

Analytic Green's Function for Radiative Transfer in Plane-Parallel Atmospheres

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ABSTRACT

Green's function is a widely used approach for boundary value problems. In problems related to radiative transfer, Green's function has been found to be useful in land, ocean, and atmosphere remote sensing. It is also a key element in higher order perturbation theory. This paper presents an explicit expression of the Green's function, in terms of the source and radiation field variables, for a plane-parallel atmosphere with either vacuum boundaries or a reflecting [atmosphere–bidirectional reflectance distribution function (BRDF)] surface. A FORTRAN 95 code, Green's function and discrete ordinate method (GDOM), has been developed to efficiently compute the Green's function. This code also integrates with an implementation of the discrete ordinate method with several extensions and improvements. Computing complexity of the Green's function algorithm is analyzed, and validation of the code is discussed.

1. Introduction

The Green's function, originated from the work on potential theory by G. Green, "An essay on the application of mathematical analysis to the theories of electricity and magnetism," has been widely used to solve boundary value problems (cf. Stakgold 1979). For a given linear differential operator, L , the Green's function of this operator is the solution to the linear differential equation, $LG(x, x_0) = \delta(x - x_0)$, defined on given domain and satisfies given boundary conditions. Using the Green's function, the solution to any inhomogeneous equation of the same operator, $Lf(x) = h(x)$, can then be found to be the convolution of $G(x, x_0)$ with the inhomogeneous (source) term, $h(x)$, that is, $f(x) = \int G(x, x')h(x') dx'$, for the same domain and boundary conditions. This last expression is sometimes also used as another definition of the Green's function. We note, however, that a Green's function is not only associated with a linear differential operator, but also with certain domain and boundary conditions.

The concept of Green's function has been introduced into linear transport theory, the generalized theory

dealing with radiative transfer and neutron transport, etc., by Case and Zweifel (1967) and Bell and Glasstone (1970). In particular, Case and Zweifel (1967) developed an explicit expression of the Green's function for infinite, homogeneous, and isotropically scattering media with vanishing boundary conditions at infinity.

By generalizing from isotropic scattering to the anisotropic case, the infinite medium Green's function (IMGF) has recently been used to compute the particular solution of the discrete ordinate method (DOM; Siewert 2000; Barichello et al. 2000; Spurr 2002), which provides a universal approach for any sources. However, applications of the IMGF in finite media is limited in that it cannot be used directly, by means of convolution, to find the solution of radiative transfer problems in finite medium, because of different domain and boundary conditions.

In many cases it is desirable to have an explicit expression for the finite medium Green's function (FMGF). The most direct application of FMGF is, of course, in forward radiative transfer computations using convolution. This will be discussed in more details later in this paper. In some atmosphere correction schemes for remote sensing images, for example SeaWiFS (Wang 2003), lookup tables for a set of solar zenith angles are needed. In such cases, FMGF may be used to build up such lookup tables much more efficiently.

In surface remote sensing, the so-called atmosphere–bidirectional reflectance distribution function (BRDF)

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coupling has been a challenging task in the past. By means of the FMGF, Lyapustin and Knyazikhin (2001, 2002) showed that the radiance observed from space can be expressed in explicit terms of the surface BRDF, which generalizes the expression for Lambertian surfaces (Liou 1980). This formulation allows for recomputing the radiance for updated surface parameters without resolving the atmosphere radiative transfer equation. Therefore, it allows for quick trial evaluation loops. Landgraf et al. (2002) also used FMGF in surface remote sensing in connection with perturbation theory (Box et al. 1988; Trautmann et al. 1992). However, although the concept of the Green's function is used in these works, the explicit expression for the FMGF is not provided. In Lyapustin and Knyazikhin (2001) it is briefly mentioned that a standard radiative transfer code is used to compute the Green's function, while in Landgraf et al. (2002) the method is not discussed.

In the computation of the higher order radiative perturbation (Box et al. 1988, 2003; Polonsky and Box 2002), the Green's function is a key step that requires us to compute the FMGF. We may use a standard radiative transfer code (assuming it supports beam sources of arbitrary position and direction) to accumulate a numerical Green's function by solving the radiative transfer equation for a set of beam sources of different angles and positions. However, this approach is, at least, inefficient even after extending the DOM for fast multisource solutions (Qin et al. 2002, 2004). Furthermore, a numerical Green's function does not allow for analytical calculations on the source variables. Such ability could be critical, for example, in higher order perturbation computation where, by employing the explicit FMGF expression (to be presented in this paper), we have demonstrated very significant CPU-time reduction (Qin et al. 2005).

Green's function was used by Benedetti et al. (2002) to investigate the influence of cloud/aerosol's vertical (extinction coefficient) variation on remotely sensed reflected sunlight. An explicit expression of FMGF was developed in this work using matrix exponential together with a doubling-adding approach. However, this complicated expression is derived for a single layer only, and the radiance (or equivalently the source) is restricted to be at the two boundaries of the layer. The work by Benedetti et al. (2002) therefore provides a special case of the FMGF but (unfortunately) it is not what we were searching for, and the approach used by them probably is also difficult to be generalized for arbitrary radiance (or source) position in multilayered media.

Applications of the Green's function concept are explored by several other authors as well, for example, in

cloud remote sensing (Davis and Marshak 2002; Davis et al. 1999), surface BRDF modeling (Knyazikhin and Marshak 2000), and the application of the IMGF in neutron transport problems (Tezcan et al. 2003; Hong and Cho 2001). These works however also did not provide an explicit expression for the FMGF.

The purpose of this paper is to present an explicit expression of the finite medium Green's function, in terms of the source and radiance position and direction, for a vertically varying and anisotropically scattering atmosphere with two boundary types including reflective (BRDF) surface. We will also present a FORTRAN 95 code for the computation of the FMGF. We note that the main purpose of this paper is not to present an alternative algorithm for solving normal forward radiative transfer problems, such as the discrete ordinate method (Chandrasekhar 1960; Liou 1980; Stamnes et al. 1988), which considers the source as fixed (direction/position) rather than as variables. But we point out that the Green's function algorithm to be presented does have a deep root in DOM, which is now rather mature with proven numerical stability (Stamnes et al. 1988).

Although many of the techniques used to process the radiative transfer equation, especially those related to the DOM, may already be familiar to many readers, some other parts may be less familiar, so we use appendices to provide a self-contained development of the formulation. In the main body, we will then only present and briefly discuss the final FMGF expressions for the two boundary types (section 2). In section 3, we will illustrate how the FMGF may be used, by using the computations of the radiation fields generated by common sources as examples. Following this, we will discuss an implementation in section 4 and provide an analysis of the computing complexity compared to that of DOM. Validation of the code, including comparisons with the discrete ordinates model DISORT (Stamnes et al. 1988), will also be discussed in this section. We summarize finally in section 5.

2. The finite medium Green's function

In this section, we present the two FMGF expressions, for vertically varying media with two boundary types respectively, that is, all vacuum boundaries, or an upper vacuum boundary and a reflective (BRDF) surface at the lower boundary. Since the complete development is provided in appendix C, we give a summary of the major steps that lead to the final results.

a. FMGF for vacuum boundaries

In handling the vertical variation of the atmosphere, the atmosphere is modeled as a stack of layers of ho-

mogeneous scattering properties (Liou 1973, 1975); therefore, we will only solve the transfer equation for constant single scattering albedo and phase function, which may be written in the form of a linear differential operator, L , as (Bell and Glasstone 1970):

$$LG(\tau_0, \mu_0, \phi_0; \tau, \mu, \phi) = \delta(\mu - \mu_0)\delta(\phi - \phi_0)\delta(\tau - \tau_0), \quad (1)$$

where G is the Green's function, δ is the Dirac delta function, and (τ, μ, ϕ) are the optical depth, the cosine of zenith angle, and the azimuth angle for the radiation field, respectively. Corresponding to these radiation field variables is the set of source parameters, identified by the subscript 0. We note that the right-hand side of Eq. (1) represents a beam source of unit flux, not intensity. The linear operator, L , is defined as (Bell and Glasstone 1970)

$$L \equiv \mu \frac{d}{d\tau} - 1 + \frac{\tilde{\omega}_0}{4\pi} \int_0^{2\pi} d\phi' \int_{-1}^1 d\mu' P(\mu', \phi'; \mu, \phi)^\circ, \quad (2)$$

where $\tilde{\omega}_0$ and P are the single scattering albedo and phase function, respectively. The symbol $^\circ$ in the last term denotes the object on which the integral operator acts, and when G is inserted into the integration, (μ, ϕ_0) should be replaced by (μ', ϕ') .

The transfer equation is decomposed into a set of independent subequations of the zenith angles and optical thickness only, by expanding the Green's function (as well as the phase function) into Fourier cosine series of the azimuth angle (Chandrasekhar 1960),

$$G(\tau_0, \mu_0, \phi_0; \tau, \mu, \phi) = \sum_{m=0}^{N_m} G^m(\tau_0, \mu_0; \tau, \mu) \cos m(\phi_0 - \phi), \quad (3)$$

and by replacing the angular integration with Gaussian quadrature. The subequations can then be solved independently. In the remainder of this section, we will only deal with $G^m(\tau_0, \mu_0; \tau, \mu)$, and the superscript m will be omitted for simplicity.

The above steps essentially used the same techniques as of DOM (Chandrasekhar 1960). A major difference in the following steps is that, rather than directly seeking the solution for the finite layers as in DOM, we start from the infinite medium with vanishing boundary conditions at infinity. The infinite medium Green's function is first obtained by following Case and Zweifel (1967), and by generalizing isotropic scattering to the anisotropic case using the matrix eigenvalue approach (Stamnes et al. 1988). The obtained IMGf expression is

shown in Eqs. (B24) and (B25), which reveal an explicit relation of radiation field with the source position and direction.

The radiation field of a finite layer with vacuum boundaries can then be expressed in terms of the IMGf in a form of an integral equation, by applying the Placzek lemma (Bell and Glasstone 1970) and introducing (yet to be decided) pseudosources on the boundaries of each layer. The pseudosources are then found by solving the integral equations in accordance with the boundary (and radiance continuity) conditions (see appendix C). The key point here is to derive the explicit relation of the radiation field with the source parameters, τ_0 and μ_0 , in order to form a Green's function. Analyzing the integral equations reveals that pseudosources are composed of an unknown constant kernel and a known function of τ_0 and μ_0 . By multiplying the inverse of this known function on both sides of the integral equations, we eventually arrive at a set of linear equations of the unknown kernels. The coefficient matrix of this system has a block-band diagonal structure similar to that of the integral constants equations in the DOM (Stamnes et al. 1988), which can be solved numerically using, for example, LAPACK (Anderson et al. 1999).

Once the constant kernels are found, the expression for FMGF is obtained. For l ($\tau^{l-1} < \tau \leq \tau^l$) and l_0 ($\tau^{l_0-1} < \tau_0 \leq \tau^{l_0}$), $l, l_0 = 1, 2, \dots, N$, where N is the total number of layers and τ^l is the optical depth at the bottom of layer l ; we found that for vacuum boundaries the Green's function can be expressed as

$$\mathbf{G}^{l,l_0}(\tau_0, \mu_0; \tau, \mu) = \mathbf{\Gamma}^l(\tau, \mu) \tilde{\mathbf{T}}^{l,l_0}(\tau, \tau_0) \mathbf{\Gamma}_0^{l_0}(\tau_0, \mu_0), \quad (4)$$

where the $\tilde{\mathbf{T}}^{l,l_0}$, shown in Eq. (C21), are matrices satisfying $(\tilde{\mathbf{T}}^{l,l_0})^T = \tilde{\mathbf{T}}^{l_0,l}$. When $l \neq l_0$, $\tilde{\mathbf{T}}^{l,l_0}$ depends only on l and l_0 , but are independent of τ and τ_0 . When $l = l_0$, $\tilde{\mathbf{T}}^{l,l_0}$ is also constant in the sections of $\tau^{l-1} < \tau < \tau_0$ and $\tau_0 < \tau < \tau^l$ respectively, but changes at $\tau = \tau_0$. This reflects the fact that the radiation field is discontinuous at the position where the beam source is imposed; $\mathbf{\Gamma}^l(\tau, \mu)$ and $\mathbf{\Gamma}_0^{l_0}(\tau_0, \mu_0)$ are given by

$$\mathbf{\Gamma}^l(\tau, \mu) = [\mathbf{\Phi}_+^l(\mu) \quad \mathbf{\Phi}_-^l(\mu)] \begin{bmatrix} e^{\lambda_+^l(\tau^{l-1}-\tau)} & \mathbf{0} \\ \mathbf{0} & e^{\lambda_-^l(\tau^l-\tau)} \end{bmatrix} \quad (5)$$

and

$$\mathbf{\Gamma}_0^{l_0}(\tau_0, \mu_0) = [\mathbf{\Gamma}^{l_0}(\tau_0, -\mu_0)]^T, \quad (6)$$

where λ_\pm^l , a diagonal matrix, and $\mathbf{\Phi}_\pm^l$, a normal real matrix, are composed of the eigenvalues and eigenvectors of the scattering matrix, Eq. (B3), of layer l .

Equation (4) shows a symmetric structure that re-

veals the general principle of reciprocity. For each term of the Fourier cosine series, Eq. (3), we have

$$G(\tau, -\mu; \tau_0, -\mu_0) = G(\tau_0, \mu_0; \tau, \mu). \quad (7)$$

We note that this FMGF expression is continuous in the positional variables, τ and τ_0 , while it is discrete in the angular variables, μ and μ_0 , and the value of the function in the angular variables is evaluated at the set of the Gaussian quadrature points.

b. FMGF for a reflective (BRDF) surface

We can extend the FMGF with vacuum boundary (FMGF-VB) to the case when a reflective (BRDF) surface is present at the lower boundary. The key point is to convert the BRDF surface problem to a vacuum boundary problem to make use of the already established result. This is done by treating the reflected radiance as a (angularly distributed) source, and the radiation field generated by this source is just its convolution with the FMGF-VB. The detailed steps for this derivation are provided in the appendix D. It is found that the final expression of the FMGF with reflective surface (FMGF-RS), shown in Eq. (D8), has exactly the same form as the FMGF-VB, Eq. (4), except that the kernel matrix, $\tilde{\mathbf{T}}^{l,l_0}$, is replaced with $\tilde{\mathbf{T}}_s^{l,l_0}$, which depends on the surface BRDF matrix: see Eqs. (D6) and (D8)–(D10).

By replacing the first term and the last factor of the second term in Eq. (D6) with the intensity generated by a given source for vacuum surface, the equation is then specialized to the radiation field generated by that source for BRDF surface, which has been developed by Lyapustin and Knyazikhin (2001). It is also not difficult to specialize further for the Lambertian surface, for which an expression has been presented by Liou [1980, Eqs. (6.182)–(6.183)].

3. Radiative computation using Green's function

Although the initial motivation to develop FMGF is for radiative perturbation computation (Box et al. 1988; Qin et al. 2005), the Green's function has more applications than that. In the introduction section we reviewed in some details the applications of the finite medium Green's function in surface remote sensing (Lyapustin and Knyazikhin 2001, 2002; Landgraf et al. 2002) and in cloud/aerosol studies by remote sensing (Benedetti et al. 2002). In all these applications, the Green's function is used in some form of convolution. In this section, we explain how the FMGF expression may be used with specific source types, including emission sources (surface, deep space, or the atmosphere)

and generalized beam sources with arbitrary direction and position. We note however, by showing how radiation field can be computed using convolution of the FMGF, we do not mean to use this approach as better alternative to normal forward radiative transfer algorithms, such as DOM.

For a general source, suppose it can be expanded as a cosine series, and the m th order of the source intensity is denoted as $Q(\tau, \mu)$, then the radiance of the same order can be calculated as

$$\begin{aligned} I(\tau, \mu) &= \int d\tau' \int_{-1}^1 G(\tau', \mu'; \tau, \mu) |\mu'| Q(\tau', \mu') d\mu' \\ &= \sum_{l'=1}^N \Gamma^{l'}(\tau) \int_{\tau_{l'-1}}^{\tau_{l'}} \mathbf{T}^{l,l'}(\tau, \tau') \Gamma_0^{l'}(\tau') \mathbf{w} |\boldsymbol{\mu}| \mathbf{Q}(\tau') d\tau', \end{aligned} \quad (8)$$

where we have replaced the integration over μ' with Gaussian quadrature, and \mathbf{w} and $\boldsymbol{\mu}$ are diagonal matrices composed of the quadrature weights and points. The term $|\mu'|$ is needed to convert Q to flux. The $\mathbf{T}^{l,l'}$ matrix can be either $\tilde{\mathbf{T}}^{l,l'}$ (for vacuum surface) or $\tilde{\mathbf{T}}_s^{l,l'}$ (for BRDF surface). We note that $\mathbf{T}^{l,l'}$ can always be pulled out of the integration, but when $l = l'$, the integration should be conducted in two sections because $\mathbf{T}^{l,l'}$ changes at $\tau = \tau'$.

For surface emission, $Q(\tau, \mu) = \delta(\tau - \tau_a) \varepsilon(\mu) B(T_s)$, where $\mu > 0$, $\varepsilon(\mu)$ is the angular emissivity and $B(T_s)$ is the Planck function at surface temperature, T_s . It is straightforward to see from Eq. (8) that

$$I(\tau, \mu) = \Gamma^l(\tau) \mathbf{T}^{l,N}(\tau, \tau_a) \Gamma_0^{+N}(\tau_a) \mathbf{w} |\boldsymbol{\mu}| \varepsilon B(T_s), \quad (9)$$

where $+$ in Γ_0^{+N} indicates the columns for $\mu' > 0$, and τ_a is the optical depth at the bottom. Similarly for isotropic emission from the deep space we have

$$I(\tau, \mu) = \Gamma^l(\tau) \mathbf{T}^{l,1}(\tau, 0) \Gamma_0^{-1}(0) \mathbf{w} |\boldsymbol{\mu}| \varepsilon_i B(T_l), \quad (10)$$

where T_l and ε_l are the temperature and emissivity of the deep space, respectively.

For atmosphere emission, the source function can be approximated as a power series in optical thickness (Stamnes et al. 1988):

$$Q^l(\tau, \mu) = (1 - \tilde{\omega}_0^l) B[T(\tau)] \approx \sum_{k=1}^{N_k} a_k^l \tau^k, \quad (11)$$

where $\tilde{\omega}_0^l$ is the single scattering albedo of layer l and a_k^l are obtained by fitting the Planck function for the given temperature profile. Insert Eq. (11) into Eq. (8), the integration over τ' can be carried out analytically, but for simplicity, we omit the final results. In Qin et al. (2004) we presented the result of the convolution of

the IMGF with Eq. (11) when deriving the particular solution for atmospheric emission.

For a generalized beam source denoted by $I_0\delta(\tau' - \tau_0)\delta(\mu' - \mu_0)$, it cannot be used directly in Eq. (8) because the Green's function, Eq. (4), can only be evaluated at the Gaussian quadrature points. However, we can use the diffuse source function of the m th order, that is [cf. Eq. (6.14), Liou 1980],

$$\mathbf{Q}^l(\tau) = \frac{\tilde{\omega}_0^l}{4\pi} H[(\tau_0 - \tau)/\mu]_0 I_0 e^{-(\tau_0 - \tau)/\mu_0} \mathbf{p}^m \boldsymbol{\omega}^{l,m} \mathbf{p}_0^m, \quad (12)$$

where \mathbf{p}^m is a matrix whose i th row contains the (0 to N_m)th order of the associated Legendre polynomial (ALP) evaluated at the i th Gaussian quadrature point, μ_i , and N_m is the order of the phase function expansion; \mathbf{p}_0^m is a column vector containing the ALP evaluated at μ_0 , and $\boldsymbol{\omega}^{l,m}$ are the phase function expansion coefficients, I_0 is the beam source intensity, $H(x)$ is the Heaviside step function that equals 1 when $x \geq 0$, and zero otherwise. Insert Eq. (12) into Eq. (8), the integration over τ' can also be carried out analytically.

We now discuss another issue regarding the using of the Green's function. We note that the Green's function itself, Eq. (4) or its counterpart for a BRDF surface, contains both diffusely and directly transmitted components. This is an essential requirement for the convolution in Eq. (8) to work. However, we should be aware that the radiation field for a source computed using Eq. (8) may only have the diffuse part, depending on the source function, \mathbf{Q} . For example, in the case of the beam source, the direct component has been removed from the source function; therefore, the result of Eq. (8) contains the diffuse part only.

In the case that we need to remove the direct component from the Green's function, for example, when we validate our implementation against standard radiative transfer codes that compute the diffuse part only, we can subtract the diagonal elements of the Green's function matrix by

$$I_{\text{dir}}(\mu_i) = \frac{1}{(1 + \delta_{0m})\pi\mu_i w_i} H[(\tau_0 - \tau)/\mu_i] e^{-(\tau_0 - \tau)/\mu_i}, \quad (13)$$

where $(1 + \delta_{0m})\pi$ results from the expansion of $\delta(\phi - \phi_0)$, see Eq. (A14). The term $1/\mu_i$ is due to the fact that the Green's function is the radiation field generated by a beam source of unit flux, or $1/\mu_i$ units of intensity, see the discussion following Eq. (1). The term $1/w_i$ can be understood as the value of the discretized Dirac delta function at $\mu = \mu_i$. This ensures the quadrature form of the integration, $\int \delta(\mu - \mu_i) d\mu$, results in unity, which is required by the definition of the Dirac delta function. All other parts in the equation should be apparent.

As shown in Eq. (13), $I_{\text{dir}}(\mu_i)$ is in fact the negative of the DOM particular solution for the beam source illuminating exactly in the direction specified by μ_i . See Eq. (40) in Qin et al. (2004) where the z vector is the part of the particular solution excluding the exponential. From this point, we can deduce the connection between the DOM general solution and the Green's function matrix

$$\mathbf{\Gamma}^l(\tau)\mathbf{Y}^l = \mathbf{\Gamma}^l(\tau)\mathbf{T}^{l_0}(\tau, \tau_0)\mathbf{\Gamma}_0^{l_0}(\tau_0), \quad (14)$$

where the columns of \mathbf{Y}^l are the integral constant vectors of the DOM method, for the set of beam sources illuminating exactly in the zenith angles specified by the quadrature points. For such beam sources, adding the particular solution to the general solution results in the removal of the directly transmitted component.

4. Implementation, computing complexity, and validation

In this section, we discuss the implementation, computing complexity, and validation of the Green's function algorithm.

a. Implementation considerations and GDOM code

A FORTRAN 95 code, Green's function and discrete ordinate method (GDOM), has been developed by the authors. This code is composed of two modes: the Green's function (GF) mode and the extended discrete ordinate method (EDOM) mode. The two integrated modes can be used to compute the Green's function and/or DOM solutions in each run. A brief description of the EDOM mode is provided here, but all the details are available from the GDOM manual. Validation of the EDOM mode will be discussed together with the GF mode in the last part of this section.

The EDOM mode is an enhanced version of the EDOM code (Qin et al. 2002). It supports generalized beam sources (of arbitrary position and direction); generalized angular sources (of arbitrary position and continuous angular intensity) including surface/deep space emission; atmosphere emission represented by power series in optical thickness of virtually any order; therefore, it is able to accurately deal with a wide range of temperature profiles. The EDOM mode implemented the analytical particular solutions (Qin et al. 2004) resulting in much faster particular solution computation. Solutions for multiple sources of (mixed) types may be computed simultaneously, costing for each extra source less than 5% of the CPU time needed for the first full solution. BRDF surface is supported and radiance at arbitrary zenith angle is implemented by source func-

tion integration (Chalhoub and Garcia 2000). Delta-M scaling (Wiscombe 1977) and radiance corrections (Nakajima and Tanaka 1986, 1988) are implemented so that reasonably accurate radiances can be obtained using fewer streams, especially in the case of strong forward scattering.

We now turn our attention to the GF mode. To compute the Green's function, the following steps are needed:

- Construct the local scattering matrix defined by Eq. (B3), and compute all of its eigenvalues and vectors.
- Construct and solve the linear system of Eqs. (C17)–(C19) with a banded diagonal coefficient matrix and multiple rhs columns.

Both problems have been proven to be numerically stable (Stamnes et al. 1988), and are solved in GDOM using LAPACK (Anderson et al. 1999), which “is a library of numerical linear algebra subroutines designed for high performance on workstations, vector computers, and shared memory multiprocessors” (<http://rib.cs.utk.edu/cgi-bin/object.pl?rh=222&class=Asset&html=1&oh=30>). FORTRAN 95 has been chosen to write GDOM because of its apparent advantages in numerical computations such as, strong support to matrix operation and implicit parallelizing at the compiler level. Other considerations on numerical calculation: optional quadrature scheme (Legendre–Gauss quadrature or double-Gauss quadrature) and optional LAPACK driver routines (simple driver or expert driver).

Differing from the EDOM mode, which normally requires one entry point, the GF mode needs to work interactively with application programs. As illustrated in the previous section, in applications it is likely that the Green's function will be involved in some analytical computations, therefore the components of the Green's function (Φ_{\pm}^l , λ_{\pm}^l , and $\tilde{\mathbf{T}}^{l,l_0}$), rather than the Green's function as whole, are actually used. Because of this, it is important to provide convenient access to these components. It is also necessary to provide elemental computation functions that manipulate those components, for example, computing $\tilde{\mathbf{T}}_s^{l,l_0}$ from $\tilde{\mathbf{T}}^{l,l_0}$ for given surface BRDF model, and combining Φ_{\pm}^l and λ_{\pm}^l to compute $\mathbf{I}^l(\tau)$ for given τ , etc.

Access to internal data items is implemented through a user derived data type (FORTRAN name for compound data structure), which packs all the input parameters, and intermediate outputs, including Φ_{\pm}^l , λ_{\pm}^l , and $\tilde{\mathbf{T}}^{l,l_0}$, as its members. An object of this data type is firstly created in an application subprogram, which is then passed to GDOM subprograms to be initialized and manipulated. In turn, all the datasets stored in this ob-

ject are made available to application programs (including EDOM mode data such as particular solutions). On the other hand, it relieves us (both authors and users of GDOM) from passing a large number of arguments, especially to those elemental computation functions, because most information required by the GDOM subprograms is stored in this data object. The drawback is that no rule can be imposed on how the data members can be accessed: for example, almost all of them should be read-only to application programs. This is because of the lack of language support and we have to rely on the application programs to behave properly.

Delta-M scaling (Wiscombe 1977) and intensity corrections (Nakajima and Tanaka 1986, 1988) will be turned off in GF mode because the intensity corrections are developed only for beam sources at the top of atmosphere, and cannot be applied to individual terms of the azimuthal cosine series. Techniques that might be applicable to Green's function problem are being investigated.

Other programming considerations include: two levels of application program support to balance flexibility and complexity of using the code; support to select BRDF model at run time rather than compiling time; targeted use of caches to substantially reduce repeated computations; configuration module for centralized code configuration at compiling or run time. A manual is available detailing the theory and the code.

b. Computing complexity

As shown in the previous part, computing the Green's function requires solving an eigenvalue problem of a general $N_s \times N_s$ real matrix to compute Φ_{\pm}^l and λ_{\pm}^l for each layer, and solving a linear system that has a banded coefficient matrix and multiple rhs columns to obtain $\tilde{\mathbf{T}}^{l,l_0}$. The order of the coefficient matrix is $N \times 2N_s$ where N is the number of layers and $2N_s$ is the number of streams, and the number of rhs columns is $N_0 \times 2N_s$ where N_0 is the number of source layers (the count of all l_0). These two steps consume most of the CPU time. Therefore, the CPU time required to solve a Green's function problem depends roughly on $N \times N_s^3$.

The complexity of GF mode is comparable to that of the DOM, which also solves the same eigenvalue problems and a linear system of exactly the same coefficient matrix, but different number of rhs columns. Normally the DOM has only one rhs column though the EDOM mode of GDOM may have multiple columns, one for each source. Another difference is that the GF problem does not require the particular solution, while the DOM does. By first lower and upper triangular matrix (LU) decomposing the coefficient matrix, a solution for

each of the rhs columns can be computed efficiently using back substitution. Tests show that each extra rhs column increases the total CPU time by a fraction of 1% depending slightly on the number of layers and streams. The time required by the EDOM mode to compute the particular solution, for each beam source, ranges from 1.3% to 3.6% of the total time (Qin et al. 2004, their Table 2, lower portion). In conclusion, the Green's function of one source layer can be obtained using roughly the same amount of computation as required to solve a DOM problem of one beam source. When the Green's functions for multiple source layers are required, the time will increase because of the increase of the rhs columns as discussed in the previous paragraph. The increase of CPU time is illustrated in Table 1 (estimated using an IBM-compatible PC with single Pentium 4 1.8GHz CPU).

c. GDOM code validation

Validation measures that apply to both the GF and EDOM modes include cross comparison between the two modes, comparison with the original EDOM code (Qin et al. 2002), using the reciprocity principle to check internal (beam) sources against external sources. In the cross comparisons, almost identical results have been obtained (with relative differences at the level of one part per million).

For the EDOM mode, intensity comparison with DISORT (Stamnes et al. 1988) has been conducted for the 13 DISORT test cases, where each case has a number of variations. It is found that, when both codes are configured consistently, the maximum relative difference is less than 0.1% for most cases, and in no case does the maximum difference exceed 1%.

For the GF mode, we have conducted a comparison with DISORT as well for three sets of problems (Table 2). The phase functions used include the Rayleigh scattering and the phase function of the Haze L aerosol model (Garcia and Siewert 1985). Sets 1 and 2 have a single layer, and set 3 has two layers of equal optical thickness and single scattering albedo. The number of streams is respectively 16 (set 1) and 48 (sets 2 and 3).

TABLE 1. CPU time needed to solve a Green's function problem of one source layer compared to that of multiple source layers.

N_s	N	Time (s)	
		$N_0 = 1$	$N_0 = N$
8	12	0.063	0.219
16	6	0.406	0.766
16	12	0.859	2.875
32	12	16.359	63.141

TABLE 2. The relative difference (%) between GDOM-GF and DISORT for three sets of test cases. Shown here are the averaged difference, std dev, and the maximum difference.

Set 1: Rayleigh scattering, 16 streams, Lambertian (albedo = 0.2)			
τ	$\tilde{\omega}_0$	$\bar{\delta} \pm \sigma$ (%)	Max $ \delta $ (%)
0.1	0.5	0.0014 \pm 0.0118	0.0534
0.1	1	-0.0032 \pm 0.0130	0.0468
1	0.5	0.0015 \pm 0.0038	0.0177
1	1	0.0038 \pm 0.0084	0.0356
20	0.5	0.0018 \pm 0.0040	0.0177
20	1	0.0040 \pm 0.0085	0.0364
Set 2: Haze L, 48 streams, Lambertian (albedo = 0.2)			
0.1	0.5	0.0001 \pm 0.0005	0.0088
0.1	1	0.0000 \pm 0.0085	0.1327
1	0.5	0.0000 \pm 0.0020	0.0784
1	1	0.0000 \pm 0.0048	0.0414
20	0.5	0.0001 \pm 0.0003	0.0042
20	1	0.0021 \pm 0.0045	0.0293
Set 3: Rayleigh scattering and Haze L, 48 streams, BRDF (Hapke)			
0.1	0.5	-0.0006 \pm 0.0010	0.0066
0.1	1	-0.0014 \pm 0.0051	0.0480
20	0.5	-0.0011 \pm 0.0024	0.0140
20	1	-0.0016 \pm 0.0052	0.0325

The surface is Lambertian with albedo 0.2 for sets 1 and 2, and Hapke model (Hapke 1993) for set 3. The comparison is made for radiance at the top (upward only) and the bottom (upward and downward), for sources on the top illuminating downward in all the angles specified by the quadrature points. The directly transmitted radiance in the GDOM-GF output has been removed before the comparison (see section 3). When computing the radiances using DISORT, two more streams are used to avoid the conflict of equal source and radiance zenith angles. Therefore the comparison is not exactly the same but the influence is very small. We show in Table 2 the averaged relative difference, $\bar{\delta}$, the standard derivation, σ , and the maximum difference for each case. The difference is generally small though in one case the maximum difference exceeds 0.1%. Considering this comparison, together with other validation measures, the algorithm is implemented correctly.

5. Summary

In this paper we presented an explicit expression for the Green's function for radiative transfer problems in plane-parallel atmospheres, where the lower boundary may be vacuum or described by bidirectional reflectance distribution function (BRDF). A FORTRAN 95

code has also been developed to compute the Green's function.

The benefit of developing such an explicit expression for the Green's function is (at least) twofold: an analytical expression allows for analytical computations when the Green's function is employed, which is impossible if the GF is represented numerically; computing the Green's function is much more efficient. In contrast, using a standard radiative transfer code such as DISORT (Stamnes et al. 1988) or the EDOM mode of GDOM to accumulate a numerical GF could be very expensive, especially when the mesh of the source optical thickness has to be dense. The algorithm presented in this paper uses the proven technology of the discrete ordinate method, in particular DISORT (Stamnes et al. 1988), which ensures the numerical stability of the computer code. The accuracy of the GF algorithm is expected to be equivalent with that of the DOM algorithm.

In section 3 we used the forward radiative transfer problems for commonly seen source types as examples to illustrate how the developed Green's function matrix may be used. Another example can be found in Qin et al. (2005). It is shown that Green's function can be used to compute the radiance generated by (virtually) any source. However, we should point out that this approach is not specialized for the best efficiency in solving normal forward radiative transfer problems. In that case, specialized code such as DISORT (Stamnes et al. 1988) or the EDOM mode of GDOM is recommended. On the other hand, the Green's function approach be-

comes useful in, for example, inversion problems where the radiation field needs be computed repeatedly for changing surface BRDF, changing surface/deep space temperature or emissivity, or changing atmosphere temperature profile. The work by Benedetti et al. (2002) showed another example where we have a changing profile of the extinction coefficient. The Green's function approach makes it possible to reveal explicitly the dependence of the radiation field on the changing parameters.

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APPENDIX A

Radiative Transfer Equation and Its Reduction

In this appendix we define the radiative transfer problem in an infinite medium and reduce it to a set of subproblems that separate the azimuth angle from other variables. In an infinite and homogeneous medium illuminated by a parallel beam of unit flux, which extends indefinitely horizontally, that is,

$$\delta(\mu - \mu_0)\delta(\phi - \phi_0)\delta(\tau - \tau_0), \quad (\text{A1})$$

the Green's function satisfies the plane-parallel radiative transfer equation, which can be written as (Chandrasekhar 1960)

$$\mu \frac{dG(\tau_0, \mu_0, \phi_0; \tau, \mu, \phi)}{d\tau} = G(\tau_0, \mu_0, \phi_0; \tau, \mu, \phi) - \frac{\tilde{\omega}_0}{4\pi} \int_0^{2\pi} d\phi' \int_{-1}^1 d\mu' P(\mu', \phi'; \mu, \phi) G(\tau_0, \mu_0, \phi_0; \tau, \mu', \phi'), \quad (\text{A2})$$

where (τ_0, μ_0, ϕ_0) are the source's spatial position (optical depth, τ_0), and the propagation direction (cosine of zenith angle, μ_0 , and azimuth angle, ϕ_0). The corresponding variables for the random field are (τ, μ, ϕ) , $P(\mu', \phi'; \mu, \phi)$ is the scattering phase function, and $\tilde{\omega}_0$ is the single scattering albedo. In the case of a finite atmosphere, the top of atmosphere (TOA) optical depth is defined to be zero. For an infinite atmosphere, $\tau = 0$ can be set at any arbitrary layer. We also define the optical depth increases downward, and $\mu = \pm 1$ as pointing respectively to the zenith and the nadir.

For the case of an infinite medium, the radiation field must vanish at an infinite distance from the source (Case and Zweifel 1967), that is,

$$\lim_{\tau - \tau_0 \rightarrow \pm\infty} G(\tau_0, \mu_0, \phi_0; \tau, \mu, \phi) = 0. \quad (\text{A3})$$

The parallel beam source can be considered by the jump condition (Case and Zweifel 1967)

$$\lim_{\tau \rightarrow \tau_0^-} G(\tau_0, \mu_0, \phi_0; \tau, \mu, \phi) - \lim_{\tau \rightarrow \tau_0^+} G(\tau_0, \mu_0, \phi_0; \tau, \mu, \phi) = \frac{\delta(\mu - \mu_0)\delta(\phi - \phi_0)}{\mu}, \quad (\text{A4})$$

which shows the discontinuity of the radiation field when the source joins in at $\tau = \tau_0$.

We note that Eq. (A2) does not contain any external source term. The only source, the parallel beam, has been considered as the jump condition. Therefore, the

transfer equation considers the total (diffusely and directly transmitted) radiation. This differs from the usual convention that separates the two components in the process of solving the radiative transfer equation.

Equations (A2)–(A4) form the IMGF problem. We now separate the azimuth of the source and radiation field from other variables in order to reduce this problem to a set of independent simpler subproblems. This procedure is rather standard, but for completeness we briefly repeat it here. We first expand the Green's function and the phase function into cosine series (Chandrasekhar 1960, section 48)

$$G(\tau_0, \mu_0, \phi_0; \tau, \mu, \phi) = \sum_{m=0}^{N_m} G^m(\tau_0, \mu_0; \tau, \mu) \cos m(\phi_0 - \phi), \quad (\text{A5})$$

$$P(\mu', \phi'; \mu, \phi) = \sum_{n=0}^{N_m} (2 - \delta_{0,n}) \sum_{l=n}^{N_m} \tilde{\omega}_l^n p_l^n(\mu) p_l^n(\mu') \cos n(\phi - \phi'), \quad (\text{A6})$$

$$\tilde{\omega}_l^n = \frac{(l-n)!}{(l+n)!} \tilde{\omega}_l, \quad (\text{A7})$$

where $\tilde{\omega}_l$ are the coefficients of the phase function's Legendre polynomial expansion defined by

$$P(\Theta) = \sum_{l=0}^{\infty} \tilde{\omega}_l p_l[\cos(\Theta)], \quad (\text{A8})$$

where

$$\cos(\Theta) = \mu\mu_0 + (1 - \mu^2)^{1/2}(1 - \mu_0^2)^{1/2} \cos(\phi - \phi_0) \quad (\text{A9})$$

is the cosine of the scattering angle and p_l are the Legendre polynomials.

Insert Eqs. (A5) and (A6) into Eq. (A2) and carry out the integration over ϕ' . From the orthogonality of the cosine functions, the terms $m \neq n$ vanish and the summation over n can be removed. Group the resulting expression around $\cos m(\phi - \phi_0)$ and compare their coefficients on both sides, we obtain a set of independent equations as

$$\mu \frac{dG^m(\tau_0, \mu_0; \tau, \mu)}{d\tau} = G^m(\tau_0, \mu_0; \tau, \mu) - \frac{\tilde{\omega}_0}{2} \sum_{l=m}^{N_m} \tilde{\omega}_l^m p_l^m(\mu) \int_{-1}^1 p_l^m(\mu') G^m(\tau_0, \mu_0; \tau, \mu') d\mu' \quad (\text{A10})$$

$m = 0, 1, \dots, N_m.$

By approximately representing the angular distribution of the function G using a vector

$$[G(-\mu_1), \dots, G(-\mu_{N_s}), G(\mu_1), \dots, G(\mu_{N_s})] \quad (\text{A11})$$

and replacing the integral in Eq. (A10) with Gaussian quadrature, we obtain (Chandrasekhar 1960, section 48.1)

$$\mu_i \frac{dG^m(\tau_0, \mu_0; \tau, \mu_i)}{d\tau} = G^m(\tau_0, \mu_0; \tau, \mu_i) - \frac{\tilde{\omega}_0}{2} \sum_{l=m}^{N_m} \tilde{\omega}_l^m p_l^m(\mu_i) \sum_{j=\pm 1}^{\pm N_s} w_j p_l^m(\mu_j) G^m(\tau_0, \mu_0; \tau, \mu_j), \quad (\text{A12})$$

where the μ_i are the Gaussian quadrature points of order $2N_s$ and the w_j the corresponding weights. Applying the same process to Eqs. (A3)–(A4), we have

$$\lim_{\tau \rightarrow \tau_0 \pm} G^m(\tau_0, \mu_0; \tau, \mu_i) = 0, \quad (\text{A13})$$

$$\lim_{\tau \rightarrow \tau_0^-} G^m(\tau_0, \mu_0; \tau, \mu_i) - \lim_{\tau \rightarrow \tau_0^+} G^m(\tau_0, \mu_0; \tau, \mu_i) = \frac{1}{(1 + \delta_{0m})\pi\mu_i} \delta(\mu_i - \mu_0). \quad (\text{A14})$$

Therefore, we can solve Eq. (A12) independently for each m and find the solution to Eq. (A2) using Eq. (A5). Because of this, we will only deal with Eq. (A12) hereafter. For simplicity, the superscript, m , in Eqs. (A12)–(A14) will be omitted.

APPENDIX B

Infinite Medium Green's Function

This section derives the analytic infinite medium Green's function (IMGF), in terms of the source variables, (τ_0, μ_0) , and radiation field variables, (τ, μ) . The contents of this section are not by any means new except that we will use the matrix eigenvalue method seen in DISORT (Stamnes et al. 1988) to generalize the work of Case and Zweifel (1967), which deals with isotropic scattering only, to anisotropically scattering medium.

a. Elemental solutions

First we seek the elemental solution to Eq. (A12) of the following form (Stamnes et al. 1988):

$$\varphi(\mu) e^{-\lambda(\tau - \tau_0)}. \quad (\text{B1})$$

By inserting this into Eq. (A12), we obtain

$$\lambda \varphi(\mu_i) = \sum_{j=\pm 1}^{\pm N_s} C_{ij} \varphi(\mu_j) \quad (\text{B2})$$

$i = \pm 1, \pm 2, \dots, \pm N_s,$

where

$$C_{ij} = \mu_i^{-1} \left[\frac{\tilde{\omega}_0}{2} w_j \sum_{l=m}^{N_m} \tilde{\omega}_l^m p_l^m(\mu_i) p_l^m(\mu_j) - \delta_{ij} \right]. \quad (\text{B3})$$

Equation (B2) can be written in matrix form as

$$\lambda \begin{pmatrix} -\varphi \\ +\varphi \end{pmatrix} = \begin{pmatrix} -\mathbf{C}_- & -\mathbf{C}_+ \\ +\mathbf{C}_- & +\mathbf{C}_+ \end{pmatrix} \begin{pmatrix} -\varphi \\ +\varphi \end{pmatrix}, \quad (\text{B4})$$

where the \mathbf{C} are N_s by N_s matrices and the φ are N_s -element column vectors. The rows of \mathbf{C} and φ correspond to μ_i with their sign indicated by the left subscript, and the columns of \mathbf{C} correspond to μ_j with their sign indicated by the right subscript. From Eq. (B3) we see the block symmetric property of \mathbf{C} : $+\mathbf{C}_+ = -\mathbf{C}_-$ and $+\mathbf{C}_- = -\mathbf{C}_+$.

Equation (B4) is the eigenproblem of a general real matrix, which can be solved using any standard numerical library, for example, LAPACK (Anderson et al. 1999). However, by using the block symmetric property of the matrices \mathbf{C} , the order of the problem can be reduced by half (Asano 1975; Stamnes et al. 1988). Specifically, from Eq. (B4) we have

$$(+\mathbf{C}_+ - +\mathbf{C}_-)(+\mathbf{C}_+ + +\mathbf{C}_-)(+\varphi + -\varphi) = \lambda^2(+\varphi + -\varphi), \quad (\text{B5})$$

$$(+\mathbf{C}_+ + +\mathbf{C}_-)(+\varphi + -\varphi) = \lambda(+\varphi - -\varphi). \quad (\text{B6})$$

We see the order of problem Eq. (B5) is half that of Eq. (B4).

It is well known that problem Eq. (B4) generates $2N_s$ paired eigenvalues (Chandrasekhar 1960, section 48.3), $\pm\lambda_j$, $j = 1, \dots, N_s$, and correspondingly $2N_s$ eigenvectors, $[+\varphi_{\pm j}^T, -\varphi_{\pm j}^T]^T$. We put all these eigenvectors into one matrix as

$$\begin{bmatrix} -\varphi_{-1} \cdots -\varphi_{-N_s} & -\varphi_1 \cdots -\varphi_{N_s} \\ +\varphi_{-1} \cdots +\varphi_{-N_s} & +\varphi_1 \cdots -\varphi_{N_s} \end{bmatrix} \equiv \begin{bmatrix} -\Phi_- & -\Phi_+ \\ +\Phi_- & +\Phi_+ \end{bmatrix}, \quad (\text{B7})$$

which forms a $2N_s \times 2N_s$ matrix. For simplicity, matrix notation will be frequently used hereafter, especially the eigenvector matrix. Corresponding to the negative and positive values of μ_i and λ_j , this matrix can be divided into four submatrices, $\pm\Phi_{\pm}$, where the rows correspond to μ_i with their sign indicated by the left subscript, and the columns correspond to λ_j with their sign indicated by the right subscript. If the left subscript is omitted, it means the $2N_s \times N_s$ matrix corresponding to the whole range of μ_i . If both subscripts are omitted, it means the whole $2N_s \times 2N_s$ eigenvector matrix. We will also frequently use the transpose, denoted by a superscript, T, of the eigenvector matrix. In that case,

because the rows will be corresponding to the λ_j and the columns to μ_i , the meaning of the left and right subscripts should also be exchanged. Also, we often use the following interchangeable notations:

$$\begin{aligned} \mu_{\pm j} &\equiv \pm\mu_j, \\ w_{\pm j} &\equiv w_j, \\ \lambda_{\pm j} &\equiv \pm\lambda_j. \end{aligned} \quad (\text{B8})$$

b. Properties of eigenvectors

Case and Zweifel (1967, sections 4.5 and 4.6) have shown that the eigenvectors are orthogonal and form a complete set. Therefore the eigenvectors form the basis of a linear orthogonal space so that any function of μ can be uniquely expressed as a linear combination of the eigenvectors. Because the orthogonality of the eigenvectors is used throughout the article, we discuss it here briefly. The solution of Eq. (A12) that also satisfies the conditions Eqs. (A13) and (A14) will be presented in the next subsection.

By inserting the elemental solution, $\varphi_j(\mu)e^{-\lambda_j(\tau-\tau_0)}$, into Eq. (A10) we obtain

$$(\lambda_j\mu + 1)\varphi_j(\mu) = \frac{\tilde{\omega}_0}{2} \int_{-1}^1 d\mu' \varphi_j(\mu') \sum_{l=m}^{N_m} \tilde{\omega}_l^m p_l^m(\mu) p_l^m(\mu'). \quad (\text{B9})$$

Similarly we have

$$(\lambda_k\mu + 1)\varphi_k(\mu) = \frac{\tilde{\omega}_0}{2} \int_{-1}^1 d\mu' \varphi_k(\mu') \sum_{l=m}^{N_m} \tilde{\omega}_l^m p_l^m(\mu) p_l^m(\mu'). \quad (\text{B10})$$

For $j \neq k$, multiply Eq. (B9) by $\varphi_k(\mu)$ and Eq. (B10) by $\varphi_j(\mu)$, subtract and integrate over μ , we have

$$(\lambda_j - \lambda_k) \int_{-1}^1 \mu \varphi_j(\mu) \varphi_k(\mu) d\mu = 0. \quad (\text{B11})$$

This proves that $\varphi(\mu)$ are orthogonal with weighting function μ . For $j = k$, we define

$$N_j = \int_{-1}^1 \mu \varphi_j^2(\mu) d\mu, \quad (\text{B12})$$

which can be rewritten in matrix notation as

$$\Phi^T \mathbf{w} \mu \Phi = \mathbf{N}, \quad (\text{B13})$$

where \mathbf{w} , μ and \mathbf{N} are diagonal matrices of order $2N_s$,

$$\mathbf{w} = \text{diag}(w_j; j = -1, \dots, -N_s, 1, \dots, N_s), \quad (\text{B14})$$

$$\mu = \text{diag}(\mu_j; j = -1, \dots, -N_s, 1, \dots, N_s), \quad (\text{B15})$$

$$\mathbf{N} = \text{diag}(N_j; j = -1, \dots, -N_s, 1, \dots, N_s). \quad (\text{B16})$$

It is straightforward to show that

$$\begin{aligned} N_{-j} &= -N_j, \\ \Phi^{-1} &= \mathbf{N}^{-1} \Phi^T \mathbf{w} \boldsymbol{\mu}, \\ (\Phi^T)^{-1} &= \mathbf{w} \boldsymbol{\mu} \Phi \mathbf{N}^{-1}. \end{aligned} \quad (\text{B17})$$

Because of the block symmetry of the matrices \mathbf{C} , the eigenvector submatrices in Eq. (B7) have the following symmetry as well:

$$\begin{aligned} \pm \Phi_{\pm} &= \mp \Phi_{\mp}, \\ \mp \Phi_{\pm} &= \pm \Phi_{\mp}. \end{aligned} \quad (\text{B18})$$

c. Uniform expression for IMGF

In the previous subsection, it has been shown that $2N_s$ eigenvalues, λ_j , and eigenvectors, $\boldsymbol{\varphi}_j$, can be found. Each pair of $(\lambda_j, \boldsymbol{\varphi}_j)$ forms an elemental solution. All the elemental solutions satisfy Eq. (A12), and so do any of their linear combinations. This section is to find such a linear combination that satisfies the conditions Eqs. (A13)–(A14), so that a solution to the IMGF problem, defined by Eqs. (A12)–(A14), can be obtained.

Because at $\tau = \tau_0$ the function G is discontinuous as shown in Eq. (A14), the solution to the IMGF problem should be expressed separately for $\tau < \tau_0$ and $\tau > \tau_0$. Also, because Eq. (A13) is always satisfied by all the elemental solutions, only N_s terms are required in the linear combination, with N_s unknown coefficients. Case and Zweifel (1967, section 5.2) have suggested the following solutions:

$$G_{-}^{\infty}(\tau_0, \mu_0; \tau, \mu) = - \sum_{j=-1}^{-N_s} L_j \varphi_j(\mu) e^{\lambda_j(\tau_0 - \tau)} \quad \tau < \tau_0 \quad (\text{B19})$$

and

$$G_{+}^{\infty}(\tau_0, \mu_0; \tau, \mu) = \sum_{j=1}^{N_s} L_j \varphi_j(\mu) e^{\lambda_j(\tau_0 - \tau)} \quad \tau > \tau_0, \quad (\text{B20})$$

where the superscript, ∞ , indicates the infinite medium, and the L_j are unknown coefficients, which are to be determined from Eq. (A14). Using Eq. (A14), we have

$$- \sum_{j=\pm 1}^{\pm N_s} L_j \varphi_j(\mu) = \frac{\delta(\mu - \mu_0)}{(1 + \delta_{0m}) \pi \mu}. \quad (\text{B21})$$

Multiply both sides with $\mu \varphi_k(\mu)$ and integrate over μ from -1 to 1 , noting the orthogonality of the eigenvectors, we find

$$L_j = - \frac{1}{(1 + \delta_{0m}) \pi N_j} \varphi_j(\mu_0). \quad (\text{B22})$$

The infinite medium Green's function can now be written as

$$G_{\mp}^{\infty}(\tau_0, \mu_0; \tau, \mu) = - \sum_{j=1}^{N_s} \frac{\varphi_{\mp j}(\mu_0) \varphi_{\mp j}(\mu) e^{\lambda_{\mp j}(\tau_0 - \tau)}}{(1 + \delta_{0m}) N_{|\mp j|}}, \quad (\text{B23})$$

where the subscript \mp corresponds to $\tau < \tau_0$ and $\tau > \tau_0$, respectively.

Special consideration should be given to the case of $\tau = \tau_0$. To maintain the principle of reciprocity, the solution depends on the sign of μ_0 : for $\mu_0 > 0$, the solution is G_{-}^{∞} , and for $\mu_0 < 0$, the solution is G_{+}^{∞} . Note that although the right subscript of G_{\mp}^{∞} is used to indicate the range of τ relative to τ_0 , it has been made to be consistent with its counterpart in φ_{\mp} and λ_{\mp} . Rewriting Eq. (B23) in matrix notation, we have [recall the convention of Φ and Φ^T described following Eq. (B7)]

$$\mathbf{G}_{\mp}^{\infty}(\tau_0, \mu_0; \tau, \mu) = \Phi_{\mp}(\mu) \tilde{\Lambda}_{\mp}(\tau, \tau_0)_{\mp} \Phi^T(\mu_0), \quad (\text{B24})$$

where $\tilde{\Lambda}_{\mp}$ is an $N_s \times N_s$ diagonal matrix

$$\tilde{\Lambda}_{\mp}(\tau, \tau_0) = \text{diag} \left[- \frac{e^{\lambda_{\mp j}(\tau_0 - \tau)}}{(1 + \delta_{0m}) N_{|\mp j|}} \quad j = 1 \cdots N_s \right]. \quad (\text{B25})$$

Equation (B24) gives the analytic solution for the infinite medium, in terms of the source and function variables τ_0 , μ_0 , τ , and μ . Recalling Eq. (B18), this symmetric expression reveals the general principle of reciprocity. For the infinite medium, it is

$$\mathbf{G}_{\mp}^{\infty}(\tau, -\mu; \tau_0, -\mu_0) = \mathbf{G}_{\pm}^{\infty}(\tau_0, \mu_0; \tau, \mu). \quad (\text{B26})$$

APPENDIX C

Finite Medium Green's Function with Vacuum Boundaries

In this section, we derive the finite medium Green's function for vacuum (free) boundaries (FMGF-VB). We assume the atmosphere is composed of a stack of plane-parallel layers, each of which is homogeneous and has finite optical thickness. The layers are numbered from top to bottom as layer 1, 2, \dots , N . Therefore, the optical thickness in layer l is $\tau^{l-1} < \tau \leq \tau^l$. We assume the optical thickness at the top of the atmosphere $\tau^0 = 0$, and at the bottom of the atmosphere the optical thickness is $\tau^N = \tau_a$.

a. Constructing FMGF-VB

The radiative transfer equation used for the infinite medium applies to plane-parallel atmospheres as well.

Therefore, the problem of FMGF-VB is constituted by Eq. (A12) and the following vacuum boundary and continuity conditions:

$$G^1(\tau_0, \mu_0; 0, \mu) = 0 \quad \mu < 0, \quad (\text{C1})$$

$$G^{l-1}(\tau_0, \mu_0; \tau^{l-1}, \mu) = G^l(\tau_0, \mu_0; \tau^{l-1}, \mu), \quad l = 2, \dots, N, \quad (\text{C2})$$

$$G^N(\tau_0, \mu_0; \tau^N, \mu) = 0 \quad \mu > 0, \quad (\text{C3})$$

where a superscript, l , is used to denote the layer, and N is the total number of layers.

We use the IMGF to construct the solution to this problem according to Placzek's lemma (Bell and Glasstone 1970, section 2.5), which states that the radiative transfer problem in a finite homogeneous layer, for a given source, is equivalent to the problem in an infinite medium with the same properties as the finite layer, for three sources: the original source and two pseudosources, which are imposed on the boundaries of the finite layer and illuminate outwards, and they should have such distributions that the boundary and continuity conditions are satisfied. The pseudosources have apparently the same effect as the integral constants in the discrete ordinate method (cf. Stamnes et al. 1988).

According to the above statement, we denote the pseudosources imposed on the upper and lower boundaries of layer l as $\delta(\tau - \tau^{l-1})S'_l(\mu)$, where $\mu > 0$, and $\delta(\tau - \tau^l)S'_b(\mu)|_{\mu < 0}$, where $\mu < 0$, respectively. Because the radiation field generated by any source can be expressed as the convolution of the Green's function (of the same domain and boundary conditions) and the source flux, the combined radiation field within layer l can be expressed as

$$\begin{aligned} G^l(\tau_0, \mu_0; \tau, \mu) &= \delta_{l,l_0} G^{l,\infty}(\tau_0, \mu_0; \tau, \mu) \\ &+ \int_0^1 G_+^{l,\infty}(\tau^{l-1}, \mu'; \tau, \mu) |\mu'| |S'_l(\mu')| d\mu' \\ &+ \int_{-1}^0 G_-^{l,\infty}(\tau^l, \mu'; \tau, \mu) |\mu'| |S'_b(\mu')| d\mu', \end{aligned} \quad (\text{C4})$$

where the first term is the radiation field generated by the original source. Because each layer is treated inde-

pendently, the original source is effective only when it is inside this layer, that is, $l = l_0$ where l_0 denotes the source layer ($\tau^{l_0-1} < \tau_0 \leq \tau^{l_0}$). The second term is the radiation field generated by $\delta(\tau - \tau^{l-1})S'_l(\mu)$ [recalling the choice of the proper IMGF expression, $G_+^{l,\infty}$ or $G_-^{l,\infty}$, explained following Eq. (B23)]. We note that the term $|\mu'|$ is required in the integration to convert the source into flux. The last term is the radiation field generated by $\delta(\tau - \tau^l)S'_b(\mu)|_{\mu < 0}$.

b. Pseudosource problem

In above subsection, we have constructed the Green's function for each layer. However, the pseudosources are still unknown. In this subsection, we will find the pseudosources so that the boundary and continuity conditions are satisfied. First, we use Gaussian quadrature to replace the integrations in Eq. (A44), and by using Eqs. (B14)–(B15) and Eq. (B24), we rewrite Eq. (C4) in matrix form

$$\begin{aligned} \mathbf{G}^l(\tau_0, \mu_0; \tau, \mu) &= \delta_{l,l_0} \mathbf{G}^{l,\infty}(\tau_0, \mu_0; \tau, \mu) \\ &+ \mathbf{\Gamma}^l(\tau, \mu) \mathbf{S}^l(\tau_0, \mu_0), \end{aligned} \quad (\text{C5})$$

where

$$\mathbf{\Gamma}^l(\tau, \mu) = \begin{bmatrix} \mathbf{\Phi}'_+(\mu) & \mathbf{\Phi}'_-(\mu) \end{bmatrix} \begin{bmatrix} \mathbf{\Lambda}'_+(\tau, \tau^{l-1}) & \mathbf{0} \\ \mathbf{0} & \mathbf{\Lambda}'_-(\tau, \tau^l) \end{bmatrix} \quad (\text{C6})$$

and

$$\mathbf{S}^l(\tau_0, \mu_0) = \begin{bmatrix} -(\mathbf{N}'_+)^{-1} & +\mathbf{\Phi}'_+{}^T \mathbf{w} \mathbf{S}'_l(\tau_0, \mu_0) \\ -(\mathbf{N}'_+)^{-1} & -\mathbf{\Phi}'_-{}^T \mathbf{w} \mathbf{S}'_b(\tau_0, \mu_0) \end{bmatrix}, \quad (\text{C7})$$

where \mathbf{S}'_l and \mathbf{S}'_b are the vector notation of the pseudosources, $S'_l(\mu)$ and $S'_b(\mu)|_{\mu < 0}$, and

$$\mathbf{\Lambda}'_{\pm}(\tau, \tau_0) = \text{diag}(e^{\lambda'_{\pm j}(\tau_0 - \tau)}, j = 1, \dots, N_s). \quad (\text{C8})$$

We further define

$$\mathbf{\Gamma}_0^{l_0}(\tau_0, \mu_0) = \begin{bmatrix} \mathbf{\Lambda}_0^{l_0}(\tau^{l_0-1}, \tau_0) & \mathbf{0} \\ \mathbf{0} & \mathbf{\Lambda}_+^{l_0}(\tau^{l_0}, \tau_0) \end{bmatrix} \begin{bmatrix} -\mathbf{\Phi}_0^{l_0 T}(\mu_0) \\ +\mathbf{\Phi}_+^{l_0 T}(\mu_0) \end{bmatrix} \quad (\text{C9})$$

and

$$\mathbf{T}^{l,\infty} = \delta_{l,l_0} \begin{bmatrix} \mathbf{0} & H(\tau - \tau_0) \mathbf{\Xi}'^l \mathbf{\Lambda}_+(\tau^{l-1}, \tau^l) \\ H(\tau_0 - \tau) \mathbf{\Xi}'^l \mathbf{\Lambda}_+(\tau^{l-1}, \tau^l) & \mathbf{0} \end{bmatrix}, \quad (\text{C10})$$

where

$$\Xi^l = [-(1 + \delta_{0m})\pi\mathbf{N}_+^l]^{-1} \quad (\text{C11})$$

and $H(x)$ is the Heaviside step function which equals 1 when $x \geq 0$ and zero otherwise. The IMGF can then be written as

$$\mathbf{G}^{l,\infty}(\tau_0, \mu_0; \tau, \mu) = \Gamma^l(\tau, \mu)\mathbf{T}^{l,\infty}\Gamma_0^{l_0}(\tau_0, \mu_0). \quad (\text{C12})$$

We note from Eq. (B18) that

$$\Gamma_0^{l_0}(\tau_0, \mu_0) = [\Gamma^{l_0}(\tau_0, -\mu_0)]^T. \quad (\text{C13})$$

Now applying Eq. (C5) to the boundary and continuity conditions, Eqs. (C1)–(C3), we obtain

$$-\Gamma^1(0, -\mu)\mathbf{S}^1(\tau_0, \mu_0) = \Gamma^1(0, -\mu)\mathbf{T}^{1,\infty}\Gamma_0^{l_0}(\tau_0, \mu_0), \quad (\text{C14})$$

$$\Gamma^{l-1}(\tau^{l-1}, \mu)\mathbf{S}^{l-1}(\tau_0, \mu_0) - \Gamma^l(\tau^{l-1}, \mu)\mathbf{S}^l(\tau_0, \mu_0) = \Gamma^l(\tau^{l-1}, \mu)\mathbf{T}^{l,\infty}\Gamma_0^{l_0}(\tau_0, \mu_0) - \Gamma^{l-1}(\tau^{l-1}, \mu)\mathbf{T}^{l-1,\infty}\Gamma_0^{l_0}(\tau_0, \mu_0), \quad (\text{C15})$$

$$l = 2, \dots, N,$$

$$\Gamma^N(\tau^N, +\mu)\mathbf{S}^N(\tau_0, \mu_0) = -\Gamma^N(\tau^N, \mu)\mathbf{T}^{N,\infty}\Gamma_0^{l_0}(\tau_0, \mu_0), \quad (\text{C16})$$

where $\pm\mu$ in $\Gamma^l(\tau, \mu)$ indicates that only the rows for $\mu > 0$ or $\mu < 0$ are included. In the above linear system, the right-hand side contains a common factor, $\Gamma_0^{l_0}(\tau_0,$

$\mu_0)$, which can be removed by denoting $\mathbf{T}^{l,l_0} \equiv \mathbf{S}^l[\Gamma_0^{l_0}(\tau_0, \mu_0)]^{-1}$. We then obtain

$$-\Gamma^1(0, -\mu)\mathbf{T}^{1,l_0} = \delta_{1,l_0}[-\Phi_-^{l_0}\Xi^{l_0} \quad \mathbf{0}], \quad (\text{C17})$$

$$\Gamma^{l-1}(\tau^{l-1}, \mu)\mathbf{T}^{l-1,l_0} - \Gamma^l(\tau^{l-1}, \mu)\mathbf{T}^{l,l_0} = \delta_{l,l_0}[\Phi_-^{l_0}\Xi^{l_0} \quad \mathbf{0}] - \delta_{l-1,l_0}[\mathbf{0} \quad \Phi_+^{l_0}\Xi^{l_0}] \quad l = 2, \dots, N, \quad (\text{C18})$$

$$\Gamma^N(\tau^N, +\mu)\mathbf{T}^{N,l_0} = -\delta_{N,l_0}[\mathbf{0} \quad \Phi_+^{l_0}\Xi^{l_0}]. \quad (\text{C19})$$

It is apparent that \mathbf{T}^{l,l_0} depends only on l and l_0 . We have therefore obtained a source-independent system of equations, with a block-band coefficient matrix. The system can be solved using a standard routine. For example, LAPACK (Anderson et al. 1999) provides a subroutine to solve a general real band system by factorizing the coefficient matrix. By doing so, the solution for many right-hand side vectors (corresponding to source layers) can be found rather efficiently using back substitution.

c. Uniform expression of FMGF-VB

Once the pseudosource kernels, \mathbf{T}^{l,l_0} , are obtained, the FMGF-VB can be readily evaluated. From Eq. (C5), and recall that $\mathbf{S}^l \equiv \mathbf{T}^{l,l_0}\Gamma_0^{l_0}(\tau_0, \mu_0)$, we have

$$\mathbf{G}^l = \Gamma^l(\tau, \mu)\tilde{\mathbf{T}}^{l,l_0}(\tau, \tau_0)\Gamma_0^{l_0}(\tau_0, \mu_0), \quad (\text{C20})$$

where $\Gamma^l(\tau, \mu)$ and $\Gamma_0^{l_0}(\tau_0, \mu_0)$ are defined in Eqs. (C6) and (C9), and the kernel $\tilde{\mathbf{T}}^{l,l_0}$ has combined the IMGF and the pseudosource kernels

$$\tilde{\mathbf{T}}^{l,l_0}(\tau, \tau_0) = \mathbf{T}^{l,l_0} + \mathbf{T}^{l,\infty}. \quad (\text{C21})$$

When $l \neq l_0$, that is, the source is not in layer l , $\tilde{\mathbf{T}}^{l,l_0}$ is independent of τ_0 and τ . When $l = l_0$, $\tilde{\mathbf{T}}^{l,l_0}$ changes at the point $\tau = \tau_0$ due to the IMGF kernel, which reflects the fact that the radiation field is discontinuous when the

beam source joins in [Eq. (A4)]. Also, it can be shown that $\mathbf{T}^{l,l_0} = (\mathbf{T}^{l_0,l})^T$, which is in agreement with the general principle of reciprocity, that is,

$$\mathbf{G}(\tau, -\mu; \tau_0, -\mu_0) = \mathbf{G}(\tau_0, \mu_0; \tau, \mu). \quad (\text{C22})$$

The major steps to obtain the FMGF include an eigenvalue problem for the matrix \mathbf{C} defined in Eq. (B3), and to solve the linear system of Eqs. (C17)–(C19). The eigenvalue problem is exactly the same as in DOM and the linear system also has the same left-hand side matrix. Both are proven to be stable for numerical calculations (Stamnes et al. 1988). However, we note that the $\mathbf{T}^{l,\infty}$ as defined in Eq. (C10) has a growing exponential term, which could cause overflow if the source layer is very thick, combined with very large eigenvalues, which occurs when a quadrature point is very close to 0.0 (or 90°) and the layer is strongly absorbing. Numerical testing shows that, when in double precision, using 48 streams and normal Gaussian quadrature, for $\tilde{\omega}_0 = 0.5$, the total optical thickness of the source layer can be as large as 10 without causing overflow. However, simple solutions exist if it does become a problem, for example, splitting the source layer into thinner sublayers when initializing input parameters, or replacing the IMGF part in Eq. (C20) with Eq. (B24).

A permanent solution, which we are considering introducing in the future, uses the layer splitting method,

but the splitting will be carried out after the eigenvalue problem and the pseudosource problem have been finished, when the maximum sublayer thickness can be determined precisely. The kernel for the new layers can then be computed from the old kernels, which involves (at most) two multiplications of a (full) matrix with diagonal matrix for each new layer. This method does not change the formulations obtained, while the extra computation is considered to be small.

APPENDIX D

Finite Medium Green's Function with Reflective Surface

In this appendix, we use Eq. (C20) to construct the Green's function with a reflective surface. The reflective surface is described by a general BRDF, with the only assumption that it depends only on the phase angle between the incidence and reflection directions. Therefore we can expand it into a Fourier cosine series, that is,

$$A_s(-\mu', \phi' \rightarrow \mu, \phi) = \sum_{m=0}^{N_m} A_s^m(-\mu' \rightarrow \mu) \cos m(\phi' - \phi), \quad (\text{D1})$$

where $(-\mu', \phi')$ denotes the incidence direction and (μ, ϕ) the reflection direction. When such a surface is present on the lower boundary, the radiation reflected back by the surface can be expressed as

$$I_r(\tau_0, \mu_0, \phi_0; \tau_a, \mu', \phi') = \int_0^{2\pi} d\phi'' \int_{-1}^0 d\mu'' A_s(\mu'', \phi'' \rightarrow \mu', \phi') |\mu''| G_s(\tau_0, \mu_0, \phi_0; \tau_a, \mu'', \phi''), \quad (\text{D2})$$

where τ_a is the optical depth at the bottom of the atmosphere and G_s is the radiation field when the reflective surface is present, which is yet to be determined. The radiative transfer problem of a reflective surface can be viewed as a problem of vacuum boundaries with two sources: the original source and a source equivalent to the reflected radiance. Therefore, the radiation field is a combination of the radiation field generated by the two sources, that is,

$$G_s(\tau_0, \mu_0, \phi_0; \tau, \mu, \phi) = G(\tau_0, \mu_0, \phi_0; \tau, \mu, \phi) + \int_0^{2\pi} d\phi' \int_0^1 d\mu' G(\tau_a, \mu', \phi'; \tau, \mu, \phi) |\mu'| I_r(\tau_0, \mu_0, \phi_0; \tau_a, \mu', \phi'). \quad (\text{D3})$$

In the above equation, the first term of the right-hand side represents the radiation generated by the original source, which is just the Green's function for vacuum boundaries. The second term is the radiation field generated by the reflected radiation. We also expand G_s into a Fourier cosine series as

$$G_s(\tau_0, \mu_0, \phi_0; \tau, \mu, \phi) = \sum_{m=0}^{N_m} G_s^m(\tau_0, \mu_0; \tau, \mu) \cos m(\phi_0 - \phi). \quad (\text{D4})$$

Insert Eqs. (A5), (D1), (D4) into Eq. (D3) and note the orthogonality of the cosine functions, two of the summations can be removed. By regrouping the resulting expression around $\cos m(\phi_0 - \phi)$ and equating their coefficients, we have

$$G_s(\tau_0, \mu_0; \tau, \mu) = G(\tau_0, \mu_0; \tau, \mu) + \pi(1 + \delta_{0m})^2 \times \int_0^1 d\mu' |\mu'| G(\tau_a, \mu'; \tau, \mu) \int_{-1}^0 d\mu'' A_s(\mu'' \rightarrow \mu') |\mu''| G_s(\tau_0, \mu_0; \tau_a, \mu''). \quad (\text{D5})$$

Note that we have again omitted the superscript, m , for simplicity. Rewriting Eq. (D5) in matrix form, the unknown term $G_s(\tau_0, \mu_0; \tau_a, \mu'')$ can be found. We finally obtain

$$\mathbf{G}_s(\tau_0, \mu_0; \tau, \mu) = \mathbf{G}(\tau_0, \mu_0; \tau, \mu) + \mathbf{G}(\tau_a, +\mu; \tau, \mu) \tilde{\mathbf{A}}_s \times (-\mu; +\mu) [\mathbf{I} - \mathbf{G}(\tau_a, +\mu; \tau_a, -\mu) \tilde{\mathbf{A}}_s] \times (-\mu; +\mu)^{-1} \mathbf{G}(\tau_0, \mu_0; \tau_a, -\mu), \quad (\text{D6})$$

where \mathbf{I} is the identity matrix, and

$$\tilde{\mathbf{A}}_s(-\mu; +\mu) = \pi(1 + \delta_{0m})^2 \mathbf{w} |\boldsymbol{\mu}| \mathbf{A}_s(-\mu; +\mu) \mathbf{w} |\boldsymbol{\mu}|, \quad (\text{D7})$$

where \mathbf{w} and $\boldsymbol{\mu}$ are diagonal matrices defined in Eqs. (B14)–(B15). Using Eq. (C20), we obtain from Eq. (D6)

$$\mathbf{G}_s^{l,l_0}(\tau_0, \mu_0; \tau, \mu) = \boldsymbol{\Gamma}^l(\tau, \mu) \tilde{\mathbf{T}}_s^{l,l_0}(\mathbf{A}_s; \tau, \tau_0) \boldsymbol{\Gamma}_0^{l_0}(\tau_0, \mu_0), \quad (\text{D8})$$

where

$$\tilde{\mathbf{T}}_s^{l,l_0} = \tilde{\mathbf{T}}^{l,l_0} + \tilde{\mathbf{T}}^{l,N} \tilde{\mathbf{T}}_{ms}^{N,N}(\mathbf{A}_s) \tilde{\mathbf{T}}^{N,l_0}, \quad (\text{D9})$$

where

$$\tilde{\mathbf{T}}_{ms}^{N,N}(\mathbf{A}_s) = \boldsymbol{\Gamma}_0^N(\tau_a, \mu_+) \tilde{\mathbf{A}}_s [\mathbf{I} - \boldsymbol{\Gamma}^N(\tau_a, \mu_-) \tilde{\mathbf{T}}^{N,N} \boldsymbol{\Gamma}_0^N] \times (\tau_a, \mu_+) \tilde{\mathbf{A}}_s^{-1} \boldsymbol{\Gamma}^N(\tau_a, \mu_-), \quad (\text{D10})$$

where N is the total number of layers of the atmosphere. We see that the Green's function with a reflective surface is similar to that for vacuum boundaries, except that the kernel matrix, $\bar{\mathbf{T}}_x^{i,j_0}$, also depends on the surface BRDF.

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