Numerical integration of the discrete-ordinate radiative transfer equation in strongly non homogeneous media.

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We consider the radiation transfer problem in the discrete-ordinate, plane-parallel approach. We introduce two benchmark problems with exact known solutions and show that for strongly non-homogeneous media the homogeneous layers approximation can lead to errors of 10% in the estimation of the intensity. We propose and validate a general purpose numerical method that transforming the two-boundary problem into an initial boundary problem, using an adaptive step integration and an interpolation of the local optical properties, can improve the accuracy of the solution up to two orders of magnitude. This is furthermore of interest for practical applications, such as atmospheric radiation transfer, where the scattering and absorbing properties of the media vary strongly with height and are only known, based on measurements or models, at certain discrete points.

I. INTRODUCTION

The mathematical modeling of radiative transfer in which the phenomena of absorption, emission and scattering are taken into account is usually made using the linearized Boltzmann equation, also known as radiation transfer equation. This equation describes the transfer of radiation, with a given wavelength, through a medium with certain absorbing and scattered properties. A particular application of this equation is the study of radiation transfer in the atmosphere, where the medium properties vary strongly with height. Getting accurate solutions of this problem is important for evaluating energy balance on planetary atmospheres as well as for the so called “inverse problem” where the boundary conditions (in particular the ground albedo properties) are deduced from measurements of radiation and knowledge of the medium characteristics.

In this work we consider the time-independent, monochromatic radiative transfer equation using the well-tested and widely used discrete-ordinate method of Stamnes et al. and the plane parallel approach where the optical properties depend only on the vertical coordinate z. The procedure requires the solution of a system of n coupled linear ordinary differential equations (one for each stream or discrete-ordinate component of the intensity). This set of equations is subject to a two-point boundary condition at the top and bottom of the medium. In the general case no analytic solutions exist for this problem since the medium optical properties (phase function, absorption and scattering coefficients) depend on the position z in the vertically inhomogeneous medium.

To obtain a formal solution, the medium is generally assumed to be layered with piecewise constant optical properties, i.e. it is divided into N adjacent homogeneous layers where the eigenvalues are computed. The
coefficients of the solution are determined by imposing the continuity condition at the boundaries between adjacent layers and the two-point boundary conditions at the top and bottom of the medium \[2, 3\].

Unfortunately in many cases the optical properties of the medium are not homogeneous, in fact they show strong variations along the vertical axis and have therefore different characteristic length scales. In these cases, as we will see below, the homogeneous layers assumption may lead to errors of 10% in the estimation of the scattered radiation. Furthermore in most practical applications the medium characteristics are only known, based on measurements or calculations, at a discrete number of points \[4\]. It is therefore required to implement a method that is able to cope both with the strong variations on the medium properties and with the discrete character of the information available.

Here we solve the discrete-ordinate approximation to the radiative transfer equation with a different approach. Since the equations and the boundary conditions are linear in the intensity, the two-point boundary problem can be solved with a shooting method. The problem is then reduced to the solution of an initial value problem which can be solved numerically. We propose a numerical integration of the initial value problem that applies an adaptive step method (such as step doubling), interpolates the optical properties from the discrete set of available data (for example using a cubic spline) and uses a weighted evaluation of the integrand along the interval (in our case a 5th order Runge-Kutta scheme). This allows the adaptation of the numerical integration to the local characteristic length-scales of the problem under consideration. The assumption of homogeneity is thus not required.

As an example we apply this method to solve the two-stream discrete ordinate version of the, non-emitting, radiative transfer equation in one spatial dimension (these results can be equivalently extended to multi-stream and emitting versions of this equation). We present two benchmark cases with known analytical solutions and compare the performance obtained when the step doubling interpolating method is used and when the piecewise homogeneity is imposed. We will show that using the same available discrete information, our method can significantly improve the accuracy of the solution. In section \[\text{III}\] we will first introduce the radiative transfer equation and the equations for the direct and diffuse intensity components in the two-stream discrete ordinate approach. In section \[\text{IV}\] we will describe two benchmark cases characterized by linear and exponential height dependence of the optical coefficients in the equations. In section \[\text{V}\] we will explain our numerical procedure and will validate our results and those obtained under the assumption of piecewise homogeneous layers against the exact analytical solutions of the benchmark problems. Finally conclusions are presented in section \[\text{VI}\].

\section{Multiple Scattering and the Radiative Transfer Equation}

Our aim is to solve the radiative transfer problem in the plane parallel approach. As represented in Figure 1, this corresponds to the case in which optical properties only depend on altitude \(z\) in a plane parallel geometry.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1.png}
\caption{Layer with altitude dependant extinction and scattering coefficients.}
\end{figure}
Following for instance [1] the radiative transfer equation in this approach is written as,

$$\cos \theta \frac{dI(z, \theta, \phi, \lambda)}{dz} = -\beta_T(z, \lambda)I(z, \theta, \phi, \lambda) + \frac{\beta_{sca}(z, \lambda)}{4\pi} \int_0^{2\pi} d\phi' \int_0^\pi \sin \theta' d\theta' p(z, \theta, \phi, z', \theta', \phi', \lambda) I(z, \theta', \phi')$$

(1)

where \( \theta \) and \( \phi \) are respectively the polar and azimuthal angles. Here \( \beta_{sca} \) represents the attenuation due to scattering effects and \( \beta_T(z, \lambda) \) is the extinction coefficient defined as \( \beta_T(z, \lambda) = \beta_{sca}(z, \lambda) + \sum_i \beta_i(z, \lambda) \) where the summation in \( i \) extends to all the molecular components considered. Here \( \beta_i(z, \lambda) = n_i(z)\sigma_i(\lambda) \) is the absorption coefficient of a given component, \( \sigma_i(\lambda) \) is the attenuation cross section due to absorption and \( n_i(z) \) the atmospheric number density for species \( i \) (which generally depends exponentially on the height \( z \)). In Eq. (1), \( p(z, \theta, \phi, z', \theta', \phi', \lambda) \) is the phase function of the scattering particles which is normalized as follows:

$$\frac{1}{4\pi} \int_0^{2\pi} d\phi \int_0^\pi p(\theta, \phi, z', \theta', \phi', \lambda) \sin(\theta) d\theta = 1. \text{ This function gives the probability for a photon of wavelength \( \lambda \) incident on the scattering particle with angles \( (\theta', \phi') \) to be scattered in the direction \( (\theta, \phi) \) and satisfies }$$

$$p(\theta, \phi, z', \theta', \phi', \lambda) = p(\cos \Theta, \lambda) \text{ where } \Theta \text{ is the scattering angle, related to the polar and azimuthal angles by }$$

$$\cos \Theta = \cos \theta' \cos \phi + \sin \theta' \sin \cos(\phi - \phi').$$

The solution of Eq. (1) is splitted into two terms

$$I(z, \theta, \phi, \lambda) = I^{dir}(z, \lambda) + I^{dif}(z, \mu, \phi, \lambda).$$

(2)

\( I^{dir}(z, \lambda) \), the direct intensity, is the solution of Eq. (1) when there is no multiple scattering (no integral term):

$$\frac{\mu_0 dI^{dir}(z)}{dz} = -\beta_T(z)I^{dir}(z)$$

(3)

where \( \mu_0 \) is the cosine of the polar angle for the incident radiation. The diffuse intensity is the solution of

$$\frac{\mu dI^{dif}(z, \mu, \phi, \lambda)}{dz} = -\beta_T(z, \lambda)I^{dif}(z, \mu, \phi, \lambda) + \frac{\beta_{sca}(z, \lambda)}{4\pi} \int_0^{2\pi} d\phi' \int_0^\pi \sin \theta' d\theta' p(z, \theta, \phi, z', \theta', \phi', \lambda) I^{dif}(z, \mu', \phi')$$

$$- \frac{\beta_{sca}(z, \lambda)I^{dir}(z, \lambda)}{4\pi} p(z, \mu, \phi, z', -|\mu_0|, \phi_0, \lambda').$$

(4)

with \( \mu = \cos \theta \). In this equation the variable \( \mu \) takes values in the range \(-1 < \mu < 1\). Negative \( \mu \) corresponds to radiation going downwards, whereas positive \( \mu \) describes radiation going upwards. In order to solve Eq. (1) the diffuse intensity is expanded in a 2n Fourier cosine series (from now on we drop the superscript \( dif \)):

$$I(z, \mu, \phi, \lambda) = \sum_{m=0}^{2n-1} I^m(z, \mu) \cos m(\phi_0 - \phi).$$

The phase function is expanded in a basis of 2n Legendre polynomials \( p(z, \mu, \phi, z', \mu', \phi', \lambda) = p(z, \cos \Theta, \lambda) = \sum_{l=0}^{2n-1} (2l+1)g_l P_l(\cos \Theta). \) With these transformations and the theorem of addition of spherical harmonics Eq. (1) becomes a set of integro-differential equations depending only on the \( z \) and \( \mu \) coordinates:

$$\mu \frac{dI^m(z, \mu)}{dz} = -\beta_T(z, \lambda)I^m(z, \mu) + J^m(z, \mu)$$

(5)

where

$$J^m(z, \mu) = \frac{\beta_{sca}(z, \lambda)}{2} \sum_{l=0}^{2n-1} (2l+1)g_l P^m_l(\mu)$$

$$\times \left( \int_1 P^m_l(\mu')I^m(z, \mu')d\mu' + \frac{I^{dir}(z, \lambda)}{2\pi} (2 - \delta_{0,m})(-1)^{(l+m)}P^m_l(|\mu_0|) \right)$$

(6)
being $P^m_\ell (\mu)$ the associated Legendre polynomial, $g^m = g_1 \frac{(m+1)!}{(m-\ell)!}$, and $g_1 = \frac{1}{2} \int_1^1 p(\cos \Theta) P_1(\cos \Theta) d(\cos \Theta)$.

In the discrete ordinate approximation the angular integral term in Eq. (6) and following the two-stream approximation we consider a weighted summation to a two-point boundary condition. Solving these equations, we will get a discrete approximation to the angular distribution of $I^m(z, \mu)$ from the top of the atmosphere to the surface level.

In this work, for simplicity, we will consider the two-stream approximation to this problem and obtain the measurement of the direct component attenuation. This is a non-dimensional variable which is defined as $\tau(\mu) = \int_0^\infty \beta_T(z) dz$. It describes the attenuation within the medium of an incident beam of radiation when emission and multiple scattering are ignored, i.e. it is a measurement of the direct component attenuation.

### III. THE BENCHMARK PROBLEMS

In this section we define three benchmark problems with an exact solution where the optical properties $\beta_T(z, \lambda)$ and $\beta_{sca}(z, \lambda)$ in Eq. (1) have different altitude ($z$) dependences. For the sake of simplicity we consider that particles scatter radiation uniformly, i.e. the scattering phase function is $p(\cos \Theta) = 1$ and that $z_{max} = 1$.

For the integral part in Eq. (6) and following the two-stream approximation we consider a weighted summation over the streams $\mu_1 = -1/\sqrt{3}$ (down) and $\mu_2 = 1/\sqrt{3}$ (up) which are the zeroes of the second order Legendre polynomial, i.e. $P_2(\mu_i) = 0$, $i = 1, 2$. Then, Eq. (6) can be transformed in two coupled ordinary differential equations for the down ($I_1$) and up ($I_2$) radiation intensity:

$$\mu_1 \frac{dI_1}{dz} = -\beta_T(z) I_1 + \frac{0.5 \beta_{sca}(z)}{2} \left( I_1 + I_2 + \frac{I^{dir}(z)}{2\pi} \right),$$

$$\mu_2 \frac{dI_2}{dz} = -\beta_T(z) I_2 + \frac{0.5 \beta_{sca}(z)}{2} \left( I_1 + I_2 + \frac{I^{dir}(z)}{2\pi} \right).$$

After a change of variables $z' = 1 - z$ (from now on dropping the prime in $z$) and taking into account that $\mu_1 = -\mu_2$ the above equations may be rewritten as,

$$\mu_0 \frac{dI^{dir}}{dz} = [A(z) - B(z)] \mu_2 I^{dir}$$

$$\frac{dI_1}{dz} = A(z) I_1 + B(z) I_2 + I^{dir}(z) \frac{B(z)}{2\pi}$$

$$\frac{dI_2}{dz} = -A(z) I_2 - B(z) I_1 - I^{dir}(z) \frac{B(z)}{2\pi}$$

where
\[
A(z) = \frac{-\beta_T(z) + 0.25\beta_{sca}(z)}{\mu_2}
\]
(14)
\[
B(z) = \frac{0.25\beta_{sca}(z)}{\mu_2}
\]
(15)
\[
I_{dir}(z) = I_0 e^{-\frac{\lambda(z) - \beta_{sca}(z)}{\mu_0} \mu_2 dz}
\]
(16)

and $I_0$ is fixed by the condition at the top $I_{dir}(z = 0)$. In the following examples we will solve this problem with the two-point boundary conditions given in Eqs. (7)-(8), which are now explicitly written as $I_1(z = 0) = 0$ (at the top) and $I_2(z = 1) = 0$ (at the bottom). The incident intensity on the top is characterized by $I_0 = 100$ and $\mu_0 = -0.788$. We will consider two different height dependences of the optical properties.

### A. Linear dependence

We propose as study-case a linear dependence on the extinction coefficients. In particular we have considered the functions $A(z)$ and $B(z)$,

\[
A(z) = \frac{z (4a^2 + c^2)}{2c}
\]
(17)
\[
B(z) = \frac{z (4a^2 - c^2)}{2c}
\]
(18)

With this choice the general solutions of Eqs. (12)-(13) for the diffuse components are,

\[
I_1(z) = e^{(-z^2a)} C_1 + e^{(z^2a)} C_2 - \frac{I_0 (\mu_0^2 - \mu_0 \mu_2) (4a^2 - c^2)}{16 \pi (-c^2 \mu_2^2 + 4a^2 \mu_0^2)} e^{\left(\frac{-c^2z^2}{2\mu_0}\right)}
\]
(19)

for the downwards radiation, and

\[
I_2(z) = -\frac{2a + c}{2a - c} e^{(-z^2a)} C_1 - \frac{2a - c}{2a + c} e^{(z^2a)} C_2 - \frac{I_0 (\mu_0^2 + \mu_0 \mu_2) (4a^2 - c^2)}{16 \pi (-c^2 \mu_2^2 + 4a^2 \mu_0^2)} e^{\left(\frac{-c^2z^2}{2\mu_0}\right)}
\]
(20)

for the upwards component. Here $C_1$ and $C_2$ are arbitrary constants fixed with the boundary conditions in Eqs. (7)-(8). The direct component of the intensity is now

\[
I_{dir}(z) = I_0 e^{\left(\frac{-c^2z^2}{2\mu_0}\right)}
\]
(21)

For the specific choice $c = -10.5, a = 4$ the constants $C_1$ and $C_2$ satisfy the boundary conditions are $C_1 = -33.0927$ and $C_2 = -6.71346e - 05$. For this particular set of parameters the total optical path is $\tau \approx 3$. The optical functions $\beta_T(z)$ and $\beta_{sca}(z)$ are shown in Fig. 2-I and in Fig. 2-II the attenuation of the direct intensity as a function of height. The two-stream components of the diffused intensity are shown in Fig. 3-I.

### B. Exponential dependence

In atmospheric layers the gas density typically depends on the altitude as a growing exponential from $z = 0$ (the top) to $z = 1$ (the bottom). For this reason the choice of exponential dependence in the extinction coefficients is very convenient as it allows us to validate our method with solutions similar to those appearing in atmospheres, where our method has been applied [4]. In particular we have chosen,
\[ A(z) = \frac{e^{(az)}}{2c} \left( a^2 b^2 + c^2 \right) \]  
\[ B(z) = \frac{e^{(az)}}{2c} \left( a^2 b^2 - c^2 \right) \]  

The general solution for the downwards intensity is,

\[ I_1(z) = e^{(az)} b \ C_2 + e^{(-az)} b \ C_1 - \frac{\left( -c^2 + a^2 b^2 \right) \left( \mu_0 \mu_2 - \mu_0 \mu_2 \right)}{16 \pi \left( -c^2 \mu_2^2 + a^2 b^2 \mu_0^2 \right)} I_0 e^{\left( -\frac{e^{az}}{\mu_0 \mu_2} \right)} \]  

and for the upwards intensity is,

\[ I_2(z) = \frac{e - ab}{c + ab} e^{(az)} b \ C_2 - \frac{c + ab}{c + ab} e^{(-az)} b \ C_1 - \frac{\left( a^2 b^2 - c^2 \right) \left( \mu_0 \mu_2 + \mu_0 \mu_2 \right)}{16 \pi \left( a^2 b^2 \mu_0^2 - c^2 \mu_2^2 \right)} I_0 e^{\left( -\frac{e^{az}}{\mu_0 \mu_2} \right)} \]  

where \( C_1 \) and \( C_2 \) are arbitrary constants fixed with the boundary conditions. The direct component of the intensity is,

\[ I_{\text{dir}}(z) = I_0 e^{\left( -\frac{e^{az}}{\mu_0 \mu_2} \right)} \]  

For the specific choice \( c = -0.8, a = 3, b = 0.2 \), the constants \( C_1 \) and \( C_2 \) that satisfy the boundary conditions are \( C_1 = -71.6787 \) and \( C_2 = -8.51812 e - 05 \). The total optical path, for this particular set of parameters, is \( \tau \approx 3 \). The optical functions \( \beta_T(z) \) and \( \beta_T(z) \) are shown in Fig. 3-I and the direct intensity in Fig. 3-II. The two-stream components of the diffused intensity are shown in Fig. 3-II.

**IV. THE NUMERICAL METHOD**

In contrast to the examples discussed above, where the optical properties of the media are known functions, in the general case the medium optical properties are only known, based on measurements or models, at a discrete set of points. In order to solve the radiative transfer equation, it is generally assumed that these optical properties are piecewise constant in a layer around the point, i.e. that the plane parallel layers are homogeneous piecewise. As we shall see later this should not be assumed in the case of atmospheric layers, where the optical properties show a strong (exponential) altitude dependence. We therefore propose to solve the problem numerically, using an adaptative step procedure and interpolating the optical values where necessary.

Equation (4) is an initial value problem and it is easily integrated knowing the incident intensity on the top \( I_0 \). Equations (12), (13) and their boundary conditions constitute a two-point boundary problem which can be solved for instance with a shooting method as those explained in [3, 4]. For problems with linear boundary conditions, shooting methods are able to get the exact solution in few steps. We choose values for all the variables at one boundary, which must be consistent with any boundary condition there, but are otherwise arranged to depend on arbitrary free parameters whose initial values are guessed. We then integrate the ordinary differential equations with initial value methods, arriving at the other boundary, and adjust the free parameters at the starting point that zeros the discrepancies at the other boundary. Thanks to this procedure the problem is reduced to the solution of an initial value problem where no assumption of piecewise homogeneity is required.

The numerical integration of the equation for the direct component (4) and of the set of \( n \) ordinary differential equations (4) for the diffused streams is done with a fifth-order Runge-Kutta (RG) scheme with variable step. For
the adaptative step control we use a "step doubling" technique: the local error is estimated by comparing a solution obtained with a fifth-order scheme and the one obtained with a fourth-order method. The integrating step is halved if this error is above a desired tolerance. Next, given the tabulated function $\beta_{T,i} = \beta_T(z_i)$ and $\beta_{sca,i} = \beta_{sca}(z_i)$ with $i = 1...N$, we interpolate to obtain the new values at the locations required by the RG and the adaptative step doubling integration scheme. We have chosen a cubic interpolating spline which allows the interpolating formula to be smooth in the first derivative, and continuous in the second derivative, both within the interval and at its boundaries [5].

As an example, next we solve for the direct and diffused intensity in the two benchmark problems explained in section III. For problems with optical depths of the order of $\tau \approx 1$, standard calculations based on the homogeneous layer approximation divide the medium into $N = 10$ homogeneous layers [2]. We will analyze problems of $\tau \approx 3$ and keep a similar ratio for our comparisons, we will then increase the number of layers. The tabulated optical properties $\beta_T(z_i), \beta_{sca}(z_i)$ at $N$ equidistant $z_i$ points are given as input.

A summary of the maximal relative error $E(I) = |I_{num} - I_{exact}| / I_{exact}$ for the benchmark problems as a function of the method and number of initial layers is given in table I. We compare the relative error in the solution where piecewise homogeneity is assumed with the one obtained with our RG, step doubling, interpolating method. Figure 4 shows the relative error as a function of height $z$ for the step doubling interpolating
technique with $N = 30$ layers, for the linear (I) and exponential case (II). For a ratio of layers $N/\tau \approx 10$ the piecewise homogeneous approximation leads to errors of the order of 10% which can be reduced to 1% by increasing this ratio to $N/\tau \approx 80$. The step doubling interpolating RG technique permits the adaption of the numerical integration to the local characteristic length-scales of the medium and, for the same input, increases the accuracy of the solution between one and two orders of magnitude allowing for fast and accurate radiative transfer calculations.

V. CONCLUSIONS AND DISCUSSION

We have considered the discrete-ordinate approach to the radiation transfer equation. In view of our calculations the error in the plane parallel approach, assuming $N$ piecewise homogeneous layers, with $N \approx 10\tau$ can go up to 10% of the diffused intensity and thus the inhomogeneities in the atmosphere cannot be ignored. We have validated a general purpose numerical method that, based on an adaptative step integration and an interpolation of the local optical properties, can significantly improve (up to two orders of magnitude) the accuracy of the solution. This is furthermore of interest for practical applications, such as atmospheric radiation transfer, where the scattering and absorbing properties of the media are only known, based on experiments or theoretical models, at certain discrete points. Furthermore, this numerical method can be straightforward extended to multiple streams, non trivial boundary conditions and non uniform scattering function allowing for fast and accurate solutions of the radiative transfer equation.

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