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A review of the deterministic solution of nonclassical transport problems

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1. Introduction

The mathematical description of the migration of small neutral particles, such as neutrons and photons, through a background material is usually referred to as Transport Theory [1]. In practical terms, in a deterministic approach, the equation that describes the interactions of these migrating particles with matter is the well-known linear Boltzmann equation (LBE) [1]. Several applications in science have been developed using the LBE as mathematical model. Examples are included in nuclear reactor physics, astrophysics, nuclear medicine, oil exploration, non-destructive test methods, among others.

The development of the LBE (also referred to as the transport equation) is based on considering that the material properties (geometry, cross sections, etc) of the background material are known. This means, that in order to determine the particle angular flux (solution of the LBE) it is required to know previously the material parameters in each point of space and time. However, in many practical situations (such as radiation transport through atmospheric clouds), the properties of the background system in which particles travel are known only in a statistical sense.

The branch of Transport Theory that deals with this type of problem is known as Stochastic Transport Theory. Hence, as the material properties are known only in a statistical sense, instead of looking for the true solution of the transport equation, the goal is to find the ensemble-average (expected value) of the particle flux. To use the LBE in this type of situation it is necessary first to use other methods, such as the atomic mix model (the most notable and widely used), to derive cross sections that are applicable (functions of space and time) to this equation. However, the atomic mix model assumes that the distribution of chord lengths between scattering centers is exponential. This assumption is very restrictive since it implies that the medium spatial heterogeneities occur on a length scale which is small compared to a typical mean free path and that the locations of the scattering centers are uncorrelated. Therefore, the LBE is unable to accurately address certain classes of stochastic problems.

By adding the term "nonclassical" to transport problems, we mean transport problems where the probability distribution function for distance-to-collision is not exponentially distributed. As the LBE inherently assumes that the particle flux is exponentially attenuated, a generalized linear Boltzmann equation (GLBE) which would accounts for situations where the particle flux is not exponentially attenuated should be derived. This was done by Larsen in the work [2] and expanded later in [3]. For monoenergetic problems, the GLBE appears as

$$\begin{aligned}&\frac{\partial}{\partial s}\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)+\boldsymbol{\Omega}\cdot\nabla\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)+\Sigma_t(\boldsymbol{\Omega},s)\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)=\\&\delta(s)\left[c\int_{4\pi}\int_0^\infty P(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\Sigma_t(\boldsymbol{\Omega}',s')\Psi(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'd\Omega'+\frac{Q(\boldsymbol{x})}{4\pi}\right],\quad \boldsymbol{x}\in V,\ \boldsymbol{\Omega}\in 4\pi,\ 0<s.\end{aligned}\tag{1}$$

This equation is similar to the LBE except for the introduction of a new independent variable s, which represents the distance traveled by the particle since its last interaction (birth or scattering), with $s = 0$ at the interaction point. The Dirac delta function $\delta(s)$ that appears in Eq. (1) follows the definition of the variable s, i.e., it resets the value of s for particles that just scattered or were born in the system through source Q. As we see in Eq. (1), both the particle angular flux (Ψ) and the macroscopic cross section (Σ_t) are functions of the variable s and direction of motion $\boldsymbol{\Omega}$. Moreover, Σ_t satisfies the relation

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

where $p(\boldsymbol{\Omega}, s)$ is the free-path distribution function in the $\boldsymbol{\Omega}$ direction. If one considers Σ_t being independent of $\boldsymbol{\Omega}$ and s, Eq. (2) is reduced to an exponential free-path distribution function and Eq. (1) is reduced to the classic LBE [2].

2. The Spectral Approach

One way to obtain the particle angular flux for nonclassical transport problems is by solving Eq. (1). As there exists an extensive number of well-established deterministic methods to solve the LBE, it is of interest to make use of a methodology that allows one to directly apply these conventional deterministic methods to the solution of the GLBE. The Spectral Approach (SA) has been developed to achieve this goal [4]. In the SA the particle angular flux is represented through the following relation:

$$\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)\equiv\psi(\boldsymbol{x},\boldsymbol{\Omega},s)e^{-\int_0^s\Sigma_t(\boldsymbol{\Omega},s')ds'}.\tag{3}$$

Function ψ is then expanded in a truncated series of Laguerre polynomials in s. That is,

$$\psi(\boldsymbol{x},\boldsymbol{\Omega},s)=\sum_{m=0}^{M}\psi_m(\boldsymbol{x},\boldsymbol{\Omega})L_m(s),\tag{4}$$

where M is the truncation order of the Laguerre series and $L_m(s)$ is the Laguerre polynomial of degree m in s. Substituting Eqs. (3) and (4) into the "initial value form" [4] of Eq. (1), it is possible to obtain, after some mathematical manipulations, a system of equation for ψ_m, i.e.,

$$\boldsymbol{\Omega}\cdot\nabla\psi_m(\boldsymbol{x},\boldsymbol{\Omega})+\sum_{j=0}^{m}\psi_j(\boldsymbol{x},\boldsymbol{\Omega})=c\int_{4\pi}P(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\sum_{k=0}^{M}\psi_k(\boldsymbol{x},\boldsymbol{\Omega}')\mathcal{L}_k(\boldsymbol{\Omega}')d\Omega'+\frac{Q(\boldsymbol{x})}{4\pi},\tag{5a}$$

where $m = 0, 1, 2, \ldots, M$ and we have defined

$$\mathcal{L}_k(\boldsymbol{\Omega})=\int_0^\infty p(\boldsymbol{\Omega},s')L_k(s')ds'.\tag{5b}$$

The system of equations represented by Eq. (5a) possesses a "classical" form. In other words, it is constituted by equations which are very similar to the LBE. In fact, once the functions described in Eq. (5b) are calculated, it is possible to solve Eq. (5a) as a slightly modified system of coupled LBEs.

3. Solving Nonclassical Problems Using the Spectral Approximation of the GLBE

In the same work where the SA was described [4], the first attempts to solve nonclassical transport problems through Eqs. (5) were made. Equations (5) were solved for one-dimensional problems making use of conventional deterministic methods, namely, the Discrete Ordinates Formulation (S_N) and the Diamond Difference method [1], for the discretization of the angular and spatial variables respectively.

The physical system considered in reference [4] is shown in Fig. 1. This system is composed of two distinct materials periodically arranged, where the period is given by $\ell = \ell_1 + \ell_2$, with ℓ_1 and ℓ_2 representing the width of each material. Material 1 is a solid with $\Sigma_{t_1} = 1$ cm^{-1}, and material 2 is defined as a void, i.e., $\Sigma_{t_2} = 0$ cm^{-1}. This periodic system is *randomly placed* in

Figure 1: One-dimensional Random Periodic Media [4].

the infinite line $-\infty < x < \infty$, such that the probability P_i of finding material $i \in \{1, 2\}$ in a given point is ℓ_i/ℓ. Therefore, material parameters (such as the cross sections) are stochastic functions of space. The ensemble-averaged free-path distribution for the problem depicted in Fig. 1, considering the case where $\ell_1 = \ell_2$ (reference [4] also describes situations where $\ell_1 \neq \ell_2$) is given through the following relation

$$p(\mu, s) = \begin{cases} \frac{\Sigma_{t1}}{\ell_1}(n\ell + \ell_1 - s|\mu|)e^{-\Sigma_{t1}(s - n\ell_2/|\mu|)}, & \text{if } n\ell \leq s|\mu| \leq n\ell + \ell_1 \\ \frac{\Sigma_{t1}}{\ell_1}(s|\mu| - n\ell - \ell_2)e^{-\Sigma_{t1}[s-(n+1)\ell_2/|\mu|]}, & \text{if } n\ell + \ell_2 \leq s|\mu| \leq (n+1)\ell \end{cases}, \quad (6)$$

where $n = 0, 1, \ldots$. Table I displays the results considering the space domain limits as $-10 \leq x \leq 10$, $\ell_1 = \ell_2 = 1$ cm and $Q(x) = \begin{cases} 0.5 \times 10^{17}\,\text{neutrons/cm}^3 \cdot \text{s, if } -0.5 \leq x \leq 0.5 \\ 0\text{, otherwise} \end{cases}$. Moreover, the angular quadrature chosen was the Gauss-Legendre S_{20} and the spatial domain was discretized such that the width of each discretization cell is 0.005 cm. The benchmarks were produced by solving 200 classical transport problems using the LBE. Thus, in each classical transport problem Σ_t is independent of μ and s (exponential free-path distribution function). Details of how to obtain the benchmark solution can be found in [5].

Table I: Ensemble-Averaged scalar fluxes for the nonclassical transport problem [4].

|x| (cm)	Benchmark (neutrons/cm^{2}s)	Solution of Eqs. (5) (neutrons/cm^{2}s)		Relative error (%)	
		M=50	M=200	M=50	M=200
			$c = 0.0$		
0.0	3.890079E+16	3.891017E+16	3.889305E+16	2.411346E-02	-1.988391E-02
5.0	6.598115E+14	6.660539E+14	6.591396E+14	9.460837E-01	-1.018436E-01
10.0	2.999265E+13	3.028603E+13	2.994294E+13	9.781649E-01	-1.657549E-01
			$c = 0.9$		
0.0	1.427736E+17	1.410333E+17	1.410050E+17	-1.218951E+00	-1.238745E+00
5.0	3.186643E+16	3.218562E+16	3.214855E+16	1.001670E+00	8.853233E-01
10.0	4.032572E+15	4.365284E+15	4.367367E+15	8.250617E+00	8.302263E+00

4. Trends in the future

After reference [4] introduced the SA and showed this methodology is interesting for the solution of the GLBE, 3 research topics emerge naturally for further development: (i) the improvement of the SA; (ii) the investigation of different deterministic methods for the solution of Eqs. (5); and (iii) the use of acceleration methods.

In research topic (i) the point is to develop useful modifications of the SA in order to make this method more efficient. An interesting work is given in reference [6], where the authors describe a slightly different representation for the particle angular flux (related to Eq. (3)) that in some cases allows a severe decreasing of the Laguerre series truncation order, required to generate accurate results. In research topic (ii), the idea is to explore deterministic methods that fit well with the GLBE characteristics. One class of such methods that has potential in this perspective is the class of the spectral nodal methods. As the ensemble-average free-path distribution function and the macroscopic cross section are not functions of space, the number of eigenvalue problems (related to the homogeneous solution of Eq. (5a)) needed to be solved is reduced to one, regardless of the problem. A first work in this path is given in [7].

Efforts should also be given at the development/application of acceleration methods. As the phase space in the GLBE is extended (in the variable s), the order of the problem needed to be solved is increased. This situation foments even more the need to accelerate the iterative schemes used to generate numerical solutions. A successful first attempt can be found in reference [8].

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