterogenous slab case semi-log relative error.

FUTURE WORK

In-depth verification is needed for the benefits of the SA method with smaller mesh sizes and $N > 16$. Additions to this project include various boundary condition such as reflective boundary treatment, multigroup and anisotropic scattering extension, multi-dimensional expansion, and *k*-eigenvalue application, etc. Optimization of the current code structure and implementation will also be pursued.

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