A Spectral Approach to the Nonclassical Transport Equation (tentative title)

R. Vasques[a,*], C.F. Segatto[b,1], R.N. Slaybaugh[a,2]

[a] *University of California, Berkeley, Department of Nuclear Engineering, 4155 Etcheverry Hall Berkeley, CA 94720-1730*
[b] *UFRGS - Federal University of Rio Grande do Sul, Av. Osvaldo Aranha 99, 90046-900 Porto Alegre, RS, Brazil*

Abstract

These notes describe an approach to manipulate the nonclassical transport equation into a classical form that can be numerically solved through traditional approaches. The approach uses a combination of the spectral method and source iteration to eliminate the s-dependence. We use the LTS$_N$ method to solve the resulting equation in a 1-D system.

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1. Introduction

2. Nonclassical Transport Equation

Consider the one-speed nonclassical transport equation with isotropic scattering given by

$$\frac{\partial}{\partial s}\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)+\boldsymbol{\Omega}\cdot\nabla\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)+\Sigma_t(\boldsymbol{\Omega},s)\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)= \\ \frac{\delta(s)}{4\pi}\left[\int_{4\pi}\int_0^\infty c\Sigma_t(\boldsymbol{\Omega}',s')\Psi(\boldsymbol{x},\boldsymbol{\Omega}',s')d\Omega' ds'+Q(\boldsymbol{x})\right],\quad \boldsymbol{x}\in V, \tag{1a}$$

subject to the vacuum boundary condition

$$\Psi(\boldsymbol{x}_b,\boldsymbol{\Omega},s)=0,\quad \boldsymbol{n}\cdot\boldsymbol{\Omega}<0,\quad \boldsymbol{x}_b\in\partial V. \tag{1b}$$

Here, $\boldsymbol{x}=(x,y,z)$, $\boldsymbol{\Omega}=(\Omega_x,\Omega_y,\Omega_z)$, s describes the free-path of a particle, Ψ is the nonclassical angular flux, c is the scattering ratio, and Q is an isotropic source. The angular-dependent nonclassical total cross section $\Sigma_t(\boldsymbol{\Omega},s)$ satisfies

$$p(\boldsymbol{\Omega},s)=\Sigma_t(\boldsymbol{\Omega},s)e^{-\int_0^s\Sigma_t(\boldsymbol{\Omega},s')ds'}, \tag{2}$$

*Corresponding author: richard.vasques@fulbrightmail.org; Tel: (510) 340 0930
Postal address: University of California, Berkeley, Department of Nuclear Engineering, 4103 Etcheverry Hall, Berkeley, CA 94720-1730
[1] cynthia.segatto@ufrgs.br
[2] slaybaugh@berkeley.edu

where $p(\boldsymbol{\Omega}, s)$ is the free-path distribution function in the direction $\boldsymbol{\Omega}$.

It is useful to work with Eq. (1a) in an equivalent "initial value" form:

$$\frac{\partial}{\partial s}\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \boldsymbol{\Omega}\cdot\nabla\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \Sigma_t(\boldsymbol{\Omega},s)\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) = 0, \tag{3a}$$

$$\Psi(\boldsymbol{x},\boldsymbol{\Omega},0) = \frac{1}{4\pi}\left[\int_{4\pi}\int_0^\infty c\Sigma_t(\boldsymbol{\Omega}',s')\Psi(\boldsymbol{x},\boldsymbol{\Omega}',s')d\Omega' ds' + Q(\boldsymbol{x})\right]. \tag{3b}$$

Let us define ψ such that

$$\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) \equiv \psi(\boldsymbol{x},\boldsymbol{\Omega},s)e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega},s')ds'}. \tag{4}$$

We can now rewrite the nonclassical problem as

$$\frac{\partial}{\partial s}\psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \boldsymbol{\Omega}\cdot\nabla\psi(\boldsymbol{x},\boldsymbol{\Omega},s) = 0, \tag{5a}$$

$$\psi(\boldsymbol{x},\boldsymbol{\Omega},0) = \frac{1}{4\pi}\left[\underbrace{\int_{4\pi}\int_0^\infty cp(\boldsymbol{\Omega}',s')\psi(\boldsymbol{x},\boldsymbol{\Omega}',s')d\Omega' ds'}_{S(\boldsymbol{x})} + Q(\boldsymbol{x})\right] = \frac{S(\boldsymbol{x})}{4\pi} + \frac{Q(\boldsymbol{x})}{4\pi}, \tag{5b}$$

$$\psi(\boldsymbol{x}_b,\boldsymbol{\Omega},s) = \quad \boldsymbol{n}\cdot\boldsymbol{\Omega} < 0, \quad \boldsymbol{x}_b \in \partial V. \tag{5c}$$

We will take advantage of the initial value form of Eqs. (5) by using source iteration. We define

$$\psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \sum_{k=0}^{K}\psi^{(k)}(\boldsymbol{x},\boldsymbol{\Omega},s), \tag{6}$$

where $\psi^{(k)}$ represents particles in the angular flux that have undergone *exactly* k collisions. It is easy to see that $\psi^{(k)}$ satisfies

$$\frac{\partial}{\partial s}\psi^{(k)}(\boldsymbol{x},\boldsymbol{\Omega},s) + \boldsymbol{\Omega}\cdot\nabla\psi^{(k)}(\boldsymbol{x},\boldsymbol{\Omega},s) = 0, \tag{7a}$$

$$\psi^{(k)}(\boldsymbol{x},\boldsymbol{\Omega},0) = F^{(k)}(\boldsymbol{x}) = \begin{cases} \frac{Q(\boldsymbol{x})}{4\pi}, & k=0, \\ \frac{S^{(k-1)}(\boldsymbol{x})}{4\pi}, & k>0, \end{cases}, \tag{7b}$$

$$\psi^{(k)}(\boldsymbol{x}_b,\boldsymbol{\Omega},s) = 0, \quad \boldsymbol{n}\cdot\boldsymbol{\Omega} < 0, \quad \boldsymbol{x}_b \in \partial V. \tag{7c}$$

where $S^{(k-1)}(\boldsymbol{x}) = \int_{4\pi}\int_0^\infty cp(\boldsymbol{\Omega}',s')\psi^{(k-1)}(\boldsymbol{x},\boldsymbol{\Omega}',s')d\Omega' ds'$.

The idea in these notes is to use the spectral method to eliminate the s-dependence in Eqs. (7).

3. The Spectral Method

To eliminate the dependence on s, we approximate $\psi^{(k)}$ by a truncated series of Laguerre polynomials $\{L_0(s), L_1(s), ..., L_M(s)\}$ such that

$$\psi^{(k)}(\boldsymbol{x},\boldsymbol{\Omega},s) = \sum_{m=0}^{M}\psi_m^{(k)}(\boldsymbol{x},\boldsymbol{\Omega})L_m(s). \tag{8}$$

The Laguerre polynomials are orthogonal with respect to the weight function e^{-s}; that is,

$$\int_0^\infty e^{-s} L_j(s) L_m(s) ds = \begin{cases} 0 & j \neq m, \\ 1 & j = m. \end{cases} \tag{9}$$

We multiply Eq. (7a) by $e^{-s} L_m(s)$ and operate on it by $\int_0^\infty (\cdot) ds$ (truncating in M) to obtain

$$\boldsymbol{\Omega} \cdot \nabla \psi_m^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}) = \sum_{j=m+1}^{M} \psi_j^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}). \tag{10}$$

Equations (7b) and (8) give us

$$\sum_{j=m+1}^{M} \psi_j^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}) = F^{(k)}(\boldsymbol{x}) - \sum_{j=0}^{m} \psi_j^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}). \tag{11}$$

We now have

$$\boldsymbol{\Omega} \cdot \nabla \psi_m^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}) + \psi_m^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}) = U_m^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}), \tag{12a}$$

$$\psi_m^{(k)}(\boldsymbol{x}_b, \boldsymbol{\Omega}) = 0, \quad \boldsymbol{n} \cdot \boldsymbol{\Omega} < 0, \quad \boldsymbol{x}_b \in \partial V, \tag{12b}$$

where

$$U_0^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}) = F^{(k)}(\boldsymbol{x}), \tag{13a}$$

$$U_m^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}) = U_{m-1}^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}) - \psi_{m-1}^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}), \quad m = 1, ..., M. \tag{13b}$$

For each step m, $U_m^{(k)}$ is a known function. Equations (12) have the form of a *classical* purely absorbing homogeneous system with a fixed source and $\Sigma_t = \Sigma_a = 1$. That is, Eqs. (12) can be solved using *any* established homogeneous solver.

A simple sketch of the algorithm follows:

- "While" loop: $k = 0, 1, 2, ...$ (uses a stopping criterion)
  - Closed loop: $m = 0, 1, ..., M$
    * Apply homogeneous solver to Eqs. (12) and obtain $\psi_m^{(k)}$
  - Check stopping criterion
- Obtain the classical angular flux:

$$\hat{\Psi}(\boldsymbol{x}, \boldsymbol{\Omega}) = \int_0^\infty \Psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) ds = \int_0^\infty \left(e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s') ds'} \sum_{k=0}^{K} \sum_{m=0}^{M} \psi_m^{(k)}(\boldsymbol{x}, \boldsymbol{\Omega}) L_m(s) \right) ds$$

In the next section we apply this approach to a 1-D problem using the LTS_N method to solve Eqs. (12).

4. The LTS$_N$ Approach

Let the coefficients μ_n and ω_n represent the zeros and weights of the Gauss-Legendre quadrature. We define

$$\psi_{m,n}^{(k)}(x) = \psi_m^{(k)}(x, \mu_n), \tag{14a}$$
$$U_{0,n}^{(k)}(x) = U_0^{(k)}(x, \mu_n) = F^{(k)}(x), \tag{14b}$$
$$U_{m,n}^{(k)}(x) = U_{m-1,n}^{(k)}(x) - \psi_{m-1,n}^{(k)}(x) = U_{m-1}^{(k)}(x, \mu_n) - \psi_{m-1}^{(k)}(x, \mu_n), \tag{14c}$$

where

$$F^{(0)}(\boldsymbol{x}) = \frac{Q(\boldsymbol{x})}{2}, \tag{14d}$$
$$F^{(k)}(\boldsymbol{x}) = \frac{c}{2}\int_0^\infty \sum_{n=1}^{N}\left(\omega_n p_n(s)\sum_{m=1}^{M}\psi_{m,n}^{(k-1)}L_m(s)\right)ds, \quad k = 1, 2, ..., \tag{14e}$$

and

$$p_n(s) = p(\mu_n, s). \tag{14f}$$

Now, we can write the corresponding 1-D S$_N$ problem to Eqs. (12) as

$$\mu_n \frac{\partial}{\partial x}\psi_{m,n}^{(k)}(x) + \psi_{m,n}^{(k)}(x) = U_{m,n}^{(k)}(x), \tag{15a}$$
$$\psi_{m,n}^{(k)}(0) = \psi_{m,N-n+1}^{(k)}(0), \quad n = 1, ..., N/2, \tag{15b}$$
$$\psi_{m,n}^{(k)}(X) = 0, \quad n = N/2+1, ..., N. \tag{15c}$$

Applying the LTS$_N$ method to this problem, we obtain an analytical formulation for $\psi_{m,n}^{(k)}$:

$$\psi_{m,n}^{(k)}(x) = \sum_{i=1}^{N/2}\Bigg[\alpha(n,i)\left(e^{\gamma(i)(x-H)} + e^{\gamma(i+N/2)x}\right)\Gamma_{m,i}^{(k)} + \tag{16}$$
$$\sum_{j=1}^{N}\alpha(n,i)\left(\int_H^x e^{\gamma(i)(x-\tau)}U_{m,j}^{(k)}(\tau)d\tau + \int_0^x e^{\gamma(i+N/2)(x-\tau)}U_{m,j}^{(k)}(\tau)d\tau\right)\beta(i,j)\Bigg],$$

where $\gamma(i)$ are the eigenvalues resulting from the diagonalization of the LTS$_N$ matrix, $\alpha(n,i)$ are the components of the eigenvector matrix, and $\beta(i,j)$ are the components of its inverse. The coefficients $\Gamma_{m,i}^{(k)}$ are determined from the boundary conditions.

5. Numerical Results

6. Conclusion

Comments

- While we do not explicitly discretize s, the following takes place:

- $\psi(x,\mu,s)$ is approximated by a truncated series of Laguerre polynomials in s
- The integral in s described in Eq. (14e) will probably need to be performed numerically
- At the end of the algorithm, we need to calculate

$$\hat{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}) = \int_0^\infty \Psi(\boldsymbol{x},\boldsymbol{\Omega},s)ds = \int_0^\infty \left(e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega},s')ds'} \sum_{k=0}^{K}\sum_{m=0}^{M} \psi_m^{(k)}(\boldsymbol{x},\boldsymbol{\Omega}) L_m(s) \right) ds,$$

which will also need to be performed numerically

- The convolution integrals in Eq. (16) will *probably* need to be solved numerically due to the recursiveness of the problem arising from the source term. **Is there a way to do that analitically?**
- Due to the source iteration approach, convergence will be slow as problems become more diffusive.
- It is not clear to me what will be the more time-consuming step. My guess is that the time to converge the source iteration will dominate in diffusive problems; for absorbing problems, I do not know.
- Nonclassical boundary conditions are tricky: incoming fluxes will have a $\delta(s)$. I need to think more about the best approach in those cases; it is possible that the best solution will be using the *forward* nonclassical equation. That, however, is beyond the current scope.
- To validate the method, we can apply the algorithm to solve a classical problem. In that case, $p(\mu,s) = \Sigma_t e^{-\Sigma_t s}$. This will also allow us to see how efficiently the solver works.
- After it is validated, we can apply the algorithm to the random periodic case we have been working on; after that, we can go for general stochastic mixtures.

References