Particular solution of the discrete-ordinate method

Yi Qin, Michael A. Box, and David L. B. Jupp

We present two methods that can be used to derive the particular solution of the discrete-ordinate method (DOM) for an arbitrary source in a plane-parallel atmosphere, which allows us to solve the transfer equation 12–18% faster in the case of a single beam source and is even faster for the atmosphere thermal emission source. We also remove the divide by zero problem that occurs when a beam source coincides with a Gaussian quadrature point. In our implementation, solution for multiple sources can be obtained simultaneously. For each extra source, it costs only 1.3–3.6% CPU time required for a full solution. The GDOM code that we developed previously has been revised to integrate with the DOM. Therefore we are now able to compute the Green's function and DOM solutions simultaneously. © 2004 Optical Society of America

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1. Introduction

Recently we have developed an algorithm to compute the Green's function for radiative transfer in a plane–parallel atmosphere,[1] and a FORTRAN 95 computer code, GDOM, has been developed to implement this algorithm. In the mean time, the EDOM code,[2] which is a special implementation of the discrete-ordinate method (DOM)[3] and is capable of computing simultaneously the radiation fields for multiple sources, has been revised and integrated into the GDOM code to form a code package that provides comprehensive functionalities for radiative transfer computation.

In the new version of GDOM, a number of improvements have been included. In this paper we discuss the improvements on the computation of the DOM particular solution. Since the DOM algorithm was developed by Chandrasekhar,[3] especially after the first numerically stable implementation, the discrete-ordinate radiative transfer (DISORT) code,[4] became available, this algorithm has become a classical method for radiative transfer computation. However, accurate radiative transfer computation is generally a time-consuming process, and improvements are always required. One of them is the particular solution, which was usually obtained by the solution of one or more linear equations systems[4] depending on the source type. Godsalve[5] has demonstrated that the order of the linear systems can be reduced by half. However, the burden of solving the linear systems can be completely avoided, for example, by use of the infinite medium Green's function.[6] It is particularly beneficial to cut back the CPU time on the particular solution computation when the solutions of the radiative transfer equation for multiple sources are sought, for example, in the computation of look-up tables for atmosphere correction[7] or the retrieval of atmospheric properties from multiangular observation[8,9] with the perturbation theory.[10] In such cases, the particular solution becomes the major consumer of CPU time (see the standard approach rows in Table 1).

In Section 2 we briefly review the standard approach used to find the particular solution for the solar beam source and demonstrate how to avoid solving the linear equations system. Then we present two generally applicable methods that can be used to derive analytic particular solutions (APSs) for any source function. Following this general discussion, the particular solutions for generalized beam sources are presented in Section 3, and the particular solution for angularly distributed sources (ADSs; an example is the thermal emission from the Earth's surface) and atmosphere thermal emission sources are presented in Section 4. In Section 5 we provide some sample results and a comparison with DISORT[4]; the paper is summarized in Section 6.

Y. Qin and M. A. Box (m.box@unsw.edu.au) are with the School of Physics, University of New South Wales, Sydney, New South Wales 2052, Australia. D. L. B. Jupp is with the Earth Observation Centre, Commonwealth Scientific and Industrial Research Organization, Australia.

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It is known that computation of the particular solution for a beam source, divide by zero, or the inverting of a singular matrix, may be encountered if the beam source happens to illuminate in a direction that coincides with one of the Gaussian quadrature points.[4] In Subsection 3.B the reason for this problem is analyzed, and a special particular solution is developed that completely removes the numerical difficulty.

2. General Discussion on the Particular Solution

In this section we first set up the context for the whole paper. After that, we briefly review the standard approach to compute the particular solution (Subsection 2.A), and two general methods are presented (Subsections 2.B and 2.C) that can be used to derive an APS for any source. To show the connection between these approaches, the solar beam source is used as an example.

The first step of the DOM is to expand the intensity into a Fourier cosine series and represent each Fourier component of the intensity as a vector of intensities at a finite number of zenith angles. This process decomposes the radiative transfer equation into a set of independent systems of linear differential equations, each for one order of the intensity series. This procedure can be found in a number of texts.[3,4] We start from the equation for the mth-order term of the intensity series, which can be written as[3]

$$\frac{\mathrm{d}I^m(\tau, \mu_i)}{\mathrm{d}\tau} = -\sum_{j=\pm 1}^{\pm N_s} C_{ij} I^m(\tau, \mu_j) - {\mu_i}^{-1} Q^m(\tau, \mu_i), \qquad i, j = \pm 1, \cdots, \pm N_s \tag{1}$$

where I^m is the coefficient of the mth term of the intensity series, τ is the optical thickness, the μ_i's are the Gaussian quadrature points, $2N_s$ is the total number of intensity streams that are used to approximately represent the intensity, and Q^m is the coefficient of the mth term of the source function's Fourier series. In Eq. (1),

$$C_{ij} = {\mu_i}^{-1} \left[\frac{\tilde{\omega}_0}{2} w_j \sum_{l=m}^{N_m} \tilde{\omega}_l{}^m p_l{}^m(\mu_i) p_l{}^m(\mu_j) - \delta_{ij} \right], \qquad i, j = \pm 1, \cdots, \pm N_s \tag{2}$$

where $\tilde{\omega}_0$ is the single-scattering albedo, the w_i's are the Gaussian quadrature weights, $\tilde{\omega}_l{}^m$ is the coefficient of the phase function's Legendre series multiplied with $(l-m)!/(l+m)!$, $p_l{}^m$ is the associated Legendre function, and δ_{ij} is the Kronecker delta that equals 1 if $l = j$ or 0 otherwise.

In Eq. (1), Q^m depends on the type of source. For the solar beam source, it can be written as

$$Q^m(\tau, \mu_i) = d_i \exp(\tau/\mu_0), \; i = \pm 1, \cdots, \pm N_s, \tag{3}$$

where

$$d_i = \frac{I_0}{\pi(1 + \delta_{0m})} \frac{\tilde{\omega}_0}{2} \sum_{l=m}^{N_m} \tilde{\omega}_l{}^m p_l{}^m(\mu_i) p_l{}^m(\mu_0), \tag{4}$$

where $\mu_0 < 0$ is the cosine of the solar zenith angle and I_0 is the solar intensity.

To simplify our notation, we rewrite Eq. (1) in matrix form and omit the superscript m:

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \mathbf{I}(\tau) = -\mathbf{C}\mathbf{I}(\tau) - \boldsymbol{\mu}^{-1}\mathbf{Q}(\tau), \tag{5}$$

where $\mathbf{I}$ and $\mathbf{Q}$ are column vectors, $\mathbf{C}$ is a square matrix, and $\mathbf{I}$ is a diagonal matrix composed of the Gaussian quadrature points. For the solar beam source, we write Eq. (3) in matrix notation as

$$\mathbf{Q}(\tau) = \mathbf{d} \exp(\tau/\mu_0), \tag{6}$$

where $\mathbf{d}$ is a column vector with its elements defined in Eq. (4).

The solution to Eqs. (1)–(5) is generally expressed as a two-term summation in the DOM: the general solution and the particular solution. The general solution is the solution to the homogeneous version of the equation (which does not consider the source term), and the particular solution is the solution to the whole equation disregarding the boundary conditions. Detailed discussions of the DOM algorithm can be found in Refs. 3 and 4. The two terms of the solution are also discussed in Subsection 2.B, in particular Eq. (19). In this paper we provide alternative, more efficient, and applicable methods to obtain the particular solution, compared with the standard approach that is reviewed in Subsection 2.A.

A. Standard Approach and Its Improvement

To compute the particular solution with the standard approach we try to find a solution that is appropriate to the specific pattern of the source function. For example, in the case of the solar beam source, the pattern of its source function Q_m in Eq. (6) suggests the following solution[4]:

$$\mathbf{I}_p(\tau) = \mathbf{z} \exp(\tau/\mu_0), \tag{7}$$

where $\mathbf{I}_p$ and $\mathbf{z}$ are column vectors. By inserting Eq. (7) into Eq. (5) and comparing the coefficients of $\exp(\tau/\mu_0)$ on both sides, we obtain

$$(\mathbf{C} + \mathbf{E}/\mu_0)\mathbf{z} = -\boldsymbol{\mu}^{-1}\mathbf{d}, \tag{8}$$

where $\mathbf{E}$ is the identity matrix.

The usual method to find the vector $\mathbf{z}$ is to solve Eq. (8) numerically,[4] which is straightforward but not an efficient method. In fact, Eq. (8) can be solved analytically. By using the eigenvalues and corresponding eigenvectors of matrix $\mathbf{C}$, which we obtained by computing the general solution,[4] we can diagonalize $\mathbf{C}$ as[1]

$$\mathbf{C} = \boldsymbol{\Phi}\boldsymbol{\lambda}\boldsymbol{\Phi}^{-1}, \tag{9}$$

where $\boldsymbol{\lambda}$ is a diagonal matrix composed of the eigenvalues of $\mathbf{C}$ and the columns of $\mathbf{U}$ are the eigenvectors corresponding to $\boldsymbol{\lambda}$. Because of the orthogonality of the eigenvectors,[11] we can compute the inverse of $\mathbf{U}$ using[1]

$$\boldsymbol{\Phi}^{-1} = \mathbf{N}^{-1}\boldsymbol{\Phi}^T\mathbf{w}\boldsymbol{\mu}, \tag{10}$$

where $\mathbf{N}$ is a diagonal matrix defined as

$$N_j = \boldsymbol{\phi}_j^{\,T}\mathbf{w}\boldsymbol{\mu}\boldsymbol{\phi}_j, \; j = \pm 1, \cdots, \pm N_s, \tag{11}$$

where $\boldsymbol{\phi}_j$ is the jth column of $\boldsymbol{\Phi}$. $\mathbf{w}$ and $\boldsymbol{\mu}$ are diagonal matrices composed of the Gaussian quadrature weights and points. Using Eqs. (9) and (10) we obtain

$$\mathbf{z} = -\boldsymbol{\Phi}[(\boldsymbol{\lambda} + \mathbf{E}/\mu_0)\mathbf{N}]^{-1}\boldsymbol{\Phi}^T\mathbf{wd}. \tag{12}$$

The particular solution for the solar beam source can then be obtained from Eq. (7). We note that, because the eigenvalues and eigenvectors are already available from the general solution, evaluating Eq. (12) involves only two matrix-vector multiplications, which needs $O(N^2)$ operations (multiplications and additions). In comparison, $O(N^3)$ operations are generally required to solve a linear equation system such as Eq. (8). Comparison computations are given in Section 5.

B. Method 1 for General Source Functions

Above we showed a method to derive an APS for the solar beam source. This approach, however, depends on the pattern of the source function Q and is not generally applicable. In this subsection we present a method that can be used to derive the APS for any source function.

Assume that $\mathbf{I}_g$ is a matrix whose columns are the solutions to the homogeneous version of Eq. (5), i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{I}_g(\tau) = -\mathbf{C}\mathbf{I}_g(\tau), \tag{13}$$

where $\mathbf{I}_g$ is of the following form[3]:

$$\mathbf{I}_g(\tau) = \boldsymbol{\Phi}\exp(-\boldsymbol{\lambda}\tau). \tag{14}$$

Because $\mathbf{I}_g$ is invertible [compare with Eq. (10)], we obtain

$$\frac{\mathrm{d}}{\mathrm{d}\tau}(\mathbf{I}_g\mathbf{I}_g^{\,-1}) = \frac{\mathrm{d}\mathbf{I}_g}{\mathrm{d}\tau}\mathbf{I}_g^{\,-1} + \mathbf{I}_g\frac{\mathrm{d}\mathbf{I}_g^{\,-1}}{\mathrm{d}\tau} \equiv 0. \tag{15}$$

By using Eq. (13) we obtain

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{I}_g^{\,-1}(\tau) = -\mathbf{I}_g^{\,-1}\frac{\mathrm{d}\mathbf{I}_g(\tau)}{\mathrm{d}\tau}\mathbf{I}_g^{\,-1} = \mathbf{I}_g^{\,-1}\mathbf{C}. \tag{16}$$

Multiplying both sides of Eq. (5) with $\mathbf{I}_g^{\,-1}$ and replacing $\mathbf{I}_g^{\,-1}\mathbf{C}$ with $(\mathrm{d}/\mathrm{d}\tau)\mathbf{I}_g^{\,-1}(\tau)$, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}\tau}[\mathbf{I}_g^{\,-1}(\tau)\mathbf{I}(\tau)] = -\mathbf{I}_g^{\,-1}(\tau)\boldsymbol{\mu}^{-1}\mathbf{Q}(\tau), \tag{17}$$

which leads to

$$\mathbf{I}_g^{\,-1}(\tau)\mathbf{I}(\tau) = \mathbf{Y} - \int_{\tau_1}^{\tau}\mathbf{I}_g^{\,-1}(t)\boldsymbol{\mu}^{-1}\mathbf{Q}(t)\mathrm{d}t, \tag{18}$$

where $\mathbf{Y}$ is any (integral) constant vector and τ_1 can be set to any value, which will only cause a difference of a constant vector. Equation (18) leads to

$$\mathbf{I}(\tau) = \mathbf{I}_g(\tau)\mathbf{Y} - \mathbf{I}_g(\tau)\int_{\tau_1}^{\tau}\mathbf{I}_g^{\,-1}(t)\boldsymbol{\mu}^{-1}\mathbf{Q}(t)\mathrm{d}t, \tag{19}$$

where the first term is the general solution and the second term is the particular solution. Using Eqs. (10) and (14), we obtain the following general expression for the particular solution:

$$\mathbf{I}_p(\tau) = -\int_{\tau_1}^{\tau}\boldsymbol{\Phi}\exp[\boldsymbol{\lambda}(t-\tau)]\mathbf{N}^{-1}\boldsymbol{\Phi}^T\mathbf{w}\mathbf{Q}(t)\mathrm{d}t. \tag{20}$$

We note again that $\boldsymbol{\lambda}$, $\mathbf{N}$, and $\mathbf{w}$ are all diagonal matrices and $\mathbf{Q}$ is a column vector.

In the case of a solar beam source, we choose τ_1 to be the optical thickness at the top of the layer in question. By inserting Eq. (6) into Eq. (20) and combining the scalar term $\exp(t/\mu_0)$ with $\exp[\boldsymbol{\lambda}(t-\tau)]$, we can carry out the integration:

$$\begin{aligned}\mathbf{I}_p(\tau) &= -\boldsymbol{\Phi}\exp(-\boldsymbol{\lambda}\tau)\\ &\quad\times\left\{\int_{\tau_1}^{\tau}\exp[(\boldsymbol{\lambda} + 1/\mu_0)t]\mathrm{d}t\right\}\mathbf{N}^{-1}\boldsymbol{\Phi}^T\mathbf{wd}\\ &= -\boldsymbol{\Phi}[(\boldsymbol{\lambda} + 1/\mu_0)\mathbf{N}]^{-1}\boldsymbol{\Phi}^T\mathbf{wd}\exp(\tau/\mu_0)\\ &\quad+\boldsymbol{\Phi}\exp(-\boldsymbol{\lambda}\tau)\mathbf{z}_g,\end{aligned} \tag{21}$$

where

$$\mathbf{z}_g = [(\boldsymbol{\lambda} + 1/\mu_0)\mathbf{N}]^{-1}\exp[(\boldsymbol{\lambda} + 1/\mu_0)\tau_1]\boldsymbol{\Phi}^T\mathbf{wd}. \tag{22}$$

We note that the second term of Eq. (21) resembles the general solution; therefore it can be dropped from the particular solution and merged with the general solution (with $\mathbf{Y} + \mathbf{z}_g$ replaced with another unknown constant vector). This shows that this method leads to the same particular solution for the solar beam source as in Subsection 2.A.

C. Method 2 for General Source Functions

Because the particular solution is just any solution to Eq. (5) disregarding any boundary conditions, the infinite medium Green's function can be used to compute the particular solution for any source function[1,6]:

$$\begin{aligned}I_p(\tau, \mu) = \int_{\tau_1}^{\tau_2}\mathrm{d}\tau'\int_{-1}^{1}\mathrm{d}\mu' G_{\mp}^{\infty}(\tau', \mu'; \tau, \mu)\\ \times|\mu'|Q(\tau', \mu'),\end{aligned} \tag{23}$$

where τ_1 and τ_2 are the optical thickness at the top and bottom of the atmosphere layer under consideration and $G_{\mp}^{\infty}$ is the infinite medium Green's function that can be written as[1]

$$\mathbf{G}_{\mp}^{\infty}(\tau', \mu'; \tau, \mu) = \boldsymbol{\Phi}_{\mp}(\mu)\tilde{\boldsymbol{\Lambda}}_{\mp}(\tau, \tau')_{\mp}\boldsymbol{\Phi}^{T}(\mu'), \tag{24}$$

where $\boldsymbol{\Phi}_{\mp}$ are the eigenvectors of $\mathbf{C}$ corresponding to the negative and positive eigenvalues, respectively, and $_{\mp}\boldsymbol{\Phi}^{T}$ are the transpose of $\boldsymbol{\Phi}_{\mp}$. $\tilde{\boldsymbol{\Lambda}}_{\mp}$ are diagonal matrices defined as[1]

$$\tilde{\boldsymbol{\Lambda}}_{\mp}(\tau, \tau') = -\frac{1}{(1 + \delta_{0m})\pi}\,\mathbf{N}_{+}^{-1}\exp[\boldsymbol{\lambda}_{\mp}(\tau' - \tau)]. \tag{25}$$

The subscript $\mp$ corresponds to $\tau < \tau'$ and $\tau > \tau'$, respectively; $\boldsymbol{\lambda}_{\mp}$ *are diagonal matrices composed of the negative and positive eigenvalues of matrix* $\mathbf{C}$, respectively; and $\mathbf{N}_{+}$ is a diagonal matrix whose diagonal elements are defined in Eq. (11) for the positive j's only ($j = 1, \ldots, N_s$). Inserting Eq. (24) into Eq. (23) and writing the result in matrix notation, we obtain

$$I_p(\tau, \mu) = \int_{\tau_1}^{\tau_2} \mathrm{d}\tau'\boldsymbol{\Phi}_{\mp}(\mu)\tilde{\boldsymbol{\Lambda}}_{\mp}(\tau, \tau')_{\mp}\boldsymbol{\Phi}^{T}(\mu')\mathbf{w}|\boldsymbol{\mu}|\mathbf{Q}(\tau'), \tag{26}$$

where $\mathbf{w}$ and $\mathbf{I}$ are diagonal matrices, $\mathbf{Q}$ is a column vector, and $|\,|$ represents the absolute value.

For the solar beam source, inserting Eq. (6) into Eq. (26), combining the scaler term $\exp(\tau'/\mu_0)$ with $\exp[\boldsymbol{\lambda}_{\mp}(\tau' - \tau)]$, we can carry out the integration in two sections, i.e., (τ_1, τ) and (τ, τ_2), which leads to

$$\begin{aligned}\mathbf{I}_p(\tau, \mu) = {} & -\boldsymbol{\Phi}[(\lambda + 1/\mu_0)\mathbf{N}]^{-1}\boldsymbol{\Phi}^{T}\mathbf{wd}\exp(\tau/\mu_0) \\ & - \boldsymbol{\Phi}\exp(-\boldsymbol{\lambda}\tau)\mathbf{z}_g,\end{aligned} \tag{27}$$

where

$$\begin{aligned}\mathbf{z}_g = {} & \begin{bmatrix} \exp[(\boldsymbol{\lambda}_{+} + 1/\mu_0)\tau_1] & 0 \\ 0 & \exp[(\boldsymbol{\lambda}_{-} + 1/\mu_0)\tau_2] \end{bmatrix} \\ & \times [(\boldsymbol{\lambda} + 1/\mu_0)\mathbf{N}]^{-1}\boldsymbol{\Phi}^{T}\mathbf{wd}.\end{aligned} \tag{28}$$

Again we can drop the second term of Eq. (27) by merging it with the general solution. This shows that this method leads to the same particular solution as in previous methods.

Equation (26) provides us another generally applicable expression to derive the particular solution for any source functions.

3. Particular Solution for the General Beam Source

In this section we generalize the particular solution for the solar beam source for beam sources that have no restrictions on their position and propagation direction. We also deal with the numerical difficulty encountered when a beam source illuminates in a direction coinciding with one of the Gaussian quadrature points.

A. Particular Solution for a Generalized Beam Source

In the previous section we showed the APS for the solar beam source, which is located at the top of the atmosphere and illuminates downwards. In this subsection we present the particular solution for a general beam source. The source function can be written as[2]

$$Q(\tau, \mu_i) = d_i U[(\tau - \tau_0)/\mu_0]\exp[(\tau - \tau_0)/\mu_0], \tag{29}$$

where τ_0 denotes the source position, $-1 < \mu_0 < 1$ is the cosine of the source zenith angle, $U(x)$ is the step function that equals 1 when $x \geq 0$ and 0 otherwise, and d_i is defined in Eq. (4). In this subsection, we also use τ_1 and τ_2 to denote the optical thickness at the top and bottom of the atmosphere layer under consideration.

For layers that are behind the source, i.e., $(\tau - \tau_0)/\mu_0 < 0$ for $\tau_1 \leq \tau \leq \tau_2$, $Q = 0$ and no particular solution is needed. For layers that are completely in front of the source, i.e., $(\tau - \tau_0)/\mu_0 > 0$ for $\tau_1 \leq \tau \leq \tau_2$, it is straightforward to write the particular solution as

$$\mathbf{I}_p(\tau, \mu) = \mathbf{z}\exp[(\tau - \tau_0)/\mu_0], \tag{30}$$

where $\mathbf{z}$ can be computed with Eq. (12).

In the case that the source is inside a layer, i.e., $\tau_1 < \tau_0 < \tau_2$, it becomes a little more complicated. We can treat this case by splitting this layer into two sublayers from $\tau = \tau_0$. Therefore the sublayers are either completely in front or behind the source, and their particular solutions can be readily obtained. However, in such cases the complete solutions for the two sublayers will be different in formalism, which consequently complicates the process to obtain the integral constants for the two sublayers. Specifically in this case, the complete solutions can be written as

$$\mathbf{I}(\tau, \mu) = \begin{cases} \boldsymbol{\Phi}\exp(-\boldsymbol{\lambda}\tau)\mathbf{Y}_1 & (\tau - \tau_0)/\mu_0 < 0 \\ \boldsymbol{\Phi}\exp(-\boldsymbol{\lambda}\tau)\mathbf{Y}_2 + \mathbf{z}\exp[(\tau - \tau_0)/\mu_0] & (\tau - \tau_0)/\mu_0 \geq 0 \end{cases}, \tag{31}$$

where $\mathbf{Y}_1$ and $\mathbf{Y}_2$ are integral constants. To simplify the process to obtain $\mathbf{Y}_1$ and $\mathbf{Y}_2$, which also improves computing efficiency, it is desirable to obtain a uniform complete solution for the whole layer. This can be achieved through the requirement that the (diffusely transmitted) radiance must be continuous at $\tau = \tau_0$, i.e.,

$$\boldsymbol{\Phi}\exp(-\boldsymbol{\lambda}\tau_0)\mathbf{Y}_1 = \boldsymbol{\Phi}\exp(-\boldsymbol{\lambda}\tau_0)\mathbf{Y}_2 + \mathbf{z}, \tag{32}$$

which leads to

$$\mathbf{Y}_1 = \mathbf{Y}_2 + \exp(\boldsymbol{\lambda}\tau_0)\boldsymbol{\Phi}^{-1}\mathbf{z}. \tag{33}$$

Inserting Eq. (12) into Eq. (33) and inserting the resulting equation into the first part of Eq. (31), we obtain the uniform complete solution as

$$\mathbf{I}(\tau, \mu) = \boldsymbol{\Phi}\exp(-\boldsymbol{\lambda}\tau)\mathbf{Y} + \mathbf{I}_p(\tau), \tag{34}$$

where we replaced $\mathbf{Y}_2$ with $\mathbf{Y}$, and

$$\mathbf{I}_p(\tau) = \mathbf{\Phi}\begin{cases} \exp[\boldsymbol{\lambda}(\tau_0 - \tau)]\boldsymbol{\xi} & (\tau - \tau_0)/\mu_0 < 0 \\ \exp[(\tau - \tau_0)/\mu_0]\boldsymbol{\xi} & (\tau - \tau_0)/\mu_0 \geq 0 \end{cases}, \tag{35}$$

where $\boldsymbol{\xi}$ is a column vector:

$$\boldsymbol{\xi} = [(\boldsymbol{\lambda} + \mathbf{E}/\mu_0)\mathbf{N}]^{-1}\mathbf{\Phi}^T\mathbf{w}\mathbf{d}. \tag{36}$$

B. Special Case of $\mu_0 = \mu_j$: Removing Divide by Zero

In Eq. (2), $\tilde{\omega}_l^m = \tilde{\omega}_l(l - m)!/(l + m)!$ where $\tilde{\omega}_l$ are the coefficients of the phase function's Legendre series. For large m, which means very large $(l + m)!$, $\tilde{\omega}_l^m$ becomes so small that $C_{ij} \approx -\delta_{ij}\mu_i^{-1}$, which means that $\boldsymbol{\lambda} \approx -\boldsymbol{\mu}^{-1}$. If $\mu_0 = \mu_j$, then $\lambda_j + 1/\mu_0 \approx 0$, which causes a divide by zero error in Eq. (12). For the same reason, the coefficient matrix of Eq. (8) is close to singular, and Eq. (8) cannot be solved accurately.

The usual solution to this problem is to change μ_0 by a tiny amount.[4] However, we have found that this problem can be completely removed. In fact, in such a case the vector $\mathbf{d}$ in Eqs. (8)–(12) is also close to zero, so Eq. (12) contains a 0/0 component. Therefore the result depends on the relative speed at which the numerator and the denominator approach zero, and the 0/0 component might be removed. When $\mu_0 = \mu_j$, by comparing Eq. (2) with Eq. (4), we find

$$\mathbf{d} = \frac{1}{\pi(1 + \delta_{0m})}\mathbf{w}^{-1}(\mathbf{C}^T\boldsymbol{\mu} + \mathbf{E})\mathbf{E}_j, \tag{37}$$

where $\mathbf{E}_j$ is the jth column of $\mathbf{E}$ (the identity matrix). Because only the jth column of the matrix $(\mathbf{C}^T\boldsymbol{\mu} + \mathbf{E})$ has any effect on $\mathbf{d}$, all diagonal elements of $\mathbf{I}$ except for the (j, j)th can be replaced by arbitrary values. By replacing them with μ_j we obtain

$$\frac{\mu_j}{\pi(1 + \delta_{0m})}\mathbf{w}^{-1}(\mathbf{C}^T + \mathbf{E}/\mu_j)\mathbf{E}_j = \mathbf{d}. \tag{38}$$

Inserting Eq. (38) into Eq. (12) [remember that $\mu_0 = \mu_j$ and recall Eq. (9)] we obtain

$$\mathbf{z} = -\frac{\mu_j}{\pi(1 + \delta_{0m})}\mathbf{\Phi}\mathbf{N}^{-1}\mathbf{\Phi}^T\mathbf{E}_j. \tag{39}$$

Using Eq. (10) we obtain

$$\mathbf{z} = -\frac{1}{\pi(1 + \delta_{0m})}\mathbf{w}^{-1}\mathbf{E}_j. \tag{40}$$

It turns out that in this case the $\mathbf{z}$ vector is only a constant vector whose jth element is $-w_j^{-1}/\pi(1 + \delta_{0m})$ and all others are zero. We therefore successfully removed the problem of divide by zero.

4. Particular Solution for Other Source Types

Both Eqs. (20) and (26) described in Section 2 can be used to derive particular solutions for general source functions. The choice between the two depends only on which one is more convenient for the given source function. In this section we derive the particular solution for two more source types: angularly distributed surface sources (Subsection 4.A) and atmosphere thermal emission sources (Subsection 4.B).

A. Particular Solution for Angularly Distributed Sources

ADSs are sources that illuminate from a surface in either or both of the hemispheres as a continuous function of zenith angle. The thermal emission from the Earth's surface is an example. For an ADS, we can write its source function as

$$Q(\tau, \mu) = \delta(\tau - \tau_0)I_0(\mu), \tag{41}$$

where τ_0 is the vertical position of the source and $I_0(\mu)$ is any function of μ.

We use Eq. (26) to derive the particular solution for ADSs because it is simpler than using Eq. (20). Inserting Eq. (41) into Eq. (26), we can show that

$$\mathbf{I}_p(\tau, \mu) = \mathbf{\Phi}_{\pm}(\mu)\tilde{\mathbf{\Lambda}}_{\pm}(\tau, \tau_0)_{\pm}\mathbf{\Phi}^T\mathbf{w}|\boldsymbol{\mu}|\mathbf{I}_0, \tag{42}$$

where $\mathbf{w}$ and $\mathbf{I}$ are diagonal matrices; $\mathbf{I}_0$ is a column vector; and the subscript $\pm$ corresponds to $\tau > \tau_0$ and $\tau < \tau_0$, respectively, which indicates that the particular solution for ADSs is discontinuous at $\tau = \tau_0$.

B. Particular Solution for Atmosphere Thermal Emission Source

The source function of the atmosphere thermal emission is a continuous function of optical thickness. This function depends on the temperature profile. It is possible for us to derive the particular solution for any given source function using the two general methods. Here we follow Stamnes *et al.*[4] to represent the atmosphere thermal emission as a polynomial in optical thickness, i.e.,

$$Q(\tau) = (1 - \tilde{\omega}_0)B(\tau) = \sum_{k=0}^{N_k} b_k\tau^k, \tag{43}$$

where $B(\tau)$ is the Planck function, and we did not assume the temperature profile.

Both Eqs. (20) and (26) can be used to derive the particular solution for the atmosphere thermal emission source. For this particular case, Eq. (20) is slightly more convenient, but the same result can be obtained with Eq. (26). Inserting Eq. (43) into Eq. (20), we obtain

$$\mathbf{I}_p(\tau) = -\mathbf{\Phi}\left(\sum_{k=0}^{N_k} b_k\mathbf{h}_k(\tau)\right)\mathbf{N}^{-1}\mathbf{\Phi}^T\mathbf{w}, \tag{44}$$

where $\mathbf{w}$ is a column vector rather than a diagonal matrix as it usually is in this paper, and $\mathbf{h}_k$ is a diagonal matrix defined by the following recursive relation:

$$\begin{aligned}\mathbf{h}_k(\tau) &= \int_0^\tau t^k \exp[\boldsymbol{\lambda}(t - \tau)]\mathrm{d}t \\ &= \begin{cases} \boldsymbol{\lambda}^{-1}\tau^k - k\boldsymbol{\lambda}^{-1}\mathbf{h}_{k-1}(\tau) & k > 0 \\ \boldsymbol{\lambda}^{-1} - \boldsymbol{\lambda}^{-1}\exp(-\boldsymbol{\lambda}\tau) & k = 0 \end{cases},\end{aligned} \tag{45}$$

where we chose the lower integral limit $\tau_1 = 0$ for convenience [see discussion following Eq. (18)]. Expanding Eq. (45), we find

$$\mathbf{h}_k(\tau) = \sum_{n=0}^{k} (-1)^{k-n} \frac{k!}{n!} \boldsymbol{\lambda}^{-(k-n+1)} \tau^n - (-1)^k k! \boldsymbol{\lambda}^{-(k+2)} \exp(-\boldsymbol{\lambda}\tau), \quad k = 0, 1, \cdots, N_k. \tag{46}$$

We note that, when Eq. (46) is inserted into Eq. (44), all the terms in the resulting equation that are associated with the second part of Eq. (46) contain $\boldsymbol{\Phi} \exp(-\boldsymbol{\lambda}\tau)$, and we can drop it from the particular solution by merging it with the general solution. Therefore we only need insert the first part of $\mathbf{h}_k$ into Eq. (44), and by collecting the coefficients of τ^n we obtain

$$\mathbf{I}_p(\tau) = -\boldsymbol{\Phi}\left(\sum_{n=0}^{N_k} \boldsymbol{\alpha}_n \tau^n\right)\mathbf{N}^{-1}\boldsymbol{\Phi}^T\mathbf{w}, \tag{47}$$

where the $\boldsymbol{\alpha}_n$ terms are diagonal matrices defined as

$$\boldsymbol{\alpha}_n = \sum_{k=n}^{N_k} (-1)^{k-n} \frac{k!}{n!} b_k \boldsymbol{\lambda}^{-(k-n+1)}, \tag{48}$$

where $\boldsymbol{\lambda}$ is a diagonal matrix. By now we have obtained the particular solution for the atmosphere thermal emission source. Because Eqs. (47) and (48) can be evaluated efficiently, we can use higher-order polynomials in Eq. (43) to achieve higher accuracy in fitting the source function, and we are able to achieve higher accuracy for a wider range of temperature profiles.

5. Numerical Computation

The APSs presented in this paper have been implemented in the new version of the GDOM[1] code. To demonstrate that we indeed can obtain the same solution using less CPU time, we present some example outputs in this section. The results are compared with the outputs from codes that use the standard approach of computing the particular solution, including EDOM[2] and particularly the DISORT[4] code.

The atmosphere is a one-layer model with an optical thickness of 0.75, a single-scattering albedo of 0.95, and a scattering phase function of the two-term Henyey–Greenstein function[12] of parameters $\alpha = 0.965$, $g_1 = 0.75$, and $g_2 = 0.65$, which represents a typical aerosol atmosphere. The lower boundary is a Lambertian surface with an albedo of 0.3. Three sources are considered: a beam source illuminating from the top of the atmosphere in a zenith angle of 45°, a surface thermal emission source with a temperature of 310 K, and an atmosphere thermal emission source with a linear temperature profile defined by the boundary temperature of 230 and 300 K. The wavelength used for the thermal sources is 4 μm.

Figure 1 shows the intensity generated by the beam source and a comparison with DISORT. For zenith angles less than 60° or larger than 120°, the difference is less than 0.1%. For zenith angles close to the horizon, the difference is still less than 0.5%. Comparison with EDOM[2] (which is implemented by the same authors of GDOM) is also conducted (but not presented), and it is found that the results match to at least six digits.

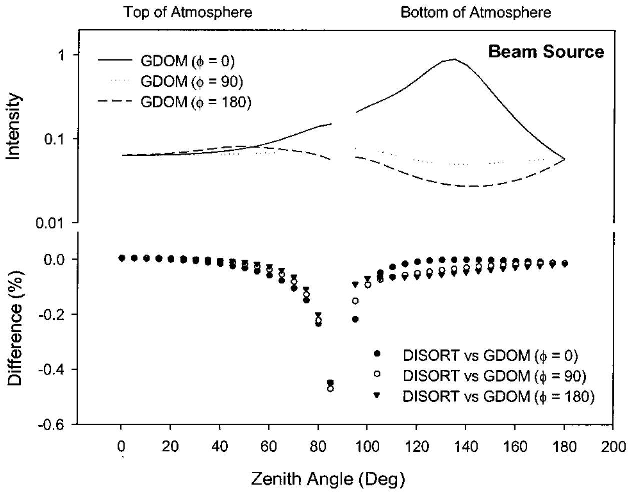

Fig. 1. Example output from GDOM and comparison with DISORT for the case of a beam source. The upper section shows the intensity (no unit) of exiting radiation at, respectively, the top and bottom of the atmosphere and in three azimuth angles ϕ; the lower section shows the difference (%) between the outputs from the two codes.

Figure 2 shows the output from GDOM and a comparison with DISORT for the case of the combined thermal emission sources. We note that GDOM generates output for each individual source, but the outputs for the two thermal sources are combined

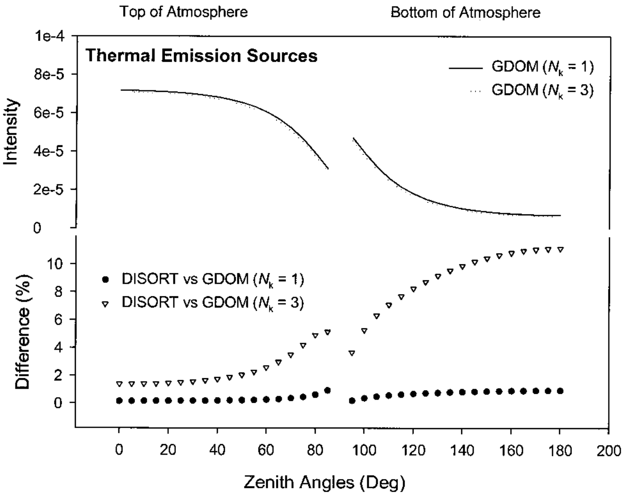

Fig. 2. Example output from the GDOM and comparison with DISORT in the case of thermal emission sources. The upper section shows the intensity [W/cm^2(sr/μm)] of exiting radiation at, respectively, the top and bottom of the atmosphere; the lower section shows the difference (%) between the outputs from the two codes. N_k [see also Eq. (43)] is the order of the source function used by GDOM.

together to compare with DISORT. Because DISORT uses a linear relation to fit the source function, Eq. (43), we also use a linear relation first and find that the two codes agree with each other quite well (with a difference less than 1%), which indicates that GDOM has computed the particular solution correctly. Following this testing, we increased the order of the source function polynomial to 3 and found (as shown in Fig. 2) a significant (up to 10%) difference between the two codes, which indicates that use of a linear relation to fit the source function could result in large errors when the temperature step is large.

6. Discussion

In this paper we have discussed two approaches to derive particular solutions for general source functions. Choosing one or the other depends only on which one is more convenient. These methods allow us to obtain an APS for any source function. The ADS case shown in Subsection 4.A has demonstrated the advantage of these approaches. It is straightforward to derive the particular solution for ADSs with Eq. (26), and it can also be obtained with Eq. (20) with a little more work. In contrast, it would be a greater challenge to use the standard approach of seeking the particular solution according to the pattern of the source function.

Because an APS can be obtained, we no longer need to solve any linear equations systems to compute the particular solution. This allows us to achieve higher efficiency. We have shown that, in the case of beam sources, the operation count to compute the particular solution has been reduced from $O(N^3)$ to $O(N^2)$. The gain of efficiency is greater when solutions for multiple sources are being sought.

In Table 1 we show the time used to compute the particular solution, as well as the total time, by the APS approach that is developed in this paper and the standard approach for the case of beam sources. Cases for various hemisphere stream numbers (16, 32, and 48), atmosphere layer numbers (1 and 10), and source numbers (1, 10, and 50) are compared in Table 1. The testing is done on a Windows 2000 system running with a 500-MHz CPU and 380-Mbyte physical memory.

In terms of the particular solution alone, over 94% CPU time can be saved with the APS. For single-source cases, the overall reduction of CPU time ranges from 12 to 18%. This percentage grows with the increasing number of sources. For example, in the case of 50 sources, 73–82% of time can be saved.

Table 1. Comparison of the CPU Time (in Seconds) Used by the Standard (STD) Approach and the APS in the Case of Beam Sources for Different (Hemisphere) Stream Numbers (N_s)

	Number of Layers					
	1			10		
	Number of Sources					
Approach	1	10	50	1	10	50
Particular Solution						
N_s16						
STD	0.0662	0.6276	2.7358	0.6359	6.3491	27.3827
APS	0.0039	0.0302	0.1469	0.0351	0.3305	1.5823
Reduced by	94%	95%	95%	94%	95%	94%
N_s32						
STD	0.6795	6.8415	27.3193	6.8398	68.9391	321.9918
APS	0.0229	0.2136	0.9589	0.2504	2.5437	12.8284
Reduced by	97%	97%	96%	96%	96%	96%
N_s48						
STD	2.9893	27.1941	125.4103	26.9588	272.8924	1393.9344
APS	0.0801	0.8212	4.0158	0.9313	8.8627	44.2436
Reduced by	97%	97%	97%	97%	97%	97%
Total						
N_s16						
STD	0.3434	0.9503	3.2131	4.0475	10.7955	35.3709
APS	0.2811	0.3530	0.6242	3.4466	4.7769	9.5704
Reduced by	18%	63%	81%	15%	56%	73%
N_s32						
STD	3.8927	10.4851	32.7170	48.1693	117.9997	398.1212
APS	3.2361	3.8572	6.3566	41.5798	51.6042	88.9579
Reduced by	17%	63%	81%	14%	56%	78%
N_s48						
STD	18.9322	44.3187	147.7625	223.1709	492.8988	1714.4453
APS	16.0230	17.9458	26.3679	197.1435	228.8691	364.7545
Reduced by	15%	60%	82%	12%	54%	79%

Table 2. Comparison of the Unit Increase by the Standard (STD) Approach and the APS in the Case of Beam Sources

	Number of Layers					
	1			10		
Approach	First Source[a]	Extra Source[b]	Unit Increase[c]	First Source	Extra Source	Unit Increase
STD						
N_s16	0.3434	0.0586	17.1	4.0475	0.6393	15.8
N_s32	3.8927	0.5883	15.1	48.1693	7.1419	14.8
N_s48	18.9322	2.6292	13.9	223.1709	30.4342	13.6
APS						
N_s16	0.2811	0.0070	2.5	3.4466	0.1250	3.6
N_s32	3.2361	0.0637	2.0	41.5798	0.9669	2.3
N_s48	16.0230	0.2111	1.3	197.1435	3.4206	1.7

[a] The CPU time (seconds) required to find the solution for the first source.
[b] The CPU time (seconds) required to find the solution for each extra source.
[c] The increase of CPU time (in percent) for each extra source relative to the first source.

In Table 2 we show the time (in percent) needed to compute the solution for each extra source relative to that for the first (full solution) source. We can see that, to compute the radiation field for each extra source, the APS approach needs only 1.3–3.6% of the full solution time. In contrast, a standard approach (suppose it has an implementation of a simultaneous multisource solution similar to that of EDOM[2]) needs 13.6–17.1% of the full solution time. As a result, in the same amount of time, 4.4–10.5 times more sources can be processed by the APS approach than by the standard approach.

In the case of atmosphere thermal emission sources, the gain of efficiency is even greater because the standard approach needs to solve at least two linear equations systems, each for one order of the source function polynomial. The particular solution developed in this paper requires only $O(N^2)$ operations, and because Eq. (48) needs only $O(N)$ operations, it can be evaluated efficiently. Our tests have shown that, with the APS, the total time is barely affected by the order of the source function polynomial (the total time increases up to 5% when the order is increased from 1 to 10). Therefore higher-order polynomials can be used, which allows us to fit the source function more accurately and to deal with a wider range of temperature profiles.

In this paper we have also presented a special particular solution for beam sources whose illumination direction coincides with a Gaussian quadrature point. In such case, divide by zero, or inverting of a singular matrix, will be encountered. The special particular solution developed in this paper removes such a problem.

With the particular solutions developed in this paper, the revised GDOM code is capable of computing the radiation field efficiently for multiple sources. The new GDOM code supports the commonly seen source types, including generalized beam sources, ADSs (including the special cases of thermal emission from the Earth's surface and from deep space), and the atmosphere thermal emission source. This GDOM code has the integrated component of the Green's function algorithm that we developed previously, which means that the Green's function and the radiation field of any number of sources can be obtained simultaneously. Radiation field angular interpolation has also been implemented to obtain the radiance at any zenith angle. Vacuum, Lambertian, and bidirectional reflectance distribution function boundaries are supported. Special consideration has been taken on the usability of this FORTRAN 95 code, in particular, internal data items can be accessed easily, and calling to subprograms has been greatly simplified. However, we would like to point out that this code is based on the plane-parallel (one-dimensional) atmosphere model, and the surface is assumed to be homogeneous. This code is a solver-style code, which requires as input the optical properties of the atmosphere and the surface. The current version of GDOM computes the intensity and scalar Green's function only, but a new version that considers the full polarization effect will be available soon.[13]

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13. The code and comprehensive documentation are available publicly. Please contact the authors to obtain a copy.