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# Mixed singular-regular boundary conditions in multislab radiation transport

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**Abstract**

This article reports a computational method for approximately solving radiation transport problems with anisotropic scattering defined on multislab domains irradiated from one side with a beam of monoenergetic neutral particles. We assume here that the incident beam may have a monodirectional component and a continuously distributed component in angle. We begin by defining the target problem representing the class of radiation transport problems that we are focused on. We then Chandrasekhar decompose the target problem into an uncollided transport problem with left singular boundary conditions and a diffusive transport problem with regular boundary conditions. We perform an analysis of these problems to derive the exact solution of the uncollided transport problem and a discrete ordinates solution in open form to the diffusive transport problem. These solutions are the basis for the definition of a computational method for approximately solving the target problem. We illustrate the numerical accuracy of our method with three basic problems in radiative transfer and neutron transport, and we conclude this article with a discussion and directions for future work.


*Keywords:* Radiation transport; Mixed beams; Multislab problems; Discrete ordinates; Analytical and numerical methods

## 1. Introduction

Basic and important problems arising in radiation transport theory are modelled by a plane-parallel stratified (multislab) domain irradiated from one side with a neutral particle beam. Such problems most often lie within a multidisciplinary scope and, from first principles and with simplifying assumptions, they are physically represented, mathematically formulated and solved, yielding a first approximation to the solution of the basic problem in question and giving us directions for the development of mathematical methods for the solution of model problems "closer" to the basic ones [27]. Representative problems in

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multidisciplinary research areas include: (i) the fundamental problem of radiation shielding – the problem of keeping a region clear of radiation by shielding the region against a one-sided radiation source [32]; (ii) the classical atmospheric radiative transfer problem of computing the distribution of radiant energy in a finite plane-parallel planetary atmosphere illuminated from the outer side by a beam of solar radiation [5,35]; (iii) the problem of estimating the spectral reflectance of forest canopies for remote sensing applications [17,18,28,29,36] and (iv) the problem of designing a neutron beam filter assembly (a stack of filtering blocks) suited for boron neutron capture therapy (BNCT) applications [20,23,26,37,39].

The problems listed in the preceding paragraph are, generally speaking, characterized by an incident beam with a monodirectional (singular) component *and/or* a continuously distributed (regular) component in angle. The mixed case (singular *and* regular) is particularly true of problems (iii) and (iv), where scattered radiation contributes significantly to the incident particle beam. For an approximate solution to multislab radiation transport problems with only a continuously distributed incident beam, some of the discrete ordinates ($S_N$) spectral methods developed over the last 10 years by the present author and former collaborators can be readily used [2–4,7–12]. For an approximate solution to multislab problems with only a monodirectional incident beam, we have recently developed (unpublished) a computational method based on $S_N$ spectral methods and inspired mostly on a decomposition technique – the radiation transport problem is decomposed into an uncollided problem with singular boundary conditions and a diffusive problem with zero incoming boundary conditions – firstly introduced by Chandrasekhar for solving the classical albedo problem in atmospheric radiative transfer [5]. It is noteworthy that the methods referred to in this paragraph do apply to multislab problems with *either* singular *or* regular boundary conditions.

In this article, we take a step further and we describe a computational method for efficiently and accurately solving radiation transport problems with anisotropic scattering defined on a multislab domain irradiated from one side with a neutral particle beam having a monodirectional component and/or a continuously distributed component in angle. The method here is essentially that recently developed by us for problems with only a monodirectional beam, with the necessary modifications to enable us to solve multislab problems with one-type (singular *or* regular) or mixed boundary conditions. We believe that the method described in the present article is relevant, for it solves multislab problems covered by the methods referred to in the preceding paragraph and multislab problems not covered so far in an efficient and accurate manner.

We outline the remaining sections of this article. In Section 2, we mathematically formulate and perform an analysis of the target problem that represents the class of radiation transport problems dealt with in this article. In Section 3, we describe a mathematical method for approximately solving the target problem. In Section 4, we discuss computational aspects of our method and we illustrate its numerical accuracy with three basic problems in atmospheric radiative transfer and neutron transport. In Section 5, we conclude this article with a discussion and directions for further developments and future work.

## 2. Formulation and analysis of the target problem

### 2.1. Problem formulation

We begin with a mathematical formulation of the target problem representing a class of radiation transport problems with anisotropic scattering defined on a multislab domain irradiated from one side with a monoenergetic neutral particle beam. We consider the slab-geometry transport equation

$$\mu\frac{\partial}{\partial z}\psi(z,\mu)+\sigma_t(z)\psi(z,\mu)=S(z,\mu),\quad z\in\Omega\equiv[z_0,z_{\mathrm{R}}],\quad -1\leqslant\mu\leqslant 1. \tag{1}$$

Here, $\Omega$ is a multislab domain with transparent boundaries [5] denoted by $z_0$ (left) and $z_{\mathrm{R}}$ (right), respectively; the quantity $\psi(z,\mu)$ is the angular flux of particles traveling in direction $\mu$ at position $z$ on $\Omega$; $\sigma_t(z)$ is

the macroscopic total cross-section at position $z$ and the remaining notation and nomenclature are standard in particle transport theory [15,38]. The quantity $S(z,\mu)$ is the scattering source given by

$$S(z,\mu)=\frac{\sigma_0(z)}{2}\sum_{\ell=0}^{\infty}(2\ell+1)\beta_\ell(z)P_\ell(\mu)\int_{-1}^{1}\mathrm{d}\mu' P_\ell(\mu')\psi(z,\mu'), \tag{2}$$

where $\sigma_0(z)$ is the macroscopic scattering cross-section at position $z$; $P_\ell(\mu)$ denotes the $\ell$th-degree Legendre polynomial and $(2\ell+1)\beta_\ell(z)$ is the $\ell$th-order component of the Legendre expansion of the scattering phase function at position $z$. Changes in the meaning of some of the terms in Eq. (1) for radiative transfer problems are due. For then $z$ is the optical variable, $\psi(z,\mu)$ denotes the specific intensity of the radiation field, $\sigma_t(z)$ is set to one and, as a result, $\sigma_0(z)$ is the single scattering albedo [5,35]. The multislab domain consists of $R$ contiguous and disjoint layers of homogeneous material each, i.e. the quantities $\sigma_t(z)$ and $\sigma_0(z)$ are nonnegative piecewise constant functions of $z$ on $\Omega$. The transport Eq. (1) is subject to the boundary conditions

$$\psi(z_0,\mu)=\psi_0\delta(\mu-\mu_0)+\gamma_0(\mu),\quad \mu>0,\quad \mu_0>0, \tag{3.1}$$

$$\psi(z_{\mathrm{R}},-\mu)=0,\quad \mu>0, \tag{3.2}$$

where $\psi_0$ is a nonnegative real; $\mu_0$ is the cosine of the polar angle defining the direction of incidence of the monodirectional component of the particle beam upon the left boundary of the multislab domain $\Omega$; $\delta$ is to denote a Dirac distribution and $\gamma_0(\mu)$, $\mu>0$, is a nonnegative function of $\mu$ representing the angularly continuous component of the incident beam. Eqs. (1–3) define the target problem representing the class of radiation transport problems dealt with in this article.

### 2.2. A basic approach to solve the target problem

The target problem (1–3) can be approximately solved as follows: (i) we Chandrasekhar decompose the target problem into, say, a problem A defined by Eq. (1) and the left singular boundary conditions $\psi_A(z_0,\mu)=\psi_0\delta(\mu-\mu_0)$, $\mu>0,\mu_0>0$, and $\psi_A(z_{\mathrm{R}},-\mu)=0$, $\mu>0$, and a problem B defined by Eq. (1) and the regular boundary conditions $\psi_B(z_0,\mu)=\gamma_0(\mu)$ and $\psi_B(z_{\mathrm{R}},-\mu)=0$, $\mu>0$; (ii) we solve problem A with the method recently developed by us (unpublished) and we solve problem B with some of the $S_N$ spectral methods developed in the past and finally (iii) we compose the obtained solutions to problems A and B. This approach allows for the use of available and accurate methods with good theoretical basis and of computer programs ready and functional. However, a closer look at such an approach reveals a serious drawback: it is concerned with the formulation (and solution) of *two* diffusive transport problems – one coming from the Chandrasekhar's decomposition of problem A and the other is just problem B. Since diffusive problems in the field are algebraically hard to work out and computationally costly [1,25], we are convinced that this is a drawback serious enough to think of a different approach as a basis for a computational method for approximately solving the target problem Eqs. (1–3). So, we discard that way leading to two diffusive transport problems and we instead directly Chandrasekhar decompose the target problem (1–3) into the uncollided transport problem

$$\mu\frac{\partial}{\partial z}\psi^{\mathrm{u}}(z,\mu)+\sigma_t(z)\psi^{\mathrm{u}}(z,\mu)=0,\quad z\in\Omega,\quad -1\leqslant\mu\leqslant 1, \tag{4}$$

with the left singular boundary conditions

$$\psi^{\mathrm{u}}(z_0,\mu)=\psi_0\delta(\mu-\mu_0);\quad \psi^{\mathrm{u}}(z_{\mathrm{R}},-\mu)=0,\quad \mu>0,\quad \mu_0>0, \tag{5}$$

and the diffusive transport problem

$$\mu\frac{\partial}{\partial z}\psi^{\mathrm{d}}(z,\mu)+\sigma_t(z)\psi^{\mathrm{d}}(z,\mu)$$
$$=\frac{\sigma_0(z)}{2}\sum_{\ell=0}^{\infty}(2\ell+1)\beta_\ell(z)P_\ell(\mu)\int_{-1}^{1}\mathrm{d}\mu' P_\ell(\mu')\psi^{\mathrm{d}}(z,\mu')+s^{\mathrm{u}}(z,\mu),\quad z\in\Omega,\quad -1\leqslant\mu\leqslant 1, \tag{6}$$

with the regular boundary conditions

$$\psi^{\mathrm{d}}(z_0,\mu)=\gamma_0(\mu);\quad \psi^{\mathrm{d}}(z_{\mathrm{R}},-\mu)=0,\quad \mu>0, \tag{7}$$

so that $\psi(z,\mu)=\psi^{\mathrm{u}}(z,\mu)+\psi^{\mathrm{d}}(z,\mu)$, $z_0\leqslant z\leqslant z_{\mathrm{R}}$, $-1\leqslant\mu\leqslant 1$. The quantity

$$s^{\mathrm{u}}(z,\mu)\equiv\frac{\sigma_0(z)}{2}\sum_{\ell=0}^{\infty}(2\ell+1)\beta_\ell(z)P_\ell(\mu)\int_{-1}^{1}\mathrm{d}\mu' P_\ell(\mu')\psi^{\mathrm{u}}(z,\mu'), \tag{8}$$

is a space-dependent anisotropic source given in terms of the solution $\psi^{\mathrm{u}}(z,\mu)$ to the uncollided transport problem (4) and (5). With this approach, we formulate and need to solve *only one* diffusive problem.

### 2.3. Analysis of the uncollided and diffusive problems

We hereafter perform an analysis of both the uncollided transport problem (4) and (5) and the diffusive transport problem (6) and (7) in order to get analytical results important to define and substantiate our computational method.

#### 2.3.1. The uncollided problem

We begin our analysis with the uncollided transport problem (4) and (5). Since the uncollided problem (4) and (5) represents an auxiliary problem defined in a purely absorbing multislab domain with transparent boundaries, with no interior source and with an incident particle beam upon the left ($z_0$) boundary only, we must have $\psi^{\mathrm{u}}(z,\mu)=0$, for $\mu<0$ and for all $z\in\Omega$. For $\mu>0$ and $z\in\Omega$, $\psi^{\mathrm{u}}(z,\mu)>0$ and we can write the uncollided transport Eq. (4) in the integral form

$$\int_{z_0}^{z}\frac{1}{\psi^{\mathrm{u}}(v,\mu)}\frac{\partial}{\partial v}\psi^{\mathrm{u}}(v,\mu)\mathrm{d}v=-\frac{1}{\mu}\int_{z_0}^{z}\sigma_t(v)\mathrm{d}v,\quad z\in\Omega,\quad \mu>0, \tag{9}$$

where the integral on the right side of the equal sign in Eq. (9) is the number of particle mean free paths [15,38] on the interval $(z_0,z)$. We solve Eq. (9) for $\psi^{\mathrm{u}}(z,\mu)$ and we successively obtain

$$\ln\psi^{\mathrm{u}}(v,\mu)\big|_{z_0}^{z}=-\frac{1}{\mu}\int_{z_0}^{z}\sigma_t(v)\mathrm{d}v, \tag{10}$$

$$\ln\frac{\psi^{\mathrm{u}}(z,\mu)}{\psi^{\mathrm{u}}(z_0,\mu)}=-\frac{1}{\mu}\int_{z_0}^{z}\sigma_t(v)\mathrm{d}v, \tag{11}$$

and

$$\psi^{\mathrm{u}}(z,\mu)=\psi^{\mathrm{u}}(z_0,\mu)\exp\left(-\frac{1}{\mu}\int_{z_0}^{z}\sigma_t(v)\mathrm{d}v\right),\quad z\in\Omega,\quad \mu>0. \tag{12}$$

We make use of the left singular boundary conditions (5) and the uncollided transport problem (4) and (5) has the closed form solution

$$\begin{cases} \psi^{\mathrm{u}}(z,\mu) = \psi_0 \delta(\mu-\mu_0)\exp\left(-\dfrac{1}{\mu}\displaystyle\int_{z_0}^{z}\sigma_t(v)\mathrm{d}v\right), \quad z\in\Omega, \mu>0, \quad \mu_0>0, \\ \psi^{\mathrm{u}}(z,\mu) = 0, \quad z\in\Omega, \quad \mu<0. \end{cases} \tag{13}$$

At this point, we may substitute the closed form solution (13) into the anisotropic source (8) to completely define the diffusive transport problem (6) and (7). Let us firstly calculate the space-dependent anisotropic source (8). We substitute solution (13) into the source (8) and we successively obtain

$$\begin{aligned} s^{\mathrm{u}}(z,\mu) &= \frac{\sigma_0(z)}{2}\sum_{\ell=0}^{\infty}(2\ell+1)\beta_\ell(z)P_\ell(\mu)\int_{-1}^{1}\mathrm{d}\mu' P_\ell(\mu')\psi^{\mathrm{u}}(z,\mu') \\ &= \frac{\sigma_0(z)}{2}\sum_{\ell=0}^{\infty}(2\ell+1)\beta_\ell(z)P_\ell(\mu)\int_{0}^{1}\mathrm{d}\mu'\left[P_\ell(\mu')\psi_0\delta(\mu'-\mu_0)\exp\left(-\frac{1}{\mu'}\int_{z_0}^{z}\sigma_t(v)\mathrm{d}v\right)\right] \\ &= \frac{\sigma_0(z)}{2}\sum_{\ell=0}^{\infty}(2\ell+1)\beta_\ell(z)P_\ell(\mu)P_\ell(\mu_0)\psi_0\exp\left(-\frac{1}{\mu_0}\int_{z_0}^{z}\sigma_t(v)\mathrm{d}v\right) \\ &= \psi_0\exp\left(-\frac{1}{\mu_0}\int_{z_0}^{z}\sigma_t(v)\mathrm{d}v\right)\frac{\sigma_0(z)}{2}\sum_{\ell=0}^{\infty}(2\ell+1)\beta_\ell(z)P_\ell(\mu)P_\ell(\mu_0). \end{aligned} \tag{14}$$

*2.3.2. The diffusive problem*

We now perform an analysis of the diffusive transport problem (6) and (7). We decompose the multislab domain $\Omega$ into $R$ contiguous and disjoint uniform subdomains (layers) and we define the local diffusive transport problems

$$\begin{aligned} \mu\frac{\partial}{\partial z}\psi_r^{\mathrm{d}}(z,\mu)+\sigma_{t,r}\psi_r^{\mathrm{d}}(z,\mu) &= \frac{\sigma_{0,r}}{2}\sum_{\ell=0}^{\infty}(2\ell+1)\beta_{\ell,r}P_\ell(\mu)\int_{-1}^{1}\mathrm{d}\mu' P_\ell(\mu')\psi_r^{\mathrm{d}}(z,\mu') \\ &\quad + s_r^{\mathrm{u}}(z,\mu), \quad z_{r-1}\leqslant z\leqslant z_r, \quad -1\leqslant\mu\leqslant 1, \quad r=1:R, \end{aligned} \tag{15}$$

with $\psi_1^{\mathrm{d}}(z_0,\mu)=\gamma_0(\mu)$; $\psi_{\mathrm{R}}^{\mathrm{d}}(z_{\mathrm{R}},-\mu)=0$, $\mu>0$, and with angular flux continuity conditions at layer interfaces, i.e.

$$\psi_j^{\mathrm{d}}(z_j,\mu)=\psi_{j+1}^{\mathrm{d}}(z_j,\mu), \quad -1\leqslant\mu\leqslant 1, \quad \mu\neq 0, \quad j=1:R-1, \tag{16}$$

where $z_j$, $j=1{:}\ R-1$, is to denote the $j$th layer interface. We remark that if $R$ is equal to 1, then the multislab domain $\Omega$ consists of one single layer. We note further that material parameters are constant within each layer, i.e. $\sigma_t(z)=\sigma_{t,r}$ and $\sigma_0(z)=\sigma_{0,r}$, $z_{r-1}\leqslant z\leqslant z_r$, for $r=1:R$, and that the space-dependent anisotropic source $s_r^{\mathrm{u}}(z,\mu)$ that appears in Eq. (15) can be expressed as

$$s_r^{\mathrm{u}}(z,\mu)=\psi_0\exp\left(-\frac{1}{\mu_0}\int_{z_0}^{z}\sigma_t(v)\mathrm{d}v\right)\frac{\sigma_{0,r}}{2}\sum_{\ell=0}^{\infty}(2\ell+1)\beta_{\ell,r}P_\ell(\mu_0)P_\ell(\mu). \tag{17}$$

Result (17) can be reformulated further and written in the form

$$s_r^{\mathrm{u}}(z,\mu) = s_r^0(\mu)\exp\left(-\frac{\sigma_{t,r}z}{\mu_0}\right), \quad -1 \leqslant \mu \leqslant 1, \quad z_{r-1} \leqslant z \leqslant z_r, \quad r = 1:R, \tag{18}$$

where

$$s_r^0(\mu) \equiv \left(\frac{\sigma_{0,r}}{2}\sum_{\ell=0}^{\infty}(2\ell+1)\beta_{\ell,r}P_\ell(\mu_0)P_\ell(\mu)\right)\psi_0\exp\left(-\frac{k_{r-1}}{\mu_0}\right), \tag{19}$$

$$k_{r-1} \equiv \Lambda_{r-1} - \sigma_{t,r}z_{r-1}, \tag{20}$$

and

$$\Lambda_{r-1} \equiv \int_{z_0}^{z_{r-1}}\sigma_t(v)\mathrm{d}v = \sum_{r'=1}^{r-1}\sigma_{t,r'}\Delta z_{r'}, \tag{21}$$

with $\Delta z_{r'} \equiv z_{r'} - z_{r'-1}$, $r' = 1:R$, and $\Lambda_0 = 0$.

We follow our analysis by considering standard $S_N$ approximations [25] to the local diffusive Eq. (15) in the form

$$\mu_m\frac{d}{\mathrm{d}z}\psi_{r,m}^{\mathrm{d}}(z) + \sigma_{t,r}\psi_{r,m}^{\mathrm{d}}(z) = \frac{\sigma_{0,r}}{2}\sum_{\ell=0}^{L_r}(2\ell+1)\beta_{\ell,r}P_\ell(\mu_m)\sum_{n=1}^{N}\omega_n P_\ell(\mu_n)\psi_{r,n}^{\mathrm{d}}(z) + s_{r,m}^{\mathrm{u}}(z),$$
$$m = 1:N, \quad z_{r-1} \leqslant z \leqslant z_r, \quad r = 1:R, \tag{22}$$

where $\psi_{r,m}^{\mathrm{d}}(z) \cong \psi_r^{\mathrm{d}}(z,\mu_m)$, $s_{r,m}^{\mathrm{u}}(z) \cong s_r^{\mathrm{u}}(z,\mu_m)$ and $\{\mu_m\}$, $m = 1:N$, is a finite set of angular directions on the interval $[-1,1]$. We remark that the nonnegative integers $L_r$ in Eq. (22), $r = 1:R$, indicate that the Legendre expansions of the scattering phase functions in corresponding layers have been truncated after $(L_r+1)$ terms. We note further that continuity conditions hold at layer interfaces and that we use here the standard discrete boundary conditions [25]

$$\psi_{1,m}^{\mathrm{d}}(z_0) = \gamma_0(\mu_m); \quad \psi_{\mathrm{R},-m}^{\mathrm{d}}(z_{\mathrm{R}}) = 0, \quad \mu_m > 0, \tag{23}$$

where the subscript $-m$ is to denote the angular direction $-\mu_m$.

Solution to the system of $S_N$ Eq. (22) can be expressed in terms of nontrivial elementary solutions to the homogeneous version of Eq. (22) and particular solutions in the open form [2,10,33]

$$\psi_{r,m}^{\mathrm{d}}(z) = \sum_{i=1}^{N}\alpha_{r,i}\psi_{r,m}^{\mathrm{d}}(z,\nu_{r,i}) + \psi_{r,m,p}^{\mathrm{d}}(z), \quad z_{r-1} \leqslant z \leqslant z_r, \quad m = 1:N, \quad r = 1:R, \tag{24}$$

where $\alpha_{r,i}$, $r = 1:R$, $i = 1:N$, are scalars depending upon the discrete boundary conditions (23);

$$\psi_{r,m}^{\mathrm{d}}(z,\nu_{r,i}) \equiv a_{r,m}(\nu_{r,i})\exp\left(\frac{\sigma_{t,r}(z-z_{r,i})}{\nu_{r,i}}\right), \quad z_{r-1} \leqslant z \leqslant z_r, \quad i = 1:N, \quad m = 1:N, \quad r = 1:R, \tag{25}$$

are elementary (exponential) solutions to the homogeneous version of the $S_N$ Eq. (22), with $z_{r,i}$, $i = 1:N$, being appropriate positions on the layer r; $\nu_{r,i}$ and $a_{r,m}(\nu_{r,i})$, $r = 1:R$, $i = 1:N$, $m = 1$ :N, are the separation constants and the angular components [10,33] of the elementary solutions (25), respectively;

$$\psi_{r,m,p}^{\mathrm{d}}(z) = f_{r,m}\exp\left(-\frac{\sigma_{t,r}z}{\mu_0}\right), \quad z_{r-1} \leqslant z \leqslant z_r, \quad m = 1:N, \quad r = 1:R, \tag{26}$$

are the particular solutions used by Chandrasekhar to express the general solution to the classical albedo problem in atmospheric radiative transfer [5] and $f_{r,m}$, $r = 1 : R$, $m = 1 : N$, are constants to be determined upon substitution of the particular solution (26) into Eq. (22). As noted by Siewert in a recent work [33], the particular solution (26) is not valid in the (unlikely) event that $\mu_0$ be equal to one of the separation constants $\nu_{r,i}$, $i = 1 : N$. So, we are assuming here that $\mu_0$ does not match any $_{r,i}$ for all $i$ and $r$. We assume further that the separation constants are bounded, i.e. there exists a positive real number K such that $|\nu_{r,i}| < K$ for all $r$ and $i$. Accordingly, the special conservative problem of radiative transfer [5,33] will not be considered in this article.

The separation constants and the angular components of the elementary solutions (25) can be generated with a method reported by the present author [10], from which we quote the main results. Upon substitution of the elementary solutions (25) into the homogeneous version of the $S_N$ Eq. (22), and after some operations, we obtain

$$\frac{\mu_m}{\nu_{r,i}} a_{r,m}(\nu_{r,i}) + a_{r,m}(\nu_{r,i}) = \sum_{\ell=0}^{L_r} \frac{(2\ell+1)}{2} c_{\ell,r} P_\ell(\mu_m) \sum_{n=1}^{N} \omega_n P_\ell(\mu_n) a_{r,n}(\nu_{r,i}),$$
$$m = 1 : N, \quad i = 1 : N, \quad r = 1 : R, \tag{27}$$

where $c_{\ell,r} \equiv (\sigma_{0,r}\beta_{\ell,r})/\sigma_{t,r}$, $r = 1 : R$, $\ell = 0 : L_r$. Since the $\ell$-dependent N-term finite series on the right hand side of Eq. (27) is just the Chandrasekhar polynomial $g^0_{r,\ell}(\nu)$ [5,33] evaluated at $\nu_{r,i}$, it is not difficult to draw from a parity analysis of Eq. (27) that the constants $\nu_{r,i}$ appear in pairs of $\pm$ numbers and that the angular components satisfy the relation $a_{r,m}(\nu_{r,i}) = a_{r,-m}(-\nu_{r,i})$, for all $r$, $m$ and $i$. The former conclusion will be helpful throughout the article whilst the later one will be brought to further discussion in the final section of this article. Further reformulation leads us to the $R$ algebraic eigenvalue problems

$$\sum_{n=1}^{N} \frac{1}{\mu_m} \left\{ -\delta_{mn} + \left[ \sum_{\ell=0}^{L_r} \frac{(2\ell+1)}{2} c_{\ell,r} P_\ell(\mu_m) P_\ell(\mu_n) \right] \omega_n \right\} a_{r,n}(\nu_{r,i}) = \frac{1}{\nu_{r,i}} a_{r,m}(\nu_{r,i}),$$
$$m = 1 : N, \quad i = 1 : N, \quad r = 1 : R, \tag{28}$$

where $\delta_{mn}$ is the Kronecker delta. In compact notation, we may write

$$\underline{\underline{A}}_r \, \vec{a}_r(\nu_{r,i}) = \frac{1}{\nu_{r,i}} \vec{a}_r(\nu_{r,i}), \quad r = 1 : R, \tag{29}$$

where $\underline{\underline{A}}_r$ with entries

$$A^r_{m,n} \equiv \frac{1}{\mu_m} \left\{ -\delta_{mn} + \left[ \sum_{\ell=0}^{L_r} \frac{(2\ell+1)}{2} c_{\ell,r} P_\ell(\mu_m) P_\ell(\mu_n) \right] \omega_n \right\}, \quad m = 1 : N, \quad n = 1 : N, \quad r = 1 : R, \tag{30}$$

is a real square matrix whose eigenvalues $(\nu_{r,i})^{-1}$, $i = 1 : N$, are the reciprocals of the separation constants $\nu_{r,i}$ and whose corresponding eigenvectors

$$\vec{a}_r(\nu_{r,i}) \equiv [a_{r,1}(\nu_{r,i}), a_{r,2}(\nu_{r,i}), \ldots, a_{r,N}(\nu_{r,i})]^{\mathrm{T}}, \quad i = 1 : N, \tag{31}$$

are ordered sets of angular components of the elementary solutions (25) in the subdomain (layer) $r$. Solution to the eigenvalue problems (29) can be achieved by means of modern mathematical software systems such as MAPLE [21] or even with conventional matrix eigensystem packages such as LINPACK and EISPACK [14,34]. Once the algebraic eigenvalue problems (29) are solved, the elementary solutions (25) become readily available. In this article, we assume that the separation constants $\nu_{r,i}$ are distinct pairs of $\pm$ real numbers and so, $\{\vec{a}_r(\nu_{r,i})\}$, $i = 1 : N$, constitute a full ($N$) set of eigenvectors [31].

The constants $f_{r,m}$, $m = 1 : N$, in the particular solution (26) can be efficiently computed with the help of the parity relation $P_\ell(-\mu_m) = (-1)^\ell P_\ell(\mu_m)$ for the Legendre polynomials and through a not-so-straightforward use of matrix algebra for splitting and handling the matrix equation resulting from the substitution of the particular solution (26) into the $S_N$ Eq. (22). A description of these algebraic steps can be found in a recent work by Siewert [33]. For the sake of continuity of presentation, we extract from [33] the main results and we quote them here. For fixed $r$, the constants $f_{r,m}$ in the particular solution (26) are the entries of the $(N/2)$-dimensional column matrices

$$\vec{f}_r^{\,+} = -\frac{1}{2}\mu_0 \underline{\underline{M}}^{-1}\left[\left(\underline{\underline{I}} - \mu_0^2 \underline{\underline{F}}_r \underline{\underline{E}}_r\right)^{-1}\left(\vec{d}_r + \mu_0 \underline{\underline{F}}_r \vec{c}_r\right) + \left(\underline{\underline{I}} - \mu_0^2 \underline{\underline{E}}_r \underline{\underline{F}}_r\right)^{-1}\left(\vec{c}_r + \mu_0 \underline{\underline{E}}_r \vec{d}_r\right)\right] \tag{32}$$

and

$$\vec{f}_r^{\,-} = -\frac{1}{2}\mu_0 \underline{\underline{M}}^{-1}\left[\left(\underline{\underline{I}} - \mu_0^2 \underline{\underline{F}}_r \underline{\underline{E}}_r\right)^{-1}\left(\vec{d}_r + \mu_0 \underline{\underline{F}}_r \vec{c}_r\right) - \left(\underline{\underline{I}} - \mu_0^2 \underline{\underline{E}}_r \underline{\underline{F}}_r\right)^{-1}\left(\vec{c}_r + \mu_0 \underline{\underline{E}}_r \vec{d}_r\right)\right], \tag{33}$$

where

$$\vec{f}_r^{\,+} \equiv \left[f_{r,1}; \cdots; f_{r,N/2}\right]^{\mathrm{T}} \tag{34}$$

and

$$\vec{f}_r^{\,-} \equiv \left[f_{r,N/2+1}; \cdots; f_{r,N}\right]^{\mathrm{T}}. \tag{35}$$

The quantities $\underline{\underline{E}}_r \equiv [\underline{\underline{I}} - (\underline{\underline{T}}_r^+ + \underline{\underline{T}}_r^-)]\underline{\underline{M}}^{-1}$ and $\underline{\underline{F}}_r \equiv [\underline{\underline{I}} - (\underline{\underline{T}}_r^+ - \underline{\underline{T}}_r^-)]\underline{\underline{M}}^{-1}$ are $(N/2)$-dimensional real square matrices. The symbol $\underline{\underline{I}}$ is to denote the $(N/2)$-dimensional identity matrix and the symbol $\underline{\underline{M}}$ is to denote the $(N/2)$-dimensional diagonal matrix whose entries are $M_{ii} = \mu_i$, $i = 1 : N/2$. The quantities $\underline{\underline{T}}_r^+$ and $\underline{\underline{T}}_r^-$ denote $(N/2)$-dimensional real square matrices with entries

$$T^+_{r,m,n} = \omega_n \left[\sum_{\ell=0}^{L_r} \frac{(2\ell+1)}{2} c_{\ell,r} P_\ell(\mu_m) P_\ell(\mu_n)\right], \quad m = 1 : N/2, \quad n = 1 : N/2, \tag{36}$$

and

$$T^-_{r,m,n} = \omega_n \left[\sum_{\ell=0}^{L_r} \frac{(2\ell+1)}{2} c_{\ell,r} (-1)^\ell P_\ell(\mu_m) P_\ell(\mu_n)\right], \quad m = 1 : N/2, \quad n = 1 : N/2, \tag{37}$$

respectively. The quantities $\vec{c}_r$ and $\vec{d}_r$ are $(N/2)$-dimensional column matrices given by

$$\left[h^0_{r,1} + h^0_{r,N/2+1}; h^0_{r,2} + h^0_{r,N/2+2}; \cdots; h^0_{r,N/2} + h^0_{r,N}\right]^{\mathrm{T}} \tag{38}$$

and

$$\left[h^0_{r,1} - h^0_{r,N/2+1}; h^0_{r,2} - h^0_{r,N/2+2}; \cdots; h^0_{r,N/2} - h^0_{r,N}\right]^{\mathrm{T}}, \tag{39}$$

respectively, with $h^0_{r,m} \equiv s^0_{r,m}/\sigma_{t,r}$ and $s^0_{r,m} \cong s^0_r(\mu_m)$, $m = 1 : N$, viz definition (19). We may run over all $r$, using results (32) through (39) to determine the constants $f_{r,m}$ in the particular solution (26) for every layer and, at this point, the open form solution (24) to the $S_N$ local Eq. (22) in every layer of the multislab domain is complete.

We now proceed to Section 3, where we describe a computational method to yield an approximate solution to the target problem (1–3).

## 3. A computational method for approximately solving the target problem

### 3.1. Basic relations

The computational method that we describe in this section is to provide an approximation to the solution $\psi(z,\mu) = \psi^{\mathrm{u}}(z,\mu) + \psi^{\mathrm{d}}(z,\mu)$ of the target problem (1–3). The approximate solution we seek is a distribution on $z$ and $\mu$ of the form

$$\psi_N(z,\mu) = \psi^{\mathrm{u}}(z,\mu) + \psi^{\mathrm{d}}_{N-1}(z,\mu), \quad z_0 \leqslant z \leqslant z_{\mathrm{R}}, \quad -1 \leqslant \mu \leqslant 1, \tag{40}$$

where $\psi^{\mathrm{u}}(z,\mu)$ means that we have directly incorporated the closed form (13) into our approximate solution (40) and $\psi^{\mathrm{d}}_{N-1}(z,\mu)$, the diffuse component of our approximate solution (40), is the well-known spherical harmonics ($P_{N-1}$) approximation [15,25] to the solution of the local diffusive Eq. (15) given by

$$\psi^{\mathrm{d}}_{N-1}(z,\mu) = \sum_{\ell=0}^{N-1} \frac{(2\ell+1)}{2} \phi^{\mathrm{d}}_{r,\ell}(z) P_\ell(\mu), \quad -1 \leqslant \mu \leqslant 1, \quad z_{r-1} \leqslant z \leqslant z_r, \quad r = 1:R, \tag{41}$$

where $\psi^{\mathrm{d}}_{N-1}(z,\mu_m) = \psi^{\mathrm{d}}_{r,m}(z)$, $m = 1:N$, $z_{r-1} \leqslant z \leqslant z_r$, $r = 1:R$. The quantities $\phi^{\mathrm{d}}_{r,\ell}(z)$, $\ell = 0:N-1$, are the $P_{N-1}$ angular moments

$$\phi^{\mathrm{d}}_{r,\ell}(z) = \sum_{t=1}^{N} \omega_t P_\ell(\mu_t) \psi^{\mathrm{d}}_{r,t}(z), \quad z_{r-1} \leqslant z \leqslant z_r, \quad r = 1:R, \tag{42}$$

and $\psi^{\mathrm{d}}_{r,t}(z)$ is given by the open form solution (24). Results (41) and (42) can be shown to come up from two equivalent formulations of the local diffusive problem (15) – the $S_N$ formulation (22) with the discrete boundary conditions (23) and the classical $P_{N-1}$ formulation with corresponding boundary conditions due to Mark [15,25]. We remark that the diffuse component (41) of our approximate solution (40) is continuous in the $z$ and $\mu$ variables. Results (40)–(42) are the basis for the method described in this section.

### 3.2. Computational method

Having in mind that the quantities of interest in a radiation transport problem may be problem-dependent [38], we have thought of a computational method having a numerical component and an analytical component. The numerical component is to provide layer-average

$$\overline{\psi}^{\mathrm{d}}_{r,m} \equiv \frac{1}{\Delta z_r} \int_{z_{r-1}}^{z_r} \mathrm{d}z \psi^{\mathrm{d}}_{r,m}(z), \quad m = 1:N, \quad r = 1:R, \tag{43}$$

and layer-edge values for $\psi^{\mathrm{d}}_{r,m}(z)$ without having to determine the scalars $\alpha_{r,i}$, $r = 1:R$, $i = 1:N$, in the open form solution (24). The numerical component is thus suited to problems where the quantities of interest are, for example, the angular distribution of particles leaving the multislab domain and layer averages such as scalar fluxes. For the angular distribution of leaving particles, we can make direct use of expressions (42) through (40) at $z = z_0$ for $\mu < 0$ and at $z = z_{\mathrm{R}}$ for $\mu > 0$. For layer-average scalar fluxes, the zeroth-order ($\ell = 0$) angular moments (42) and the layer averages (43) can be brought together to yield the diffuse contribution to the scalar flux

$$\overline{\phi}^{\mathrm{d}}_{r,0} = \sum_{t=1}^{N} \omega_t \overline{\psi}^{\mathrm{d}}_{r,t}, \quad r = 1:R. \tag{44}$$

It is not difficult to show that the uncollided contribution to the layer-average scalar flux is

$$\overline{\phi}^{\mathrm{u}}_{r,0} \equiv \frac{1}{\Delta z_r}\int_{z_{r-1}}^{z_r}\mathrm{d}z\int_{-1}^{1}\mathrm{d}\mu\psi^{\mathrm{u}}(z,\mu)$$
$$= \frac{\mu_0}{\sigma_{t,r}\Delta z_r}\psi_0\exp\left(-\frac{k_{r-1}}{\mu_0}\right)\left[\exp\left(-\frac{\sigma_{t,r}z_{r-1}}{\mu_0}\right)-\exp\left(-\frac{\sigma_{t,r}z_r}{\mu_0}\right)\right], \tag{45}$$

and so, our approximation to layer-average scalar fluxes might be $\overline{\phi}_{r,0} = \overline{\phi}^{\mathrm{u}}_{r,0} + \overline{\phi}^{\mathrm{d}}_{r,0}$, $r = 1:R$. The analytical component of our method is to close up the open form solution (24) by solving a system of linear algebraic equations whose unknowns are the scalars $\alpha_{r,i}$. Inputs to the system are layer-edge values for $\psi^{\mathrm{d}}_{r,m}(z)$ supplied by the numerical component. The analytical component is to be applied when the angular distribution of particles $\psi_N(z,\mu)$ at any position $z$ is sought, for then we can make direct use of results (24)–(26) and (42) through (40). For radiative transfer problems, the partial radiative heat fluxes [5,35]

$$q^{\pm}_N(z) = 2\pi\int_0^1\mu\psi_N(z,\pm\mu)\mathrm{d}\mu = 2\pi\left[\int_0^1\mu\psi^{\mathrm{u}}(z,\pm\mu)\mathrm{d}\mu + \int_0^1\mu\psi^{\mathrm{d}}_{N-1}(z,\pm\mu)\mathrm{d}\mu\right]$$
$$= 2\pi\left\{H^{\pm}_0\int_0^1\mu\psi_0\delta(\mu-\mu_0)\exp\left[-\frac{1}{\mu}\int_{z_0}^{z}\sigma_t(v)\mathrm{d}v\right]\mathrm{d}\mu + \sum_{\ell=0}^{N-1}\frac{(2\ell+1)}{2}\phi^{\mathrm{d}}_{r,\ell}(z)(\pm 1)^{\ell}\int_0^1\mu P_\ell(\mu)\mathrm{d}\mu\right\}$$
$$= 2\pi\left\{H^{\pm}_0\mu_0\psi_0\exp\left[-\frac{(k_{r-1}+\sigma_{t,r}z)}{\mu_0}\right] + \sum_{\ell=0}^{N-1}\frac{(2\ell+1)}{2}\phi^{\mathrm{d}}_{r,\ell}(z)\frac{(\pm 1)^{\ell}}{2}\sum_{m=1}^{N}\omega_m\frac{(\mu_m+1)}{2}P_\ell\left(\frac{\mu_m+1}{2}\right)\right\}, \tag{46}$$

where $H^{\pm}_0$ is the unit step function ($H^{+}_0 = 1$ and $H^{-}_0 = 0$), as well as the net radiative heat flux

$$q_N(z) = q^{+}_N(z) - q^{-}_N(z), \tag{47}$$

can be determined at any $z$ on a layer $r$ with results (24)–(26) and (42). We describe next either component of our computational method.

### 3.2.1. The numerical component

The numerical component of our method is a numerical method designed for solving the $S_N$ diffusive problem (22) and (23) with no spatial truncation error. That is to say, the numerical solution of the $S_N$ diffusive problem (22) and (23) generated by our numerical method agrees to the analytical solution of the same problem on corresponding layer-edge points, apart from computational finite arithmetic considerations [6] and regardless of layer thicknesses. Our numerical method is an extension to anisotropic scattering of arbitrary order and space-dependent anisotropic sources of the former spectral Green's function (SGF) method developed some years ago [2]. For this reason, we hereafter refer to our numerical method as the extended spectral Green's function (ESGF) method.

The ESGF method has two main ingredients: one is standard and the other is nonstandard. The standard ingredient is the derivation of zeroth-order spatial balance equations defined on each layer of the multislab domain $\Omega$. So, if we integrate the $S_N$ diffusive Eq. (22) for fixed $r$ over the interval $(z_{r-1}, z_r)$, divide the resulting equations by $\Delta z_r$ and let $r$ vary from 1 to $R$, then we get the spatial balance equations

$$\frac{\mu_m}{\Delta z_r}(\psi^{\mathrm{d}}_{r,m} - \psi^{\mathrm{d}}_{r-1,m}) + \sigma_{t,r}\overline{\psi}^{\mathrm{d}}_{r,m}$$
$$= \frac{\sigma_{0,r}}{2}\sum_{\ell=0}^{L_r}(2\ell+1)\beta_{\ell,r}P_\ell(\mu_m)\sum_{n=1}^{N}\omega_n P_\ell(\mu_n)\overline{\psi}^{\mathrm{d}}_{r,n} + \overline{s}^{\mathrm{u}}_{r,m}, \quad r = 1:R, \quad m = 1:N, \tag{48}$$

where $\psi^{\mathrm{d}}_{j,m} \equiv \psi^{\mathrm{d}}_{r,m}(z_j)$, $j = r-1:r$, $r = 1:R$, are layer-edge angular fluxes,

$$\overline{s}^{\mathrm{u}}_{r,m} \equiv \frac{1}{\Delta z_r}\int_{z_{r-1}}^{z_r} \mathrm{d}z s^{\mathrm{u}}_{r,m}(z) = s^0_{r,m}\frac{\mu_0}{\sigma_{t,r}\Delta z_r}\left[\exp\left(-\frac{\sigma_{t,r}z_{r-1}}{\mu_0}\right) - \exp\left(-\frac{\sigma_{t,r}z_r}{\mu_0}\right)\right], \tag{49}$$

and $\overline{\psi}^{\mathrm{d}}_{r,m}$, $r = 1:R$, $m = 1:N$, is given by definition (43). We remark that the notation used in the spatial balance Eq. (48) is well suited for indicating our assumption of angular flux continuity at layer interfaces. The standard zeroth-order spatial balance Eq. (48) together with the discrete boundary conditions (23) form a system of linear algebraic equations whose unknowns are layer-average and layer-edge angular fluxes. Such a system does not have a unique solution because there are more unknowns than equations. A simple count gives us $N(R+1)$ layer-edge angular fluxes, $NR$ layer-average angular fluxes, $NR$ balance equations and $N$ boundary equations. The net score is $N(2R+1)$ unknowns against $N(R+1)$ equations. So, a total of $N(2R+1) - N(R+1) = NR$ additional equations are needed or, equivalently, $N$ additional equations per layer relating layer-edge and layer-average fluxes.

The nonstandard ingredient is to provide $NR$ equations to the system of $N(R+1)$ equations referred to in the preceding paragraph. These $NR$ additional equations are the ESGF auxiliary equations

$$\overline{\psi}^{\mathrm{d}}_{r,m} = \sum_{u=1}^{N/2}\theta_{r,m,u}\psi^{\mathrm{d}}_{r-1,u} + \sum_{u=N/2+1}^{N}\theta_{r,m,u}\psi^{\mathrm{d}}_{r,u} + g_{r,m}, \quad r = 1:R, \quad m = 1:N, \tag{50}$$

where the layer-dependent coefficients $\theta_{r,m,u}$ and $g_{r,m}$ are determined so that the analytical solution (24) be preserved by the ESGF auxiliary Eq. (50), for arbitrary scalars $\alpha_{r,i}$ and for $\psi^{\mathrm{d}}_{r,m,p}(z)$ given by the particular solution (26). Let us firstly calculate the layer-average angular fluxes in terms of the analytical results (24)–(26). If we substitute results (24)–(26) into definition (43), then we obtain, after some Calculus,

$$\begin{aligned}\overline{\psi}^{\mathrm{d}}_{r,m} = {} & \sum_{i=1}^{N}\alpha_{r,i}a_{r,m}(v_{r,i})\frac{v_{r,i}}{\sigma_{t,r}\Delta z_r}\left[\exp\left(\frac{\sigma_{t,r}(z_r - z_{r,i})}{v_{r,i}}\right) - \exp\left(\frac{\sigma_{t,r}(z_{r-1} - z_{r,i})}{v_{r,i}}\right)\right] \\ & + \frac{\mu_0 f_{r,m}}{\sigma_{t,r}\Delta z_r}\left[\exp\left(-\frac{\sigma_{t,r}z_{r-1}}{\mu_0}\right) - \exp\left(-\frac{\sigma_{t,r}z_r}{\mu_0}\right)\right], \quad r = 1:R, \quad m = 1:N.\end{aligned} \tag{51}$$

Since the ESGF auxiliary Eq. (50) are to preserve the analytical solution (24) for arbitrary scalars $\alpha_{r,i}$ and for $\psi^{\mathrm{d}}_{r,m,p}(z)$ given by (26), we substitute results (51) and (24)–(26) evaluated at $z_{r-1}$ or $z_r$, where appropriate, into the ESGF auxiliary Eq. (50) for fixed $r$ to obtain

$$\begin{aligned}& \sum_{i=1}^{N}\alpha_{r,i}a_{r,m}(v_{r,i})\frac{v_{r,i}}{\sigma_{t,r}\Delta z_r}\left[\exp\left(\frac{\sigma_{t,r}(z_r - z_{r,i})}{v_{r,i}}\right) - \exp\left(\frac{\sigma_{t,r}(z_{r-1} - z_{r,i})}{v_{r,i}}\right)\right] \\ & \quad + \frac{\mu_0 f_{r,m}}{\sigma_{t,r}\Delta z_r}\left[\exp\left(-\frac{\sigma_{t,r}z_{r-1}}{\mu_0}\right) - \exp\left(-\frac{\sigma_{t,r}z_r}{\mu_0}\right)\right] \\ & \quad = \sum_{u=1}^{N/2}\theta_{r,m,u}\left[\sum_{i=1}^{N}\alpha_{r,i}a_{r,u}(v_{r,i})\exp\left(\frac{\sigma_{t,r}(z_{r-1} - z_{r,i})}{v_{r,i}}\right) + f_{r,u}\exp\left(-\frac{\sigma_{t,r}z_{r-1}}{\mu_0}\right)\right] \\ & \quad + \sum_{u=N/2+1}^{N}\theta_{r,m,u}\left[\sum_{i=1}^{N}\alpha_{r,i}a_{r,u}(v_{r,i})\exp\left(\frac{\sigma_{t,r}(z_r - z_{r,i})}{v_{r,i}}\right) + f_{r,u}\exp\left(-\frac{\sigma_{t,r}z_r}{\mu_0}\right)\right] + g_{r,m},\end{aligned} \tag{52}$$

for $m = 1:N$. Since Eq. (52) hold for arbitrary scalars $\alpha_{r,i}$, they must hold for $\alpha_{r,i}$ set equal to zero for all $i$ from 1 to $N$. Therefore, we must have

$$g_{r,m} = \frac{\mu_0 f_{r,m}}{\sigma_{t,r}\Delta z_r}\left[\exp\left(-\frac{\sigma_{t,r}z_{r-1}}{\mu_0}\right) - \exp\left(-\frac{\sigma_{t,r}z_r}{\mu_0}\right)\right] - \left[\exp\left(-\frac{\sigma_{t,r}z_{r-1}}{\mu_0}\right)\sum_{u=1}^{N/2}\theta_{r,m,u}f_{r,u} + \exp\left(-\frac{\sigma_{t,r}z_r}{\mu_0}\right)\sum_{u=N/2+1}^{N}\theta_{r,m,u}f_{r,u}\right], \quad m = 1:N. \tag{53}$$

We substitute result (53) into Eq. (52), we simplify terms and we arrive at

$$\sum_{i=1}^{N}\alpha_{r,i}a_{r,m}(v_{r,i})\frac{v_{r,i}}{\sigma_{t,r}\Delta z_r}\left[\exp\left(\frac{\sigma_{t,r}(z_r - z_{r,i})}{v_{r,i}}\right) - \exp\left(\frac{\sigma_{t,r}(z_{r-1} - z_{r,i})}{v_{r,i}}\right)\right] = \sum_{i=1}^{N}\alpha_{r,i}\left[\exp\left(\frac{\sigma_{t,r}(z_{r-1} - z_{r,i})}{v_{r,i}}\right)\sum_{u=1}^{N/2}\theta_{r,m,u}a_{r,u}(v_{r,i}) + \exp\left(\frac{\sigma_{t,r}(z_r - z_{r,i})}{v_{r,i}}\right)\sum_{u=N/2+1}^{N}\theta_{r,m,u}a_{r,u}(v_{r,i})\right], \tag{54}$$

for $m = 1:N$. Since Eq. (54) hold for arbitrary scalars $\alpha_{r,i}$, they must hold for the $N$ ordered sets of scalars $(\delta_{1j}, \delta_{2j}, \delta_{3j}, \ldots, \delta_{Nj})$, $j = 1:N$. These ordered sets of scalars yield, for fixed m, the system of $N$ linear algebraic equations

$$\frac{v_{r,j}a_{r,m}(v_{r,j})}{\sigma_{t,r}\Delta z_r}\left[\exp\left(\frac{\sigma_{t,r}(z_r - z_{r,j})}{v_{r,j}}\right) - \exp\left(\frac{\sigma_{t,r}(z_{r-1} - z_{r,j})}{v_{r,j}}\right)\right] = \exp\left(\frac{\sigma_{t,r}(z_{r-1} - z_{r,j})}{v_{r,j}}\right)\sum_{u=1}^{N/2}\theta_{r,m,u}a_{r,u}(v_{r,j}) + \exp\left(\frac{\sigma_{t,r}(z_r - z_{r,j})}{v_{r,j}}\right)\sum_{u=N/2+1}^{N}\theta_{r,m,u}a_{r,u}(v_{r,j}), \quad j = 1:N, \tag{55}$$

in the $N$ unknowns $\theta_{r,m,u}$, $u = 1:N$.

We now choose appropriate positions $z_{r,j}$, $j = 1:N$. Once we have assumed that the layer-dependent separation constants are pairs of $\pm$ real numbers, we set $z_{r,j} = z_r$ for $v_{r,j} > 0$ and $z_{r,j} = z_{r-1}$ for $v_{r,j} < 0$. With this choice, the arguments of the exponentials in Eq. (55) are nonpositive real numbers. This makes all exponential evaluations lie within the interval (0,1] and precludes possible computer overflow exceptions when solving the system (55) on a digital computer. With our choice, Eq. (55) may be written with respect to the sign of the separation constants as

$$\frac{v_{r,j}a_{r,m}(v_{r,j})}{\sigma_{t,r}\Delta z_r}\left[1 - \exp\left(-\frac{\sigma_{t,r}\Delta z_r}{v_{r,j}}\right)\right] = \exp\left(-\frac{\sigma_{t,r}\Delta z_r}{v_{r,j}}\right)\sum_{u=1}^{N/2}\theta_{r,m,u}a_{r,u}(v_{r,j}) + \sum_{u=N/2+1}^{N}\theta_{r,m,u}a_{r,u}(v_{r,j}), \quad v_{r,j} > 0, \tag{56}$$

and

$$\frac{|v_{r,j}|a_{r,m}(v_{r,j})}{\sigma_{t,r}\Delta z_r}\left[1 - \exp\left(-\frac{\sigma_{t,r}\Delta z_r}{|v_{r,j}|}\right)\right] = \sum_{u=1}^{N/2}\theta_{r,m,u}a_{r,u}(v_{r,j}) + \exp\left(-\frac{\sigma_{t,r}\Delta z_r}{|v_{r,j}|}\right)\sum_{u=N/2+1}^{N}\theta_{r,m,u}a_{r,u}(v_{r,j}), \quad v_{r,j} < 0. \tag{57}$$

With $r$ fixed in Eqs. (56) and (57), we may run over all $m$ and, for each $m$, we obtain a corresponding system of $N$ linear algebraic equations in the $N$ unknowns $\theta_{r,m,u}$, $u = 1 : N$. With the coefficients $\theta_{r,m,u}$, $m = 1 : N$, $u = 1 : N$, determined, we may go back to expression (53) to calculate the coefficients $g_{r,m}$, $m = 1 : N$. We run over all $r$, calculating the layer-dependent coefficients $\theta_{r,m,u}$ and $g_{r,m}$ and completely defining the ESGF auxiliary Eq. (50). Eqs. (48) and (50) and the boundary Eq. (23) constitute the ESGF equations of the $S_N$ diffusive problem (22) and (23). For the numerical solution of the ESGF equations, we use the one-cell block inversion (CBI) iterative scheme [2,7,9] and we determine the layer-average $\overline{\psi}^{\mathrm{d}}_{r,m}$ and the layer-edge angular fluxes $\psi^{\mathrm{d}}_{r,m}(z_{r-1})$ and $\psi^{\mathrm{d}}_{r,m}(z_r)$ for all $r$ and $m$ with no spatial truncation error.

### 3.2.2. The analytical component

The analytical component of our method is a local reconstruction scheme of the analytical solution (24). It is based upon solving an r-local system of $N$ linear algebraic equations whose unknowns are the scalars $\alpha_{r,i}$, r fixed, $i = 1 : N$. Inputs to the system are the layer-edge angular fluxes $\psi^{\mathrm{d}}_{r,m}(z_j)$, $j = r - 1 : r$, that are incident upon the layer of interest [4,8]. Here, the layer-edge angular fluxes are those generated by the ESGF method. Since the numerical solution of the $S_N$ diffusive problem (22) and (23) generated by the ESGF method is free from spatial truncation error, the numerical values for layer-edge angular fluxes generated by the ESGF method are exactly the same as those generated by the analytical solution (24) in closed form on corresponding layer-edge points. Accordingly, the system of $N$ linear algebraic equations

$$\psi^{\mathrm{d}}_{r-1,m} = \sum_{i=1}^{N} \alpha_{r,i} a_{r,m}(\nu_{r,i}) \exp\left(\frac{\sigma_{t,r}(z_{r-1} - z_{r,i})}{\nu_{r,i}}\right) + f_{r,m} \exp\left(-\frac{\sigma_{t,r} z_{r-1}}{\mu_0}\right), \quad \mu_m > 0, \tag{58}$$

and

$$\psi^{\mathrm{d}}_{r,m} = \sum_{i=1}^{N} \alpha_{r,i} a_{r,m}(\nu_{r,i}) \exp\left(\frac{\sigma_{t,r}(z_r - z_{r,i})}{\nu_{r,i}}\right) + f_{r,m} \exp\left(-\frac{\sigma_{t,r} z_r}{\mu_0}\right), \quad \mu_m < 0, \tag{59}$$

in the $N$ unknowns $\alpha_{r,i}$, $i = 1 : N$, must hold for arbitrary $r$. With the system (58) and (59) solved and the scalars $\alpha_{r,i}$, $i = 1 : N$, determined, we can make direct use of results (24)–(26) and (42) through (40) to reconstruct the angular distribution $\psi_N(z, \mu)$ at any position $z$ on the layer of interest. We stress here that our reconstruction scheme is local in the sense that calculation of the scalars $\alpha_{r,i}$ and later reconstruction of the angular distribution $\psi_N(z, \mu)$ are confined to the layer of interest. We may reconstruct over as many layers as we wish in this layer-by-layer process. It is important to note here that if $r = 1$, then $\psi^{\mathrm{d}}_{r-1,m} = \gamma_0(\mu_m)$, $\mu_m > 0$, and that if $r = R$, then $\psi^{\mathrm{d}}_{r,m} = 0$, $\mu_m < 0$.

In the next section, we illustrate the numerical accuracy of our computational method with numerical results for basic problems in atmospheric radiative transfer and neutron beam transport.

## 4. Computational aspects and numerical results

### 4.1. Test problems and numerical results

We now illustrate the numerical accuracy of our method with three basic problems: two problems of atmospheric radiative transfer and one problem of neutron beam transport. We should notice that the numerical results reported here come from the execution of our FORTRAN [30] program on an IBM-compatible PC (1.4 GHz-clock Intel Pentium 4 processor and 256 Mb of RAM) running on GNU/Linux, version 0.2. The executable file of our program has been generated with the g77 GNU Fortran package, release 2.95. The execution (CPU) times for the three problems were 189.4, 7.5 and 53.1 s, respectively. These times were generated with the TIME GNU internal routine, option $-S$.

#### 4.1.1. Test problem 1

The first problem is a challenging test problem based on a haze $L = 82$ scattering model posed in 1977 by the Radiation Commission of the International Association of Meteorology and Atmospheric Physics [24]. The problem here is the second of the five test problems posed by the Commission. The haze is modelled by a single homogeneous plane-parallel layer with optical thickness $\Delta z_1 = 1$ and single scattering albedo $\sigma_{0,1} = 0.9$. The haze 83-term scattering phase function data have been extracted from a work of Garcia and Siewert [19]. The boundary conditions here are defined by $z_0 = 0$, $z_1 = 1$, $\psi_0 = 0.5$ in units of power per unit area per unit frequency interval per steradian, $\mu_0 = 1$ and $\gamma_0(\mu) = 0$ (no regular component) in Eq.(3). In Tables 1 and 2, we present numerical results for the diffuse component $\psi^{\mathrm{d}}_{399}(z,\mu)$ of our approximate solution $\psi_{400}(z,\mu)$ and for the radiant heat fluxes $q^{\pm}_{400}(z)$ and $q_{400}(z)$ in units of power per unit area per unit frequency interval, respectively. We are happy to notice that, except for the $\mu = 0$ boundary values, at which the intensity of the radiation field is expected to be discontinuous (and therefore the finite Legendre series (41) is not expected to work soundly), the results in Table 1 agree to within $\pm 1$ in the fourth figures with corresponding $N$-converged results generated with the facile ($F_N$) method [19]. Also, the results in Table 2 agree in all figures given to corresponding converged $F_N$ results quoted in [19].

#### 4.1.2. Test problem 2

The second problem is actually a set of three multislab radiative transfer problems all based on a six-layer model for a stratified atmosphere described in a work of Devaux et al. [13]. Each of the six layers has the same scattering law but the single scattering albedo is allowed to be different in each layer. The optical thickness $\Delta z_r$ and single scattering albedo $\sigma_{0,r}$ for each layer are provided in Table 3. The scattering law is approximated by the $L = 8$ scattering phase function data given in Table 4. The boundary data defining the problems in the set are $z_0 = 0$, $z_6 = 21$, $\psi_0 = 0$ (no singular component) and $\gamma_0(\mu) = \mu^{\mathrm{b}}$ in units of power per unit area per unit frequency interval per steradian, $\mu > 0$, where the integer $b$ specifies each problem in the set, $b = 0 : 2$.

Table 1
Numerical results for the diffuse component $\psi^{\mathrm{d}}_{399}(z,\mu)$

| $\mu$ | $z = 0$ | $z = 1/10$ | $z = 1/2$ | $z = 3/4$ | $z = 1$ |
|---|---|---|---|---|---|
| −1.0 | 0.0263486 | 0.0251844 | 0.0137540 | 0.0067054 | |
| −0.8 | 0.0313669 | 0.0286420 | 0.0160966 | 0.0078552 | |
| −0.6 | 0.0390112 | 0.0365141 | 0.0220980 | 0.0110620 | |
| −0.4 | 0.0534913 | 0.0521415 | 0.0368542 | 0.0202307 | |
| −0.2 | 0.0667894 | 0.0705000 | 0.0666970 | 0.0463003 | |
| −0.0 | 0.0341578 | 0.0680172 | 0.0939988 | 0.0974843 | |
| 0.0 | | 0.0680172 | 0.0939988 | 0.0974843 | 0.0404453 |
| 0.2 | | 0.0253403 | 0.0915927 | 0.1138156 | 0.1239562 |
| 0.4 | | 0.0190679 | 0.0883332 | 0.1225035 | 0.1482369 |
| 0.6 | | 0.0249089 | 0.1153349 | 0.1622289 | 0.2005148 |
| 0.8 | | 0.0560207 | 0.2384866 | 0.3225506 | 0.3867963 |
| 1.0 | | 0.6290471 | 2.2483366 | 2.7414049 | 2.9750950 |

Table 2
Numerical results for radiant heat fluxes

| | $z = 0$ | $z = 1/10$ | $z = 1/2$ | $z = 3/4$ | $z = 1$ |
|---|---|---|---|---|---|
| $q^{+}_{400}(z)$ | 3.141592 | 3.100743 | 2.920648 | 2.799232 | 2.671269 |
| $q^{-}_{400}(z)$ | 0.123665 | 0.117603 | 0.078869 | 0.044545 | 0.0 |
| $q_{400}(z)$ | 3.017927 | 2.983141 | 2.841779 | 2.754687 | 2.671269 |

Table 3
Optical thickness and single scattering albedo

| $r$ | $\Delta z_r$ | $\sigma_{0,r}$ |
|---|---|---|
| 1 | 1.0 | 0.65 |
| 2 | 2.0 | 0.70 |
| 3 | 3.0 | 0.75 |
| 4 | 4.0 | 0.80 |
| 5 | 5.0 | 0.85 |
| 6 | 6.0 | 0.90 |

Table 4
Scattering phase function data

| $\ell$ | $(2\ell+1)\beta_\ell$ |
|---|---|
| 0 | 1 |
| 1 | 2.00916 |
| 2 | 1.56339 |
| 3 | 0.67407 |
| 4 | 0.22215 |
| 5 | 0.04725 |
| 6 | 0.00671 |
| 7 | 0.00068 |
| 8 | 0.00005 |

In Table 5, we present numerical results for the plane albedo and transmission factors defined in [13]. We are happy to notice that our $S_{32}$ results in Table 5 for the albedo and transmission factors are in very close agreement to corresponding converged $F_N$ results extracted from the work of Devaux et al. [13]. To illustrate the numerical merit of our mathematical method in the $S_N$ framework, we also show in Table 5 corresponding $S_{32}$ results for the above quantities generated by the Oak Ridge National Laboratory one-dimensional $S_N$ computer code ANISN [16]. The ANISN results in Table 5 were generated with a fine-mesh grid defining six mesh cells per unit vertical optical length and were also extracted from the work of Devaux et al. It is noteworthy that our results for the albedo factor are as accurate as those generated by ANISN, while ANISN results for the transmission factor are less accurate than those generated by our method. This happens because the model atmosphere is optically thick ($z_6 = 21$) and ANISN uses a first-order polynomial approximation – the diamond-difference approximation [15,25] – for the optical dependence of the intensity of the radiation field in the $S_N$ Eq. (22). The effect of the optical truncation error in the intensity is more pronounced in the regions of the medium far from the boundary source (as we move from left to right), and this explains the loss of accuracy in the transmission factor results generated by ANISN. In contrast, the results generated by our method do not degrade because our $S_N$ method is free from optical truncation error.

Table 5
Numerical results for albedo and transmission factors

| $b$ | Albedo | | | Transmission | | |
|---|---|---|---|---|---|---|
| | Present method | Converged $F_N$ | ANISN | Present method | Converged $F_N$ | ANISN |
| 0 | 0.10002 | 0.1001 | 0.1001 | 7.4185E − 05[a] | 7.419E − 05 | 7.391E − 05 |
| 1 | 0.08059 | 0.08058 | 0.08059 | 8.5431E − 05 | 8.543E − 05 | 8.512E − 05 |
| 2 | 0.07053 | 0.07052 | 0.07051 | 9.3074E − 05 | 9.307E − 05 | 9.274E − 05 |

[a] Should be read as $7.4185 \times 10^{-5}$.

#### 4.1.3. Test problem 3

The third problem is a plane-parallel, constant energy version of a neutron beam transport problem basic to the design and optimisation of a neutron filter assembly for BNCT applications [26,37]. The problem here is to determine the angular distribution of neutrons on the right boundary of the filter assembly ($z = z_R$) due to a high-energy neutron beam normally incident upon the left boundary ($z = z_0$). With that angular distribution determined, we might evaluate quantities of interest such as beam attenuation and current-to-flux ratio at $z = z_R$. For the filter assembly, we have considered a three-block filter with materials and dimensions adapted from the assembly described in a work of Ingersoll et al. for studies of potential conversion of the Tower Shielding Facility (TSF) at Oak Ridge National Laboratory to BNCT applications [22]. Here, the leftmost (reactor side) block is an 80 cm-thick layer of aluminium, the middle block is a 9.2 cm-thick layer of sulfur and the rightmost (patient side) block is a 10 cm-thick layer of bismuth. The boundary conditions for this third problem are defined by $z_0 = 0$, $z_3 = 99.2$ cm, $\psi_0 = 1 \times 10^{11}$ cm$^{-2}$ s$^{-1}$ steradian$^{-1}$, $\mu_0 = 1$ and we have chosen $\gamma_0(\mu) = 1 \times 10^9\ \mu^2$ cm$^{-2}$ s$^{-1}$ steradian$^{-1}$, $\mu > 0$, to represent a continuously distributed, forwardly peaked component in the high-energy incident beam. As the constant energy assumption leads to a poor representation of the scattering events taking place (neutron energy losses are of the very greatest importance here), this third problem is of theoretical rather than practical value. So, we feel free to select a representative energy from the high-energy neutron beam and, for the select energy, generate temperature-dependent neutron cross-sections from the online version of the Evaluated Nuclear Data File library (ENDF/B-VI, MF = 3, MT = 1,2), available at http://www-nds.iaea.org. We remark that we have neglected resonance and nonelastic contributions to the cross-sections to facilitate data handling. Since the source of the neutron beam is a nuclear fission reactor (TSF), we choose 1 MeV of energy and we generate the 300 K macroscopic cross-sections (in cm$^{-1}$) provided in Table 6. In Table 7, we tabulate the scattering phase function data for

Table 6
Macroscopic cross-sections

| | $r = 1$ (Al) | $r = 2$ (S) | $r = 3$ (Bi) |
|---|---|---|---|
| $\sigma_{t,r}$ | 0.143731 | 0.067836 | 0.147094 |
| $\sigma_{0,r}$ | 0.141566 | 0.067446 | 0.145463 |

Table 7
Scattering phase function data

| $\ell$ | $\beta_{\ell,1}$ (Al) | $\beta_{\ell,2}$ (S) | $\beta_{\ell,3}$ (Bi) |
|---|---|---|---|
| 0 | 1 | 1 | 1 |
| 1 | 3.14359E − 1[a] | 0.30940E + 0 | 1.53700E − 1 |
| 2 | 9.35187E − 2 | 0.15601E + 0 | 1.37000E − 1 |
| 3 | 6.74197E − 3 | 3.42150E − 3 | 1.22100E − 1 |
| 4 | 7.23405E − 4 | 4.72620E − 3 | 4.25600E − 2 |
| 5 | 1.35765E − 5 | 4.14010E − 5 | |
| 6 | 9.26126E − 6 | 1.90490E − 4 | |
| 7 | 2.36402E − 8 | | |
| 8 | 3.60216E − 8 | | |
| 9 | 8.05308E − 8 | | |
| 10 | 1.07452E − 8 | | |
| 11 | 3.75038E − 8 | | |
| 12 | 3.88242E − 8 | | |
| 13 | 1.49097E − 8 | | |
| 14 | 2.74337E − 8 | | |
| 15 | 4.91905E − 8 | | |
| 16 | 3.65227E − 8 | | |

[a] Should be read as $3.14359 \times 10^{-1}$.

Table 8
Numerical results for the diffuse component $\psi^{d}_{199}(z_3, \mu)$

| $\mu$ | $\psi^{d}_{199}(z_3, \mu)$ | $\mu$ | $\psi^{d}_{199}(z_3, \mu)$ |
|---|---|---|---|
| $\mu_4$ | 5.47061477E + 09 | $\mu_{38}$ | 1.04862179E + 10 |
| 0.1 | 5.95413167E + 09 | 0.6 | 1.09398636E + 10 |
| $\mu_{10}$ | 6.51454734E + 09 | $\mu_{46}$ | 1.14302885E + 10 |
| 0.2 | 7.10267319E + 09 | 0.7 | 1.18667439E + 10 |
| $\mu_{17}$ | 7.60969449E + 09 | $\mu_{55}$ | 1.23781367E + 10 |
| 0.3 | 8.05397797E + 09 | 0.8 | 1.28342778E + 10 |
| $\mu_{23}$ | 8.48861871E + 09 | $\mu_{66}$ | 1.33497501E + 10 |
| 0.4 | 8.99564725E + 09 | 0.9 | 1.37825913E + 10 |
| $\mu_{30}$ | 9.45611393E + 09 | $\mu_{81}$ | 1.42908573E + 10 |
| 0.5 | 9.97726223E + 09 | 1.0 | 1.45482592E + 10 |

each layer. These data were extracted directly from ENDF/B-VI, MF = 4, MT = 2 at 1 MeV and 300 K. In Table 8, we present results for the diffuse component $\psi^{d}_{199}(z_3, \mu)$ of our approximate solution $\psi_{200}(z_3, \mu)$. We remark that that the labelled directions $\mu_m$, $m \in C \equiv \{4, 10, 17, 23, 30, 38, 46, 55, 66, 81\}$, in Table 8 are positive directions in the $S_{200}$ Gauss-Legendre quadrature set. Therefore, $\psi^{d}_{199}(z_3, \mu_m) = \psi^{d}_{3,m}(z_3)$, $m \in C$, where the angular fluxes $\psi^{d}_{3,m}(z_3)$ are exactly those generated by the ESGF method, viz result (41). The values for $\psi^{d}_{199}(z_3, \mu_m)$, $m \in C$, in Table 8 are in very close agreement to corresponding fine-mesh $S_{200}$ results generated with an ANISN-like code developed some years ago by the present author and former collaborators [8].

At this point we proceed to Section 5, where we give a discussion and directions for further developments and future work.

## 5. Discussion

We have described a computational method for approximately solving multislab radiation transport problems with azimuthal symmetry, with anisotropic scattering of arbitrary (Legendre) order and with no internal source of radiation other than redistribution by scattering. We have assumed that the multislab domain is irradiated from one side with a (rather) mixed neutral particle beam. We have considered here a mathematical formulation general enough to accommodate a number of basic and important problems in neutron and photon transport theory, as well as in radiative heat transfer. From a conceptual viewpoint, the computational method described in this article is a threefold method, in the following sense: (i) the multislab target problem (1)–(3) is suitably Chandrasekhar decomposed into two basic transport problems – the uncollided transport problem (4) and (5) with left singular boundary conditions and the diffusive transport problem (6) and (7) with regular boundary conditions; (ii) the uncollided problem is considered as is and it is solved rather easily and straightforwardly, whilst the diffusive problem is considered approximately through a standard $S_N$ formulation and the approximate $S_N$ diffusive problem is solved exactly with $S_N$ analytical and numerical methods and (iii) solutions to the two problems are composed through basic relations in order to yield an approximate solution to the multislab target problem. From a practical standpoint, the method described here is a constructive method designed to conform to the type of incident beam and to the quantities we are looking at. Owing to its two-component nature, our method can be used for generating spatially localized quantities, such as the angular distribution of radiation leaving the multislab domain, without having to worry about the detailed distribution of radiation in space. This is accomplished by the numerical component of our computational method. When the detailed space-angle distribution of radiation on a specific layer is required, the layer-edge values generated by the numerical component for the layer of interest are the inputs to a local reconstruction scheme of the angular distribution of radiation at any position on the layer of interest. This is accomplished by the analytical

component of our computational method. The reconstruction scheme is local in that computations are confined to the layer of interest. So, we can get space-angle distributions of radiation over as many layers as we wish on a layer-by-layer basis.

We believe that the method described in this article can be substantially improved as regarding computational efficiency. For example, in Section 2, we have stated that the angular components $a_{r,m}(\nu_{r,i})$ of the elementary solutions (25) satisfy the relation $a_{r,m}(\nu_{r,i}) = a_{r,-m}(-\nu_{r,i})$ for all $r$, $m$ and $i$. Let us explore one such relation a bit further. The above relation for the angular components can be readily obtained from a simple parity analysis of the $S_N$ Eq. (27). It can be obtained by replacing $\nu_{r,i}$ with $(-\nu_{r,i})$, $\mu_m$ with $(-\mu_m)$ and using the parity relations $P_\ell(-\mu_m) = (-1)^\ell P_\ell(\mu_m)$ and $g^0_{r,\ell}(-\nu_{r,i}) = (-1)^\ell g^0_{r,\ell}(\nu_{r,i})$ for Legendre and Chandrasekhar polynomials, respectively. And so it could have been used in our program to save some computer memory by storing only half of the separation constants (positive or negative) and the corresponding angular components. But, instead of formulating an eigenvalue problem defined in the full-range $\mu$-interval [−1,1] (as we did in Section 2) and only then saving some computer memory, we are rather thinking of implementing the half-range eigenvalue formulation for $\nu_{r,i}$ and $a_{r,m}(\nu_{r,i})$ described by Siewert in a recent article [33] in connection to double Gauss ($DP_N$) quadrature sets [15,25,35]. With this half-range formulation, we expect to increase the computational efficiency of our program and to report on $S_N$ results for the model problems considered in Section 4 (and others) for $N$ about twice as higher as those in Section 4 in near future.

We are currently working on the extension of the method described in this article to target problems defined on a multislab domain with *interacting boundaries* [5,35]. This would enlarge the applicability of our method to problems of theoretical and practical interest not covered so far, e.g. radiative transfer and neutron transport problems with specularly and/or diffusely reflective boundary conditions [5,15,25,35]. Target problems with reflecting boundaries are generally more complicated to formulate and solve than those with transparent ones, for the implicit boundary conditions induced. We intend to report our findings on these lines in forthcoming articles.

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